

## LAMPIRAN

### Lampiran 1 Surat Izin Penelitian

MAJELIS PENDIDIKAN TINGGI, PENELITIAN DAN PENGEMBANGAN  
**UNIVERSITAS MUHAMMADIYAH PALOPO**  
 LEMBAGA PENELITIAN DAN PENGABDIAN KEPADA  
 MASYARAKAT (LPPM)  
 Lt. 2 Gedung MKU, Universitas Muhammadiyah Palopo  
 Jl. Jend. Sudirman Km. 03 Buntan, Kota Palopo (91939) – Telp/Fax: (0471) 327429

Nomor : 710/III.3.AU/LPPM/F/2025  
 Lampiran : -  
 Perihal : Permohonan Izin Penelitian

Palopo, 28 November 2025

Kepada Yth  
**Kepala Lab Farmasi UM.Palopo**  
 Di \_\_\_\_\_  
 Tempat \_\_\_\_\_

*Assalamu 'alaikum warahmatullahi wabarakatuh*

Dengan hormat, disampaikan bahwa dalam rangka pelaksanaan penelitian Mahasiswa Universitas Muhammadiyah Palopo, mohon kiranya diberikan izin untuk melakukan kegiatan penelitian kepada:

Nama : Aisyah Yadin  
 NIM : 221320082  
 Jurusan : SI Farmasi  
 Alamat : Karetan, Kab. Luwu  
 Jenis Kelamin : Perempuan  
 No.Hp/Wa : 081523951639

Untuk melengkapi data penelitian yang berkaitan dengan Judul "**Pengembangan Tablet Brotowali (Tinospora Crispa) Sebagai Agen Antimalaria Berdasarkan Hasil Skrining In Silico Dan Uji Stabilitas Fisik Sediaan**" yang akan dilakukan pada November-Desember 2025

Demikian permohonan dari kami, atas kerjasama yang baik diucapkan terima kasih.

*Wassalamu 'alaikum warahmatullahi wabarakatuh*

Ka.L.PPM,  
  
 Junaidi, SE, AK, M. Ak., C.A., Ph.D.  
 NIDN: 0910067705

Tembusan:  
 - Dekan Bersangkutan

### Lampiran 2 Perhitungan Maserasi

Perbandingan 1:10

Ekstrak batang brotowali = 300 mg

Etanol = 70%

Vol Pelarut = Berat Simplisia  $\times$  10

$$= 300 \times 10$$

$$= 3000 \text{ ml}$$

### Lampiran 3 Perhitungan Formula

#### A. Formula 1

|                          |                                     |
|--------------------------|-------------------------------------|
| Ekstrak batang brotowali | $= 50 \times 30 = 1500 \text{ mg}$  |
| Gelatin                  | $= 60 \times 30 = 1800 \text{ mg}$  |
| Avicel                   | $= 60 \times 30 = 1800 \text{ mg}$  |
| Aerosil                  | $= 3 \times 30 = 90 \text{ mg}$     |
| Mg stearat               | $= 6 \times 30 = 180 \text{ mg}$    |
| Laktosa                  | $= 221 \times 30 = 6630 \text{ mg}$ |

#### B. Formula 2

|                          |                                     |
|--------------------------|-------------------------------------|
| Ekstrak batang brotowali | $= 60 \times 30 = 1800 \text{ mg}$  |
| Gelatin                  | $= 60 \times 30 = 1800 \text{ mg}$  |
| Avicel                   | $= 60 \times 30 = 1800 \text{ mg}$  |
| Aerosil                  | $= 3 \times 30 = 90 \text{ mg}$     |
| Mg stearat               | $= 6 \times 30 = 180 \text{ mg}$    |
| Laktosa                  | $= 211 \times 30 = 6330 \text{ mg}$ |

#### C. Formula 3

|                          |                                     |
|--------------------------|-------------------------------------|
| Ekstrak batang brotowali | $= 70 \times 30 = 2100 \text{ mg}$  |
| Gelatin                  | $= 60 \times 30 = 1800 \text{ mg}$  |
| Avicel                   | $= 60 \times 30 = 1800 \text{ mg}$  |
| Aerosil                  | $= 3 \times 30 = 90 \text{ mg}$     |
| Mg stearat               | $= 6 \times 30 = 180 \text{ mg}$    |
| Laktosa                  | $= 201 \times 30 = 6030 \text{ mg}$ |

## Lampiran 4 Perhitungan Uji Granul

### A. Perhitungan Uji Kadar Air

Rumus kadar air

$$\text{Kadar air (\%)} = \frac{W_o - W_t}{W_o} \times 100\%$$

Keterangan:

W<sub>o</sub> = berat granul sebelum pengeringan

W<sub>t</sub> = berat granul sesudah pengeringan

#### Formula 1

Dik: W<sub>o</sub> = 5 kg

W<sub>t</sub> = 4,8 kg

Dit: kadar air (%) ?

$$\text{Peny: kadar air (\%)} = \frac{W_o - W_t}{W_o} \times 100\%$$

$$\text{kadar air (\%)} = \frac{5 - 4,8}{5} \times 100\%$$

$$\begin{aligned} \text{kadar air (\%)} &= \frac{0,2}{5} \times 100\% \\ &= 0,04 \times 100\% \\ &= 4\% \end{aligned}$$

#### Formula 2

Dik: W<sub>o</sub> = 5 kg

W<sub>t</sub> = 4,8 kg

Dit: kadar air (%) ?

$$\text{Peny: kadar air (\%)} = \frac{W_o - W_t}{W_o} \times 100\%$$

$$\text{kadar air (\%)} = \frac{5 - 4,8}{5} \times 100\%$$

$$\begin{aligned} \text{kadar air (\%)} &= \frac{0,2}{5} \times 100\% \\ &= 0,04 \times 100\% \\ &= 4\% \end{aligned}$$

**Formula 3**

Dik:  $W_o = 5 \text{ kg}$

$$W_t = 4,8 \text{ kg}$$

Dit: kadar air (%) ?

$$\text{Peny: kadar air (\%)} = \frac{W_o - W_t}{W_o} \times 100\%$$

$$\text{kadar air (\%)} = \frac{5 - 4,8}{5} \times 100\%$$

$$\begin{aligned} \text{kadar air (\%)} &= \frac{0,2}{5} \times 100\% \\ &= 0,04 \times 100\% \\ &= 4\% \end{aligned}$$

**B. Perhitungan Uji Sudut Diam**

Rumus sudut diam

$$\tan(\alpha) = \frac{h}{r}$$

Keterangan:

$\alpha$  = sudut diam ( $^{\circ}$ )

$h$  = tinggi granul (cm)

$r$  = jari-jari granul (cm)

**Formula 1**

Dik:  $d_1 = 7 \text{ cm}$

$$d_2 = 5 \text{ cm}$$

$$t = 1,8 \text{ cm}$$

Dit :  $r$  ?

$$\alpha ?$$

$$\text{Peny : } t = \frac{d_1 + d_2}{2}$$

$$= \frac{7 + 5}{2}$$

$$= \frac{12}{2}$$

$$= 6$$

$$\begin{aligned}
 \tan \alpha &= \frac{h}{r} \\
 &= \frac{1,8}{6} \\
 &= 0,3 \\
 &= 17,19^\circ
 \end{aligned}$$

### Formula 2

Dik:  $d_1 = 9 \text{ cm}$

$$d_2 = 5 \text{ cm}$$

$$t = 1,9 \text{ cm}$$

Dit :  $r$  ?

$$\alpha?$$

$$\begin{aligned}
 \text{Peny : } t &= \frac{d_1 + d_2}{2} \\
 &= \frac{9 + 5}{2} \\
 &= \frac{14}{2} \\
 &= 7
 \end{aligned}$$

$$\begin{aligned}
 \tan \alpha &= \frac{h}{r} \\
 &= \frac{1,9}{7} \\
 &= 0,27 \\
 &= 15,47^\circ
 \end{aligned}$$

### Formula 3

Dik:  $d_1 = 9 \text{ cm}$

$$d_2 = 5 \text{ cm}$$

$$t = 1,9 \text{ cm}$$

Dit :  $r$  ?

$$\alpha?$$

$$\begin{aligned}
 \text{Peny : } t &= \frac{d_1 + d_2}{2} \\
 &= \frac{9 + 5}{2} \\
 &= \frac{14}{2} \\
 &= 7
 \end{aligned}$$

$$\begin{aligned}
 \tan \alpha &= \frac{h}{r} \\
 &= \frac{1,9}{7} \\
 &= 0,27 \\
 &= 15,47^\circ
 \end{aligned}$$

### C. Perhitungan Uji Kompresibilitas

Rumus kompresibilitas

$$\% = \frac{V_o - V_t}{V_o} \times 100\%$$

Keterangan:

$V_o$  = volume awal granul

$V_t$  = volume setelah diketuk/ditap

#### Formula 1

Dik:  $V_o = 12$

$V_t = 11$

Dit: % ?

$$\text{Peny: } \% = \frac{V_o - V_t}{V_o} \times 100\%$$

$$\% = \frac{12 - 11}{12} \times 100\%$$

$$\% = \frac{1}{12} \times 100\%$$

$$= 8,33\%$$

#### Formula 2

Dik:  $V_o = 14$

$V_t = 12$

Dit: % ?

$$\text{Peny: } \% = \frac{V_o - V_t}{V_o} \times 100\%$$

$$\% = \frac{14 - 12}{14} \times 100\%$$

$$\% = \frac{2}{14} \times 100\%$$

$$= 14,2\%$$

**Formula 3**

Dik:  $V_o = 12$

$V_t = 11$

Dit: % ?

$$\text{Peny: \%} = \frac{V_o - V_t}{V_o} \times 100\%$$

$$\% = \frac{12 - 11}{12} \times 100\%$$

$$\% = \frac{1}{12} \times 100\%$$

$$= 8,33\%$$

**Lampiran 5 Perhitungan Uji Sifat Fisik****A. Uji Keseragaman Bobot**

| Tablet | F1 (gr) | F2 (gr) | F3 (gr) |
|--------|---------|---------|---------|
| 1      | 0,44    | 0,45    | 0,44    |
| 2      | 0,45    | 0,44    | 0,45    |
| 3      | 0,44    | 0,45    | 0,46    |
| 4      | 0,45    | 0,44    | 0,45    |
| 5      | 0,44    | 0,45    | 0,44    |
| 6      | 0,45    | 0,46    | 0,45    |
| 7      | 0,45    | 0,45    | 0,46    |
| 8      | 0,44    | 0,44    | 0,45    |
| 9      | 0,45    | 0,45    | 0,44    |
| 10     | 0,44    | 0,44    | 0,45    |
| 11     | 0,45    | 0,45    | 0,46    |
| 12     | 0,44    | 0,46    | 0,45    |
| 13     | 0,45    | 0,45    | 0,44    |
| 14     | 0,44    | 0,44    | 0,45    |
| 15     | 0,45    | 0,45    | 0,46    |
| 16     | 0,45    | 0,45    | 0,45    |
| 17     | 0,44    | 0,44    | 0,44    |

|           |       |       |       |
|-----------|-------|-------|-------|
| 18        | 0,45  | 0,45  | 0,45  |
| 19        | 0,44  | 0,44  | 0,46  |
| 20        | 0,45  | 0,45  | 0,45  |
| Jumlah    | 8,90  | 8,96  | 9,00  |
| Rata-rata | 0,445 | 0,448 | 0,450 |

Rumus yang digunakan:

Menghitung bobot rata-rata tablet

$$\bar{x} = \frac{\sum x}{n}$$

Keterangan:

$\bar{x}$  = rata-rata bobot tablet

$\sum x$  = jumlah seluruh bobot tablet

n = jumlah tablet

Menghitung batas penyimpangan  $\pm 5\% = \bar{x} \pm (0,05 \times \bar{x})$

Menghitung batas penyimpangan  $\pm 10\% = \bar{x} \pm (0,10 \times \bar{x})$

### Formula 1

Bobot rata-rata:

$$\bar{x} = \frac{8,90}{20} = 0,445 \text{ g}$$

**Batas penyimpangan  $\pm 5\%$**

$$= 0,445 \pm (0,05 \times 0,445)$$

$$= 0,445 \pm 0,02225$$

$$\text{Batas minimum} = 0,445 - 0,02225 = 0,42275 \text{ g}$$

$$\text{Batas maksimum} = 0,445 + 0,02225 = 0,46725 \text{ g}$$

**Batas penyimpangan  $\pm 10\%$**

$$= 0,445 \pm (0,10 \times 0,445)$$

$$= 0,445 \pm 0,0445$$

$$\text{Batas minimum} = 0,445 - 0,0445 = 0,4005 \text{ g}$$

$$\text{Batas maksimum} = 0,445 + 0,0445 = 0,4895 \text{ g}$$

### Formula 2

Bobot rata-rata:



$$\bar{x} = \frac{8,96}{20} = 0,448 \text{ g}$$

**Batas penyimpangan  $\pm 5\%$**

$$= 0,448 \pm (0,05 \times 0,448)$$

$$= 0,448 \pm 0,0224$$

$$\text{Batas minimum} = 0,448 - 0,0224 = 0,4256 \text{ g}$$

$$\text{Batas maksimum} = 0,448 + 0,0224 = 0,4704 \text{ g}$$

**Batas penyimpangan  $\pm 10\%$**

$$= 0,448 \pm (0,10 \times 0,448)$$

$$= 0,448 \pm 0,0448$$

$$\text{Batas minimum} = 0,448 - 0,0448 = 0,4032 \text{ g}$$

$$\text{Batas maksimum} = 0,448 + 0,0448 = 0,4928 \text{ g}$$

### **Formula 3**

Bobot rata-rata:

$$\bar{x} = \frac{9,00}{20} = 0,450 \text{ g}$$

**Batas penyimpangan  $\pm 5\%$**

$$= 0,450 \pm (0,05 \times 0,450)$$

$$= 0,450 \pm 0,0225$$

$$\text{Batas minimum} = 0,450 - 0,0225 = 0,4275 \text{ g}$$

$$\text{Batas maksimum} = 0,450 + 0,0225 = 0,4725 \text{ g}$$

**Batas penyimpangan  $\pm 10\%$**

$$= 0,450 \pm (0,10 \times 0,450)$$

$$= 0,450 \pm 0,045$$

$$\text{Batas minimum} = 0,450 - 0,045 = 0,405 \text{ g}$$

$$\text{Batas maksimum} = 0,450 + 0,045 = 0,495 \text{ g}$$

## **B. Uji keseragaman Ukuran**

| Tablet | Keseragaman ukuran |        |           |        |           |        |
|--------|--------------------|--------|-----------|--------|-----------|--------|
|        | Formula 1          |        | Formula 2 |        | Formula 3 |        |
|        | D (mm)             | T (mm) | D (mm)    | T (mm) | D (mm)    | T (mm) |

|           |        |       |        |       |        |       |
|-----------|--------|-------|--------|-------|--------|-------|
| 1         | 12,01  | 4,52  | 12,03  | 4,55  | 12,05  | 4,58  |
| 2         | 12,00  | 4,50  | 12,02  | 4,54  | 12,04  | 4,57  |
| 3         | 12,02  | 4,53  | 12,01  | 4,56  | 12,06  | 4,59  |
| 4         | 12,01  | 4,51  | 12,03  | 4,55  | 12,05  | 4,58  |
| 5         | 12,00  | 4,50  | 12,02  | 4,54  | 12,04  | 4,57  |
| 6         | 12,01  | 4,52  | 12,04  | 4,56  | 12,05  | 4,58  |
| 7         | 12,02  | 4,53  | 12,03  | 4,55  | 12,06  | 4,59  |
| 8         | 12,00  | 4,50  | 12,01  | 4,54  | 12,04  | 4,57  |
| 9         | 12,01  | 4,52  | 12,03  | 4,55  | 12,05  | 4,58  |
| 10        | 12,00  | 4,51  | 12,02  | 4,54  | 12,04  | 4,57  |
| Rata-rata | 12,008 | 4,514 | 12,024 | 4,548 | 12,048 | 4,578 |

Rumus yang digunakan:

$$\text{Perbandingan} = \frac{\text{Diameter Tablet}}{\text{Tebal Tablet}}$$

#### Formula 1

$$\text{Perbandingan} = \frac{12,008}{4,514} = 2,66$$

#### Formula 2

$$\text{Perbandingan} = \frac{12,024}{4,548} = 2,64$$

#### Formula 3

$$\text{Perbandingan} = \frac{12,048}{4,578} = 2,63$$

### C. Uji Kerapuhan

Rumus yang digunakan:

$$\text{Kerapuhan \%} = \frac{W_0 - W_1}{W_0} \times 100\%$$

Keterangan:

$W_0$  = berat total tablet sebelum pengujian

$W_1$  = berat total tablet setelah pengujian

**Formula 1**

Dik:  $W_0 = 9$  gr

$$W_1 = 8,5 \text{ gr}$$

Dit: Kerapuhan (%) ?

Penye:

$$\begin{aligned} \text{Kerapuhan \%} &= \frac{W_0 - W_1}{W_0} \times 100\% \\ &= \frac{9 - 8,5}{9} \times 100\% \\ &= 0,05\% \end{aligned}$$

**Formula 2**

Dik:  $W_0 = 9$  gr

$$W_1 = 8,6 \text{ gr}$$

Dit: Kerapuhan (%) ?

$$\begin{aligned} \text{Kerapuhan \%} &= \frac{W_0 - W_1}{W_0} \times 100\% \\ &= \frac{9 - 8,6}{9} \times 100\% \\ &= 0,04\% \end{aligned}$$

**Formula 3**

Dik:  $W_0 = 9$  gr

$$W_1 = 8,3 \text{ gr}$$

Dit: Kerapuhan (%) ?

$$\begin{aligned} \text{Kerapuhan \%} &= \frac{W_0 - W_1}{W_0} \times 100\% \\ &= \frac{9 - 8,3}{9} \times 100\% \\ &= 0,07\% \end{aligned}$$

**Lampiran 6 Pengambilan dan Pengolahan Sampel**

|                                                                                     |                                                                          |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------|
|    | <p>Pengambilan sampel batang Brotowali<br/>(<i>Tinospora crispa</i>)</p> |
|   | <p>Pencucian</p>                                                         |
|  | <p>Perajangan</p>                                                        |



Pengeringan



Penghalusan sampel



Penimbangan sampel untuk maserasi



Maserasi



Penyaringan



Pemisahan pelarut  
(*Rotary evaporator*)



Ekstrak kental

#### Lampiran 7 Pembuatan Sediaan Tablet



Penyiapan alat dan bahan



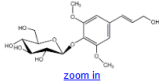
Pembuatan granul

|                                                                                     |                                 |
|-------------------------------------------------------------------------------------|---------------------------------|
|    | <p>Hasil granul Formula I</p>   |
|   | <p>Hasil granul Formula II</p>  |
|  | <p>Hasil granul Formula III</p> |
|  | <p>Proses pencetakan tablet</p> |

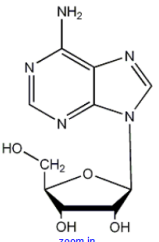


|                                                                                     |                                 |
|-------------------------------------------------------------------------------------|---------------------------------|
|    | <p>Hasil tablet Formula I</p>   |
|   | <p>Hasil tablet Formula II</p>  |
|  | <p>Hasil tablet Formula III</p> |

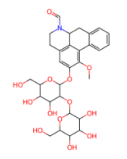
Lampiran 8 Uji Studi *In Silico* KNAPSACK

| Metabolite information                         |                                                                                                                                                               | Structural formula                                                                                            |
|------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------|
| Name                                           | Syringin                                                                                                                                                      | <br><a href="#">zoom in</a> |
| Formula                                        | C17H24O9                                                                                                                                                      |                                                                                                               |
| Mw                                             | 372.14203237                                                                                                                                                  |                                                                                                               |
| CAS RN                                         | 118-34-3                                                                                                                                                      |                                                                                                               |
| C_ID                                           | C00000010 , <a href="#">Twins (%)</a>                                                                                                                         |                                                                                                               |
| InChIKey                                       | QJVKXWHHAMZTBY-MAWHBGBXNA-N                                                                                                                                   |                                                                                                               |
| InChICode                                      | InChI=1S/C17H24O9/c1-23-10-6-9(4-3-5-18)7-11(24-2)16(10)26-17-15(22)14(21)13(20)12(8-19)25-17h3-4,6-7,12-15,17-22h,5,8h2,1-2h3b4-3+1t2-,13-,14-,15+,17-/m0/s1 |                                                                                                               |
| SMILES                                         | COc1cc(C=C(CO)cc(OC)c1O[C@@H]1OC(CO)[C@@H](O)[C@@H](O)C1O                                                                                                     |                                                                                                               |
| Start Substs in Alk. Biosynthesis (Prediction) |                                                                                                                                                               |                                                                                                               |

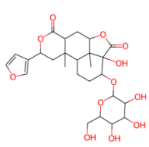
Syringin

| Metabolite Information                         |                                                                                                                                     | Structural formula                                                                                             |
|------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------|
| Name                                           | Adenosine                                                                                                                           | <br><a href="#">zoom in</a> |
| Formula                                        | C10H13N5O4                                                                                                                          |                                                                                                                |
| Mw                                             | 267.09675394                                                                                                                        |                                                                                                                |
| CAS RN                                         | 58-61-7                                                                                                                             |                                                                                                                |
| C_ID                                           | C00007444 , <a href="#">Twins (%)</a>                                                                                               |                                                                                                                |
| InChIKey                                       | OIRDTQYFTABQOQ-CDACIVGJNA-N                                                                                                         |                                                                                                                |
| InChICode                                      | InChI=1S/C10H13N5O4/c11,8-5-9(13-2-12-8)15(3-14-5)10-7(18)6(17)4(1-16)19-10h2-4-6-7,10,16-18h,1H2,(H2,11,12,13)/t4-,6-,7-,10-/m0/s1 |                                                                                                                |
| SMILES                                         | Nc1ncnc2c1ncn2[C@@H]1O[C@H](CO)[C@@H](O)[C@@H](O)C1O                                                                                |                                                                                                                |
| Start Substs in Alk. Biosynthesis (Prediction) | <a href="#">L-Asp</a> <a href="#">L-Phe</a>                                                                                         |                                                                                                                |

Adenosine

| Metabolite Information                         |                                                                                                                                                                                                                                                                                 | Structural formula                                                                                              |                      |         |           |         |                |                                      |                      |
|------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------|----------------------|---------|-----------|---------|----------------|--------------------------------------|----------------------|
| Name                                           | Tinoscorside A                                                                                                                                                                                                                                                                  | <br><a href="#">zoom in</a> |                      |         |           |         |                |                                      |                      |
| Formula                                        | C30H37NO13                                                                                                                                                                                                                                                                      |                                                                                                                 |                      |         |           |         |                |                                      |                      |
| Mw                                             | 619.22649028                                                                                                                                                                                                                                                                    |                                                                                                                 |                      |         |           |         |                |                                      |                      |
| CAS RN                                         | 1257394-26-5                                                                                                                                                                                                                                                                    |                                                                                                                 |                      |         |           |         |                |                                      |                      |
| C_ID                                           | C00063744                                                                                                                                                                                                                                                                       |                                                                                                                 |                      |         |           |         |                |                                      |                      |
| InChIKey                                       | JCMMRXKMSLWARH-JINFIROUSA-N                                                                                                                                                                                                                                                     |                                                                                                                 |                      |         |           |         |                |                                      |                      |
| InChICode                                      | InChI=1S/C30H37NO13/c1-40-27-17(9-14-6-7-31(12-34)16-8-13-4-2-3-5-15(13)21(27)20(14)16)41-30-28(25)38(32)36(19(11-33)43-30)44-29-26(39)24(37)22(35)18(10-32)42-29h2-5,9,12,16,18-19,22-26,28-30,32-33,35-39H,6-8,10-11H2,1H3/t16-,18-,19-,22-,23-,24+,25+,26-,28-,29+,30-/m1/s1 |                                                                                                                 |                      |         |           |         |                |                                      |                      |
| SMILES                                         | COc1c(OC2OC(CO)C(O)C(O)C2OC2OC(CO)C(O)C(O)C2O)cc2c3c1-c1cccc1CC3N(C=O)CC2                                                                                                                                                                                                       |                                                                                                                 |                      |         |           |         |                |                                      |                      |
| Start Substs in Alk. Biosynthesis (Prediction) |                                                                                                                                                                                                                                                                                 |                                                                                                                 |                      |         |           |         |                |                                      |                      |
| Organism                                       | <table><tr><th>Kingdom</th><th>Family</th><th>Species</th><th>Reference</th></tr><tr><td>Plantae</td><td>Menispermaceae</td><td>Tinospora crispa <a href="#">(U)</a></td><td><a href="#">Ref.</a></td></tr></table>                                                             | Kingdom                                                                                                         | Family               | Species | Reference | Plantae | Menispermaceae | Tinospora crispa <a href="#">(U)</a> | <a href="#">Ref.</a> |
| Kingdom                                        | Family                                                                                                                                                                                                                                                                          | Species                                                                                                         | Reference            |         |           |         |                |                                      |                      |
| Plantae                                        | Menispermaceae                                                                                                                                                                                                                                                                  | Tinospora crispa <a href="#">(U)</a>                                                                            | <a href="#">Ref.</a> |         |           |         |                |                                      |                      |

Tinoscorside A

| Metabolite Information                         |                                                                                                                                                                                                                                                   |                |                                        |                      | Structural formula                                                                                            |
|------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------|----------------------------------------|----------------------|---------------------------------------------------------------------------------------------------------------|
| Name                                           | Borapetoside A                                                                                                                                                                                                                                    |                |                                        |                      | <br><a href="#">zoom in</a> |
| Formula                                        | C26H34O12                                                                                                                                                                                                                                         |                |                                        |                      |                                                                                                               |
| Mw                                             | 538.20502655                                                                                                                                                                                                                                      |                |                                        |                      |                                                                                                               |
| CAS RN                                         | 100202-29-7                                                                                                                                                                                                                                       |                |                                        |                      |                                                                                                               |
| C_ID                                           | C00063584                                                                                                                                                                                                                                         |                |                                        |                      |                                                                                                               |
| InChIKey                                       | GCXIISOWSXMCD-MZYRCUENSA-N                                                                                                                                                                                                                        |                |                                        |                      |                                                                                                               |
| InChICode                                      | InChI=1S/C26H34O12/c1-24-8-13(11-5-6-34-10-11)35-21(31)12(24)7-17-25(2)15(24)3-4-16(26)25-33(23)32(38-17)37-22-20(30)19(29)18(26)14(9-27)36-22/h5-6,10,12-20,22,27-30,33H,3-4,7-9H2,1-2H3/t12-,13-,14+,15-,16-,17-,18+,19-,20+22-,24+25-,26-/m/s1 |                |                                        |                      |                                                                                                               |
| SMILES                                         | CC12CC(c3ccc3)OC(=O)C1CC1OC(=O)C3(O)C(OC4OC(CO)C(O)C(O)C4O)CC2C13C                                                                                                                                                                                |                |                                        |                      |                                                                                                               |
| Start Substs in Aib. Biosynthesis (Prediction) |                                                                                                                                                                                                                                                   |                |                                        |                      |                                                                                                               |
| Organism                                       | Kingdom                                                                                                                                                                                                                                           | Family         | Species                                | Reference            |                                                                                                               |
|                                                | Plantae                                                                                                                                                                                                                                           | Menispermaceae | Tinospora crispa ( <a href="#">W</a> ) | <a href="#">Ref.</a> |                                                                                                               |

Borapetoside A

| Metabolite Information                         |                                                           | Structural formula |
|------------------------------------------------|-----------------------------------------------------------|--------------------|
| Name                                           | Tyramine                                                  |                    |
| Formula                                        | C8H11NO                                                   |                    |
| Mw                                             | 137.08406398                                              |                    |
| CAS RN                                         | 51-67-2                                                   |                    |
| C_ID                                           | C00001435 , <a href="#">Twins (%)</a>                     |                    |
| InChIKey                                       | DZGWFCGJZKJUFU-UHFFFAOYSA-N                               |                    |
| InChICode                                      | InChI=1S/C8H11NO/c9-6-5-7-1-3-8(10)4-2-7/h1-4,10H,5-6,9H2 |                    |
| SMILES                                         | NCCc1ccc(O)cc1                                            |                    |
| Start Substs in Aib. Biosynthesis (Prediction) |                                                           |                    |

Tyramine

### Lampiran 9 Uji Studi In Silico Way2Drug

| <div><div><div><div><div><div></div><div>All</div></div><div><div></div><div>Pa&gt;Pi</div></div><div><div></div><div>Pa&gt;0,3</div></div><div><div></div><div>Pa&gt;0,7</div></div><div><div></div><div>ok</div></div></div></div></div></div>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |       |                                                  |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------|--------------------------------------------------|----------------------------------|-------|-------|--------------------------------------------------|-------|-------|-----------------------------------|-------|-------|--------------------------------------------------|-------|-------|----------------------------------|-------|-------|------------------------------------------|-------|-------|--------------------------------------------------|-------|-------|--------------------------------------------------|-------|-------|---------------------------------------------|-------|-------|-------------------------------------------|-------|-------|-----------------------------------|----------------|-------|---------------------------|-------|-------|-------------------------------|-----------|
| <div><table><tr><th>Pa</th><th>Pi</th><th>Activity</th></tr><tr><td>0,953</td><td>0,000</td><td>4-Coumarate-CoA ligase inhibitor</td></tr><tr><td>0,948</td><td>0,004</td><td>Membrane integrity agonist</td></tr><tr><td>0,943</td><td>0,004</td><td>CDP-glycerol glycerophosphotransferase inhibitor</td></tr><tr><td>0,932</td><td>0,002</td><td>Vasoprotector</td></tr><tr><td>0,922</td><td>0,003</td><td>Antiprotozoal (Leishmania)</td></tr><tr><td>0,918</td><td>0,004</td><td>Sugar-phosphatase inhibitor</td></tr><tr><td>0,917</td><td>0,004</td><td>Alkenylglycerophosphocholine hydrolase inhibitor</td></tr><tr><td>0,916</td><td>0,004</td><td>G-protein-coupled receptor kinase inhibitor</td></tr><tr><td>0,916</td><td>0,004</td><td>Beta-adrenergic receptor kinase inhibitor</td></tr><tr><td>0,905</td><td>0,004</td><td>Anaphylatoxin receptor antagonist</td></tr></table></div>                                                                                                                                                   | Pa    | Pi                                               | Activity                         | 0,953 | 0,000 | 4-Coumarate-CoA ligase inhibitor                 | 0,948 | 0,004 | Membrane integrity agonist        | 0,943 | 0,004 | CDP-glycerol glycerophosphotransferase inhibitor | 0,932 | 0,002 | Vasoprotector                    | 0,922 | 0,003 | Antiprotozoal (Leishmania)               | 0,918 | 0,004 | Sugar-phosphatase inhibitor                      | 0,917 | 0,004 | Alkenylglycerophosphocholine hydrolase inhibitor | 0,916 | 0,004 | G-protein-coupled receptor kinase inhibitor | 0,916 | 0,004 | Beta-adrenergic receptor kinase inhibitor | 0,905 | 0,004 | Anaphylatoxin receptor antagonist | Syringin       |       |                           |       |       |                               |           |
| Pa                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | Pi    | Activity                                         |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,953                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,000 | 4-Coumarate-CoA ligase inhibitor                 |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,948                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,004 | Membrane integrity agonist                       |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,943                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,004 | CDP-glycerol glycerophosphotransferase inhibitor |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,932                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,002 | Vasoprotector                                    |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,922                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,003 | Antiprotozoal (Leishmania)                       |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,918                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,004 | Sugar-phosphatase inhibitor                      |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,917                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,004 | Alkenylglycerophosphocholine hydrolase inhibitor |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,916                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,004 | G-protein-coupled receptor kinase inhibitor      |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,916                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,004 | Beta-adrenergic receptor kinase inhibitor        |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,905                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,004 | Anaphylatoxin receptor antagonist                |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| <div><table><tr><td>0,927</td><td>0,001</td><td>Pyruvate dehydrogenase inhibitor</td></tr><tr><td>0,926</td><td>0,001</td><td>Benzoylformate decarboxylase inhibitor</td></tr><tr><td>0,925</td><td>0,001</td><td>tRNA adenyltransferase inhibitor</td></tr><tr><td>0,923</td><td>0,002</td><td>D-lactaldehyde dehydrogenase inhibitor</td></tr><tr><td>0,922</td><td>0,001</td><td>Glutathione peroxidase inhibitor</td></tr><tr><td>0,921</td><td>0,001</td><td>Aldehyde dehydrogenase (NADP+) inhibitor</td></tr><tr><td>0,926</td><td>0,006</td><td>CDP-glycerol glycerophosphotransferase inhibitor</td></tr><tr><td>0,922</td><td>0,003</td><td>Cytostatic</td></tr><tr><td>0,918</td><td>0,003</td><td>Cyclic AMP phosphodiesterase inhibitor</td></tr><tr><td>0,918</td><td>0,003</td><td>Vasodilator, coronary</td></tr><tr><td>0,915</td><td>0,001</td><td>Lipotropic</td></tr><tr><td>0,914</td><td>0,000</td><td>3'-Nucleotidase inhibitor</td></tr><tr><td>0,914</td><td>0,001</td><td>Uric acid excretion stimulant</td></tr></table></div> | 0,927 | 0,001                                            | Pyruvate dehydrogenase inhibitor | 0,926 | 0,001 | Benzoylformate decarboxylase inhibitor           | 0,925 | 0,001 | tRNA adenyltransferase inhibitor  | 0,923 | 0,002 | D-lactaldehyde dehydrogenase inhibitor           | 0,922 | 0,001 | Glutathione peroxidase inhibitor | 0,921 | 0,001 | Aldehyde dehydrogenase (NADP+) inhibitor | 0,926 | 0,006 | CDP-glycerol glycerophosphotransferase inhibitor | 0,922 | 0,003 | Cytostatic                                       | 0,918 | 0,003 | Cyclic AMP phosphodiesterase inhibitor      | 0,918 | 0,003 | Vasodilator, coronary                     | 0,915 | 0,001 | Lipotropic                        | 0,914          | 0,000 | 3'-Nucleotidase inhibitor | 0,914 | 0,001 | Uric acid excretion stimulant | Adenosine |
| 0,927                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,001 | Pyruvate dehydrogenase inhibitor                 |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,926                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,001 | Benzoylformate decarboxylase inhibitor           |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,925                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,001 | tRNA adenyltransferase inhibitor                 |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,923                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,002 | D-lactaldehyde dehydrogenase inhibitor           |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,922                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,001 | Glutathione peroxidase inhibitor                 |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,921                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,001 | Aldehyde dehydrogenase (NADP+) inhibitor         |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,926                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,006 | CDP-glycerol glycerophosphotransferase inhibitor |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,922                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,003 | Cytostatic                                       |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,918                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,003 | Cyclic AMP phosphodiesterase inhibitor           |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,918                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,003 | Vasodilator, coronary                            |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,915                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,001 | Lipotropic                                       |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,914                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,000 | 3'-Nucleotidase inhibitor                        |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,914                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,001 | Uric acid excretion stimulant                    |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| <div><div><div><div><div><div></div><div>All</div></div><div><div></div><div>Pa&gt;Pi</div></div><div><div></div><div>Pa&gt;0,3</div></div><div><div></div><div>Pa&gt;0,7</div></div><div><div></div><div>ok</div></div></div></div></div></div>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |       |                                                  |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| <div><table><tr><th>Pa</th><th>Pi</th><th>Activity</th></tr><tr><td>0,910</td><td>0,008</td><td>CDP-glycerol glycerophosphotransferase inhibitor</td></tr><tr><td>0,889</td><td>0,004</td><td>Anaphylatoxin receptor antagonist</td></tr><tr><td>0,792</td><td>0,019</td><td>CYP2H substrate</td></tr><tr><td>0,790</td><td>0,018</td><td>Benzoate-CoA ligase inhibitor</td></tr><tr><td>0,765</td><td>0,004</td><td>Antitussive</td></tr><tr><td>0,762</td><td>0,004</td><td>Lactase inhibitor</td></tr><tr><td>0,758</td><td>0,002</td><td>Laxative</td></tr><tr><td>0,764</td><td>0,008</td><td>Nucleotide metabolism regulator</td></tr><tr><td>0,729</td><td>0,004</td><td>Histamine release stimulant</td></tr><tr><td>0,719</td><td>0,003</td><td>CYP2E1 inducer</td></tr></table></div>                                                                                                                                                                                                                                                           | Pa    | Pi                                               | Activity                         | 0,910 | 0,008 | CDP-glycerol glycerophosphotransferase inhibitor | 0,889 | 0,004 | Anaphylatoxin receptor antagonist | 0,792 | 0,019 | CYP2H substrate                                  | 0,790 | 0,018 | Benzoate-CoA ligase inhibitor    | 0,765 | 0,004 | Antitussive                              | 0,762 | 0,004 | Lactase inhibitor                                | 0,758 | 0,002 | Laxative                                         | 0,764 | 0,008 | Nucleotide metabolism regulator             | 0,729 | 0,004 | Histamine release stimulant               | 0,719 | 0,003 | CYP2E1 inducer                    | Tinoscorside A |       |                           |       |       |                               |           |
| Pa                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | Pi    | Activity                                         |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,910                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,008 | CDP-glycerol glycerophosphotransferase inhibitor |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,889                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,004 | Anaphylatoxin receptor antagonist                |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,792                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,019 | CYP2H substrate                                  |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,790                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,018 | Benzoate-CoA ligase inhibitor                    |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,765                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,004 | Antitussive                                      |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,762                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,004 | Lactase inhibitor                                |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,758                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,002 | Laxative                                         |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,764                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,008 | Nucleotide metabolism regulator                  |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,729                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,004 | Histamine release stimulant                      |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |
| 0,719                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 0,003 | CYP2E1 inducer                                   |                                  |       |       |                                                  |       |       |                                   |       |       |                                                  |       |       |                                  |       |       |                                          |       |       |                                                  |       |       |                                                  |       |       |                                             |       |       |                                           |       |       |                                   |                |       |                           |       |       |                               |           |



### Lampiran 10 Uji Studi *In Silico* SwissAdme

| <table> <tr> <th colspan="2">Pharmacokinetics</th></tr> <tr> <td>GI absorption</td><td>Low</td></tr> <tr> <td>BBB permeant</td><td>No</td></tr> <tr> <td>P-gp substrate</td><td>No</td></tr> <tr> <td>CYP1A2 inhibitor</td><td>No</td></tr> <tr> <td>CYP2C19 inhibitor</td><td>No</td></tr> <tr> <td>CYP2C9 inhibitor</td><td>No</td></tr> <tr> <td>CYP2D6 inhibitor</td><td>No</td></tr> <tr> <td>CYP3A4 inhibitor</td><td>No</td></tr> <tr> <td>Log <math>K_p</math> (skin permeation)</td><td>-9.50 cm/s</td></tr> <tr> <th colspan="2">Druglikeness</th></tr> <tr> <td>Lipinski</td><td>Yes; 0 violation</td></tr> <tr> <td>Ghose</td><td>No; 1 violation: WLOGP&lt;-0.4</td></tr> <tr> <td>Veber</td><td>Yes</td></tr> <tr> <td>Egan</td><td>No; 1 violation: TPSA&gt;131.6</td></tr> <tr> <td>Muegge</td><td>Yes</td></tr> <tr> <td>Bioavailability Score</td><td>0.55</td></tr> </table>                                                                                                                                                                   | Pharmacokinetics                                        |  | GI absorption | Low | BBB permeant | No | P-gp substrate | No  | CYP1A2 inhibitor | No | CYP2C19 inhibitor | No | CYP2C9 inhibitor | No | CYP2D6 inhibitor | No | CYP3A4 inhibitor | No | Log $K_p$ (skin permeation) | -9.50 cm/s  | Druglikeness |  | Lipinski | Yes; 0 violation                            | Ghose | No; 1 violation: WLOGP<-0.4                             | Veber | Yes                       | Egan | No; 1 violation: TPSA>131.6 | Muegge | Yes                                                   | Bioavailability Score | 0.55 | Syringin       |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------|--|---------------|-----|--------------|----|----------------|-----|------------------|----|-------------------|----|------------------|----|------------------|----|------------------|----|-----------------------------|-------------|--------------|--|----------|---------------------------------------------|-------|---------------------------------------------------------|-------|---------------------------|------|-----------------------------|--------|-------------------------------------------------------|-----------------------|------|----------------|
| Pharmacokinetics                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                         |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| GI absorption                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Low                                                     |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| BBB permeant                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| P-gp substrate                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| CYP1A2 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| CYP2C19 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| CYP2C9 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| CYP2D6 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| CYP3A4 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Log $K_p$ (skin permeation)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | -9.50 cm/s                                              |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Druglikeness                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                         |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Lipinski                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Yes; 0 violation                                        |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Ghose                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | No; 1 violation: WLOGP<-0.4                             |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Veber                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | Yes                                                     |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Egan                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | No; 1 violation: TPSA>131.6                             |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Muegge                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | Yes                                                     |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Bioavailability Score                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 0.55                                                    |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| <table> <tr> <th colspan="2">Pharmacokinetics</th></tr> <tr> <td>GI absorption</td><td>Low</td></tr> <tr> <td>BBB permeant</td><td>No</td></tr> <tr> <td>P-gp substrate</td><td>No</td></tr> <tr> <td>CYP1A2 inhibitor</td><td>No</td></tr> <tr> <td>CYP2C19 inhibitor</td><td>No</td></tr> <tr> <td>CYP2C9 inhibitor</td><td>No</td></tr> <tr> <td>CYP2D6 inhibitor</td><td>No</td></tr> <tr> <td>CYP3A4 inhibitor</td><td>No</td></tr> <tr> <td>Log <math>K_p</math> (skin permeation)</td><td>-8.68 cm/s</td></tr> <tr> <th colspan="2">Druglikeness</th></tr> <tr> <td>Lipinski</td><td>Yes; 0 violation</td></tr> <tr> <td>Ghose</td><td>No; 1 violation: WLOGP&lt;-0.4</td></tr> <tr> <td>Veber</td><td>Yes</td></tr> <tr> <td>Egan</td><td>No; 1 violation: TPSA&gt;131.6</td></tr> <tr> <td>Muegge</td><td>Yes</td></tr> <tr> <td>Bioavailability Score</td><td>0.55</td></tr> </table>                                                                                                                                                                   | Pharmacokinetics                                        |  | GI absorption | Low | BBB permeant | No | P-gp substrate | No  | CYP1A2 inhibitor | No | CYP2C19 inhibitor | No | CYP2C9 inhibitor | No | CYP2D6 inhibitor | No | CYP3A4 inhibitor | No | Log $K_p$ (skin permeation) | -8.68 cm/s  | Druglikeness |  | Lipinski | Yes; 0 violation                            | Ghose | No; 1 violation: WLOGP<-0.4                             | Veber | Yes                       | Egan | No; 1 violation: TPSA>131.6 | Muegge | Yes                                                   | Bioavailability Score | 0.55 | Adenosine      |
| Pharmacokinetics                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                         |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| GI absorption                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Low                                                     |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| BBB permeant                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| P-gp substrate                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| CYP1A2 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| CYP2C19 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| CYP2C9 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| CYP2D6 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| CYP3A4 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Log $K_p$ (skin permeation)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | -8.68 cm/s                                              |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Druglikeness                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                         |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Lipinski                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Yes; 0 violation                                        |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Ghose                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | No; 1 violation: WLOGP<-0.4                             |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Veber                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | Yes                                                     |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Egan                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | No; 1 violation: TPSA>131.6                             |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Muegge                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | Yes                                                     |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Bioavailability Score                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 0.55                                                    |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| <table> <tr> <th colspan="2">Pharmacokinetics</th></tr> <tr> <td>GI absorption</td><td>Low</td></tr> <tr> <td>BBB permeant</td><td>No</td></tr> <tr> <td>P-gp substrate</td><td>Yes</td></tr> <tr> <td>CYP1A2 inhibitor</td><td>No</td></tr> <tr> <td>CYP2C19 inhibitor</td><td>No</td></tr> <tr> <td>CYP2C9 inhibitor</td><td>No</td></tr> <tr> <td>CYP2D6 inhibitor</td><td>No</td></tr> <tr> <td>CYP3A4 inhibitor</td><td>No</td></tr> <tr> <td>Log <math>K_p</math> (skin permeation)</td><td>-10.66 cm/s</td></tr> <tr> <th colspan="2">Druglikeness</th></tr> <tr> <td>Lipinski</td><td>No; 3 violations: MW&gt;500, NorO&gt;10, NHorOH&gt;5</td></tr> <tr> <td>Ghose</td><td>No; 4 violations: MW&gt;480, WLOGP&lt;-0.4, MR&gt;130, #atoms&gt;70</td></tr> <tr> <td>Veber</td><td>No; 1 violation: TPSA&gt;140</td></tr> <tr> <td>Egan</td><td>No; 1 violation: TPSA&gt;131.6</td></tr> <tr> <td>Muegge</td><td>No; 4 violations: MW&gt;600, TPSA&gt;150, H-acc&gt;10, H-don&gt;5</td></tr> <tr> <td>Bioavailability Score</td><td>0.17</td></tr> </table> | Pharmacokinetics                                        |  | GI absorption | Low | BBB permeant | No | P-gp substrate | Yes | CYP1A2 inhibitor | No | CYP2C19 inhibitor | No | CYP2C9 inhibitor | No | CYP2D6 inhibitor | No | CYP3A4 inhibitor | No | Log $K_p$ (skin permeation) | -10.66 cm/s | Druglikeness |  | Lipinski | No; 3 violations: MW>500, NorO>10, NHorOH>5 | Ghose | No; 4 violations: MW>480, WLOGP<-0.4, MR>130, #atoms>70 | Veber | No; 1 violation: TPSA>140 | Egan | No; 1 violation: TPSA>131.6 | Muegge | No; 4 violations: MW>600, TPSA>150, H-acc>10, H-don>5 | Bioavailability Score | 0.17 | Tinoscorside A |
| Pharmacokinetics                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                         |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| GI absorption                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Low                                                     |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| BBB permeant                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| P-gp substrate                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | Yes                                                     |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| CYP1A2 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| CYP2C19 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| CYP2C9 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| CYP2D6 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| CYP3A4 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | No                                                      |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Log $K_p$ (skin permeation)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | -10.66 cm/s                                             |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Druglikeness                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                         |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Lipinski                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | No; 3 violations: MW>500, NorO>10, NHorOH>5             |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Ghose                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | No; 4 violations: MW>480, WLOGP<-0.4, MR>130, #atoms>70 |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Veber                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | No; 1 violation: TPSA>140                               |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Egan                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | No; 1 violation: TPSA>131.6                             |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Muegge                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | No; 4 violations: MW>600, TPSA>150, H-acc>10, H-don>5   |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |
| Bioavailability Score                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 0.17                                                    |  |               |     |              |    |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |             |              |  |          |                                             |       |                                                         |       |                           |      |                             |        |                                                       |                       |      |                |

| <table> <tr> <th colspan="2">Pharmacokinetics</th></tr> <tr> <td>GI absorption </td><td>Low</td></tr> <tr> <td>BBB permeant </td><td>No</td></tr> <tr> <td>P-gp substrate </td><td>Yes</td></tr> <tr> <td>CYP1A2 inhibitor </td><td>No</td></tr> <tr> <td>CYP2C19 inhibitor </td><td>No</td></tr> <tr> <td>CYP2C9 inhibitor </td><td>No</td></tr> <tr> <td>CYP2D6 inhibitor </td><td>No</td></tr> <tr> <td>CYP3A4 inhibitor </td><td>No</td></tr> <tr> <td>Log <math>K_p</math> (skin permeation) </td><td>-9.79 cm/s</td></tr> <tr> <th colspan="2">Druglikeness</th></tr> <tr> <td>Lipinski </td><td>No; 2 violations: MW&gt;500, NorO&gt;10</td></tr> <tr> <td>Ghose </td><td>No; 3 violations: MW&gt;480, WLOGP&lt;-0.4, #atoms&gt;70</td></tr> <tr> <td>Veber </td><td>No; 1 violation: TPSA&gt;140</td></tr> <tr> <td>Egan </td><td>No; 1 violation: TPSA&gt;131.6</td></tr> <tr> <td>Muegge </td><td>No; 2 violations: TPSA&gt;150, H-acc&gt;10</td></tr> <tr> <td>Bioavailability Score </td><td>0.17</td></tr> </table> | Pharmacokinetics                                |  | GI absorption | Low  | BBB permeant | No  | P-gp substrate | Yes | CYP1A2 inhibitor | No | CYP2C19 inhibitor | No | CYP2C9 inhibitor | No | CYP2D6 inhibitor | No | CYP3A4 inhibitor | No | Log $K_p$ (skin permeation) | -9.79 cm/s | Druglikeness |  | Lipinski | No; 2 violations: MW>500, NorO>10 | Ghose | No; 3 violations: MW>480, WLOGP<-0.4, #atoms>70 | Veber | No; 1 violation: TPSA>140 | Egan | No; 1 violation: TPSA>131.6 | Muegge | No; 2 violations: TPSA>150, H-acc>10 | Bioavailability Score | 0.17 | Borapetoside A |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------|--|---------------|------|--------------|-----|----------------|-----|------------------|----|-------------------|----|------------------|----|------------------|----|------------------|----|-----------------------------|------------|--------------|--|----------|-----------------------------------|-------|-------------------------------------------------|-------|---------------------------|------|-----------------------------|--------|--------------------------------------|-----------------------|------|----------------|
| Pharmacokinetics                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                 |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| GI absorption                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | Low                                             |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| BBB permeant                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | No                                              |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| P-gp substrate                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | Yes                                             |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| CYP1A2 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | No                                              |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| CYP2C19 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | No                                              |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| CYP2C9 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | No                                              |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| CYP2D6 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | No                                              |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| CYP3A4 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | No                                              |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Log $K_p$ (skin permeation)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -9.79 cm/s                                      |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Druglikeness                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                 |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Lipinski                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | No; 2 violations: MW>500, NorO>10               |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Ghose                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | No; 3 violations: MW>480, WLOGP<-0.4, #atoms>70 |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Veber                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | No; 1 violation: TPSA>140                       |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Egan                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | No; 1 violation: TPSA>131.6                     |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Muegge                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | No; 2 violations: TPSA>150, H-acc>10            |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Bioavailability Score                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 0.17                                            |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| <table> <tr> <th colspan="2">Pharmacokinetics</th></tr> <tr> <td>GI absorption </td><td>High</td></tr> <tr> <td>BBB permeant </td><td>Yes</td></tr> <tr> <td>P-gp substrate </td><td>No</td></tr> <tr> <td>CYP1A2 inhibitor </td><td>No</td></tr> <tr> <td>CYP2C19 inhibitor </td><td>No</td></tr> <tr> <td>CYP2C9 inhibitor </td><td>No</td></tr> <tr> <td>CYP2D6 inhibitor </td><td>No</td></tr> <tr> <td>CYP3A4 inhibitor </td><td>No</td></tr> <tr> <td>Log <math>K_p</math> (skin permeation) </td><td>-6.36 cm/s</td></tr> <tr> <th colspan="2">Druglikeness</th></tr> <tr> <td>Lipinski </td><td>Yes; 0 violation</td></tr> <tr> <td>Ghose </td><td>No; 1 violation: MW&lt;160</td></tr> <tr> <td>Veber </td><td>Yes</td></tr> <tr> <td>Egan </td><td>Yes</td></tr> <tr> <td>Muegge </td><td>No; 1 violation: MW&lt;200</td></tr> <tr> <td>Bioavailability Score </td><td>0.55</td></tr> </table>                                                                                                                         | Pharmacokinetics                                |  | GI absorption | High | BBB permeant | Yes | P-gp substrate | No  | CYP1A2 inhibitor | No | CYP2C19 inhibitor | No | CYP2C9 inhibitor | No | CYP2D6 inhibitor | No | CYP3A4 inhibitor | No | Log $K_p$ (skin permeation) | -6.36 cm/s | Druglikeness |  | Lipinski | Yes; 0 violation                  | Ghose | No; 1 violation: MW<160                         | Veber | Yes                       | Egan | Yes                         | Muegge | No; 1 violation: MW<200              | Bioavailability Score | 0.55 | Tyramine       |
| Pharmacokinetics                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                 |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| GI absorption                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | High                                            |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| BBB permeant                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Yes                                             |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| P-gp substrate                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | No                                              |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| CYP1A2 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | No                                              |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| CYP2C19 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | No                                              |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| CYP2C9 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | No                                              |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| CYP2D6 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | No                                              |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| CYP3A4 inhibitor                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | No                                              |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Log $K_p$ (skin permeation)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | -6.36 cm/s                                      |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Druglikeness                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                 |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Lipinski                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | Yes; 0 violation                                |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Ghose                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | No; 1 violation: MW<160                         |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Veber                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | Yes                                             |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Egan                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | Yes                                             |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Muegge                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | No; 1 violation: MW<200                         |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |
| Bioavailability Score                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 0.55                                            |  |               |      |              |     |                |     |                  |    |                   |    |                  |    |                  |    |                  |    |                             |            |              |  |          |                                   |       |                                                 |       |                           |      |                             |        |                                      |                       |      |                |

### Lampiran 11 Uji Studi *In Silico* ProTox-3.0

Predicted LD50: 4000mg/kg

Predicted Toxicity Class: 5

Toxicity Model Report

Copy

Excel

CSV

PDF

| Classification      | Target          | Shorthand | Prediction | Probability |
|---------------------|-----------------|-----------|------------|-------------|
| Organ toxicity      | Hepatotoxicity  | dili      | Inactive   | 0.83        |
| Toxicity end points | Carcinogenicity | carcino   | Inactive   | 0.85        |
| Toxicity end points | Immunotoxicity  | immuno    | Active     | 0.92        |
| Toxicity end points | Mutagenicity    | mutagen   | Inactive   | 0.80        |
| Toxicity end points | Cytotoxicity    | cyto      | Inactive   | 0.76        |

Syringin

Predicted LD50: 8mg/kg

Predicted Toxicity Class: 2

Toxicity Model Report

Copy

Excel

CSV

PDF

| Classification      | Target          | Shorthand | Prediction | Probability |
|---------------------|-----------------|-----------|------------|-------------|
| Organ toxicity      | Hepatotoxicity  | dili      | Inactive   | 0.84        |
| Toxicity end points | Carcinogenicity | carcino   | Inactive   | 0.71        |
| Toxicity end points | Immunotoxicity  | immuno    | Inactive   | 0.99        |
| Toxicity end points | Mutagenicity    | mutagen   | Inactive   | 0.87        |
| Toxicity end points | Cytotoxicity    | cyto      | Active     | 0.74        |

Adenosine

Predicted LD50: 240mg/kg

Predicted Toxicity Class: 3

Toxicity Model Report

Copy

Excel

CSV

PDF

| Classification      | Target          | Shorthand | Prediction | Probability |
|---------------------|-----------------|-----------|------------|-------------|
| Organ toxicity      | Hepatotoxicity  | dili      | Inactive   | 0.88        |
| Toxicity end points | Carcinogenicity | carcino   | Inactive   | 0.66        |
| Toxicity end points | Immunotoxicity  | immuno    | Active     | 0.99        |
| Toxicity end points | Mutagenicity    | mutagen   | Inactive   | 0.69        |
| Toxicity end points | Cytotoxicity    | cyto      | Inactive   | 0.66        |

Tinoscorside A

Predicted LD50: 244mg/kg

Predicted Toxicity Class: 3

Toxicity Model Report

Copy

Excel

CSV

PDF

| Classification      | Target          | Shorthand | Prediction | Probability |
|---------------------|-----------------|-----------|------------|-------------|
| Organ toxicity      | Hepatotoxicity  | dili      | Inactive   | 0.91        |
| Toxicity end points | Carcinogenicity | carcino   | Inactive   | 0.83        |
| Toxicity end points | Immunotoxicity  | immuno    | Active     | 0.99        |
| Toxicity end points | Mutagenicity    | mutagen   | Inactive   | 0.74        |
| Toxicity end points | Cytotoxicity    | cyto      | Active     | 0.62        |

Borapetoside A



Predicted LD50: 1090mg/kg

Predicted Toxicity Class: 4

Toxicity Model Report

Copy

Excel

CSV

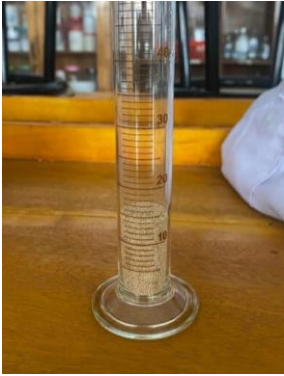
PDF

| Classification      | Target          | Shorthand | Prediction | Probability |
|---------------------|-----------------|-----------|------------|-------------|
| Organ toxicity      | Hepatotoxicity  | dili      | Inactive   | 0.95        |
| Toxicity end points | Carcinogenicity | carcino   | Inactive   | 0.68        |
| Toxicity end points | Immunotoxicity  | immuno    | Inactive   | 0.99        |
| Toxicity end points | Mutagenicity    | mutagen   | Inactive   | 0.62        |
| Toxicity end points | Cytotoxicity    | cyto      | Inactive   | 0.80        |

Tyramine

## Lampiran 12 Uji Stabilitas Fisik Sediaan

|                                                                                     |                              |
|-------------------------------------------------------------------------------------|------------------------------|
|   | <p>Uji kadar air granul</p>  |
|  | <p>Uji waktu alir granul</p> |

|                                                                                                                                                                                                                                                                                                       |                                   |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------|
|  A photograph showing a granule angle test. A metal funnel is positioned above a yellow circular target with concentric circles. A conical pile of brown granules has been poured onto the target, forming a peak.   | <p>Uji sudut diam granul</p>      |
|  A photograph of a granule compressibility test. A clear cylindrical tube with a scale inside is placed on a wooden surface. The tube is partially filled with brown granules, and a plunger is visible at the top. | <p>Uji kompresibilitas granul</p> |
|  A photograph showing three small glass petri dishes arranged in a row. Each dish contains a small pile of light-colored, spherical granules, used for organoleptic testing.                                       | <p>Uji organoleptik</p>           |
|  A photograph of a weight uniformity test. A single light-colored granule is placed on a white weighing paper. Below the paper is a digital scale with a display showing '0.44'.                                   | <p>Uji keseragaman bobot</p>      |

|                                                                                                                                                                                                                                                                                                                                            |                               |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------|
|  A digital caliper is shown measuring a small, light-colored cylindrical object. The digital display shows the number 12.01. The caliper has a silver body and a black digital screen.                                                                    | <p>Uji keseragaman ukuran</p> |
|  A vertical metal rod is shown with a white cloth wrapped around its middle section. The rod has a threaded top and bottom section.                                                                                                                      | <p>Uji kekerasan</p>          |
|  A BIOBASE environmental test chamber is shown. It has a white body with a blue digital display on the front. The display shows the numbers 20.0 and 20.0. The chamber has two large circular doors on the sides.                                       | <p>Uji kerapuhan</p>          |
|  A BIOBASE environmental test chamber is shown with two test samples inside. The chamber has a white body with a blue digital display on the front. The display shows the numbers 20.0 and 20.0. The chamber has two large circular doors on the sides. | <p>Uji waktu hancur</p>       |

**Aisyah Yadin**

**(1) PENGEMBANGAN TABLET EKSTRAK BROTOWALI  
(Tinospora crispa) SEBAGAI AGEN ANTIMALARIA BERDASAR ...**

 Farmasi  
 Fak. Ilmu Kesehatan  
 LLDIKTI IX Turnitin Consortium Part III

**Document Details**

Submission ID  
trn:old::1:3604479224

Submission Date  
Jul 1, 2026, 8:12 AM GMT+7

Download Date  
Jul 1, 2026, 8:20 AM GMT+7

File Name  
SKRIPSI\_AISYAH\_YADINN\_2026\_-\_Meisya\_Azahrah\_C3.pdf

File Size  
3.6 MB



127 Pages  
17,849 Words  
120,694 Characters

Page 2 of 133 - Integrity Overview

Submission ID trnoid::1:3604479224

## 10% Overall Similarity

The combined total of all matches, including overlapping sources, for each database.

### Filtered from the Report

- Bibliography
- Quoted Text
- Small Matches (less than 12 words)

### Top Sources

|    |                                                                                                                    |
|----|--------------------------------------------------------------------------------------------------------------------|
| 7% |  Internet sources                 |
| 4% |  Publications                     |
| 4% |  Submitted works (Student Papers) |

### Integrity Flags

**0 Integrity Flags for Review**

No suspicious text manipulations found.

Our system's algorithms look deeply at a document for any inconsistencies that would set it apart from a normal submission. If we notice something strange, we flag it for you to review.

A Flag is not necessarily an indicator of a problem. However, we'd recommend you focus your attention there for further review.

Page 2 of 133 - Integrity Overview

Submission ID trnoid::1:3604479224