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LAMPIRAN

Lampiran 1. Surat Izin Penelitian di Laboratorium Penelitian UMY



LABORATORIUM FITOMEDISINAL
 PRODI FARMASI FKIK UMY
 Jl. Lingkar Selatan, Tamantirto, Kasihan, Bantul, Yogyakarta 55183
 Telp. (0274) 387656, Fax. (0274) 387646

PRODI FARMASI FAKULTAS KEDOKTERAN DAN ILMU KESEHATAN UMY FORMULIR PENDAFTARAN "PEMBUATAN EKSTRAK"	No. Dokumen : 4/FITO/FKUMY/I/2012
	Tanggal Terbit : 1 Januari 2012
	No. Revisi : 0
	Halaman : 1 dari 1

Nama	Dita Prabaningrum Handayani
Alamat	Petum Winong FG II 1A15 Kotagede Yogyakarta
Instansi	Farmasi
No. Telp/ HP	081229 77 85 44
Nama sampel	Mengkeudu
Kode sampel	
Pengujian	
Tanggal masuk	24 Februari 2014
Tanggal jadi	

Yogyakarta, 19 Februari 2014

Petugas penerima,

(Linggar W. U)

Yang mengajukan

(Dita P.H.)

Menyetujui,
 Kepala Lab. Fitomedisinal

(Rifki F, M.Sc, Apt.)

Lampiran 2. Surat Izin Penelitian di Laboratorium Parasitologi, Kedokteran UGM



BAGIAN PARASITOLOGI
FAKULTAS KEDOKTERAN UNIVERSITAS GADJAH MADA
Gedung Prof. Drs. R. Radlopoetro Lt. IV Sayap Timur, Sekip, Yogyakarta 55281.
Telp. (0274) 546215. Fax. 546215. E-mail : parasitfkugm@yahoo.com

Nomor : UGM/KU/Prst/ 525 /M/05/07
Hal : Ijin Penelitian. 4 November 2014

Kepada Yth. : DITA PRABANINGRUM HANDAYANI
PS Farmasi Fakultas Kedokteran dan Ilmu Kesehatan
Universitas Muhammadiyah Yogyakarta

Dengan hormat,

Menanggapi surat saudara tertanggal 8 Oktober 2014 tentang ijin untuk melakukan penelitian di Laboratorium Parasitologi yang berjudul:

"UJI KOMBINASI EKSTRAK ETIL ASETAT BUAH MENKUDU (*Morinda citrifolia* L.) DENGAN SENYAWA DOXORUBICIN PADA SEL KANKER PAYUDARA MCF-7 SECARA *IN VITRO* DAN *IN SILICO*"

Kami dapat mengijinkan penelitian tersebut dilakukan di Bag. Parasitologi FK. UGM., dengan catatan :

1. Mentaati peraturan yang berlaku di FK. UGM. dan Bag. Parasitologi FK. UGM.
2. Sebagai supervisor dalam melaksanakan penelitian ini adalah Prof. dr. Supargiyono, DTM&H., SU., PhD., SpParK., dengan Teknisi: Rumbiwati.
3. Menulis semua kegiatan dan hasil penelitian yang dilakukan di laboratorium dalam buku Log Penelitian; buku Log ditinggal di Laboratorium.
4. Menerapkan prinsip **Good Clinical Laboratory Practice** pada saat bekerja di laboratorium.
5. Setelah selesai melaporkan hasilnya kepada Kepala Bagian.

Atas perhatian dalam hal ini kami ucapkan terima kasih.

Kepala Bagian,

dr. Tri Baskoro T. Satoto, MSc., PhD.
NIP. 19580412 198601 1 001.

Tembusan Yth. : 1. Prof. dr. Supargiyono, DTM&H., SU., PhD., SpParK.
2. Rumbiwati
3. Arsip

Lampiran 3. Surat Determinasi Tanaman



BAGIAN BIOLOGI FARMASI
FAKULTAS FARMASI
UNIVERSITAS GADJAH MADA YOGYAKARTA
Alamat: Sekip Utara Jl. Katurang Km 4, Yogyakarta 55281
Telp. : 0274.542738, 0274.649.2568 Fax. +274-543120

SURAT KETERANGAN
No. : BF/285/ Ident/Det/VI/2014

Kepada Yth. :
Sdr/Sdr. Rajendra Agillion
NIM. 20130350068
Fakultas Farmasi UMY
Di Yogyakarta

Dengan hormat,

Bersama ini kami sampaikan hasil identifikasi/determinasi sampel yang Saudara kirimkan ke Bagian Biologi Farmasi, Fakultas Farmasi UGM, adalah :

No.Pendaftaran	Jenis	Suku
285	<i>Morinda citrifolia</i> L.	Rubiaceae

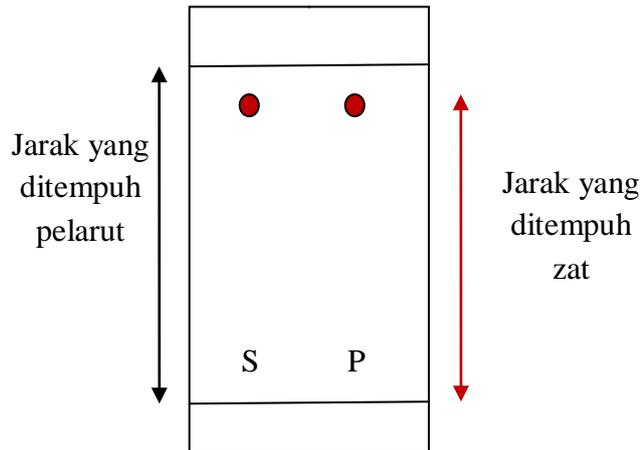
Demikian, semoga dapat digunakan sebagaimana mestinya.

Yogyakarta, 26 Juni 2014
Ketua


Prof. Dr. Wahyono, SU., Apt.
NIP. 195007011977021001

Lampiran 4. Perhitungan Hasil Uji KLT

Pengukuran nilai R_f KLT sebagai berikut :



$$R_f = \frac{\text{Jarak yang ditempuh zat}}{\text{jarak yang ditempuh pelarut}}$$

- $R_f = \frac{3,5}{8} = 0,44$
- $R_f = \frac{6}{8} = 0,75$
- $R_f = \frac{7}{8} = 0,87$

Lampiran 5. Perhitungan Hasil Uji Sitotoksik

a. Uji tunggal

- Ekstrak etil asetat buah mengkudu

Replikasi	Dosis ($\mu\text{g/mL}$)					
	750	375	187,5	93,75	46,88	23,44
1	0,115	0,116	0,315	0,546	0,484	0,466
2	0,114	0,107	0,412	0,452	0,484	0,44
3	0,119	0,126	0,289	0,447	0,448	0,401
Rata-rata	0,116	0,116	0,339	0,482	0,472	0,436
% Hidup	18,314	18,437	99,877	152,258	144,717	135,409

KONTROL	SEL	MEDIA
1	0,33	0,06
2	0,369	0,065
3	0,32	0,073
Rata rata	0,339	0,066

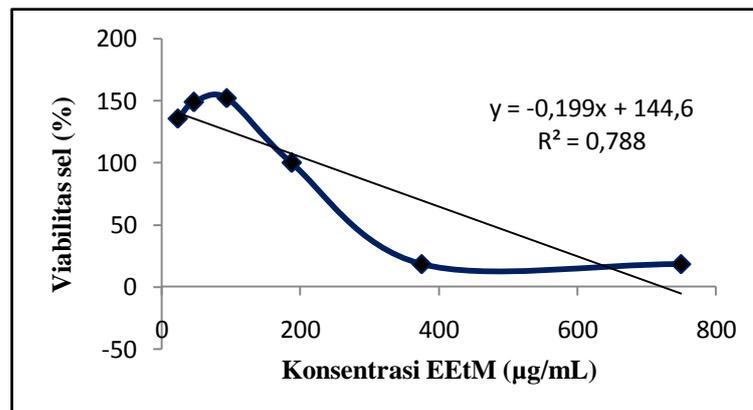
1. Rata-rata absorbansi tiap dosis

- Dosis 750 $= \frac{0,115+0,114+0,119}{3} = 0,116 \mu\text{g/ml}$
- Dosis 375 $= \frac{0,116+0,107+0,126}{3} = 0,116 \mu\text{g/ml}$
- Dosis 187,5 $= \frac{0,315+0,412+0,289}{3} = 0,339 \mu\text{g/ml}$
- Dosis 93,75 $= \frac{0,546+0,452+0,447}{3} = 0,482 \mu\text{g/ml}$
- Dosis 46,88 $= \frac{0,484+0,484+0,448}{3} = 0,472 \mu\text{g/ml}$
- Dosis 23,44 $= \frac{0,466+0,44+0,401}{3} = 0,436 \mu\text{g/ml}$

2. Presentasi Hidup Sel MCF-7

$$\% \text{ Hidup} = \frac{\text{Absorbansi perlakuan} - \text{Absorbansi kontrol media}}{\text{Absorbansi kontrol sel} - \text{Absorbansi kontrol media}} \times 100\%$$

- Dosis 750 = $\frac{0,116 - 0,066}{0,339 - 0,066} \times 100\% = 18,314 \%$
- Dosis 375 = $\frac{0,116 - 0,066}{0,339 - 0,066} \times 100\% = 18,437 \%$
- Dosis 187,5 = $\frac{0,339 - 0,066}{0,339 - 0,066} \times 100\% = 99,877 \%$
- Dosis 93,75 = $\frac{0,482 - 0,066}{0,339 - 0,066} \times 100\% = 152,258 \%$
- Dosis 46,88 = $\frac{0,472 - 0,066}{0,339 - 0,066} \times 100\% = 148,717 \%$
- Dosis 23,44 = $\frac{0,436 - 0,066}{0,339 - 0,066} \times 100\% = 135,409 \%$



Persamaan regresi linier : $Y = - 0,199x + 144,6$

$$Y = - 0,199x + 144,6$$

$$50 = - 0,199x + 144,6$$

$$X = \frac{144,6 - 50}{0,199}$$

$$X = 475 \mu\text{g/ml}$$

- *Doxorubicin*

Replikasi	Dosis ($\mu\text{g/mL}$)					
	25	12,5	6,25	3,125	1,563	0,782
1	0,071	0,099	0,207	0,27	0,264	0,259
2	0,083	0,097	0,197	0,222	0,261	0,226
3	0,074	0,104	0,231	0,256	0,269	0,247
Rata-rata	0,076	0,1	0,212	0,249	0,265	0,244
% Hidup	3,663	12,454	53,357	67,155	73	65,201

KONTROL	SEL	MEDIA
1	0,33	0,06
2	0,369	0,065
3	0,32	0,073
Rata rata	0,339	0,066

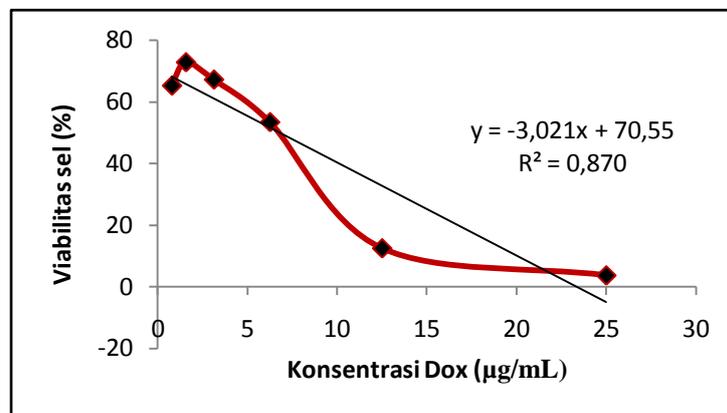
1. Rata-rata absorbansi tiap dosis

- Dosis 25 $= \frac{0,071+0,083+0,074}{3} = 0,076 \mu\text{g/ml}$
- Dosis 12,5 $= \frac{0,099+0,097+0,104}{3} = 0,1 \mu\text{g/ml}$
- Dosis 6,25 $= \frac{0,207+0,197+0,231}{3} = 0,212 \mu\text{g/ml}$
- Dosis 3,125 $= \frac{0,27+0,222+0,256}{3} = 0,249 \mu\text{g/ml}$
- Dosis 1,563 $= \frac{0,264+0,261+0,269}{3} = 0,265 \mu\text{g/ml}$
- Dosis 0,782 $= \frac{0,259+0,226+0,247}{3} = 0,244 \mu\text{g/ml}$

2. Presentasi Hidup Sel MCF-7

$$\% \text{ Hidup} = \frac{\text{Absorbansi perlakuan} - \text{Absorbansi kontrol media}}{\text{Absorbansi kontrol sel} - \text{Absorbansi kontrol media}} \times 100\%$$

- Dosis 25 = $\frac{0,076 - 0,066}{0,339 - 0,066} \times 100\% = 3,663 \%$
- Dosis 12,5 = $\frac{0,1 - 0,066}{0,339 - 0,066} \times 100\% = 12,454 \%$
- Dosis 6,25 = $\frac{0,212 - 0,066}{0,339 - 0,066} \times 100\% = 53,357 \%$
- Dosis 3,125 = $\frac{0,249 - 0,066}{0,339 - 0,066} \times 100\% = 67,155 \%$
- Dosis 1,563 = $\frac{0,265 - 0,066}{0,339 - 0,066} \times 100\% = 73 \%$
- Dosis 0,782 = $\frac{0,244 - 0,066}{0,339 - 0,066} \times 100\% = 65,201 \%$



Persamaan regresi linier : $Y = - 0,3021x + 70,55$

$$Y = - 0,3021x + 70,55$$

$$50 = - 0,3021x + 70,55$$

$$X = \frac{70,55 - 50}{0,3021}$$

$$X = 6,8 \mu\text{g/ml}$$

b. Uji Kombinasi

- Absorbansi

		Dox 0 µg/mL	Dox 0,875 µg/mL	Dox 1,75 µg/mL	Dox 2,625 µg/mL	Dox 3,5 µg/mL
	0	-	0,219	0,266	0,274	0,3
	60	0,391	0,227	0,271	0,229	0,256
EEtM	120	0,395	0,251	0,267	0,23	0,269
(µg/mL)	180	0,355	0,193	0,263	0,244	0,263
	240	0,384	0,257	0,258	0,251	0,249

KONTROL	SEL	MEDIA
1	0,527	0,124
2	0,482	0,122
3	0,445	0,134
Rata rata	0,485	0,127

- Viabilitas sel (%)

		Dox 0 µg/mL	Dox 0,875 µg/mL	Dox 1,75 µg/mL	Dox 2,625 µg/mL	Dox 3,5 µg/mL
	0	100	25,98	39,11	41,25	48,52
	60	74,02	28,12	40,32	28,77	36,22
EEtM	120	74,95	34,92	37,99	28,86	39,94
(µg/mL)	180	63,87	28,58	38,08	32,68	38,08
	240	71,97	36,87	36,78	34,64	34,26

- CI (*Combination Index*)

		Dox 0,875 µg/mL	Dox 1,75 µg/mL	Dox 2,625 µg/mL	Dox 3,5 µg/mL
	60	0,90	0,83	2,59	2,13
EEtM	120	0,59	0,97	2,58	1,69
(µg/mL)	180	0,88	0,97	2,02	1,91
	240	0,54	1,06	1,79	2,44

1. Rata-rata absorbansi tiap dosis

- EEtM 60µg/mL- Dox 0µg/mL $= \frac{0,399+0,406+0,37}{3} = 0,391 \mu\text{g/ml}$

- EEtM 60 μ g/mL- Dox 0,875 μ g/mL = $\frac{0,185+0,243+0,254}{3}$ = 0,227 μ g/ml
- EEtM 60 μ g/mL- Dox 1,75 μ g/mL = $\frac{0,307+0,251+0,255}{3}$ = 0,271 μ g/ml
- EEtM 60 μ g/mL- Dox 2,625 μ g/mL = $\frac{0,226+0,25+0,213}{3}$ = 0,229 μ g/ml
- EEtM 60 μ g/mL- Dox 3,5 μ g/mL = $\frac{0,247+0,267+0,255}{3}$ = 0,256 μ g/ml
- EEtM 120 μ g/mL- Dox 0 μ g/mL = $\frac{0,402+0,411+0,372}{3}$ = 0,395 μ g/ml
- EEtM 120 μ g/mL- Dox 0,875 μ g/mL = $\frac{0,252+0,253+0,25}{3}$ = 0,251 μ g/ml
- EEtM 120 μ g/mL- Dox 1,75 μ g/mL = $\frac{0,257+0,268+0,263}{3}$ = 0,267 μ g/ml
- EEtM 120 μ g/mL- Dox 2,625 μ g/mL = $\frac{0,241+0,254+0,222}{3}$ = 0,23 μ g/ml
- EEtM 120 μ g/mL- Dox 3,5 μ g/mL = $\frac{0,281+0,265+0,263}{3}$ = 0,269 μ g/ml
- EEtM 180 μ g/mL- Dox 0 μ g/mL = $\frac{0,358+0,355+0,353}{3}$ = 0,355 μ g/ml
- EEtM 180 μ g/mL- Dox 0,875 μ g/mL = $\frac{0,241+0,217}{2}$ = 0,193 μ g/ml
- EEtM 180 μ g/mL- Dox 1,75 μ g/mL = $\frac{0,261+0,278+0,25}{3}$ = 0,263 μ g/ml
- EEtM 180 μ g/mL- Dox 2,625 μ g/mL = $\frac{0,249+0,247+0,235}{3}$ = 0,244 μ g/ml
- EEtM 180 μ g/mL- Dox 3,5 μ g/mL = $\frac{0,26+0,267+0,262}{3}$ = 0,263 μ g/ml
- EEtM 240 μ g/mL- Dox 0 μ g/mL = $\frac{0,389+0,38+0,384}{3}$ = 0,384 μ g/ml
- EEtM 240 μ g/mL- Dox 0,875 μ g/mL = $\frac{0,255+0,273+0,248}{3}$ = 0,257 μ g/ml

- EEtM 240 μ g/mL- Dox 1,75 μ g/mL $= \frac{0,296+0,23+0,249}{3} = 0,258 \mu\text{g/ml}$
- EEtM 240 μ g/mL- Dox 2,625 μ g/mL $= \frac{0,244+0,262+0,246}{3} = 0,251 \mu\text{g/ml}$
- EEtM 240 μ g/mL- Dox 3,5 μ g/mL $= \frac{0,263+0,245+0,24}{3} = 0,249 \mu\text{g/ml}$
- EEtM 0 μ g/mL- Dox 0,875 μ g/mL $= \frac{0,215+0,225+0,219}{3} = 0,219 \mu\text{g/ml}$
- EEtM 0 μ g/mL- Dox 1,75 μ g/mL $= \frac{0,287+0,249+0,264}{3} = 0,266 \mu\text{g/ml}$
- EEtM 0 μ g/mL- Dox 2,625 μ g/mL $= \frac{0,288+0,272+0,263}{3} = 0,274 \mu\text{g/ml}$
- EEtM 0 μ g/mL- Dox 3,5 μ g/mL $= \frac{0,305+0,278+0,318}{3} = 0,3 \mu\text{g/ml}$

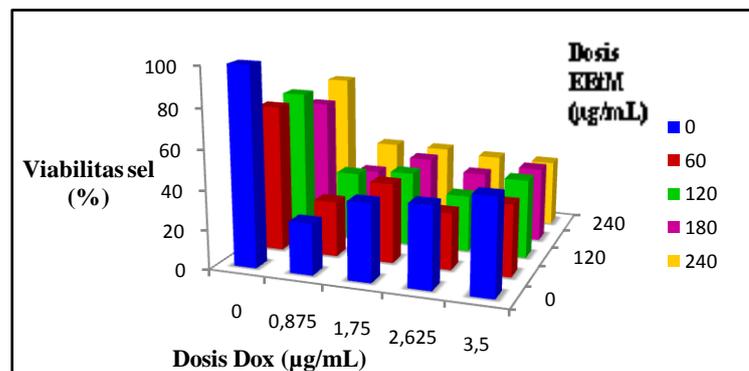
2. Presentasi Hidup Sel MCF-7

$$\% \text{ Hidup} = \frac{\text{Absorbansi perlakuan} - \text{Absorbansi kontrol media}}{\text{Absorbansi kontrol sel} - \text{Absorbansi kontrol media}} \times 100\%$$

- EEtM 60 μ g/mL- Dox 0 μ g/mL $= \frac{0,391 - 0,127}{0,485 - 0,127} \times 100\% = 74,02 \%$
- EEtM 60 μ g/mL- Dox 0,875 μ g/mL $= \frac{0,227 - 0,127}{0,485 - 0,127} \times 100\% = 28,12 \%$
- EEtM 60 μ g/mL- Dox 1,75 μ g/mL $= \frac{0,271 - 0,127}{0,485 - 0,127} \times 100\% = 40,32 \%$
- EEtM 60 μ g/mL- Dox 2,625 μ g/mL $= \frac{0,229 - 0,127}{0,485 - 0,127} \times 100\% = 28,77 \%$
- EEtM 60 μ g/mL- Dox 3,5 μ g/mL $= \frac{0,256 - 0,127}{0,485 - 0,127} \times 100\% = 36,22 \%$

- EEtM 120 μ g/mL- Dox 0 μ g/mL $= \frac{0,395 - 0,127}{0,485 - 0,127} \times 100\% = 74,95 \%$
- EEtM 120 μ g/mL- Dox 0,875 μ g/mL $= \frac{0,251 - 0,127}{0,485 - 0,127} \times 100\% = 34,92 \%$
- EEtM 120 μ g/mL- Dox 1,75 μ g/mL $= \frac{0,267 - 0,127}{0,485 - 0,127} \times 100\% = 37,99 \%$
- EEtM 120 μ g/mL- Dox 2,625 μ g/mL $= \frac{0,23 - 0,127}{0,485 - 0,127} \times 100\% = 28,86 \%$
- EEtM 120 μ g/mL- Dox 3,5 μ g/mL $= \frac{0,269 - 0,127}{0,485 - 0,127} \times 100\% = 39,94 \%$
- EEtM 180 μ g/mL- Dox 0 μ g/mL $= \frac{0,335 - 0,127}{0,485 - 0,127} \times 100\% = 63,87 \%$
- EEtM 180 μ g/mL- Dox 0,875 μ g/mL $= \frac{0,193 - 0,127}{0,485 - 0,127} \times 100\% = 28,58 \%$
- EEtM 180 μ g/mL- Dox 1,75 μ g/mL $= \frac{0,263 - 0,127}{0,485 - 0,127} \times 100\% = 38,08 \%$
- EEtM 180 μ g/mL- Dox 2,625 μ g/mL $= \frac{0,244 - 0,127}{0,485 - 0,127} \times 100\% = 32,68 \%$
- EEtM 180 μ g/mL- Dox 3,5 μ g/mL $= \frac{0,263 - 0,127}{0,485 - 0,127} \times 100\% = 38,08 \%$
- EEtM 240 μ g/mL- Dox 0 μ g/mL $= \frac{0,384 - 0,127}{0,485 - 0,127} \times 100\% = 71,97 \%$
- EEtM 240 μ g/mL- Dox 0,875 μ g/mL $= \frac{0,257 - 0,127}{0,485 - 0,127} \times 100\% = 36,87 \%$
- EEtM 240 μ g/mL- Dox 1,75 μ g/mL $= \frac{0,258 - 0,127}{0,485 - 0,127} \times 100\% = 36,78 \%$
- EEtM 240 μ g/mL- Dox 2,625 μ g/mL $= \frac{0,251 - 0,127}{0,485 - 0,127} \times 100\% = 34,64 \%$

- EEtM 240 μ g/mL- Dox 3,5 μ g/mL $= \frac{0,249 - 0,127}{0,485 - 0,127} \times 100\% = 34,26 \%$
- EEtM 0 μ g/mL- Dox 0,875 μ g/mL $= \frac{0,219 - 0,127}{0,485 - 0,127} \times 100\% = 25,98 \%$
- EEtM 0 μ g/mL- Dox 1,75 μ g/mL $= \frac{0,266 - 0,127}{0,485 - 0,127} \times 100\% = 39,11 \%$
- EEtM 0 μ g/mL- Dox 2,625 μ g/mL $= \frac{0,274 - 0,127}{0,485 - 0,127} \times 100\% = 41,52 \%$
- EEtM 0 μ g/mL- Dox 3,5 μ g/mL $= \frac{0,3 - 0,127}{0,485 - 0,127} \times 100\% = 48,52 \%$

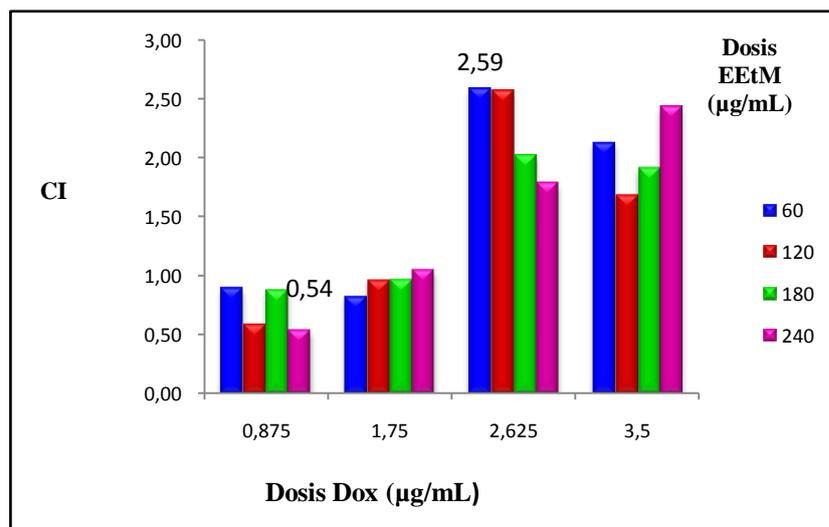


3. Nilai Index Kombinasi

$$CI = \frac{(D)1}{(Dx)1} + \frac{(D)2}{(Dx)2}$$

- EEtM 60 μ g/mL- Dox 0,875 μ g/mL $= \frac{60}{21564,3} + \frac{0,875}{0,972} = 0,90$
- EEtM 60 μ g/mL- Dox 1,75 μ g/mL $= \frac{60}{4779,3} + \frac{1,75}{2,151} = 0,83$
- EEtM 60 μ g/mL- Dox 2,625 μ g/mL $= \frac{60}{19896,1} + \frac{2,625}{1,014} = 2,59$
- EEtM 60 μ g/mL- Dox 3,5 μ g/mL $= \frac{60}{7927,8} + \frac{3,5}{1,647} = 2,13$
- EEtM 120 μ g/mL- Dox 0,875 μ g/mL $= \frac{120}{9312,9} + \frac{0,875}{1,513} = 0,59$

- EEtM 120 μ g/mL- Dox 1,75 μ g/mL $= \frac{120}{6371,5} + \frac{1,75}{1,848} = 0,97$
- EEtM 120 μ g/mL- Dox 2,625 μ g/mL $= \frac{120}{19668,6} + \frac{2,625}{1,020} = 2,58$
- EEtM 120 μ g/mL- Dox 3,5 μ g/mL $= \frac{120}{5004,3} + \frac{3,5}{2,099} = 1,69$
- EEtM 180 μ g/mL- Dox 0,875 μ g/mL $= \frac{180}{20359,1} + \frac{0,875}{1,002} = 0,88$
- EEtM 180 μ g/mL- Dox 1,75 μ g/mL $= \frac{180}{6298,7} + \frac{1,75}{1,859} = 0,97$
- EEtM 180 μ g/mL- Dox 2,625 μ g/mL $= \frac{180}{12273,6} + \frac{2,625}{1,308} = 2,02$
- EEtM 180 μ g/mL- Dox 3,5 μ g/mL $= \frac{180}{6298,7} + \frac{3,5}{1,859} = 1,91$
- EEtM 240 μ g/mL- Dox 0,875 μ g/mL $= \frac{240}{7314,5} + \frac{0,875}{1,718} = 0,54$
- EEtM 240 μ g/mL- Dox 1,75 μ g/mL $= \frac{240}{7399,1} + \frac{1,75}{1,708} = 1,06$
- EEtM 240 μ g/mL- Dox 2,625 μ g/mL $= \frac{240}{9639,9} + \frac{2,625}{1,486} = 1,79$
- EEtM 240 μ g/mL- Dox 3,5 μ g/mL $= \frac{240}{10093,7} + \frac{3,5}{1,450} = 2,44$



Lampiran 6. Hasil Perhitungan RMSD untuk Protein ER α

```
61 Hz Mem 98 Sys L YASARA View 58 Atoms
WARNING - Calculating RMSD between different atoms 28 ' C21' and 57 ' C25'
WARNING - Calculating RMSD between different residues 'OHT A 600' and 'non A 0'
WARNING - Calculating RMSD between different atoms 29 ' C22' and 58 ' C26'
WARNING - Calculating RMSD between different residues 'OHT A 600' and 'non A 0'
Molecule A and Molecule A have 1.7250 A RMSD
>
_
```

Lampiran 7. Hasil Perhitungan RMSD untuk Protein Bcl-xl

```
60 Hz Mem 98 Sys L YASARA View 32 Atoms
WARNING - Calculating RMSD between different residues '4FC A 1000' and 'non A 0'
WARNING - Calculating RMSD between different residues '4FC A 1000' and 'non A 0'
WARNING - Calculating RMSD between different residues '4FC A 1000' and 'non A 0'
WARNING - Calculating RMSD between different residues '4FC A 1000' and 'non A 0'
Molecule A and Molecule A have 0.3111 A RMSD
>
_
```

Lampiran 8. Hasil *Molecular Docking Native Ligand* dengan ER α

```
argevollen@argevollen-Satellite-L645: ~/docking/results
argevollen@argevollen-Satellite-L645:~/docking$ cd results
argevollen@argevollen-Satellite-L645:~/docking/results$ more bestranking.csv
TOTAL_SCORE,SCORE_RB_PEN,SCORE_NORM_HEVATOMS,SCORE_NORM_CRT_HEVATOMS,SCORE_NORM_WEIGHT,SCORE_NORM_CRT_WEIGHT,SCORE_RB_PEN_NORM_CRT_HEVATOMS,SCORE_NORM_CONTACT,EVAL,TIME
PROTEIN (ESTROGEN RECEPTOR ALPHA)_entry_00001_conf_01,-101.267,-83.2675,-3.49198,-32.9613,-0.260656,-13.8783,-27.1025,-3.26669,4916292,43.256
PROTEIN (ESTROGEN RECEPTOR ALPHA)_entry_00002_conf_01,-100.846,-82.8456,-3.47743,-32.8239,-0.25957,-13.8205,-26.9652,-3.25308,4791226,44.764
PROTEIN (ESTROGEN RECEPTOR ALPHA)_entry_00003_conf_01,-104.261,-86.2614,-3.59522,-33.9358,-0.268362,-14.2886,-28.077,-3.36327,4743809,41.796
PROTEIN (ESTROGEN RECEPTOR ALPHA)_entry_00004_conf_01,-99.1274,-81.1274,-3.41819,-32.2647,-0.255148,-13.585,-26.4059,-3.19766,4847420,42.772
PROTEIN (ESTROGEN RECEPTOR ALPHA)_entry_00005_conf_01,-100.862,-82.862,-3.478,-32.8293,-0.259612,-13.8227,-26.9705,-3.25361,5027965,44.68
PROTEIN (ESTROGEN RECEPTOR ALPHA)_entry_00006_conf_01,-100.886,-82.8862,-3.47884,-32.8372,-0.259675,-13.826,-26.9784,-3.25439,4786595,42.312
PROTEIN (ESTROGEN RECEPTOR ALPHA)_entry_00007_conf_01,-104.722,-86.7219,-3.6111,-34.0856,-0.269548,-14.3517,-28.2269,-3.37813,5034162,44.3
PROTEIN (ESTROGEN RECEPTOR ALPHA)_entry_00008_conf_01,-103.003,-85.0029,-3.55182,-33.5261,-0.265123,-14.1161,-27.6673,-3.32267,4780651,42.24
PROTEIN (ESTROGEN RECEPTOR ALPHA)_entry_00009_conf_01,-100.515,-82.5151,-3.46604,-32.7164,-0.25872,-13.7752,-26.8576,-3.24242,4819490,42.448
argevollen@argevollen-Satellite-L645:~/docking/results$
```

Lampiran 9. Hasil *Molecular Docking Native Ligand* dengan Bcl-xl

```
zephyrus@zephyrus-K43BY: ~/Docking/results
zephyrus@zephyrus-K43BY:~/Docking$ cd results
zephyrus@zephyrus-K43BY:~/Docking/results$ more bestranking.csv
TOTAL_SCORE,SCORE_RB_PEN,SCORE_NORM_HEVATOMS,SCORE_NORM_CRT_HEVATOMS,SCORE_NORM_WEIGHT,SCORE_NORM_CRT_WEIGHT,SCORE_RB_PEN_NORM_CRT_HEVATOMS,SCORE_NORM_CONTACT, EVAL, TIME
APOPTOSIS REGULATOR BCL-X_entry_00001_conf_01,-83.6148,-77.6148,-5.22592,-33.1825,-0.386744,-13.9315,-30.8014,-5.22592,1132249,10.608
APOPTOSIS REGULATOR BCL-X_entry_00002_conf_01,-83.4667,-77.4667,-5.21667,-33.1238,-0.386059,-13.9068,-30.7427,-5.21667,1141475,12.388
APOPTOSIS REGULATOR BCL-X_entry_00003_conf_01,-83.4712,-77.4712,-5.21695,-33.1256,-0.38608,-13.9075,-30.7445,-5.21695,1165378,12.56
APOPTOSIS REGULATOR BCL-X_entry_00004_conf_01,-83.4002,-77.4002,-5.21251,-33.0974,-0.385751,-13.8957,-30.7163,-5.21251,1138294,12.244
APOPTOSIS REGULATOR BCL-X_entry_00005_conf_01,-83.4053,-77.4053,-5.21283,-33.0994,-0.385775,-13.8966,-30.7183,-5.21283,1155458,12.592
APOPTOSIS REGULATOR BCL-X_entry_00006_conf_01,-83.4621,-77.4621,-5.21638,-33.122,-0.386038,-13.906,-30.7409,-5.21638,1153514,12.728
APOPTOSIS REGULATOR BCL-X_entry_00007_conf_01,-83.4266,-77.4266,-5.21416,-33.1079,-0.385873,-13.9001,-30.7267,-5.21416,1169508,12.54
APOPTOSIS REGULATOR BCL-X_entry_00008_conf_01,-83.4856,-77.4856,-5.21785,-33.1313,-0.386146,-13.9099,-30.7502,-5.21785,1153320,12.588
APOPTOSIS REGULATOR BCL-X_entry_00009_conf_01,-83.542,-77.542,-5.22138,-33.1537,-0.386407,-13.9193,-30.7726,-5.22138,1130720,12.424
zephyrus@zephyrus-K43BY:~/Docking/results$
```

Lampiran 10. Skor *Docking* antara *Doxorubicin* dan ER α

```
argevollen@argevollen-Satellite-L645: ~/docking/results
TOTAL_SCORE,SCORE_RB_PEN,SCORE_NORM_HEVATOMS,SCORE_NORM_CRT_HEVATOMS,SCORE_NORM_WEIGHT,SCORE_NORM_CRT_WEIGHT,SCORE_RB_PEN_NORM_CRT_HEVATOMS,SCORE_NORM_CONTACT, EVAL, TIME
_entry_00001_conf_01,-68.869,-46.869,-1.76587,-20.3081,-0.126477,-8.43372,-13.8207,-1.60161,6320955,78.548
_entry_00002_conf_01,-67.871,-45.871,-1.74028,-20.0138,-0.124644,-8.31151,-13.5264,-1.61598,6540667,81.584
_entry_00003_conf_01,-65.67,-43.67,-1.68385,-19.3648,-0.120602,-8.04197,-12.8774,-1.60171,6515757,80.024
_entry_00004_conf_01,-63.941,-41.941,-1.63951,-18.8549,-0.117426,-7.83024,-12.3676,-1.59853,6173987,75.66
_entry_00005_conf_01,-67.1072,-45.1072,-1.7207,-19.7886,-0.123241,-8.21797,-13.3012,-1.59779,6428356,79.928
_entry_00006_conf_01,-68.7631,-46.7631,-1.76316,-20.2769,-0.126282,-8.42076,-13.7895,-1.67715,6725796,82.992
_entry_00007_conf_01,-67.2526,-45.2526,-1.72442,-19.8314,-0.123508,-8.23577,-13.3441,-1.64031,6299832,77.232
_entry_00008_conf_01,-70.7854,-48.7854,-1.81501,-20.8732,-0.129996,-8.6684,-14.3858,-1.68537,6491710,79.876
_entry_00009_conf_01,-65.2153,-43.2153,-1.67219,-19.2307,-0.119767,-7.98629,-12.7433,-1.59062,6559980,80.352
argevollen@argevollen-Satellite-L645:~/docking/results$
argevollen@argevollen-Satellite-L645:~/docking/results$
```

Lampiran 11. Skor Docking antara Doxorubicin dan Bcl-xl

```
argevollen@argevollen-Satellite-L645: ~/docking/results
argevollen@argevollen-Satellite-L645:~/docking$ cd results
argevollen@argevollen-Satellite-L645:~/docking/results$ more bestranking.csv
TOTAL_SCORE,SCORE_RB_PEN,SCORE_NORM_HEVATOMS,SCORE_NORM_CRT_HEVATOMS,SCORE_NORM_
WEIGHT,SCORE_NORM_CRT_WEIGHT,SCORE_RB_PEN_NORM_CRT_HEVATOMS,SCORE_NORM_CONTACT,E
VAL,TIME
_entry_00001_conf_01,-77.0892,-55.0892,-1.97665,-22.732,-0.141573,-9.44036,-16.2
447,-2.08349,6220206,72.836
_entry_00002_conf_01,-76.7634,-54.7634,-1.96829,-22.636,-0.140974,-9.40047,-16.1
486,-2.07469,6176570,72.3
_entry_00003_conf_01,-77.2205,-55.2205,-1.98001,-22.7708,-0.141814,-9.45644,-16.
2834,-1.93051,6067442,70.972
_entry_00004_conf_01,-77.5441,-55.5441,-1.98831,-22.8662,-0.142408,-9.49607,-16.
3788,-1.98831,6132318,71.528
_entry_00005_conf_01,-77.265,-55.265,-1.98115,-22.7839,-0.141896,-9.46189,-16.29
65,-2.03329,6395685,74.948
_entry_00006_conf_01,-77.2821,-55.2821,-1.98159,-22.7889,-0.141927,-9.46399,-16.
3016,-2.03374,6129845,71.608
_entry_00007_conf_01,-77.5672,-55.5672,-1.9889,-22.873,-0.142451,-9.4989,-16.385
6,-2.09641,5941803,69.632
_entry_00008_conf_01,-76.7997,-54.7997,-1.96922,-22.6467,-0.141041,-9.40491,-16.
1593,-2.07567,6030216,70.852
_entry_00009_conf_01,-77.3254,-55.3254,-1.9827,-22.8017,-0.142007,-9.46929,-16.3
143,-1.9827,6212126,72.62
argevollen@argevollen-Satellite-L645:~/docking/results$
```

Lampiran 12. Skor Docking antara Skopoletin dan ERα

```
argevollen@argevollen-Satellite-L645: ~/docking/results
argevollen@argevollen-Satellite-L645:~/docking$ cd results
argevollen@argevollen-Satellite-L645:~/docking/results$ more bestranking.csv
TOTAL_SCORE,SCORE_RB_PEN,SCORE_NORM_HEVATOMS,SCORE_NORM_CRT_HEVATOMS,SCORE_NORM_
WEIGHT,SCORE_NORM_CRT_WEIGHT,SCORE_RB_PEN_NORM_CRT_HEVATOMS,SCORE_NORM_CONTACT,E
VAL,TIME
22. Buah Mengkudu.cdx_entry_00001_conf_01,-56.3957,-52.3957,-4.02826,-23.3993,-0
.293477,-9.77286,-21.7397,-4.02826,1026907,4.288
22. Buah Mengkudu.cdx_entry_00002_conf_01,-56.6726,-52.6726,-4.04805,-23.5142,-0
.294918,-9.82086,-21.8546,-3.77818,1026530,4.276
22. Buah Mengkudu.cdx_entry_00003_conf_01,-56.2614,-52.2614,-4.01867,-23.3436,-0
.292778,-9.7496,-21.684,-4.01867,1031303,4.296
22. Buah Mengkudu.cdx_entry_00004_conf_01,-56.7535,-52.7535,-4.05382,-23.5478,-0
.295339,-9.83487,-21.8881,-3.78357,1033602,4.316
22. Buah Mengkudu.cdx_entry_00005_conf_01,-56.0689,-52.0689,-4.00492,-23.2637,-0
.291776,-9.71624,-21.6041,-4.00492,1039773,4.392
22. Buah Mengkudu.cdx_entry_00006_conf_01,-58.6543,-54.6543,-4.18959,-24.3364,-0
.30523,-10.1643,-22.6768,-4.18959,1011476,4.192
22. Buah Mengkudu.cdx_entry_00007_conf_01,-58.9069,-54.9069,-4.20763,-24.4412,-0
.306545,-10.208,-22.7816,-3.92712,1037921,4.356
22. Buah Mengkudu.cdx_entry_00008_conf_01,-59.3852,-55.3852,-4.2418,-24.6397,-0.
309034,-10.2909,-22.9801,-3.95902,1026159,4.32
22. Buah Mengkudu.cdx_entry_00009_conf_01,-58.0562,-54.0562,-4.14687,-24.0883,-0
.302118,-10.0606,-22.4286,-3.87041,1062268,4.524
argevollen@argevollen-Satellite-L645:~/docking/results$
```

Lampiran 13. Skor *Docking* antara Skopoletin dan Bcl-xl

```
argevollen@argevollen-Satellite-L645: ~/docking/results
argevollen@argevollen-Satellite-L645:~/docking$ cd results
argevollen@argevollen-Satellite-L645:~/docking/results$ more bestranking.csv
TOTAL_SCORE,SCORE_RB_PEN,SCORE_NORM_HEVATOMS,SCORE_NORM_CRT_HEVATOMS,SCORE_NORM_
WEIGHT,SCORE_NORM_CRT_WEIGHT,SCORE_RB_PEN_NORM_CRT_HEVATOMS,SCORE_NORM_CONTACT,E
VAL,TIME
22. Buah Mengkudu.cdx_entry_00001_conf_01,-70.7573,-66.7573,-5.0541,-29.3582,-0.
368213,-12.2616,-27.6985,-5.0541,816862,2.78
22. Buah Mengkudu.cdx_entry_00002_conf_01,-70.2597,-66.2597,-5.01855,-29.1517,-0
.365624,-12.1754,-27.492,-5.01855,818834,2.812
22. Buah Mengkudu.cdx_entry_00003_conf_01,-70.7418,-66.7418,-5.05298,-29.3517,-0
.368132,-12.2589,-27.692,-5.05298,798964,2.776
22. Buah Mengkudu.cdx_entry_00004_conf_01,-70.6176,-66.6176,-5.04411,-29.3002,-0
.367486,-12.2374,-27.6405,-5.04411,809669,2.844
22. Buah Mengkudu.cdx_entry_00005_conf_01,-70.2807,-66.2807,-5.02005,-29.1604,-0
.365733,-12.179,-27.5007,-5.02005,815441,2.864
22. Buah Mengkudu.cdx_entry_00006_conf_01,-72.6331,-68.6331,-5.18808,-30.1364,-0
.377975,-12.5867,-28.4768,-5.18808,789553,2.772
22. Buah Mengkudu.cdx_entry_00007_conf_01,-72.5184,-68.5184,-5.17988,-30.0888,-0
.377378,-12.5668,-28.4292,-5.17988,796046,2.784
22. Buah Mengkudu.cdx_entry_00008_conf_01,-73.8583,-69.8583,-5.2756,-30.6448,-0.
384351,-12.799,-28.9851,-5.2756,821161,2.88
22. Buah Mengkudu.cdx_entry_00009_conf_01,-72.627,-68.627,-5.18765,-30.1339,-0.3
77943,-12.5856,-28.4743,-5.18765,802636,2.836
argevollen@argevollen-Satellite-L645:~/docking/results$
```

Lampiran 14. Skor *Docking* antara Umbeliferon dan ER α

```
argevollen@argevollen-Satellite-L645: ~/docking/results
total virtual screening time: 24.04s
Ligands skipped due to errors: 0
argevollen@argevollen-Satellite-L645:~/docking$ cd results
argevollen@argevollen-Satellite-L645:~/docking/results$ more bestranking.csv
TOTAL_SCORE,SCORE_RB_PEN,SCORE_NORM_HEVATOMS,SCORE_NORM_CRT_HEVATOMS,SCORE_NORM_
WEIGHT,SCORE_NORM_CRT_WEIGHT,SCORE_RB_PEN_NORM_CRT_HEVATOMS,SCORE_NORM_CONTACT,E
VAL,TIME
_entry_00001_conf_01,-66.2475,-64.2475,-5.52063,-28.9363,-0.408587,-12.149,-28.0
627,-5.09596,719512,2.716
_entry_00002_conf_01,-66.3019,-64.3019,-5.52516,-28.96,-0.408923,-12.159,-28.086
4,-5.10014,705270,2.66
_entry_00003_conf_01,-66.0715,-64.0715,-5.50596,-28.8594,-0.407502,-12.1167,-27.
9858,-5.08242,705277,2.664
_entry_00004_conf_01,-66.174,-64.174,-5.5145,-28.9041,-0.408134,-12.1355,-28.030
6,-5.0903,705990,2.68
_entry_00005_conf_01,-66.2298,-64.2298,-5.51915,-28.9285,-0.408478,-12.1458,-28.
055,-5.0946,691983,2.62
_entry_00006_conf_01,-66.2478,-64.2478,-5.52065,-28.9364,-0.408589,-12.1491,-28.
0628,-5.09598,715419,2.708
_entry_00007_conf_01,-66.2524,-64.2524,-5.52103,-28.9384,-0.408617,-12.1499,-28.
0648,-5.09634,725098,2.752
_entry_00008_conf_01,-66.2012,-64.2012,-5.51677,-28.916,-0.408302,-12.1405,-28.0
425,-5.0924,689418,2.616
argevollen@argevollen-Satellite-L645:~/docking/results$
```

Lampiran 15. Skor *Docking* antara Umbeliferon dan Bcl-xl

```
argevollen@argevollen-Satellite-L645: ~/docking/results
total virtual screening time: 13.04s
Ligands skipped due to errors: 0
argevollen@argevollen-Satellite-L645:~/docking$ cd results
argevollen@argevollen-Satellite-L645:~/docking/results$ more bestranking.csv
TOTAL_SCORE,SCORE_RB_PEN,SCORE_NORM_HEVATOMS,SCORE_NORM_CRT_HEVATOMS,SCORE_NORM_
WEIGHT,SCORE_NORM_CRT_WEIGHT,SCORE_RB_PEN_NORM_CRT_HEVATOMS,SCORE_NORM_CONTACT,E
VAL,TIME
_entry_00001_conf_01,-71.5027,-69.5027,-5.95856,-31.2317,-0.440999,-13.1128,-30.
3581,-5.50021,491918,1.4
_entry_00002_conf_01,-71.7619,-69.7619,-5.98016,-31.3449,-0.442598,-13.1603,-30.
4713,-5.52014,510698,1.468
_entry_00003_conf_01,-71.3903,-69.3903,-5.94919,-31.1826,-0.440306,-13.0921,-30.
309,-5.49156,501753,1.448
_entry_00004_conf_01,-71.5092,-69.5092,-5.9591,-31.2345,-0.441039,-13.114,-30.36
09,-5.50071,519319,1.48
_entry_00005_conf_01,-71.9896,-69.9896,-5.99914,-31.4444,-0.444002,-13.2021,-30.
5708,-5.53766,516906,1.484
_entry_00006_conf_01,-71.8384,-69.8384,-5.98653,-31.3783,-0.443069,-13.1743,-30.
5047,-5.52603,526133,1.504
_entry_00007_conf_01,-71.481,-69.481,-5.95675,-31.2222,-0.440865,-13.1088,-30.34
86,-5.49854,504575,1.436
_entry_00008_conf_01,-71.2881,-69.2881,-5.94068,-31.138,-0.439676,-13.0734,-30.2
644,-5.4837,517077,1.488
argevollen@argevollen-Satellite-L645:~/docking/results$
```