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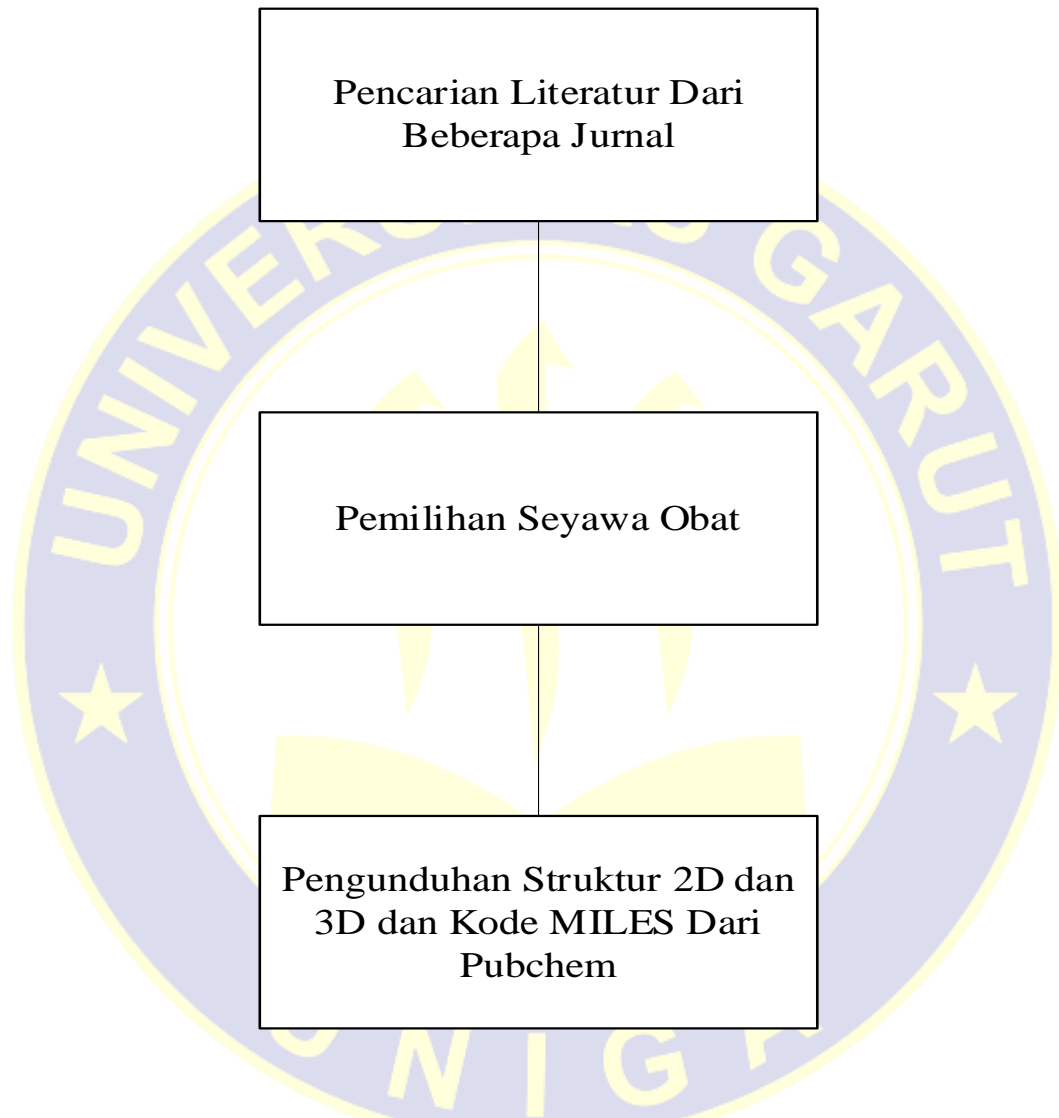
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LAMPIRAN 1

ALUR PENGUMPULAN DATA

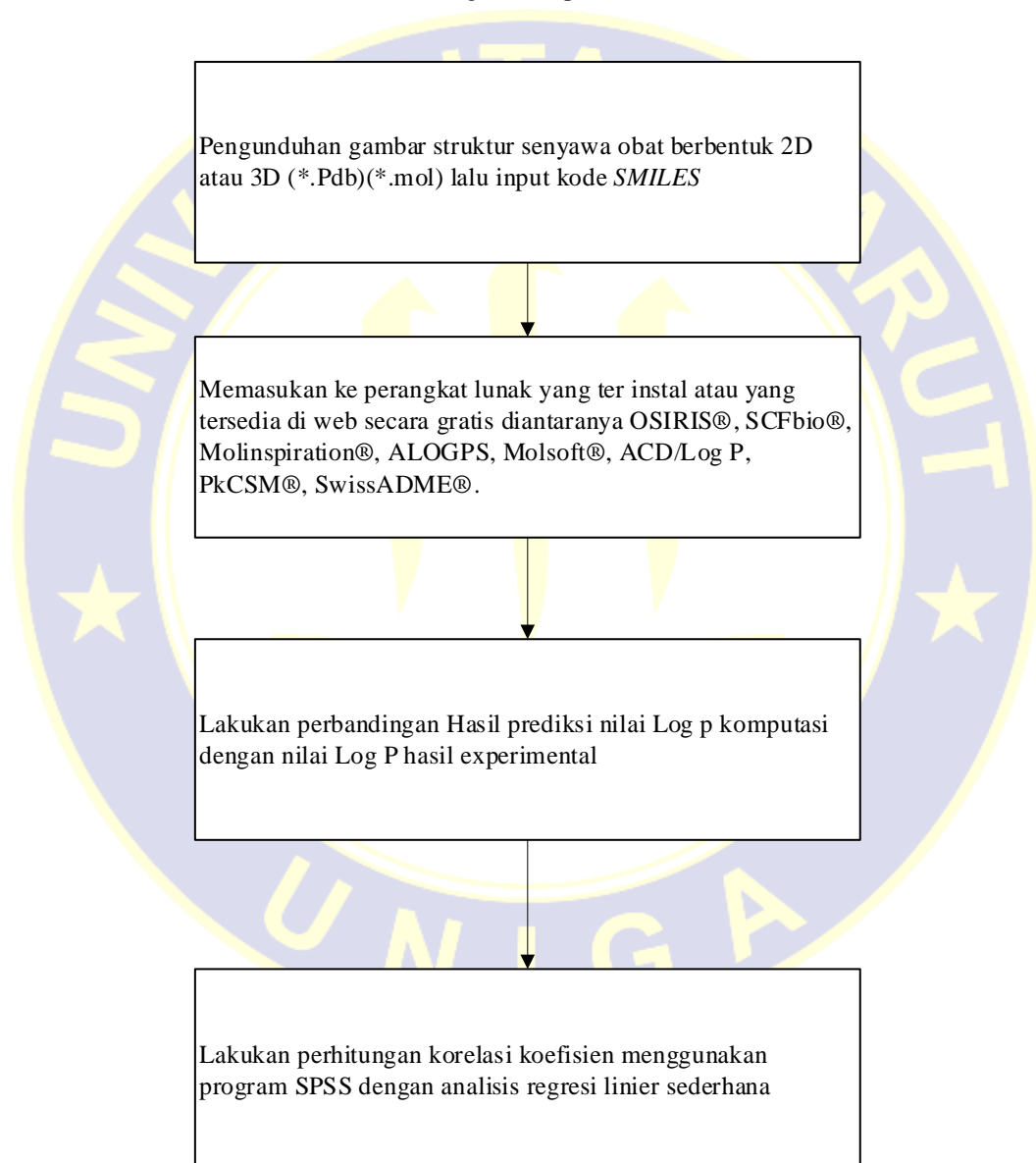


Gambar VII. 1 Pengumpulan data nilai log p senyawa obat hasil eksperimen dari beberapa jurnal

LAMPIRAN 2

ALUR PENENTUAN PREDIKSI NILAI LOG P DENGAN KOMPUTASI

Alur Penentuan Prediksi Nilai Log p
dengan Komputasi



Gambar VII. 2 Alur penentuan prediksi nilai Log P dengan beberapa komputasi

LAMPIRAN 3

DATA SENYAWA OBAT NILAI LOG P HASIL

EKSPERIMENTAL

Tabel VII. 1

Daftar Senyawa Obat Uji Hasil Eksperimental

No	Nama senyawa obat	Log P Eksp	Ref	No	Nama senyawa obat	Log P Eksp	Ref
1	Acetaminophen	0.49	³²	26	kortikosteron	1.94	⁵²
2	Alprazolam	2.12	³³	27	Librium	2.44	⁵³
3	Alprenolol	3.10	²	28	Lidocain	2.26	⁵⁴
4	Amfetamin	1.76	³⁴	29	Mebendazol	2.83	⁵⁵
5	Amobarbital	2.07	³⁵	30	metamfetamine	2.07	³⁴
6	Asam klorofibrat	3.30	³⁶	31	Metronidazole	-0.02	⁵⁶
7	Betametason	1.83	³⁷	32	Nifedipine	2.20	⁴⁷
8	Bromazepam	2.05	³⁸	33	Nitrazepam	2.25	³³
9	Cimetidine	0.40	⁷	34	Oxazepam	2.24	⁵⁷
10	Clobazam	2.12	³⁹	35	Phenytoin	2.47	⁵³
11	Demoxepam	1.41	⁴⁰	36	Pindolol	1.75	⁵⁸
12	Diazepam	2.82	³³	37	Prednisolone	1.62	⁵⁹
13	Diphenhydramine	3.27	⁴¹	38	prednisone	1.46	⁶⁰
14	Disopiramida	2.58	⁴²	39	Progesterone	3.87	⁶¹
15	Droperidol	3.50	⁴³	40	Propranolol	3.48	⁶²
16	Flurbiprofen	4.16	⁷	41	Pseudoephedrine	0.89	⁶³
17	Furosemide	2.03	⁴⁴	42	Quinidine	3.44	⁶⁴
18	Ibuprofen	3.97	⁴⁵	43	Simvastatin	4.68	⁶⁵
19	Imipramine	4.80	⁴⁶	44	Spirolactone	2.78	³⁷
20	Indometasin	4.27	⁴⁷	45	Sulfadiazine	-0.09	⁶⁶
21	Kafein	-0.09	⁴⁸	46	Sulfamethoxazole	0.89	⁶⁷
22	Kaptopil	0.34	⁴⁹	47	Sulfanilamide	-0.62	⁶⁸
23	Ketoprofen	3.12	⁴⁵	48	Tetrasiklin	-1.30	⁶⁹
24	Kloramfenikol	1.14	⁵⁰	49	Tetrazepam	3.20	⁵⁶
25	Kodein	1.19	⁵¹	50	Verapamil	3.79	⁶⁰

LAMPIRAN 4

DAFTAR NOTASI SMILES SENYAWA OBAT

Tabel VII. 2
Notasi SMILES Senyawa Obat dari Pubchem

No	Nama Senyawa	NOTASI SMILES
1	Acetaminophen	<chem>CC(=O)NC1=CC=C(C=C1)O</chem>
2	Alprazolam	<chem>CC1=NN=C2N1C3=C(C=C(C=C3)Cl)C(=NC2)C4=CC=CC=C4</chem>
3	Alprenolol	<chem>CC(C)NCC(COC1=CC=CC=C1CC=C)O</chem>
4	Amfetamin	<chem>CC(CC1=CC=CC=C1)N</chem>
5	Amobarbital	<chem>CCC1(C(=O)NC(=O)NC1=O)CCC(C)C</chem>
6	Asam klofibrat	<chem>CCOC(=O)C(C)(C)OC1=CC=C(C=C1)Cl</chem>
7	Betametason	<chem>CC1CC2C3CCC4=CC(=O)C=CC4(C3(C(CC2(C1(C(=O)CO)O)C)O)F)C</chem>
8	Bromazepam	<chem>C1C(=O)NC2=C(C=C(C=C2)Br)C(=N1)C3=CC=CC=N3</chem>
9	Cimetidine	<chem>CC1=C(N=CN1)CSCCNC(=NC)NC#N</chem>
10	Clobazam	<chem>CN1C(=O)CC(=O)N(C2=C1C=CC(=C2)Cl)C3=CC=CC=C3</chem>
11	Demoxepam	<chem>C1C(=O)N=C2C=CC(=CC2=C(N1O)C3=CC=CC=C3)Cl</chem>
12	Diazepam	<chem>CN1C(=O)CN=C(C2=C1C=CC(=C2)Cl)C3=CC=CC=C3</chem>
13	Diphenhydramine	<chem>CN(C)CCOC(C1=CC=CC=C1)C2=CC=CC=C2</chem>
14	Disopiramida	<chem>CC(C)N(CCC(C1=CC=CC=C1)(C2=CC=CC=N2)C(=O)N)C(C)C</chem>
15	Droperidol	<chem>C1CN(CC=C1N2C3=CC=CC=C3NC2=O)CCCC(=O)C4=CC=C(C=C4)F</chem>
16	Flurbiprofen	<chem>CC(C1=CC(=C(C=C1)C2=CC=CC=C2)F)C(=O)O</chem>
17	Furosemide	<chem>C1=COC(=C1)CNC2=CC(=C(C=C2C(=O)O)S(=O)(=O)N)Cl</chem>
18	Ibuprofen	<chem>CC(C)CC1=CC=C(C=C1)C(C)C(=O)O</chem>
19	Imipramine	<chem>CN(C)CCCN1C2=CC=CC=C2CCC3=CC=CC=C31</chem>
20	Indometasin	<chem>CC1=C(C2=C(N1C(=O)C3=CC=C(C=C3)Cl)C=CC(=C2)OC)CC(=O)O</chem>
21	Kafein	<chem>CN1C=NC2=C1C(=O)N(C(=O)N2C)C</chem>
22	Kaptopril	<chem>CC(CS)C(=O)N1CCCC1C(=O)O</chem>
23	Ketoprofen	<chem>CC(C1=CC(=CC=C1)C(=O)C2=CC=CC=C2)C(=O)O</chem>
24	Kloramfenikol	<chem>C1=CC(=CC=C1C(C(=O)NC(=O)C(Cl)Cl)O)[N+](=O)[O-]</chem>
25	Kodein	<chem>CN1CCC23C4C1CC5=C2C(=C(C=C5)OC)OC3C(C=C4)O</chem>

LAMPIRAN 4

(LANJUTAN)

Tabel VII.2
Lanjutan

No	Nama Senyawa	NOTASI SMILES
26	kortikosteron	<chem>CC12CCC(=O)C=C1CCC3C2C(CC4(C3CCC4C(=O)CO)C)O</chem>
27	Librium	<chem>CN=C1CN(C(=C2C=C(C=CC2=N1)Cl)C3=CC=CC=C3)O</chem>
28	Lidocain	<chem>CCN(CC)CC(=O)NC1=C(C=CC=C1C)C</chem>
29	Mebendazol	<chem>COC(=O)NC1=NC2=C(N1)C=C(C=C2)C(=O)C3=CC=CC=C3</chem>
30	metamfetamine	<chem>CC(CC1=CC=CC=C1)NC</chem>
31	Metronidazole	<chem>CC1=NC=C(N1CCO)[N+](=O)[O-]</chem>
32	Nifedipine	<chem>CC1=C(C(C(=C(N1)C)C(=O)OC)C2=CC=CC=C2[N+](=O)[O-])C(=O)OC</chem>
33	Nitrazepam	<chem>C1C(=O)NC2=C(C=C(C=C2)[N+](=O)[O-])C(=N1)C3=CC=CC=C3</chem>
34	Oxazepam	<chem>C1=CC=C(C=C1)C2=NC(C(=O)NC3=C2C=C(C=C3)Cl)O</chem>
35	Phenytoin	<chem>C1=CC=C(C=C1)C2(C(=O)NC(=O)N2)C3=CC=CC=C3</chem>
36	Pindolol	<chem>CC(C)NCC(COC1=CC=CC2=C1C=CN2)O</chem>
37	Prednisolone	<chem>CC12CC(C3C(C1CCC2(C(=O)CO)O)CCC4=CC(=O)C=CC34C)O</chem>
38	prednison	<chem>CC12CC(=O)C3C(C1CCC2(C(=O)CO)O)CCC4=CC(=O)C=CC34C</chem>
39	Progesteron	<chem>CC(=O)C1CCC2C1(CCC3C2CCC4=CC(=O)CCC34C)C</chem>
40	Propranolol	<chem>CC(C)NCC(COC1=CC=CC2=CC=CC=C21)O</chem>
41	Pseudoephedrin	<chem>CC(C(C1=CC=CC=C1)O)NC</chem>
42	Quinidine	<chem>COC1=CC2=C(C=CN=C2C=C1)C(C3CC4CCN3CC4=C)O</chem>
43	Simvastatin	<chem>CCC(C)(C)C(=O)OC1CC(C=C2C1C(C(C=C2)C)CCC3CC(CC(=O)O3)O)C</chem>
44	Spironolacton	<chem>CC(=O)SC1CC2=CC(=O)CCC2(C3C1C4CCC5(C4(CC3)C)CCC(=O)O5)C</chem>
45	Sulfadiazin	<chem>C1=CN=C(N=C1)NS(=O)(=O)C2=CC=C(C=C2)N</chem>
46	Sulfamethoxazol	<chem>CC1=CC(=NO1)NS(=O)(=O)C2=CC=C(C=C2)N</chem>
47	Sulfanilamid	<chem>C1=CC(=CC=C1N)S(=O)(=O)N</chem>
48	Tetrasiklin	<chem>CC1(C2CC3C(C(=O)C(=C(C3(C(=O)C2=C(C4=C1C=CC=C4O)O)O)O)C(=O)N)N(C)C)O</chem>
49	Tetrazepam	<chem>CN1C(=O)CN=C(C2=C1C=CC(=C2)Cl)C3=CCCCC3</chem>
50	Verapamil	<chem>CC(C)C(CCCN(C)CCC1=CC(=C(C=C1)OC)OC)(C#N)C2=CC(=C(C=C2)O)C)OC</chem>

LAMPIRAN 5

HASIL PREDIKSI LOG P DENGAN KOMPUTASI

Tabel VII. 3
Data Hasil Prediksi Senyawa Obat dengan Komputasi

No	Nama senyawa obat	LogP Eksp	ClogP	SCF bio	Mi logp	Alog ps	molL ogP	ACD Logp	pkC SM	Swiss ADME
1	Acetaminofen	0.49	1.02	1.35	0.68	0.51	0.79	0.34	1.35	0.93
2	Alprazolam	2.12	2.62	3.49	2.29	2.23	2.06	2.50	3.58	2.50
3	Alprenolol	3.10	2.25	2.15	2.58	2.59	2.94	2.88	2.15	2.13
4	Amfetamin	1.76	1.45	1.57	1.32	1.85	1.79	1.81	1.57	1.91
5	Amobarbital	2.07	1.30	1.18	1.78	1.87	2.02	2.05	1.18	1.03
6	As. klofibrat	3.30	2.90	3.06	3.72	3.99	3.52	3.32	3.06	3.02
7	Betametason	1.83	1.29	1.89	2.06	1.93	2.07	1.87	1.89	2.14
8	Bromazepam	2.05	1.80	2.63	2.41	2.09	2.08	1.65	2.63	2.18
9	Cimetidin	0.40	0.17	0.59	0.14	0.44	0.18	0.07	0.59	0.63
10	Clobazam	2.12	2.89	3.37	2.55	2.14	2.11	1.69	3.37	2.01
11	Demoxepam	1.41	1.32	1.89	3.13	2.50	2.71	1.23	1.34	2.48
12	Diazepam	2.82	2.98	2.89	2.74	2.63	2.86	2.91	3.15	2.44
13	Diphenhydramine	3.27	2.91	3.35	3.50	3.44	3.40	3.66	3.35	2.58
14	Disopiramida	2.58	2.21	3.36	2.78	3.21	2.64	2.86	3.36	3.00
15	Droperidol	3.50	3.46	4.43	3.40	3.93	3.46	3.51	3.67	3.06
16	Flurbiprofen	4.16	3.33	3.68	4.05	3.57	3.98	4.12	3.68	3.18
17	Furosemid	2.03	0.77	2.97	1.77	2.71	2.10	3.10	1.89	0.86
18	Ibuprofen	3.97	3.00	3.07	3.46	3.50	3.85	3.72	3.07	2.57
19	Imipramin	4.80	3.89	3.87	4.16	4.53	4.83	4.80	3.87	3.80
20	Indometasin	4.27	4.00	3.92	3.99	4.25	4.00	3.10	3.92	3.08
21	Kafein	-0.09	-0.18	0.06	0.06	0.24	-0.08	-0.13	1.02	-0.28
22	Kaptopril	0.34	0.37	0.62	1.09	1.02	0.41	0.27	0.62	0.62
23	Ketoprofen	3.12	2.70	3.10	3.59	3.29	3.19	2.81	3.10	2.84
24	Kloramfenikol	1.14	-0.42	0.90	0.73	1.15	-0.16	1.02	0.90	0.30
25	Kodein	1.19	1.12	1.75	1.41	1.20	1.10	1.20	1.50	1.80

LAMPIRAN 5

(LANJUTAN)

Tabel VII.3
Lanjutan

No	Nama senyawa obat	LogP Eksp	Clog P	SCF bio	Mi logp	Alog ps	molL ogP	ACD Logp	PkC SM	Swiss ADME
26	kortikosteron	1.94	2.24	2.66	1.88	2.09	1.59	1.76	2.66	2.41
27	Librium	2.44	1.45	3.03	3.73	2.98	3.05	1.82	1.84	2.66
28	Lidocain	2.26	2.16	3.00	2.13	1.81	2.55	2.36	3.00	2.31
29	Mebendazol	2.83	2.67	2.97	2.89	2.95	3.13	2.83	2.97	2.30
30	metamfetamin	2.07	1.81	1.83	2.23	2.23	2.21	1.94	1.83	1.75
31	Metronidazol	-0.02	1.05	0.09	-0.47	0.15	-0.95	-0.01	0.09	-0.47
32	Nifedipin	2.20	1.55	2.17	3.07	2.49	1.51	2.97	2.17	1.07
33	Nitrazepam	2.25	1.10	2.38	2.14	1.95	1.10	2.18	2.38	1.50
34	Oxazepam	2.24	2.28	2.44	1.84	2.01	2.01	2.31	2.44	2.28
35	fenitoin	2.47	1.67	1.76	2.18	2.26	2.31	2.52	1.76	1.56
36	Pindolol	1.75	1.26	1.90	1.98	2.17	1.97	1.97	1.90	1.42
37	Prednisolon	1.62	1.14	1.55	1.59	1.66	1.89	1.49	1.55	1.31
38	prednison	1.46	1.29	1.76	1.41	2.07	1.72	1.57	1.76	1.42
39	Progesteron	3.87	4.02	4.72	3.81	3.58	3.52	4.04	4.72	4.03
40	Propranolol	3.48	2.42	2.57	2.97	3.03	3.42	3.10	2.57	2.84
41	Pseudoefedrin	0.89	0.74	1.32	1.24	1.00	1.15	1.05	1.32	1.46
42	Quinidin	3.44	2.61	3.17	3.06	2.82	3.21	3.44	3.17	2.81
43	Simvastatin	4.68	4.46	4.58	4.76	4.51	4.80	4.42	4.58	3.36
44	Spironolacton	2.78	3.21	4.85	3.03	3.10	2.40	3.12	4.85	3.77
45	Sulfadiazine	-0.09	0.09	1.94	-0.04	0.25	-0.30	-0.12	0.85	0.24
46	Sulfametoxazol	0.89	0.44	2.44	0.61	0.79	0.90	0.89	1.36	0.71
47	Sulfanilamid	-0.62	0.25	0.99	-0.29	0.16	-0.53	-0.72	0.08	-0.01
48	Tetrasiklin	-1.30	1.26	0.60	-0.24	0.73	-1.44	-0.07	0.37	-0.58
49	Tetrazepam	3.20	2.88	3.34	3.84	3.53	3.24	2.88	3.60	2.62
50	Verapamil	3.79	4.93	5.09	4.55	5.23	3.87	3.90	5.09	4.45

LAMPIRAN 6

HASIL DATA STATISTIK KOEFISIEN KORELASI

Tabel VII. 4
Hasil Korelasi Nilai Clogp dengan Eksperimental

		clogp	ekperimental
clogp	Pearson Correlation	1	.924**
	Sig. (2-tailed)		.000
	N	50	50
ekperimental	Pearson Correlation	.924**	1
	Sig. (2-tailed)	.000	
	N	50	50

** . Correlation is significant at the 0.01 level (2-tailed).

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.924 ^a	.853	.850	.54100

a. Predictors: (Constant), ekperimental

Coefficients^a

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.
		B	Std. Error	Beta		
1	(Constant)	-.159	.143		-1.111	.272
	ekperimental	.933	.056	.924	16.688	.000

a. Dependent Variable: clogp

ANOVA^a

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	81.507	1	81.507	278.485	.000 ^b
	Residual	14.049	48	.293		
	Total	95.556	49			

a. Dependent Variable: clogp

b. Predictors: (Constant), ekperimental

LAMPIRAN 6

HASIL DATA STATISTIK KOEFISIEN KORELASI

Tabel VII. 5
Hasil Korelasi SCFBio dengan Eksperimental

		SCFBio	ekperimental
SCFBio	Pearson Correlation	1	.849**
	Sig. (2-tailed)		.000
	N	50	50
ekperimental	Pearson Correlation	.849**	1
	Sig. (2-tailed)	.000	
	N	50	50

** . Correlation is significant at the 0.01 level (2-tailed).

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.849 ^a	.722	.716	.68275

a. Predictors: (Constant), ekperimental

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.
		B	Std. Error	Beta		
1	(Constant)	.759	.181		4.200	.000
	ekperimental	.786	.071	.849	11.151	.000

a. Dependent Variable: SCFBio

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	57.968	1	57.968	124.355	.000 ^b
	Residual	22.375	48	.466		
	Total	80.344	49			

a. Dependent Variable: SCFBio

b. Predictors: (Constant), ekperimental

LAMPIRAN 6

HASIL DATA STATISTIK KOEFISIEN KORELASI

Tabel VII. 6
Hasil Korelasi *MiLogP* dengan Eksperimental

		miLogp	ekperimental
miLogp	Pearson Correlation	1	.931**
	Sig. (2-tailed)		.000
	N	50	50
ekperimental	Pearson Correlation	.931**	1
	Sig. (2-tailed)	.000	
	N	50	50

** . Correlation is significant at the 0.01 level (2-tailed).

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.931 ^a	.867	.864	.52400

a. Predictors: (Constant), ekperimental

Model		Unstandardized Coefficients		Standardized Coefficients	T	Sig.
		B	Std. Error	Beta		
1	(Constant)	.149	.139		1.074	.288
	ekperimental	.957	.054	.931	17.690	.000

a. Dependent Variable: miLogp

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	85.923	1	85.923	312.932	.000 ^b
	Residual	13.180	48	.275		
	Total	99.103	49			

a. Dependent Variable: miLogp

b. Predictors: (Constant), ekperimental

LAMPIRAN 6

HASIL DATA STATISTIK KOEFISIEN KORELASI

Tabel VII. 7
Hasil Korelasi ALOGPS dengan Eksperimental

		Alogps	ekperimental
Alogps	Pearson Correlation	1	.953**
	Sig. (2-tailed)		.000
	N	50	50
ekperimental	Pearson Correlation	.953**	1
	Sig. (2-tailed)	.000	
	N	50	50

** . Correlation is significant at the 0.01 level (2-tailed).

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.953 ^a	.907	.905	.41221

a. Predictors: (Constant), ekperimental

Coefficients^a

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.
		B	Std. Error	Beta		
1	(Constant)	.276	.109		2.535	.015
	ekperimental	.923	.043	.953	21.687	.000

a. Dependent Variable: Alogps

ANOVA^a

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	79.919	1	79.919	470.343	.000 ^b
	Residual	8.156	48	.170		
	Total	88.075	49			

a. Dependent Variable: Alogps

b. Predictors: (Constant), ekperimental

LAMPIRAN 6

HASIL DATA STATISTIK KOEFISIEN KORELASI

Tabel VII. 8
Hasil Korelasi *MolLogP* dengan Eksperimental

		molLogp	ekperimental
molLogp	Pearson Correlation	1	.961**
	Sig. (2-tailed)		.000
	N	50	50
ekperimental	Pearson Correlation	.961**	1
	Sig. (2-tailed)	.000	
	N	50	50

** . Correlation is significant at the 0.01 level (2-tailed).

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.961 ^a	.924	.923	.40401

a. Predictors: (Constant), ekperimental

Coefficients^a

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.
		B	Std. Error	Beta		
1	(Constant)	-.061	.107		-.572	.570
	ekperimental	1.009	.042	.961	24.177	.000

a. Dependent Variable: molLogp

ANOVA^a

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	95.413	1	95.413	584.545	.000 ^b
	Residual	7.835	48	.163		
	Total	103.248	49			

a. Dependent Variable: molLogp

b. Predictors: (Constant), ekperimental

LAMPIRAN 6

HASIL DATA STATISTIK KOEFESIEN KORELASI

Tabel VII. 9
Hasil Korelasi *ACDLog P* dengan Eksperimental

		ACDlogp	ekperimental
ACDlogp	Pearson Correlation	1	.963**
	Sig. (2-tailed)		.000
	N	50	50
ekperimental	Pearson Correlation	.963**	1
	Sig. (2-tailed)	.000	
	N	50	50

** . Correlation is significant at the 0.01 level (2-tailed).

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.963 ^a	.928	.926	.36208

a. Predictors: (Constant), ekperimental

Coefficients^a

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.
		B	Std. Error	Beta		
1	(Constant)	.152	.096		1.582	.120
	ekperimental	.928	.037	.963	24.800	.000

a. Dependent Variable: ACDlogp

ANOVA^a

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	80.634	1	80.634	615.042	.000 ^b
	Residual	6.293	48	.131		
	Total	86.927	49			

a. Dependent Variable: ACDlogp

b. Predictors: (Constant), ekperimental

LAMPIRAN 6

HASIL DATA STATISTIK KOEFESIEN KORELASI

Tabel VII. 10
Hasil Korelasi *PkCSM* dengan Eksperimental

		pkcsm	ekperimental
pkcsm	Pearson Correlation	1	.883**
	Sig. (2-tailed)		.000
	N	50	50
ekperimental	Pearson Correlation	.883**	1
	Sig. (2-tailed)	.000	
	N	50	50

** . Correlation is significant at the 0.01 level (2-tailed).

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.883 ^a	.780	.775	.65307

a. Predictors: (Constant), ekperimental

Coefficients^a

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.
		B	Std. Error	Beta		
1	(Constant)	.407	.173		2.355	.023
	ekperimental	.880	.067	.883	13.042	.000

a. Dependent Variable: pkcsm

ANOVA^a

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	72.544	1	72.544	170.089	.000 ^b
	Residual	20.472	48	.427		
	Total	93.016	49			

a. Dependent Variable: pkcsm

b. Predictors: (Constant), ekperimental

LAMPIRAN 6

HASIL DATA STATISTIK KOEFESIEN KORELASI

Tabel VII. 11
Hasil Korelasi *SwissADME* dengan Eksperimental

Correlations

		swissADME	ekperimental
swissADME	Pearson Correlation	1	.887**
	Sig. (2-tailed)		.000
	N	50	50
ekperimental	Pearson Correlation	.887**	1
	Sig. (2-tailed)	.000	
	N	50	50

** . Correlation is significant at the 0.01 level (2-tailed).

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.887 ^a	.787	.783	.55095

a. Predictors: (Constant), ekperimental

Coefficients^a

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.
		B	Std. Error	Beta		
1	(Constant)	.320	.146		2.193	.033
	ekperimental	.758	.057	.887	13.316	.000

a. Dependent Variable: swissADME

ANOVA^a

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	53.819	1	53.819	177.304	.000 ^b
	Residual	14.570	48	.304		
	Total	68.389	49			

a. Dependent Variable: swissADME

b. Predictors: (Constant), ekperimental

LAMPIRAN 7

KESIMPULAN HASIL KORELASI

Tabel VII. 12 Kesimpulan Hasil Koefisien Korelasi Nilai Log P Eksperimental dengan Komputasi

No	variabel	Hasil korelasi	Nilai person coralate	Korelasi	Koefisien determinasi (R^2)
1	CLogP	+	0,924	Korelasi Sempurna	85,3%
2	SCFbio	+	0,849	Korelasi Sempurna	72,2%
3	miLogP	+	0,931	Korelasi Sempurna	86,7%
4	AlogPS	+	0,935	Korelasi Sempurna	90,7%
5	MolLogP	+	0,961	Korelasi Sempurna	92,4%
6	ACDlogP	+	0,963	Korelasi Sempurna	92,8%
7	pkCSM	+	0,883	Korelasi Sempurna	78,0%
8	Swiss ADME	+	0,887	Korelasi Sempurna	78,7%

Ket :

Dengan keterangan Pada penelitian yang dilakukan diambil dengan dasar pengambilan keputusan dengan nilai ketelitian $\alpha = 0,01$ (1%) dengan tingkat kepercayaan (99%) dengan data hasil penelitian.

Jika nilai sig. < 0,01 maka berkorelasi

Jika nilai sig. > 0,01 maka tidak berkorelasi

Menggunakan Pedoman derajat hubungan sebagai berikut :

Nilai person corelate : 0,00-0,20 = tidak ada korelasi

Nilai person corelate : 0,21-0,40 = korelasi lemah

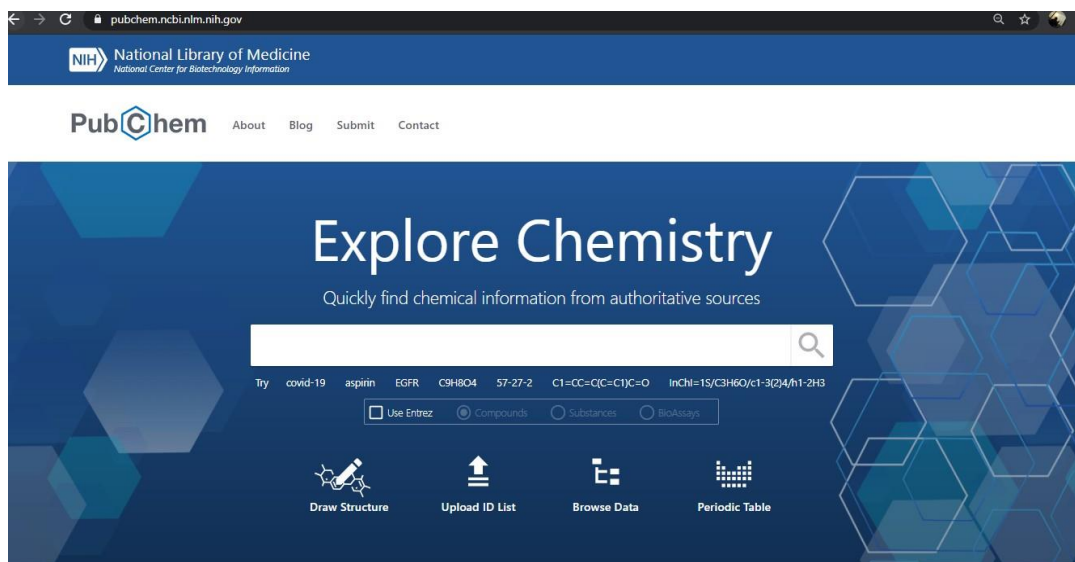
Nilai person corelate : 0,41-0,60 = korelasi sedang

Nilai person corelate : 0,61-0,80 = korelasi kuat

Nilai person corelate : 0,81-1,00 = korelasi sempurna

LAMPIRAN 8

SITUS DAN APLIKASI



Gambar VII. 3 Tampilan situs *pubchem*



Gambar VII. 4 Tampilan aplikasi OSIRIS property explorer

LAMPIRAN 8

(LANJUTAN)

scfbio-iitd.res.in/software/drugdesign/lipinski.jsp

Supercomputing Facility for Bioinformatics & Computational Biology, IIT Delhi

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Lipinski Rule of Five

Lipinski rule of 5 helps in distinguishing between drug like and non drug like molecules. It predicts high probability of success or failure due to drug likeness for molecules complying with 2 or more of the following rules

- Molecular mass less than 500 Dalton
- High lipophilicity (expressed as LogP less than 5)
- Less than 5 hydrogen bond donors
- Less than 10 hydrogen bond acceptors
- Molar refractivity should be between 40-130

These filters help in early preclinical development and could help avoid costly late-stage preclinical and clinical failures .To draw a chemical structure [Click Here](#) and follow the instructions given.

Step 1: Input Drug File.

Input PDB file No file chosen

Step 2 : Input pH Value

pH Value [Value ranges from 0.0 to 14.0]

Step 3: Click on 'Submit' to submit your job

How to Use the Tool

OPTION 1:-

- The input File should be in the following formats[*pdb, *.mol, *.mol2, *.xyz, *.sdf, *.smi]
- The input file name should not contain whitespace(s).

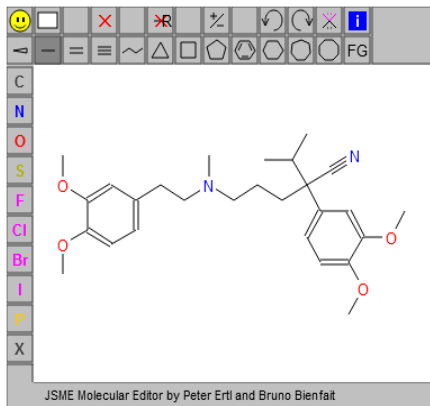
Gambar VII. 5 Tampilan situs SCFbio (Lipinski rule of five)

← → ↻ 🏠 🔒 https://www.molinspiration.com/cgi-bin/properties ☆ 🗂️ 📄 📱 📄 ☰

molinspiration Calculation of Molecular Properties and Bioactivity Score

Enter SMILES [Clear](#)

or draw molecule below



JSME Molecular Editor by Peter Ertl and Bruno Bienfait

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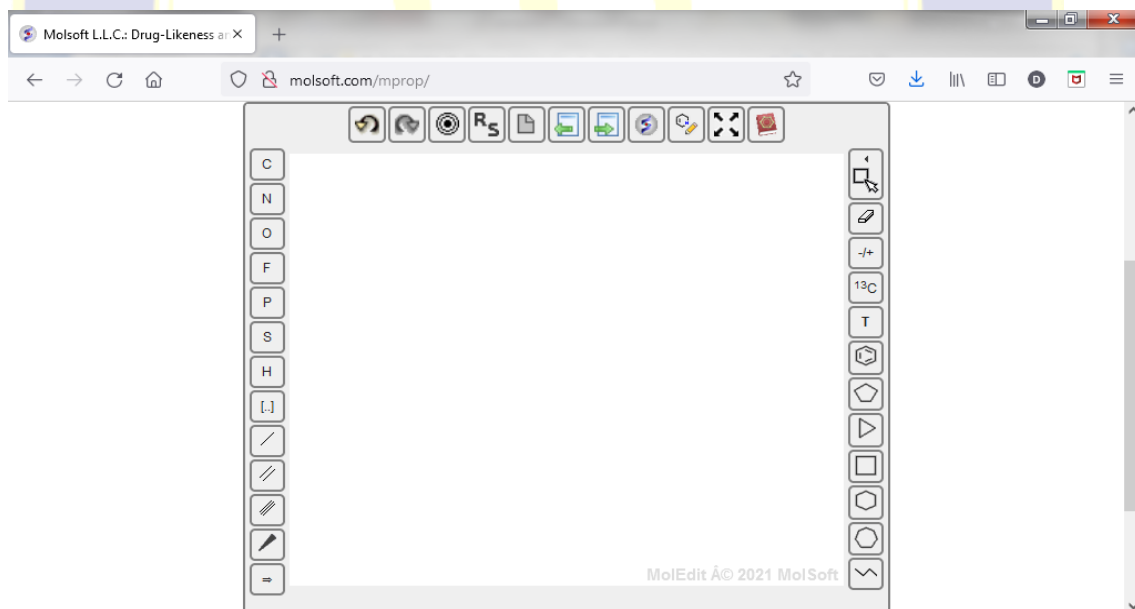
Gambar VII. 6 Tampilan situs Molinspiration

LAMPIRAN 8

(LANJUTAN)



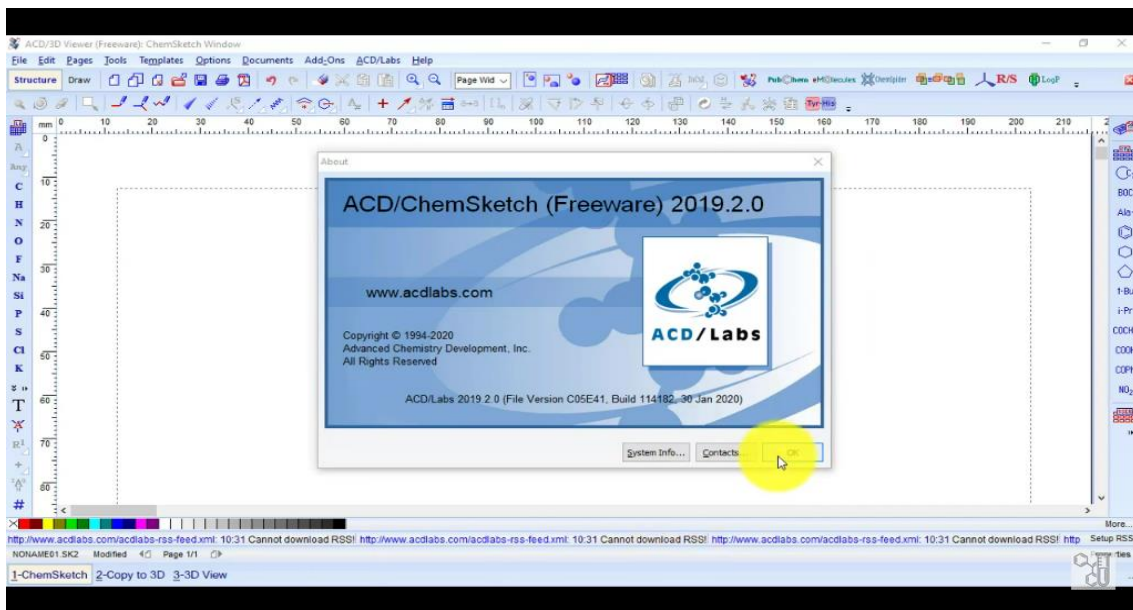
Gambar VII. 7 Tampilan situs ALOGPS2.1



Gambar VII. 8 Tampilan situs MolSoft

LAMPIRAN 8

(LANJUTAN)



Gambar VII. 9 Tampilan Aplikasi ACD/LABS

pkCSM

biosig.unimelb.edu.au/pkcsm/prediction

pkCSM Predict Theory Help Contact Acknowledgements Related Resources License

Pharmacokinetic properties

Input Molecule → Calculate All-Pair Shortest Paths → ADMET Train, Test Predict

Calculate Properties

Run example

Disclaimer

Step 1: Please provide a set of molecules (SMILES format)

Description

Upload your SMILES file: No file selected.

Files are expected to have headers identifying the columns [File limits](#)

OR

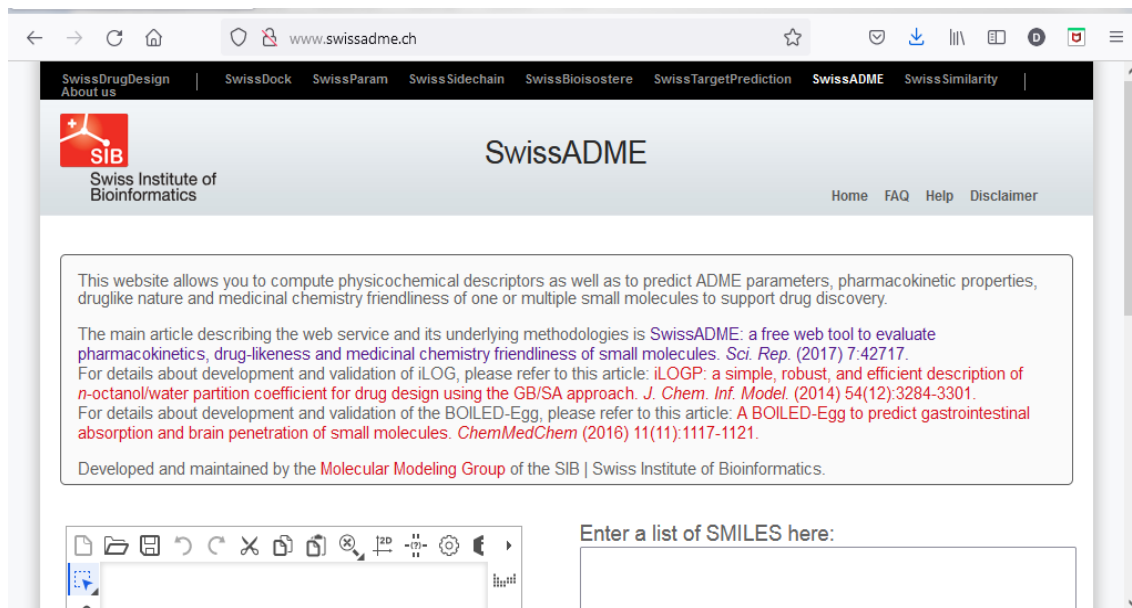
Provide a SMILES string:

Example:
CC(=O)OC1=CC=CC=C1C(=O)O

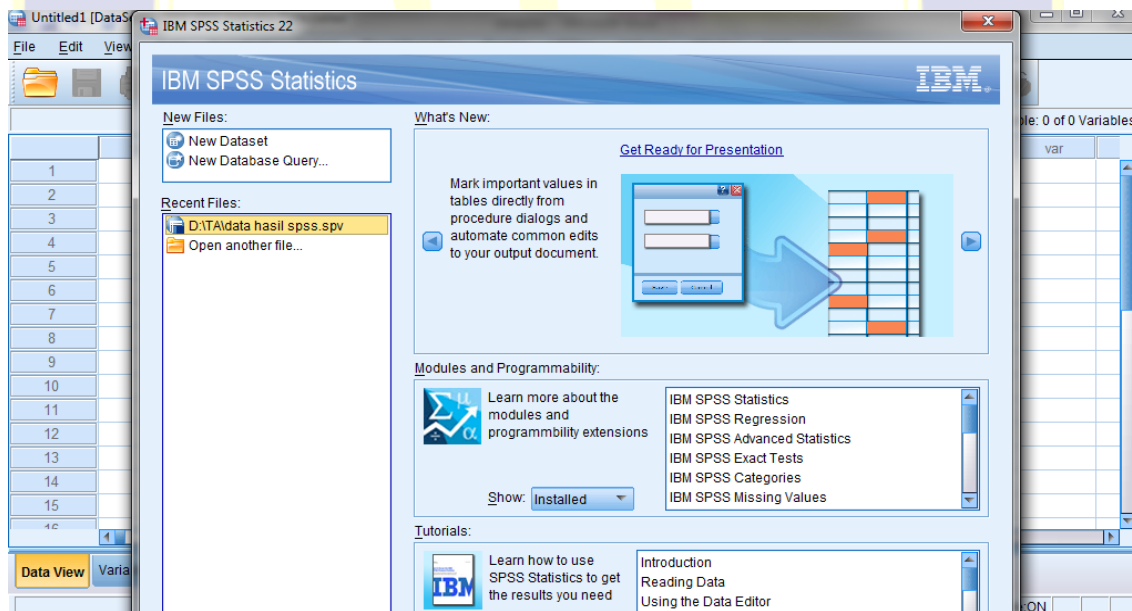
Gambar VII. 10 Tampilan situs pkCSM

LAMPIRAN 8

(LANJUTAN)

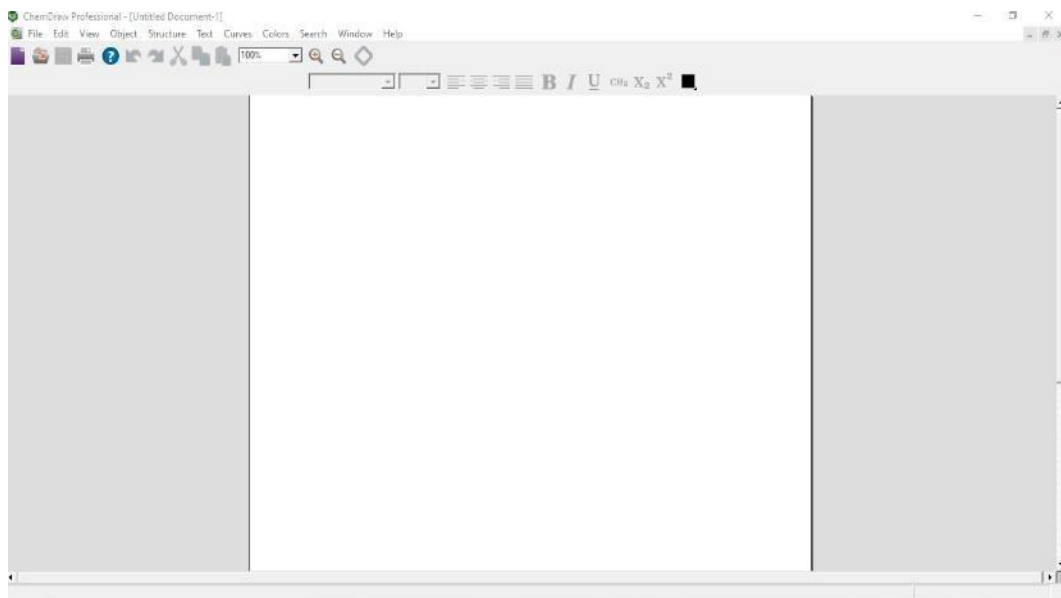


Gambar VII. 11 Tampilan situs *swissADME*

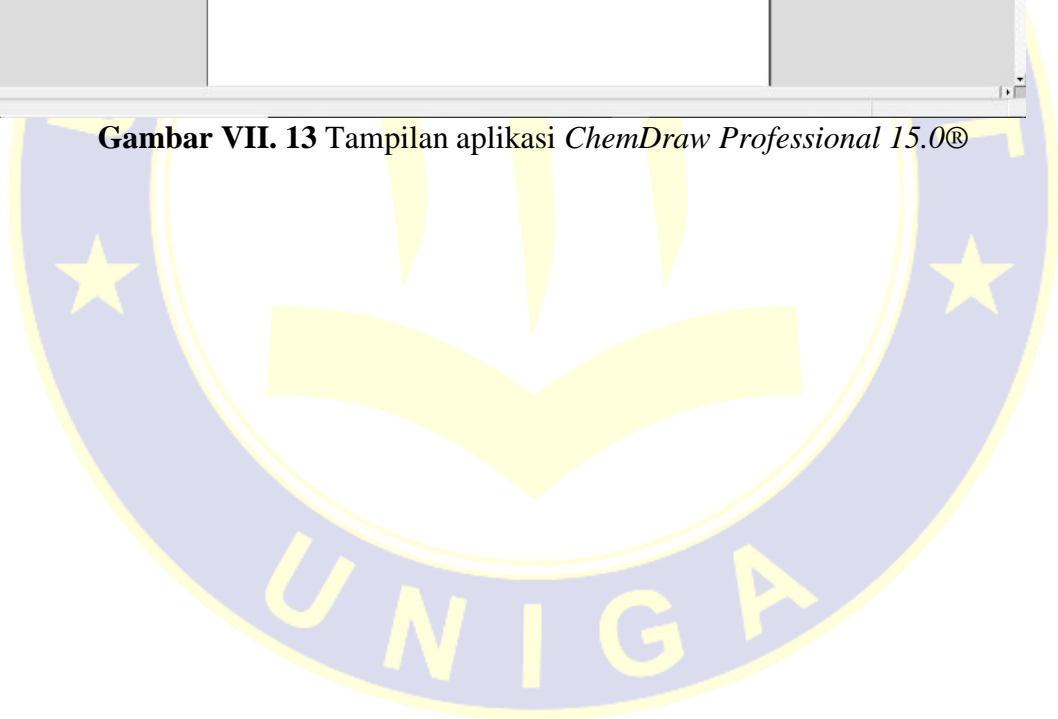


Gambar VII. 12 Tampilan program SPSS

LAMPIRAN 8
(LANJUTAN)



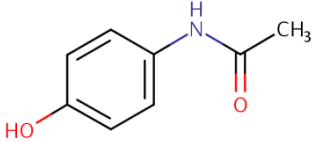
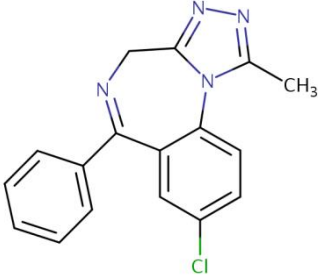
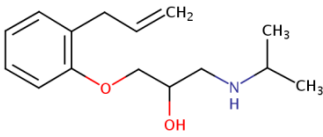
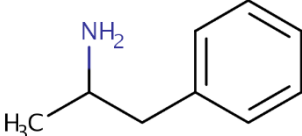
Gambar VII. 13 Tampilan aplikasi *ChemDraw Professional 15.0*®



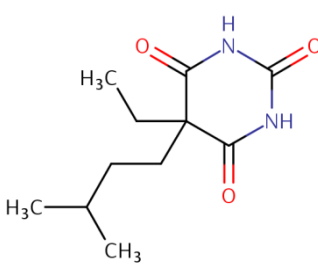
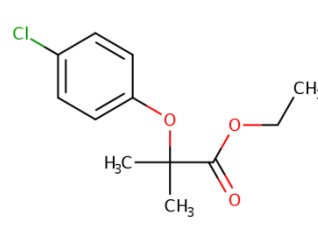
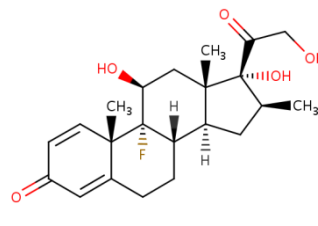
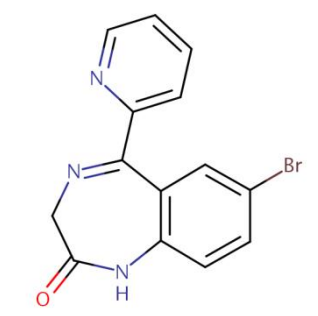
LAMPIRAN 9

STRUKTUR SENYAWA OBAT

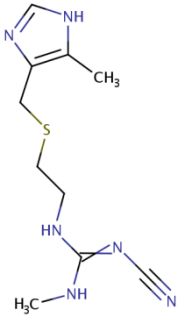
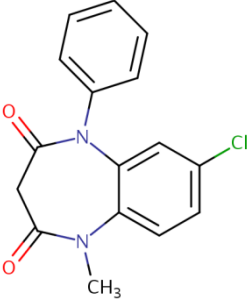
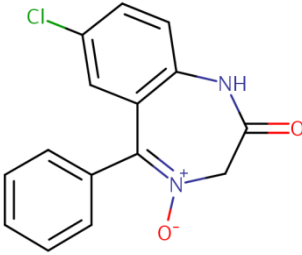
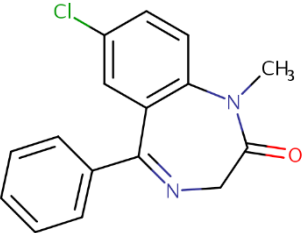
Tabel VII. 13
Struktur 2D dan *Compound CID* Senyawa Obat

No	Nama senyawa obat	Struktur 2D	<i>Compound CID</i>
1	Acetaminofen		163158
2	Alprazolam		2118
3	Alprenolol		2119
4	Amfetamin		3007

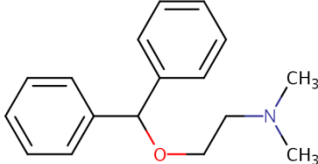
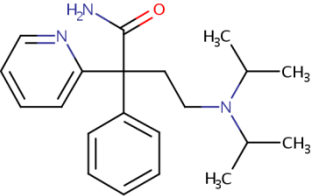
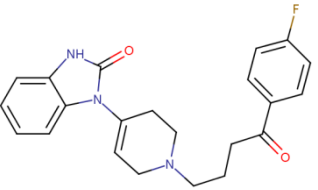
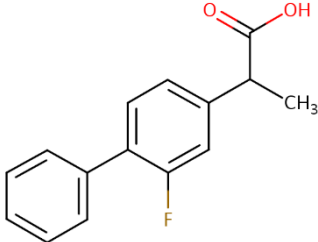
LAMPIRAN 9**(LANJUTAN)****Tabel VII.13**
Lanjutan

No	Nama senyawa obat	Struktur 2D	Compound CID
5	Amobarbital		2164
6	Asam klofibrat		2796
7	Betametason		9782
8	Bromazepam		2441

LAMPIRAN 9**(LANJUTAN)****Tabel VII.13**
Lanjutan

No	Nama senyawa obat	Struktur 2D	Compound CID
9	Cimetidin		2756
10	Clobazam		2789
11	Demoxepam		13756
12	Diazepam		3016

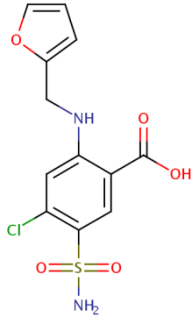
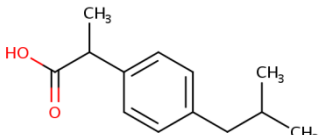
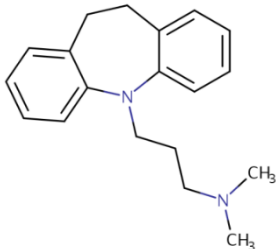
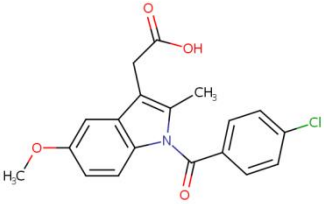
LAMPIRAN 9**(LANJUTAN)****Tabel VII.13**
Lanjutan

No	Nama senyawa obat	Struktur 2D	Compound CID
13	Dipfenidramin		3100
14	Disopiramida		3114
15	Droperidol		3168
16	Flurbiprofen		3394

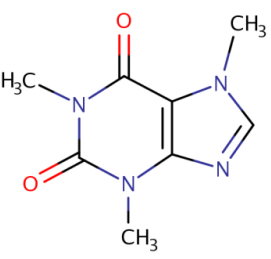
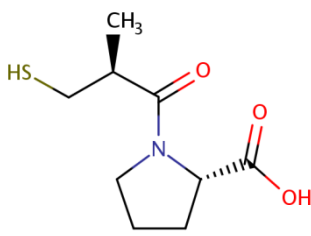
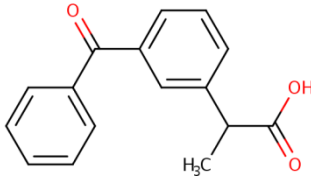
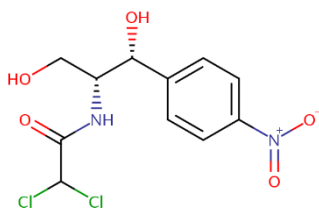
LAMPIRAN 9

(LANJUTAN)

Tabel VII.13
Lanjutan

No	Nama senyawa obat	Struktur 2D	Compound CID
17	Furosemid		3440
18	Ibuprofen		3672
19	Imipramin		3696
20	Indometasin		3715

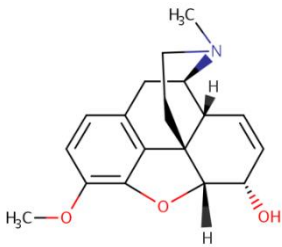
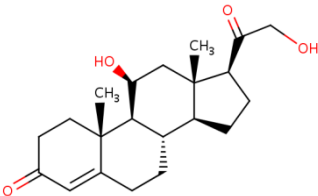
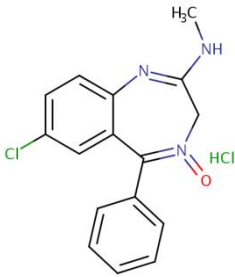
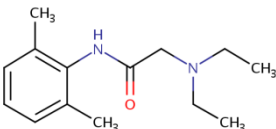
LAMPIRAN 9**(LANJUTAN)****Tabel VII.13**
Lanjutan

No	Nama senyawa obat	Struktur 2D	Compound CID
21	Kafein		2519
22	Kaptopril		44093
23	Ketoprofen		3825
24	Kloramfenikol		5959

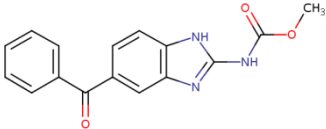
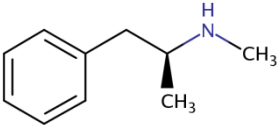
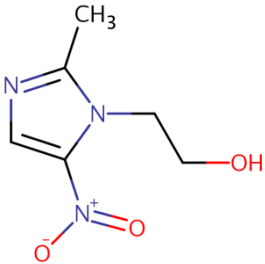
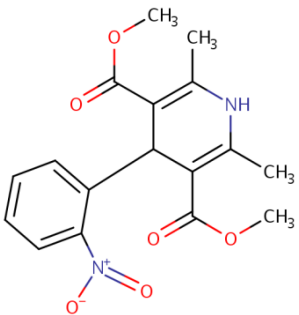
LAMPIRAN 9

(LANJUTAN)

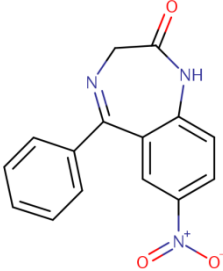
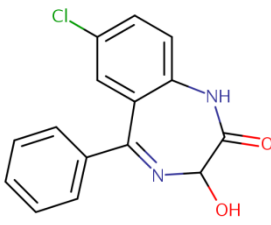
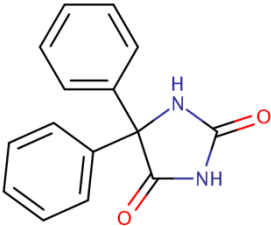
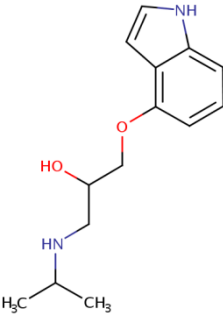
Tabel VII.13
Lanjutan

No	Nama senyawa obat	Struktur 2D	Compound CID
25	Kodein	 <p>The structure shows a complex pentacyclic ring system. It features a methyl group (H₃C) attached to a nitrogen atom, a methoxy group (H₃C-O) on one of the aromatic rings, and a hydroxyl group (OH) on another ring. Stereochemistry is indicated with wedges and dashes.</p>	5284371
26	korticosteron	 <p>The structure is a steroid nucleus with four fused rings. It has a ketone group (=O) at C3, a hydroxyl group (OH) at C11, a methyl group (CH₃) at C13, and a side chain at C17 consisting of a methyl group (CH₃) and a hydroxymethyl group (-CH₂OH).</p>	5753
27	Librium	 <p>The structure is a benzodiazepine derivative. It features a seven-membered diazepine ring fused to a benzene ring. Substituents include a methylamino group (-NHCH₃), a chlorine atom (Cl), and a benzamide group (-NH-C(=O)-C₆H₅). The structure is shown as a hydrochloride salt (HCl).</p>	2712
28	Lidocain	 <p>The structure shows a benzamide core with two methyl groups (CH₃) on the benzene ring. The amide nitrogen is attached to a propyl chain that ends in a diethylamino group (-N(CH₂CH₃)₂).</p>	3676

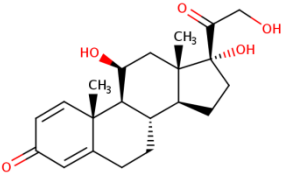
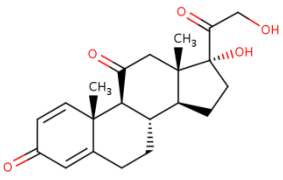
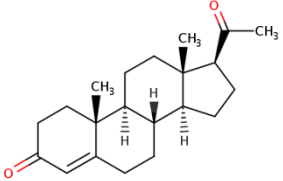
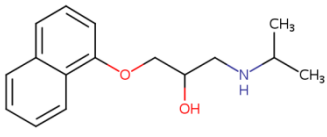
LAMPIRAN 9**(LANJUTAN)****Tabel VII.13**
Lanjutan

No	Nama senyawa obat	Struktur 2D	Compound CID
29	Mebendazol		4030
30	metamfetamin		10836
31	Metronidazol		4173
32	Nifedipine		4485

LAMPIRAN 9**(LANJUTAN)****Tabel VII.13**
Lanjutan

No	Nama senyawa obat	Struktur 2D	Compound CID
33	Nitrazepam		4506
34	Oxazepam		4616
35	phenytoin		1775
36	Pindolol		4828

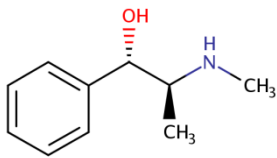
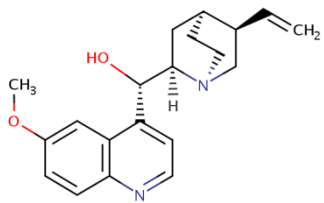
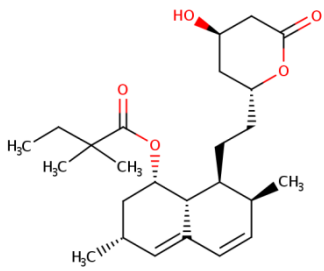
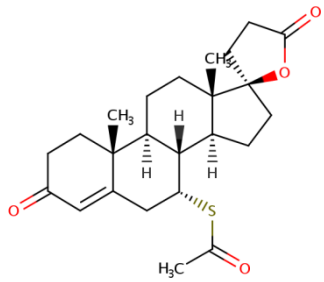
LAMPIRAN 9**(LANJUTAN)****Tabel VII.13**
Lanjutan

No	Nama senyawa obat	Struktur 2D	Compound CID
37	Prednisolon	 The structure shows a steroid nucleus with a ketone at C3, a double bond at C4, and a methyl group at C10. At C17, there is a side chain consisting of a methyl group, a hydroxyl group, and a dihydroxyethyl group.	5755
38	prednison	 The structure is identical to Prednisolon, showing a steroid nucleus with a ketone at C3, a double bond at C4, a methyl group at C10, and a side chain at C17 with a methyl group, a hydroxyl group, and a dihydroxyethyl group.	5865
39	Progesteron	 The structure shows a steroid nucleus with a ketone at C3, a double bond at C4, and methyl groups at C10 and C13. At C17, there is an acetyl group.	5994
40	Propranolol	 The structure consists of a naphthalene ring system connected via an ether linkage to a propanol chain. The propanol chain has a hydroxyl group at the second carbon and is terminated by an isopropylamino group.	4946

LAMPIRAN 9

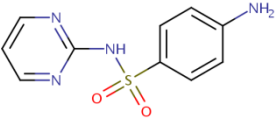
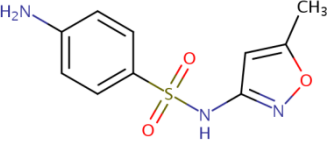
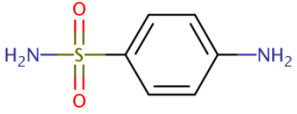
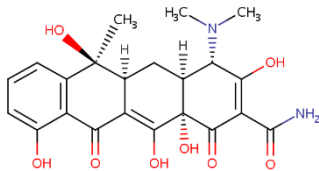
(LANJUTAN)

Tabel VII.13
Lanjutan

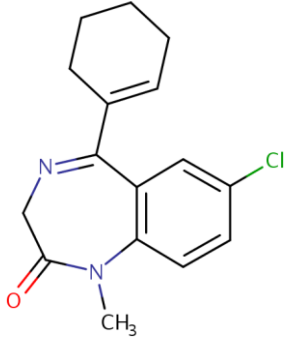
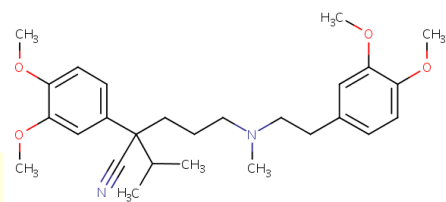
No	Nama senyawa obat	Struktur 2D	Compound CID
41	Pseudoefedrin		9581
42	Quinidin		441074
43	Simvastatin		54454
44	spironolactone		5833

LAMPIRAN 9
(LANJUTAN)

Tabel VII.13
Lanjutan

No	Nama senyawa obat	Struktur 2D	Compound CID
45	Sulfadiazine		5215
46	Sulfamethoxazol		5329
47	Sulfanilamid		5333
48	Tetrasiklin		54675776

LAMPIRAN 9**(LANJUTAN)****Tabel VII.13**
Lanjutan

No	Nama senyawa obat	Struktur 2D	Compound CID
49	Tetrazepam		25215
50	Verapamil		2520