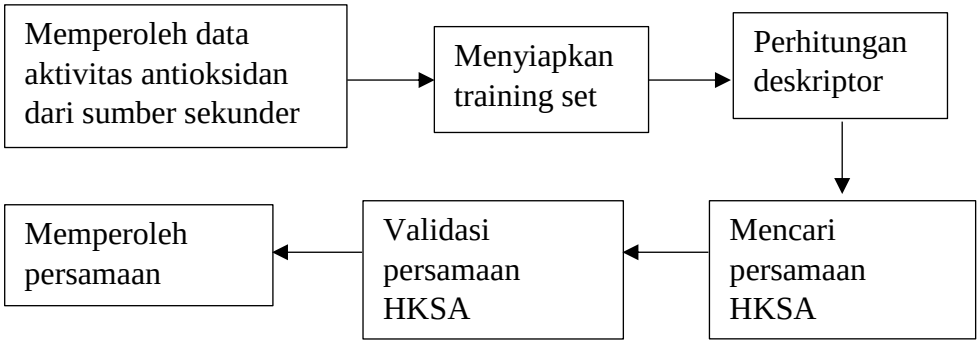
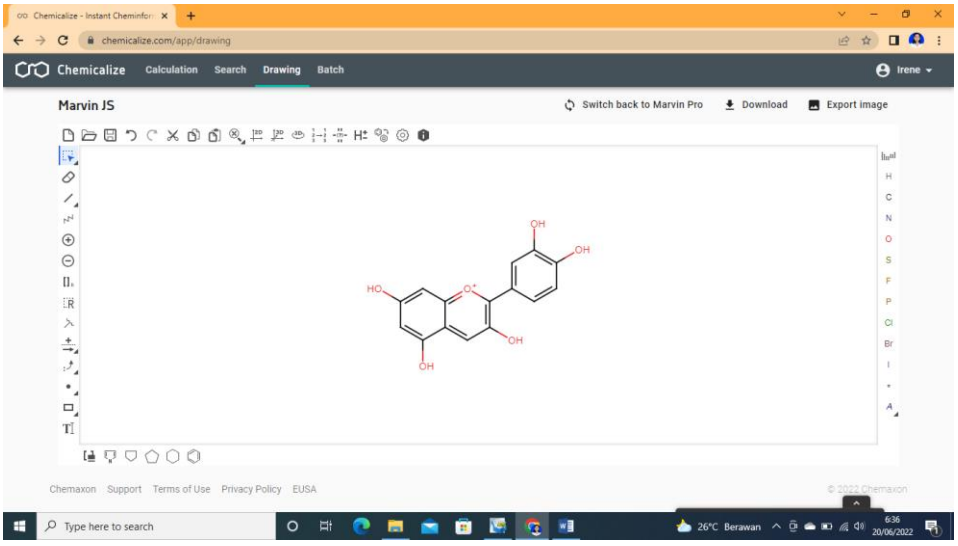
LAMPIRAN

1. Alur penelitian



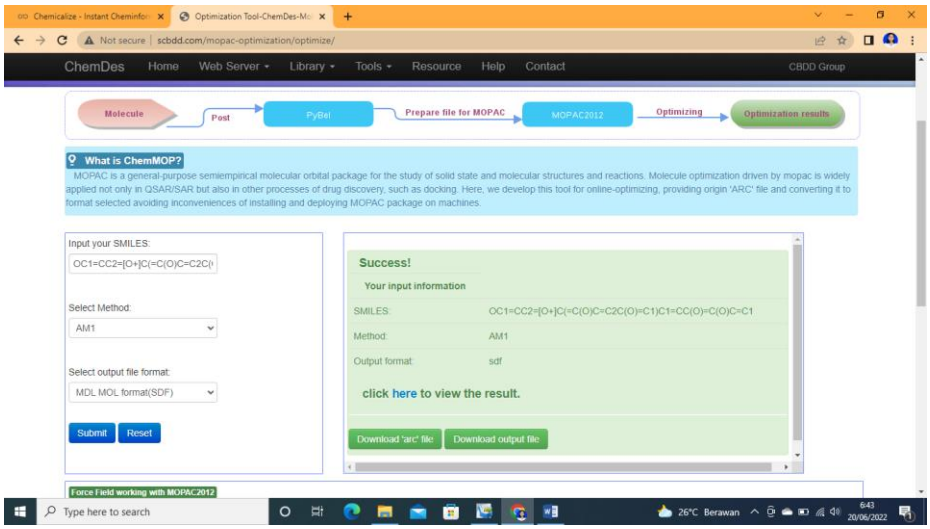
2. Langkah kerja HKSA

2.1.Menggambar menggunakan website *marvin sketch*



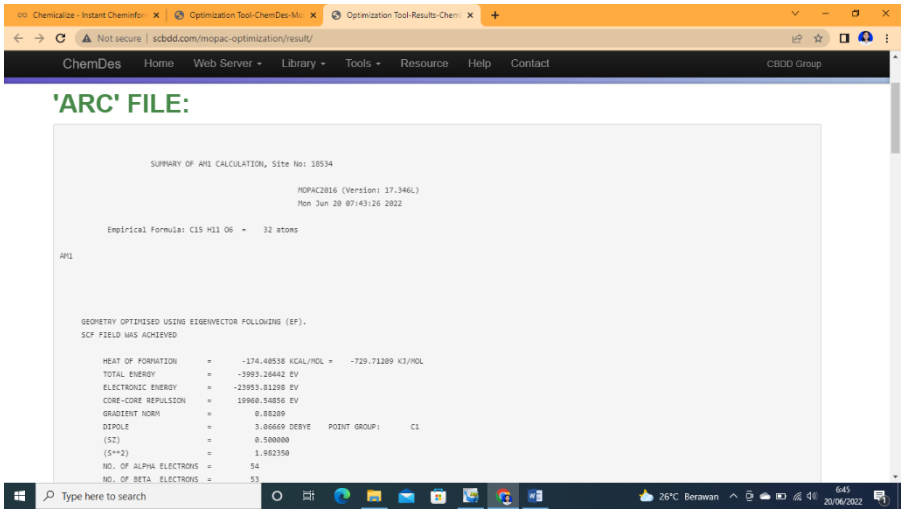
Mengetikan *marvin sketch* pada mesin pencarian → kemudian masuk *website chemaxon* → mencari *bagian supporting and education* → pilih bagian *try online* → kemudian pilih *sign up for free* → pilih *draw* → gunakan marvin JS → gambar struktur → pilih *export* kemudian di simpan menggunakan jenis file *.sdf* dan *export* ke file SMILE

2.2. Penggunaan metode semiempiris AM-1



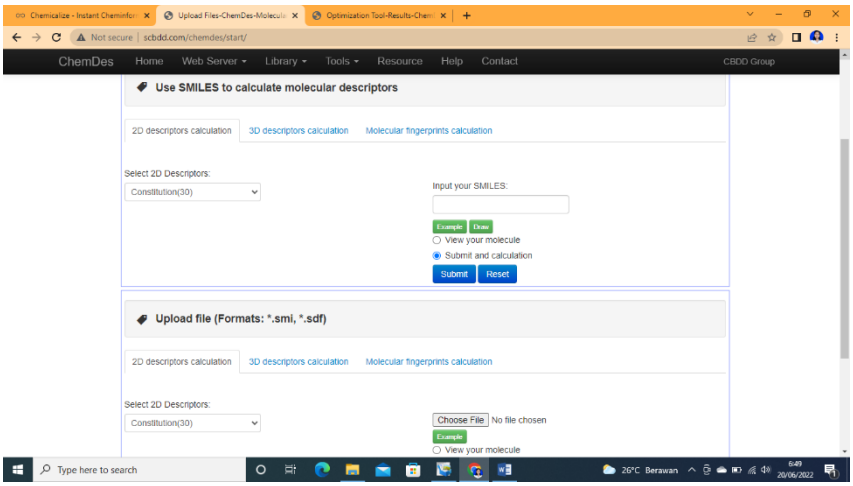
Ketikan *Chemdes* pada mesin pencarian → masuk website → kemudian pilih *tools* → pilih *ChemMop* → *output format* pilih MDL MOL format (SDF) → masukkan SMILES yang didapatkan dari *marvin sketch* → *submit*

2.3. Hasil perhitungan AM-1



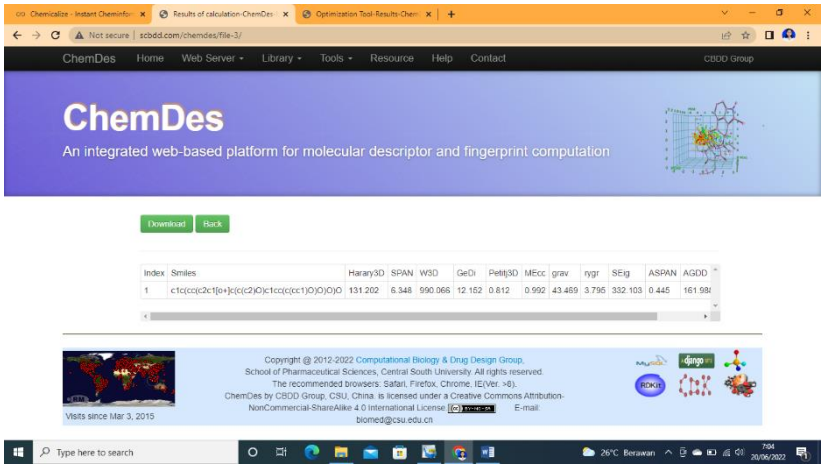
Pilih *click here* → kemudian akan muncul beberapa deskriptor.

2.4. Perhitungan deskriptor



Pilih menu *web server* → pilih *custom computation* → masukkan file struktur atau SMILE → menghitung deskriptor 2D dan 3D deskriptor → untuk 3D deskriptor dapat memilih metode semiempiris → pilih *calculate*.

2.5.Hasil perhitungan deskriptor



hasil perhitungan muncul → pilih *download*.

3. nilai IC50 antosianin dan turunannya dari Kahkonen, M dan M, Heinonen (2003).

compound	DPPH	MeLo emulsion		LDL			MeLo bulk
	17µM	50 µM	250 µM	2,5 µM	10 µM	25 µM	50 µM
Pelargonidin	31 ± 0	45± 0	49± 1	8 ± 1	31 ± 4	92 ± 0	-3±0
Cyanidin	33 ± 0	56±5	84±0	-3 ± 1	94 ± 0	98 ± 0	-18±1
Delphinidin	42 ± 1	67±5	83±1	-3 ± 0	94 ± 0	98 ± 0	14±2
Peonidin	33 ± 0	49±2	84±1	6 ± 0	59 ± 1	95 ± 1	21±15
Petunidin	10 ± 1	38±2	74±3	-2 ± 1	-7 ± 1	-3 ± 4	-22±7
Malvidin	24 ± 1	63±1	88±0	24 ± 2	84 ± 1	97 ± 0	-21±3
Pelargonidin-3-glucoside	20 ± 0	44±3	68±0	-17 ± 1	-23 ± 2	-2 ± 1	33±2
Cyanidin-3-glucoside	32 ± 1	52±2	83±0	-9 ± 1	92 ± 0	92 ± 0	20±1
Delphinidin-3-glucoside	42 ± 1	51±4	70±1	-5 ± 1	90 ± 1	93 ± 0	18±15
Peonidin-3-glucoside	26 ± 1	43±1	47±3	-5 ± 9	7 ± 1	97 ± 0	
Petunidin-3-glucoside	23 ± 1	60±4	87±2	-20 ± 1	59 ± 5	83 ± 0	33±10
Malvidin-3-glucoside	26 ± 1	82±0	90±1	-17 ± 1	-13 ± 1	14 ± 1	-13±1
Cyanidin-3-galactoside	25 ± 0	47±1	85±0		86 ± 1	89 ± 0	
Peonidin-3-galactoside	20 ± 1	-6±4	88±1		-8 ± 2	97 ± 0	
Malvidin-3-galactoside	22 ± 0	25±3	77±2		91 ± 2	98 ± 0	
Cyanidin-3-arabinoside	26 ± 0	50±5	76±0		98 ± 0	99 ± 0	
Peonidin-3-arabinoside	6 ± 0	20±6	72±3		-19 ± 1	94 ± 0	
Cyanidin-3-rutinoside	25 ± 0	21±6	78±4		11 ± 3	77 ± 0	
Delphinidin-3-rutinoside	32 ± 2	-57 ±13	47±6		98 ± 0	98 ± 0	
Cyanidin-3,5-diglucoside	21 ± 0	40 ±2	77±1		11 ± 1	53 ± 2	
Malvidin-3,5-diglucoside	14 ± 0	49 ±0	73±0		10 ± 0	25 ± 2	
Cyanidin-3-(xylosyl-glucoside)-5-galactoside	22 ± 0	37 ±7	94±3		-4 ± 1	98 ± 0	
Cyanidin-3-(coumaroyl-xylosyl-glucoside)-5-galactoside	26 ± 0	38 ±4	74 ± 1		98 ± 0	97 ± 1	

4. Hasil Analisis LOO

4.1.Hasil LOO Persamaan 1

senyawa	Log IC50 eksperimen (Y)	koefisien	polarity number (chemopy)		energi pembentukan		TASA (total hydrofobic surface area)	
			koefisien	nilai	koefisien	nilai	koefisien	nilai
Cyanidin	1.519	1.538070266	0.06825525	36	0.00373299	-173.83468	-0.0086675	226.963
Delphinidin	1.623	1.504558438	0.076833465	39	0.00395593	-221.62713	-0.0099935	191.351
cyanidin-3-glucoside	1.505	1.443881201	0.069623194	59	0.0036266	-367.41803	-0.0087981	287.729
delphinidin-3-glucoside	1.623	1.529088267	0.066879181	62	0.00360783	-454.35412	-0.0085982	247.227
malvidin-3-glucoside	1.415	1.508086536	0.059840081	66	0.00299371	-324.25053	-0.0082452	388.083
pelargonidin-3-glucoside	1.301	1.544572758	0.067017145	54	0.00362878	-359.70066	-0.0085997	292.715
petunidin-3-glucoside	1.362	1.528424158	0.066758266	64	0.00360777	-442.27463	-0.0085836	317.327
cyanidin-3-galactoside	1.398	1.46981824	0.073747092	59	0.00398495	-409.35047	-0.0091939	287.618
peonidin-3-arabinoside	0.778	1.411281393	0.02989902	56	0.00135547	-351.07820	-0.0041722	351.042
cyanidin-3-rutinoside	1.398	1.82496928	0.071744287	79	0.0051615	-403.34717	-0.0086936	381.211
delphinidin-3-rutinoside	1.505	1.520049036	0.068011429	82	0.0036175	-616.64253	-0.0087524	326.251
cyanidin 3-O-[6-O-((E)-p-coumaroyl)-2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	1.415	2.212751914	0.059827609	115	0.00403032	-780.02942	-0.0086238	502.724
cyanidin 3-O-[2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	1.342	1.587220196	0.065115676	100	0.00351373	-819.73951	-0.0085313	359.373

4.2.Hasil LOO persamaan 1

Senyawa	dipole (debye)		Log P		y'	y-y'	$(y-y')^2$	Y rata-rata	Y-$Y_{rata-rata}$	$(Y-Y_{rata-rata})^2$	Q^2
	Koefisien	nilai	koefisien	nilai							
Cyanidin	-0.06448443	5.36959	0.12376864	2.909	1.392914	0.126	0.015774254	1.399	0.120	0.01432984	
Delphinidin	-0.06478572	5.24562	0.18673993	2.615	1.860531	-0.237	0.056314209	1.399	0.224	0.05036537	
cyanidin-3-glucoside	-0.06632374	5.83077	0.15495867	0.382	1.360186	0.145	0.021014446	1.399	0.106	0.01130975	
delphinidin-3-glucoside	-0.05816452	5.09956	0.13447655	0.088	1.625867	-0.003	0.000006 8488	1.399	0.224	0.05037659	
malvidin-3-glucoside	-0.03869973	2.80887	0.13133512	0.694	1.269432	0.146	0.021181252	1.399	0.016	0.00026138	
pelargonidin-3-glucoside	-0.06071 69	1.59217	0.13333 83	0.634	1.328824	-0.028	0.000772492	1.399	-0.098	0.00955 95	
petunidin-3-glucoside	-0.05752749	3.16209	0.13367393	0.391	1.351889	0.010	0.0001	1.399	-0.037	0.00137438	
cyanidin-3-galactoside	-0.07002635	5.24819	0.15266552	0.382	1.236133	0.162	0.026181539	1.399	-0.001	0.00000 1	
peonidin-3-arabinoside	-0.01318581	4.28020	0.09835157	1.324	1.218912	-0.441	0.194270729	1.399	-0.621	0.38520976	
cyanidin-3-rutinoside	-0.02972449	8.47743	0.02558 36	-0.766	1.825211	-0.427	0.182560881	1.399	-0.001	0.00000 1	-0.23073
delphinidin-3-rutinoside	-0.06024318	5.10776	0.13970665	-1.061	1.554878	-0.050	0.002472882	1.399	0.106	0.01130975	
cyanidin 3-O-[6-O-((E)-p-coumaroyl)-2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	-0.06348284	8.25901	0.02451997	-1.712	1.047474	0.367	0.135053202	1.399	0.016	0.00026138	
cyanidin 3-O-[2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	-0.05704177	5.24813	0.11790638	-3.682	1.419019	-0.077	0.005867416	1.399	-0.056	0.00317901	
		Jumlah					0.661566994			0.53753821	

4.3.Hasil LOO persamaan 2

senyawa	Log IC50 Eksperimen (Y)	koefisien	energi pembentukan		TASA (total hydrofobic surface area)		dipole (debye)		ionization potentional (EV)	
			koefisien	nilai	koefisien	nilai	koefisien	nilai	koefisien	nilai
cyanidin	1.519	1.510101	0.00629341	-173.83468	-0.01136	226.963	-0.15521	5.36959	0.32899	8.0008
pelargonidin	1.491	1.187133	0.00591631	-132.76618	-0.01065	262.375	-0.15231	4.00476	0.347338	7.9126
petunidin	1.000	0.965887	0.00549025	-211.83601	-0.01005	270.994	-0.13664	6.39999	0.354904	8.0558
cyanidin-3-glucoside	1.505	0.917407	0.00574693	-367.41803	-0.01042	287.729	-0.14985	5.83077	0.372935	8.0365
delphinidin-3-glucoside	1.623	1.579452	0.00585042	-454.35412	-0.01026	247.227	-0.14703	5.09956	0.283532	8.2384
malvidin-3-glucoside	1.415	0.913376	0.00589221	-324.25053	-0.01054	388.083	-0.15556	2.80887	0.37999	8.1629
petunidin-3-glucoside	1.362	1.501744	0.00601828	-442.27463	-0.01077	317.327	-0.14344	3.16209	0.303793	8.1056
cyanidin-3-galactoside	1.398	-0.50258	0.00593574	-409.35047	-0.01055	287.618	-0.16029	5.24819	0.557638	7.8669
peonidin-3-arabinoside	0.778	1.15696	0.00514534	-351.07820	-0.0093	351.042	-0.13627	4.28020	0.311919	7.9522
cyanidin-3-rutinoside	1.398	1.923322	0.00584586	-403.34717	-0.01069	381.211	-0.15643	8.47743	0.256181	8.5063
cyanidin 3-O-[6-O-((E)-p-coumaroyl)-2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	1.415	0.668139	0.00564129	-780.02942	-0.01046	502.724	-0.15103	8.25901	0.409242	8.2179
cyanidin 3-O-[2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	1.342	1.086848	0.00541904	-819.73951	-0.01094	359.373	-0.15709	5.24813	0.361648	8.1324

4.4. hasil LOO persamaan 2

senyawa	gravitational 3D index		y'	y-y'	$(y-y')^2$	$Y_{rata-rata}$	$Y-Y_{rata-rata}$	$(Y-Y_{rata-rata})^2$	Q^2
	koefisien	nilai							
cyanidin	0.046552	43.469	1.6592	-0.141	0.019794	1.354	0.165	0.0271077	
pelargonidin	0.043987	40.365	1.520296	-0.029	0.000837	1.354	0.137	0.01890465	
petunidin	0.040854	49.467	1.083795	-0.084	0.007022	1.354	-0.354	0.12522103	
cyanidin-3-glucoside	0.04289	82.536	1.470969	0.034	0.001168	1.354	0.151	0.0228869	
delphinidin-3-glucoside	0.043246	82.519	1.539766	0.083	0.00697	1.354	0.269	0.07256783	
malvidin-3-glucoside	0.043778	88.440	1.448569	-0.034	0.001129	1.354	0.061	0.00373372	
petunidin-3-glucoside	0.044611	85.548	1.248412	0.113	0.012841	1.354	0.008	0.00006	
cyanidin-3-galactoside	0.043822	82.537	1.195233	0.203	0.04109	1.354	0.044	0.00194253	
peonidin-3-arabinoside	0.038397	76.069	0.902884	-0.125	0.015559	1.354	-0.576	0.33144872	
cyanidin-3-rutinoside	0.043959	112.981	1.309963	0.088	0.00774	1.354	0.044	0.00194253	0.687414
cyanidin 3-O-[6-O-((E)-p-coumaroyl)-2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	0.042106	195.226	1.345491	0.069	0.004827	1.354	0.061	0.00373372	
cyanidin 3-O-[2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	0.043117	157.248	1.610005	-0.268	0.071601	1.354	-0.011	0.00013101	
	jumlah				0.190578			0.60968218	

4.5.Hasil LOO Persamaan 3

Senyawa	Log IC50 eksperimen (Y)	koefisien	energi pembentukan		TASA		dipole (debye)		TPSA	
			koefisien	nilai	koefisien	nilai	koefisien	nilai	koefisien	nilai
cyanidin	1.519	2.678221	0.005852	-173.83468	-0.00725	-226.963	-0.07911	5.36959	0.010092	112.450
pelargonidin	1.491	1.670766	0.005504	-132.76618	-0,00484	-262.375	-0.03063	4.00476	0.016582	92.220
cyanidin-3-glucoside	1.505	2.435516	0.005912	-367.41803	-0.00668	-287.729	-0.06734	5.83077	0.012006	191.600
delphinidin-3-glucoside	1.623	2.557598	0.005693	-454.35412	-0.00686	-247.227	-0.07779	5.09956	0.010439	211.830
malvidin-3-glucoside	1.415	2.521685	0.006722	-324.25053	-0.00675	-388.083	-0.10193	2.80887	0.01329	189.830
petunidin-3-glucoside	1,362	2.531165	0.005753	-442.27463	-0.00689	-317.327	-0.07233	3.16209	0.010547	200.830
cyanidin-3-galactoside	1.398	2.571278	0.005724	-409.35047	-0.00691	-287.618	-0.07961	5.24819	0.010398	191.600
cyanidin-3-arabinoside	1.415	2.834494	0.006129	-355.64682	-0.00776	-283.448	-0.10644	5.52027	0.009593	171.370
peonidin-3-arabinoside	0.778	1.972653	0.002956	-351.07820	-0.00343	-351.042	-0.02295	4.28020	0.005769	160.370
delphinidin-3-rutinoside	1.505	2.751258	0.005879	-616.64253	-0.00754	-326.251	-0.09091	5.10776	0.009846	270.750
cyanidin-3,5-diglucoside	1.322	2.664399	0.005838	-632.62119	-0.00726	-364.321	-0.07628	3.31224	0.00967	270.750
cyanidin 3-O-[6-O-((E)-p-coumaroyl)-2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	1.415	2.99197	0.005151	-780.02942	-0.00761	-502.724	-0.11976	8.25901	0.010432	355.970
cyanidin 3-O-[2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	1.342	2.742196	0.005496	-819.73951	-0.00738	-359.373	-0.08847	5.24813	0.008869	329.670

4.6.Hasil LOO persamaan 3

Senyawa	gravitational		y'	y-y'	$(y-y')^2$	$Y_{rata-rata}$	$Y-Y_{rata-rata}$	$(Y-Y_{rata-rata})^2$	Q^2
	koefisien	nilai							
Cyanidin	0.020266	43.469	1.607026	-0.089	0.007835	1.392	0.127	0.01610634	
Pelargonidin	0.004047	40.365	1.240196	0.251	0.063083	1.392	0.100	0.00995221	
cyanidin-3-glucoside	0.016378	82.536	1.600217	-0.095	0.009038	1.392	0.114	0.01289378	
delphinidin-3-glucoside	0.01858	82.519	1.622351	0.0009	0.00000081	1.392	0.232	0.05366208	
malvidin-3-glucoside	0.018505	88.440	1.594827	-0.180	0.032349	1.392	0.023	0.00054619	
petunidin-3-glucoside	0.018653	85.548	1.285971	0.076	0.005739	1.392	-0.030	0.00089217	
cyanidin-3-galactoside	0.018898	82.537	1.375992	0.022	0.000482	1.392	0.006	0.00003606	
cyanidin-3-arabinoside	0.023941	72.696	1.251442	0.164	0.026741	1.392	0.023	0.00054619	
peonidin-3-arabinoside	0.008133	76.069	1.175669	-0.398	0.158022	1.392	-0.613	0.37631996	
delphinidin-3-rutinoside	0.021744	125.703	1.602282	-0.097	0.009435	1.392	0.114	0.01289378	
cyanidin-3,5-diglucoside	0.021006	120.233	1.218332	0.104	0.010793	1.392	-0.069	0.00481348	-0.09144
cyanidin 3-O-[6-O-((E)-p-coumaroyl)-2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	0.015836	195.226	0.962156	0.453	0.205041	1.392	0.023	0.00054619	
cyanidin 3-O-[2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	0.021552	157.248	1.432014	-0.090	0.008027	1.392	-0.049	0.00241826	
	Jumlah				0.536585			0.49163118	

4.7.Hasil LOO persamaan 4

senyawa	Log IC50 Eksperimen (Y)	koefisien	energi pembentukan		TASA		dipole (debye)		gravitational	
			koefisien	nilai	koefisien	Nilai	koefisien	nilai	koefisien	nilai
cyanidin	1.519	2.033968	0.001951	-173.83468	-0.00343	226.963	-0.03448	5.36959	0.01341	43.469
delphinidin	1.623	2.062866	0.002014	-221.62713	-0.00356	191.351	-0.03788	5.24562	0.01401	46.705
Pelargonidin	1.491	1.950541	0.002084	-132.76618	-0.0035	262.375	-0.03957	4.00476	0.01419	40.365
peonidin	1.519	2.189465	0.00183	-163.11151	-0.00349	300.921	-0.03258	3.39667	0.01319	46.147
cyanidin-3-glucoside	1.505	1.63288	0.00203	-367.41803	-0.0034	287.729	-0.03883	5.83077	0.01394	82.536
delphinidin-3-glucoside	1.623	2.362536	0.002043	-454.35412	-0.00327	247.227	-0.03833	5.09956	0.01382	82.519
malvidin-3-glucoside	1.415	1.975992	0.001853	-324.25053	-0.00332	388.083	-0.03241	2.80887	0.01269	88.440
petunidin-3-glucoside	1.362	1.950534	0.001906	-442.27463	-0.00336	317.327	-0.03594	3.16209	0.01306	85.548
cyanidin-3-galactoside	1.398	1.994567	0.001811	-409.35047	-0.00326	287.618	-0.0312	5.24819	0.01244	82.537
cyanidin-3-arabinoside	1.415	2.034208	0.001921	-355.64682	-0.00338	283.448	-0.03518	5.52027	0.01322	72.696
cyanidin-3-rutinoside	1.398	2.006639	0.001808	-403.34717	-0.00315	381.211	-0.02756	8.47743	0.01354	112.981
delphinidin-3-rutinoside	1.505	1.895332	0.001838	-616.64253	-0.00318	326.251	-0.03124	5.10776	0.01519	125.703
cyanidin-3,5-diglucoside	1.322	2.032991	0.001919	-632.62119	-0.00338	364.321	-0.03489	3.31224	0.01294	120.233
malvidin-3,5-diglucoside	1.146	2.018148	0.001829	-636.72646	-0.00323	450.238	-0.03381	1.88490	0.01258	127.020
cyanidin 3-O-[6-O-((E)-p-coumaroyl)-2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	1.415	2.299668	0.001578	-780.02942	-0.00317	502.724	-0.03128	8.25901	0.01089	195.226
cyanidin 3-O-[2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	1.342	2.070034	0.001935	-819.73951	-0.00366	359.373	-0.0392	5.24813	0.01403	157.248

4.8.Hasil LOO persamaan 4

Senyawa	somo (beta) (EV) koefisien	nilai	y'	y-y'	$(y-y')^2$	$Y_{rata-rata}$	$Y-Y_{rata-rata}$	$(Y-Y_{rata-rata})_2$	Q^2
cyanidin	-0.03038	-8.766	1.580571	-0.062	0.003852	1.437	0.081	0.006578376	
delphinidin	-0.03038	-8.837	1.658806	-0.036	0.001266	1.437	0.186	0.034529885	
Pelargonidin	-0.04353	-8.893	1.55719	-0.066	0.004334	1.437	0.054	0.002911378	
peonidin	-0.00884	-8.843	1.417843	0.101	0.010134	1.437	0.081	0.006578376	
cyanidin-3-glucoside	-0.07503	-8.036	1.434717	0.070	0.004961	1.437	0.068	0.004589681	
delphinidin-3-glucoside	0.012401	-9.139	1.45697	0.166	0.027649	1.437	0.186	0.034539177	
malvidin-3-glucoside	-0.03225	-8.242	1.399467	0.0155	0.00024	1.437	-0.022	0.000503231	
petunidin-3-glucoside	-0.03786	-9.051	1.401235	-0.040	0.001561	1.437	-0.076	0.005726375	
cyanidin-3-galactoside	-0.02919	-8.838	1.444395	-0.046	0.002158	1.437	-0.039	0.001557314	
cyanidin-3-arabinoside	-0.02808	-8.800	1.413133	0.002	0.000004	1.437	-0.022	0.000503231	
cyanidin-3-rutinoside	-0.02354	-8.506	1.438082	-0.040	0.001611	1.437	-0.039	0.001557314	
delphinidin-3-rutinoside	-0.03853	-8.498	1.465711	0.039	0.001555	1.437	0.068	0.004589681	0.625512
cyanidin-3,5-diglucoside	-0.02803	-8.836	1.318747	0.003	0.000009	1.437	-0.115	0.01326708	
malvidin-3,5-diglucoside	-0.02621	-8.677	1.17124	-0.025	0.000631	1.437	-0.291	0.084839851	
cyanidin 3-O-[6-O-((E)-p-coumaroyl)-2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	0.004816	-8.913	1.317793	0.097	0.009443	1.437	-0.022	0.000503231	
cyanidin 3-O-[2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	-0.02961	-8.894	1.441957	-0.100	0.009908	1.437	-0.095	0.009021735	
	Jumlah				0.079315			0.211795916	

4.9.Hasil LOO Persamaan 5

senyawa	Log IC50 Eksperimen (Y)	koefisien	energi pembentukan		TASA		dipole (debye)		gravitational	
			koefisien	nilai	koefisien	nilai	koefisien	nilai	koefisien	nilai
pelargonidin	1.491	5.130045	0.008107	-132.76618	-0.01377	262.375	-0.18443	4.00476	0.045012	40.365
petunidin	1.000	3.896798	0.005562	-211.83601	-0.01014	270.994	-0.10867	6.39999	0.035757	49.467
cyanidin-3-glucoside	1.505	4.077949	0.006081	-367.41803	-0.01089	287.729	-0.13361	5.83077	0.040247	82.536
delphinidin-3-glucoside	1.623	3.905199	0.005967	-454.35412	-0.01034	247.227	-0.12991	5.09956	0.04061	82.519
malvidin-3-glucoside	1.415	3.996006	0.005712	-324.25053	-0.01088	388.083	-0.11473	2.80887	0.037932	88.440
petunidin-3-glucoside	1.362	4.077656	0.006333	-442.27463	-0.01122	317.327	-0.12601	3.16209	0.04291	85.548
cyanidin-3-galactoside	1.398	4.080509	0.00612	-409.35047	-0.0109	287.618	-0.13489	5.24819	0.040277	82.537
cyanidin-3-arabinoside	1.415	4.142664	0.006395	-355.64682	-0.01119	283.448	-0.1441	5.52027	0.042537	72.696
peonidin-3-arabinoside	0.778	3.477186	0.004764	-351.07820	-0.00847	351.042	-0.11073	4.28020	0.033314	76.069
cyanidin-3-rutinoside	1.398	4.110525	0.005952	-403.34717	-0.01091	381.211	-0.14479	8.47743	0.040252	112.981
delphinidin-3-rutinoside	1.505	3.980308	0.006244	-616.64253	-0.01126	326.251	-0.13539	5.10776	0.050369	125.703
cyanidin 3-O-[6-O-((E)-p-coumaroyl)-2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	1.415	4.072898	0.006112	-780.02942	-0.01089	502.724	-0.13348	8.25901	0.040309	195.226
cyanidin 3-O-[2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	1.342	4.240398	0.005613	-819.73951	-0.01119	359.373	-0.14389	5.24813	0.033119	157.248

4.10. Hasil LOO persamaan 5

Senyawa	energi elektronik		y'	y-y'	$(y-y')^2$	$Y_{rata-rata}$	$Y-Y_{rata-rata}$	$(Y-Y_{rata-rata})^2$	Q^2
	koefisien	nilai							
pelargonidin	-0.000015	-21800.7306	1.837168	-0.346	0.119583	1.358	0.134	0.017908	
petunidin	-0.0000056	-28315.9951	1.201512	-0.202	0.040607	1.358	-0.358	0.127834	
cyanidin-3-glucoside	-0.0000052	-48209.4010	1.50516	0.000	0	1.358	0.148	0.021789	
delphinidin-3-glucoside	-0.0000034	-55356.7793	1.514477	0.109	0.011832	1.358	0.266	0.070603	
malvidin-3-glucoside	-0.0000057	-57861.8005	1.282945	0.132	0.01743	1.358	0.057	0.003298	
petunidin-3-glucoside	-0.0000039	-57398.8547	1.210394	0.151	0.022902	1.358	0.004	0.00002	
cyanidin-3-galactoside	-0.0000055	-52713.4649	1.34675	0.051	0.00262	1.358	0.040	0.001632	
cyanidin-3-arabinoside	-0.0000051	-46220.5989	1.229452	0.186	0.034417	1.358	0.057	0.003298	
peonidin-3-arabinoside	-0.0000021	-47962.6800	0.992213	-0.214	0.045823	1.358	-0.579	0.335691	
cyanidin-3-rutinoside	-0.0000047	-83795.1989	1.267518	0.130	0.01701	1.358	0.040	0.001632	0.28481
delphinidin-3-rutinoside	0.00000476	-79396.8272	1.717249	-0.212	0.044986	1.358	0.148	0.021789	
cyanidin 3-O-[6-O-((E)-p-coumaroyl)-2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	-0.0000055	-154280.6988	1.437537	-0.023	0.000509	1.358	0.057	0.003298	
cyanidin 3-O-[2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	-0.000013	-121562.1553	1.621432	-0.279	0.077848	1.358	-0.015	0.000229	
		Jumlah			0.43557			0.60902218	

4.11. Hasil LOO persamaan 6

senyawa	Log IC50 Eksperimen (Y)	koefisien	energi pembentukan		TASA		dipole (debye)		gravitational	
			koefisien	nilai	koefisien	nilai	koefisien	nilai	koefisien	nilai
cyanidin	1.519	2.118557	0.002119	-173.83468	-0.00429	226.963	-0.04506	5.36959	0.006691	43.469
delphinidin	1.623	2.126001	0.002324	-221.62713	-0.00484	191.351	-0.05441	5.24562	0.005601	46.705
pelargonidin	1.491	2.132635	0.002168	-132.76618	-0.0043	262.375	-0.04761	4.00476	0.007162	40.365
Peonidin	1.519	1.929091	0.0022	-163.11151	-0.00511	300.921	-0.05353	3.39667	0.000916	46.147
cyanidin-3-glucoside	1.505	2.070911	0.002134	-367.41803	-0.00438	287.729	-0.04824	5.83077	0.005559	82.536
delphinidin-3-glucoside	1.623	2.394897	0.001945	-454.35412	-0.00264	247.227	-0.03045	5.09956	0.019266	82.519
malvidin-3-glucoside	1.415	2.103776	0.002292	-324.25053	-0.00456	388.083	-0.05364	2.80887	0.006097	88.440
petunidin-3-glucoside	1.362	2.02604	0.002156	-442.27463	-0.00461	317.327	-0.05175	3.16209	0.003474	85.548
cyanidin-3-galactoside	1.398	2.086971	0.002017	-409.35047	-0.00415	287.618	-0.04273	5.24819	0.006304	82.537
peonidin-3-galactoside	1.301	2.081994	0.002098	-396.06605	-0.00428	361.868	-0.04652	2.42715	0.005965	83.132
cyanidin-3-arabinoside	1.415	2.083501	0.002108	-355.64682	-0.00431	283.448	-0.04647	5.52027	0.006	72.696
cyanidin-3-rutinoside	1.398	1.988655	0.00199	-403.34717	-0.00406	381.211	-0.03739	8.47743	0.004521	112.981
delphinidin-3-rutinoside	1.505	1.92287	0.002041	-616.64253	-0.00435	326.251	-0.04467	5.10776	0.00161	125.703
cyanidin-3,5-diglucoside	1.322	2.084934	0.002121	-632.62119	-0.00432	364.321	-0.04655	3.31224	0.006048	120.233
malvidin-3,5-diglucoside	1.146	2.061629	0.002053	-636.72646	-0.00422	450.238	-0.04577	1.88490	0.005565	127.020
cyanidin 3-O-[6-O-((E)-p-coumaroyl)-2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	1.415	2.106347	0.0019	-780.02942	-0.00406	502.724	-0.04295	8.25901	0.005872	195.226
cyanidin 3-O-[2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	1.342	2.186383	0.002046	-819.73951	-0.00426	359.373	-0.046	5.24813	0.008906	157.248

4.12. Hasil LOO persamaan 6

Senyawa	atomic polarizability		y'	y-y'	$(y-y')^2$	$Y_{rata-rata}$	$Y-Y_{rata-rata}$	$(Y-Y_{rata-rata})^2$	Q^2
	koefisien	nilai							
Cyanidin	0.023905	31.212	1.572141	-0.054	0.002876	1.429	0.089	0.007944	
Delphinidin	0.031952	32.014	1.684061	-0.061	0.003701	1.429	0.194	0.037575542	
Pelargonidin	0.023469	30.410	1.528873	-0.038	0.001407	1.429	0.062	0.003841411	
Peonidin	0.044846	32.972	1.372745	0.146	0.021248	1.429	0.089	0.007944	
Cyandin-3-glucoside	0.027892	45.782	1.480087	0.025	0.000628	1.429	0.076	0.005740959	
Delphinidin-3-glucoside	-0.01852	46.584	1.429664	0.194	0.037475	1.429	0.194	0.037585235	
Malvidin-3-glucoside	0.02932	50.104	1.447373	-0.032	0.00105	1.429	-0.014	0.000207674	
Petunidin-3-glucoside	0.034694	48.344	1.420925	-0.059	0.003504	1.429	-0.068	0.004576642	
Cyanidin-3-galactoside	0.023229	45.782	1.428126	-0.030	0.000911	1.429	-0.031	0.000988529	0.598777
Peonidin-3-galactoside	0.025857	47.542	1.313157	-0.012	0.000147	1.429	-0.128	0.016473949	
Cyanidin-3-arabinoside	0.026023	43.220	1.415426	0	0	1.429	-0.014	0.000207674	
Cyanidin-3-rutinoside	0.027194	59.550	1.452344	-0.054	0.00296	1.429	-0.031	0.000988529	
Delphinidin-3-rutinoside	0.036731	60.352	1.435904	0.069	0.004795	1.429	0.076	0.005740959	
Cyanidin-3,5-diglucoside	0.02608	60.352	1.314844	0.007	0.000049	1.429	-0.107	0.011483455	
Malvidin-3,5-diglucoside	0.026153	64.674	1.165835	-0.020	0.000388	1.429	-0.283	0.080231062	

4.13. Hasil LOO persamaan 6

Senyawa	Atomic Polarizability		y'	y-y'	$(y-y')^2$	$Y_{rata-rata}$	$Y-Y_{rata-rata}$	$(Y-Y_{rata-rata})^2$	Q^2
	koefisien	nilau							
Cyanidin-3-O-[6-O-((E)-p-coumaroyl)-2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	0.022001	89.804	1.350702	0.064	0.00413	1.429	-0.014	0.000207674	0.598777
Cyanidin-3-O-[2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	0.017766	72.360	1.424454	-0.082	0.00673	1.429	-0.087	0.007562195	
Jumlah					0.092000311			0.229299487	

4.14. Hasil LOO persamaan 7

senyawa	Log IC50 eksperimen (Y)	koefisien	log P		energi pembentukan		TASA		Dipole (debye)	
			koefisien	nilai	koefisien	nilai	koefisien	nilai	koefisien	nilai
cyanidin	1.519	4.092723	-0.05305	2.909	0.006554	-173.83468	-0.01072	226.963	-0.11778	5.36959
pelargonidin	1.491	3.962425	-0.06258	3.203	0.006261	-132.76618	-0.01003	262.375	-0.11553	4.00476
petunidin	1.000	3.717189	-0.04799	2.918	0.005645	-211.83601	-0.00936	270.994	-0.09639	6.39999
cyanidin-3-glucoside	1.505	3.95551	-0.06838	0.382	0.006227	-367.41803	-0.00997	287.729	-0.11213	5.83077
delphinidin-3-glucoside	1.623	3.819709	-0.06545	0.088	0.006219	-454.35412	-0.00948	247.227	-0.11101	5.09956
malvidin-3-glucoside	1.415	3.718065	-0.04235	0.694	0.005536	-324.25053	-0.01005	388.083	-0.08158	2.80887
cyanidin-3-galactoside	1.398	3.921039	-0.06331	0.382	0.006223	-409.35047	-0.00994	287.618	-0.11334	5.24819
cyanidin-3-arabinoside	1.415	4.039014	-0.06625	1.021	0.006631	-355.64682	-0.0104	283.448	-0.12415	5.52027
peonidin-3-arabinoside	0.778	3.506411	-0.05468	1.324	0.00503	-351.07820	-0.00805	351.042	-0.10018	4.28020
cyanidin-3-rutinoside	1.398	3.996607	-0.10751	-0.766	0.00659	-403.34717	-0.00971	381.211	-0.09566	8.47743
delphinidin-3-rutinoside	1.505	3.982058	-0.05876	-1.061	0.006223	-616.64253	-0.01023	326.251	-0.11833	5.10776
cyanidin 3-O-[6-O-((E)-p-coumaroyl)-2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	1.415	4.719204	-0.22438	-1.712	0.006214	-780.02942	-0.0094	502.724	-0.11789	8.25901
cyanidin 3-O-[2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	1.342	3.99053	-0.09378	-3.682	0.005851	-819.73951	-0.00977	359.373	-0.11551	5.24813

4.15. Hasil LOOpersamaan 7

Senyawa	gravitational koefisien	nilai	y'	y-y'	$(y-y')^2$	$Y_{rata-rata}$	$Y-Y_{rata-rata}$	$(Y-Y_{rata-rata})^2$	Q^2
cyanidin	0.044365	43.469	1.661295	-0.143	0.020388	1.370	0.149	0.022174646	
pelargonidin	0.041895	40.365	1.526767	-0.035	0.001254	1.370	0.122	0.014825872	
petunidin	0.03832	49.467	1.124108	-0.124	0.015403	1.370	-0.370	0.136603023	
cyanidin-3-glucoside	0.04144	82.536	1.538042	-0.033	0.001082	1.370	0.136	0.01837422	
delphinidin-3-glucoside	0.040896	82.519	1.454154	0.169	0.028594	1.370	0.254	0.064339103	
malvidin-3-glucoside	0.039042	88.440	1.217473	0.197	0.039005	1.370	0.045	0.002058577	
cyanidin-3-galactoside	0.041634	82.537	1.332616	0.065	0.004267	1.370	0.028	0.000803243	
cyanidin-3-arabinoside	0.04431	72.696	1.201388	0.214	0.045617	1.370	0.045	0.002058577	
peonidin-3-arabinoside	0.033634	76.069	0.972448	-0.194	0.037752	1.370	-0.591	0.349811283	
cyanidin-3-rutinoside	0.041016	112.981	1.541351	-0.143	0.020567	1.370	0.028	0.000803243	-0.15507
delphinidin-3-rutinoside	0.0424	125.703	1.593616	-0.088	0.007826	1.370	0.136	0.01837422	
cyanidin 3-O-[6-O-((E)-p-coumaroyl)-2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	0.031693	195.226	0.742773	0.672	0.451849	1.370	0.045	0.002058577	
cyanidin 3-O-[2-O-(beta-D-xylopyranosyl)-beta-D-glucopyranoside]-5-O-beta-D-galactopyranoside	0.039185	157.248	1.582391	-0.240	0.057586	1.370	-0.027	0.000738669	
	Jumlah				0.731189			0.63302325	

5. Persamaan HKSA

NO	Persamaan	r
1	log p + energi pembentukan + dipole + TASA +grav	0.570347
2	apol + log p + TASA + ion + dipole	0.549792
3	log p + TASA + ion + dipole +grav	0.547284
4	log p + somo beta + dipole + TASA +grav	0.546684
5	log p + pol + dipole + TASA +grav	0.521253
6	ion+ energi pembentukan + dipole + TASA +grav	0.590783
7	Somo beta + energi pembentukan + dipole + TASA +grav	0.578372
8	energi elektronik + energi pembentukan + dipole + TASA +grav	0.572152
9	apol+ energi pembentukan + dipole + TASA +grav	0.570794
10	TPSA+ energi pembentukan + dipole + TASA +grav	0.580515
11	ion+ log P + dipole + TASA +grav	0.547284
12	ion + dipole + Qmin + TASA + grav	0.525955
13	ion + energi pembentukan + Qmin + TASA + grav	0.558844
14	ion + QHmin + QHmax + TASA + grav	0.518397
15	ion + pol + energi pembentukan + TASA + grav	0.558502
16	ion + lumo beta + somo alpha + TASA + grav	0.530066
17	ion + Qmin + dipole + TASA + grav	0.525955
18	Log P + PSA + dipole + TASA + grav	0.527772
19	Log P + Qmin + dipole + TASA + grav	0.500035
20	Log P + QHmax + QHmin + TASA + grav	0.516786
21	Log P + lumo beta + somo alpha + TASA + grav	0.551983
22	Log P + dipole + energi elektronik + TASA + grav	0.500767
23	log P + TPSA + dipole + TASA + grav	0.540453
24	Log P + energi pembentukan + apol + TASA + grav	0.543465
25	Log P + energi pembentukan + pol + TASA + grav	0.558407
26	TPSA + PSA + TASA + dipole + energi pembentukan	0.548728
27	energi pembentukan + energi elektronik + dipole + log P + ion	0.289741
28	TPSA + PSA + TASA + pol + energi pembentukan	0.544809
29	TPSA + PSA + pol+ dipol + energi pembentukan	0.526475
30	TPSA + PSA + dipol + TASA + pol	0.468833
31	QCmin + QCmax + PSA + energi elektronik + TPSA	0.448641
32	QCmin + QCmax +QHmin + QHmax + Qmin	0.275989
33	lomo alpha + Somo beta+ PSA + energi elektronik + TPSA	0.480531
34	log P + MR + QOmin + QOmax + apol	0.319631
35	MR +apol + energi pembentukan + energi total + Molecular weight	0.492696
36	TASA + ion + Qcmin + Qcmax + dipole	0.496406
37	Log P + Pol + energi pembentukan + TASA + dipole	0.593432
38	Log P + Pol + energi pembentukan + TASA + PSA	0.558293
39	Log P + Pol + energi pembentukan + TASA + somo beta	0.54231

6. Tabel persamaan HKSA

No	Persamaan	r
40	Lumo alpha + somo beta + energi pembentukan + pol + PSA	0.533817
41	Lumo alpha + somo beta + ion + pol + PSA	0.532907
42	Log P + Pol + energi pembentukan + TASA + dipole	0.593432
43	Log P + Pol + energi pembentukan + TASA + PSA	0.558293
44	Log P + Pol + energi pembentukan + TASA + somo beta	0.54231
45	Lumo alpha + somo beta + energi pembentukan + pol + PSA	0.533817
46	Lumo alpha + somo beta + ion + pol + PSA	0.532907
47	Lumo alpha + somo beta + energi pembentukan + grav + TPSA	0.42793
48	energi total + molecular weight + MR + TPSA + grav	0.426848
49	Ion + Log P + PSA + TPSA + dipole	0.442345
50	Ion + Log P + Qomax + Qomin + dipole	0.270416