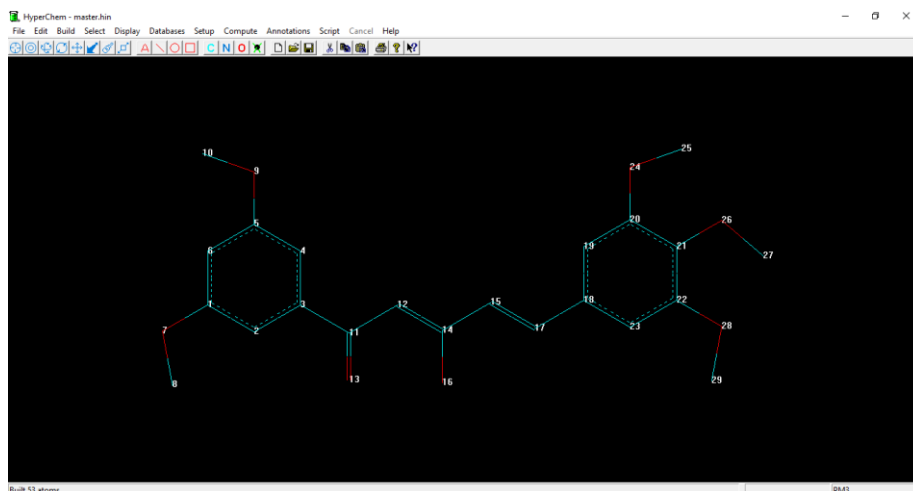
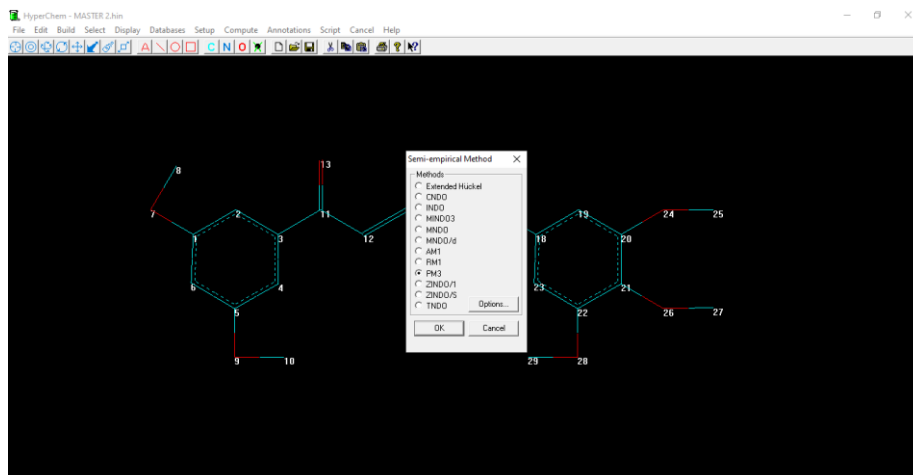


LAMPIRAN

Lampiran 1. Desain Senyawa dengan Aplikasi *Hyperchem*



Lampiran 2. Pemilihan metode semiempiris PM3



Lampiran 3. Hasil Optimasi Geometri dan Deskriptor-deskriptor dari Senyawa

Hs-055 - Notepad

File Edit Format View Help

HyperChem log start -- Tue May 17 12:35:16 2022.

Single Point, SemiEmpirical, molecule = D:\data terbaru\Hs-055.hin.

PM3

Convergence limit = 0.0100000 Iteration limit = 50

Accelerate convergence = YES

RHF Calculation:

Singlet state calculation

Number of electrons = 136

Number of Double Occupied Levels = 68

Charge on the System = 0

Total Orbitals = 124

Starting PM3 calculation with 124 orbitals

Iteration = 1 Difference = 24104.53635

Iteration = 2 Difference = 187.40817

Iteration = 3 Difference = 30.40451

Iteration = 4 Difference = 6.51567

Iteration = 5 Difference = 0.40101

Iteration = 6 Difference = 0.06115

Energy = -102335.6946911 kcal/mol Gradient = 0.0171705 Symmetry = CS

ENERGIES AND GRADIENT

Total Energy = -102335.6946911 (kcal/mol)

Total Energy = -163.082290037 (a.u.)

Binding Energy = -4969.5698591 (kcal/mol)

Isolated Atomic Energy = -97366.1248320 (kcal/mol)

Electronic Energy = -719075.4744648 (kcal/mol)

Core-Core Interaction = 616739.7797737 (kcal/mol)

Heat of Formation = -152.3758591 (kcal/mol)

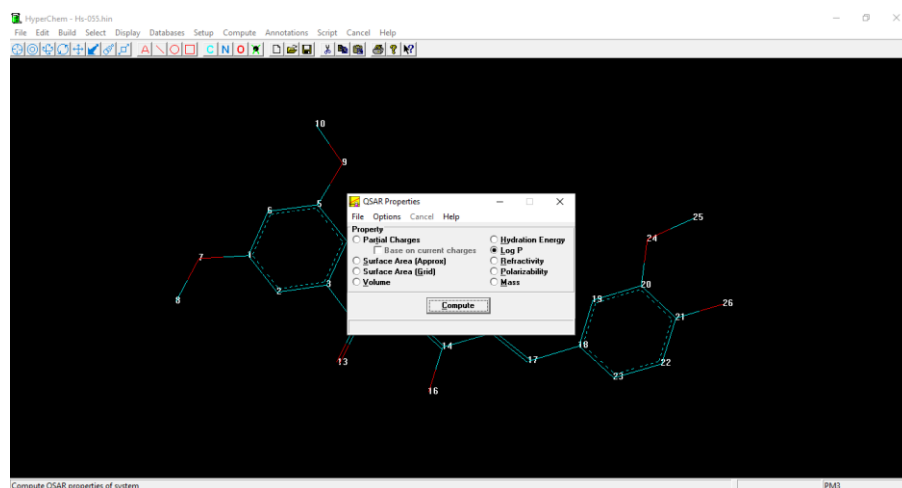
Gradient = 0.0171705 (kcal/mol/Ang)

MOLECULAR POINT GROUP

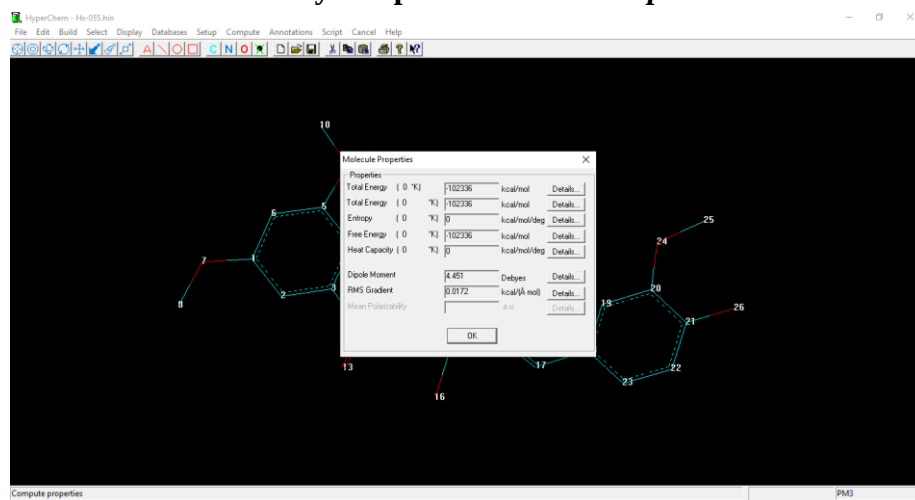
CS

<

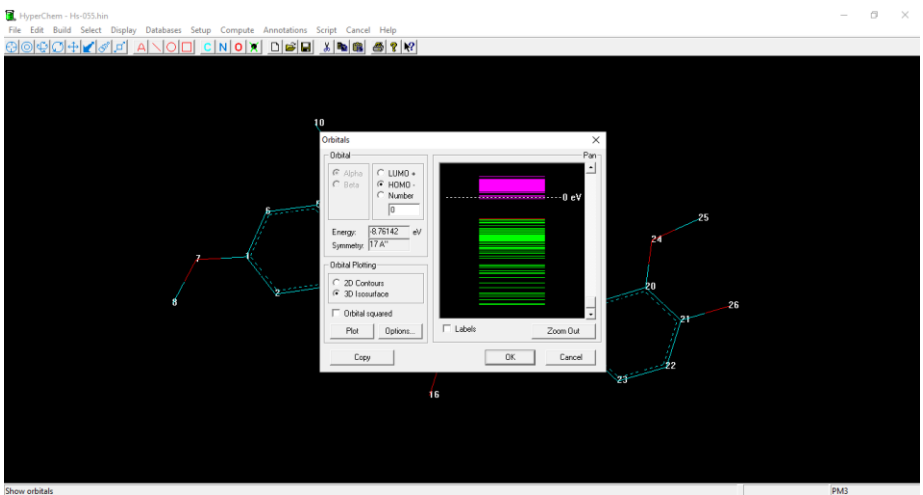
Lampiran 4. Hasil Optimasi Geometri dan Deskriptor-deskriptor dari Senyawa pada QSAR Properties



Lampiran 5. Hasil Optimasi Geometri dan Deskriptor-deskriptor dari Senyawa pada *Molecule Properties*



Lampiran 6. Hasil Optimasi Geometri dan Deskriptor-deskriptor dari Senyawa pada *Orbitals*



Lampiran 7. Mencari persamaan HKSA terbaik dengan Aplikasi *BuildQSAR*

BuildQSAR - [Data Atomik dan Molekuler Derivat Kurkumin 10 Senyawa.bqj]

File Edit View Dataset QSAR Tools Windows Help

PATH: D:\data terbaru

	ID	Structure	Comment	Log 1/C50	qC1	qC2	qC3	qC4	qC5	qC6	qC7	qC8	qC9	qC10	qC11	qC12	qC13	qC14	qC15	qC16	qC17	E HOMO	E LUMO	Log P	E Hd	a	MR
1	He-047			-1.1335	0.11304	-0.17259	-0.07818	-0.15079	0.10815	-0.20524	0.37289	-0.30847	0.16053	-0.15595	-0.06682	0.00826	-0.16639	0.12659	-0.2158	0.12834	-0.20718	-0.9595	-1.055	2.17	-14.35	39.5	104
2	He-054			-1.0755	0.12789	-0.18664	-0.06908	-0.15838	0.12332	-0.22216	0.37188	-0.30746	0.16016	-0.15189	-0.07013	0.01891	-0.17432	0.14198	-0.23287	0.1434	-0.22321	-0.0779	-1.1458	2.05	-34.54	32.16	85.5
3	He-055			-1.3385	0.11274	-0.17268	-0.07783	-0.15073	0.10788	-0.2055	0.37344	-0.31252	0.16481	-0.1684	-0.05304	-0.0676	-0.1029	0.06769	0.05034	-0.16516	-0.07733	-0.7614	-1.0129	2.14	-17.28	37.66	99.6
4	He-056			-1.5717	0.11297	-0.17259	-0.07753	-0.15124	0.1078	-0.20542	0.37366	-0.31471	0.16711	-0.17588	-0.04575	-0.10835	-0.04688	-0.14262	0.11506	-0.19948	-0.03452	-0.8347	-1.0192	2.39	-18.31	35.19	93.4
5	He-057			-0.9435	0.11748	-0.17225	-0.07984	-0.15453	0.11392	-0.20882	0.37778	-0.29911	0.14756	-0.14941	-0.06941	-0.01824	-0.13812	0.07047	0.01448	0.08667	-0.17293	-0.9923	-1.1024	1.92	-14.48	41.97	111
6	He-062			-1.2395	0.12748	-0.18653	-0.06862	-0.1582	0.12296	-0.22256	0.37261	-0.31262	0.168	-0.16882	-0.05461	-0.06188	-0.1091	0.07703	0.02492	-0.15315	-0.08171	-0.8416	-1.0797	2.05	-33.83	32.16	85.5
7	He-054			-1.0963	0.11021	-0.17271	-0.07802	-0.15583	0.10905	-0.2054	0.37338	-0.31091	0.16313	-0.16437	-0.05732	-0.0237	-0.13366	0.0883	-0.02169	-0.05445	-0.16229	-0.7162	-1.0224	1.89	-17.96	40.13	106
8	He-073			-1.5788	0.12789	-0.18669	-0.06827	-0.15861	0.12385	-0.22256	0.37304	-0.31625	0.16717	-0.17734	-0.04423	-0.10914	-0.04651	-0.14262	0.11548	-0.19957	-0.03419	-0.8577	-1.0476	2.33	-38.38	31.52	93.4
9	He-089			-0.9805	0.05995	-0.12307	-0.12385	-0.08788	-0.10065	0.04052	0.3818	-0.30236	0.15146	-0.15105	-0.06867	0.00925	-0.16751	0.12674	-0.216	0.12865	-0.20722	-0.0421	-1.0292	2.17	-13.7	39.5	104
10	He-140			-1.1959	0.01043	-0.08868	-0.15787	-0.08514	-0.14071	0.09709	0.38186	-0.31178	0.16395	-0.16872	-0.05288	-0.06761	-0.10324	0.06771	0.05059	-0.16501	-0.07716	-0.7655	-1.0248	2.11	-21.87	35.93	95.1

Activities = 1 Descriptors = 29 Compounds = 10

Lampiran 8. Mencari persamaan HKSA terbaik dengan Aplikasi BuildQSAR secara Systemic Search dan Genetic Algorithm

BuildQSAR - [Data Atomik dan Molekuler Derivat Kurkumin 10 Senyawa.bqs]

File Edit View Dataset QSAR Tools Windows Help

PATH: D:\data terbaru

Plot Variables...
Correlation Matrix...
Covariance Matrix...
Variable Selection
Systematic Search...
Genetic Algorithm...

ID	Struture	Cor	qC3	qC4	qC5	qC6	qC7	qC8	qC9	qC10	qC11	qC12	qC13	qC14	qC15	qC16	qC17	E Homo	E Lumo	Log P	E Hid	a	MR				
1	Hu-047		20524	0.37289	-0.30847	0.16053	-0.15595	-0.06682	0.00826	-0.16639	0.12659	-0.2158	0.12834	-0.20718	-0.9595	-1.055	2.17	-14.35	39.5	104							
2	Hu-054		22216	0.37188	-0.30746	0.16016	-0.15189	-0.07013	0.01891	-0.17432	0.14198	-0.23287	0.1434	-0.22321	-9.0779	-1.1450	2.05	-34.54	32.16	85.5							
3	Hu-055		88	-0.07783	-0.15073	0.10788	-0.2095	0.37344	-0.31252	0.16481	-0.1684	-0.05304	-0.0676	-0.1029	0.06769	0.05034	-0.16516	-0.07733	-0.7614	-0.0129	2.14	-17.28	37.66	99.0			
4	Hu-056		89	-0.07753	-0.15124	0.1078	-0.20542	0.37366	-0.31471	0.16711	-0.17996	-0.04575	-0.10035	-0.04688	-0.14262	0.11506	-0.19940	-0.04352	-0.8347	-0.0192	2.39	-18.31	35.19	93.4			
5	Hu-057		8	-0.08338	-0.17125	-0.07964	-0.15453	0.11392	-0.20882	0.37778	-0.29911	0.14765	-0.14941	-0.06041	-0.01024	-0.13812	0.07047	0.01448	0.08867	-0.17291	-0.8923	-1.1024	1.92	-14.48	41.97	111	
6	Hu-062		1	1.2395	0.12748	-0.19683	-0.06862	0.1582	0.12296	-0.22256	0.37261	-0.31362	0.1655	-0.16682	-0.05461	-0.06186	0.1051	0.07703	0.03482	-0.15315	-0.06171	-0.8416	-0.0757	2.06	33.03	32.16	95.5
7	Hu-064		1	-1.0969	0.11283	-0.17271	-0.07802	-0.15068	0.10806	-0.2054	0.37336	-0.31051	0.16313	-0.16437	-0.05732	-0.0337	-0.13266	0.0893	0.02169	0.03545	-0.16225	-0.7162	-0.0224	1.89	-17.96	40.13	106
8	Hu-073		1	-1.5786	0.12759	-0.19863	-0.06827	-0.15861	0.12265	-0.22256	0.37304	-0.31625	0.16917	-0.17734	-0.04423	-0.10914	-0.04651	-0.14262	0.11549	-0.19957	-0.03419	-0.8577	-0.0476	2.33	-28.38	31.53	83.0
9	Hu-089		1	-0.9005	-0.05995	-0.12207	-0.12265	-0.09788	-0.10065	0.04052	0.3818	-0.30236	0.15146	-0.15105	-0.06867	0.00925	-0.16751	0.12674	-0.216	0.12865	-0.20722	-0.0421	-0.0292	2.17	-13.7	39.5	104
10	Hu-140		1	-1.1959	0.01043	-0.08868	-0.15757	-0.06514	-0.14071	0.09709	0.38186	-0.31178	0.16395	-0.16872	-0.05288	-0.06761	-0.10324	0.06771	0.05099	-0.16501	-0.07716	-0.7655	-0.0248	2.11	-21.87	35.03	95.1

Activities = 1 Descriptors = 29 Compounds = 10

Lampiran 9. Hasil Semua Persamaan dengan Systemic Search

Variable selection results

	X-1	X-2	X-3	X-4	X-5	R	s	F	Q ²	SPress	SDep
1	qC1	qC8	qC12	E Homo	E Lumo	0.991	0.045	42.665	0.527	0.229	0.153
2	qC1	qC8	qC12	E Homo	Log P	0.997	0.027	117.002	0.939	0.083	0.055
3	qC1	qC8	qC12	E Homo	E Hid	0.998	0.023	166.305	0.975	0.053	0.035
4	qC1	qC8	qC12	E Homo	a	0.996	0.028	109.061	0.966	0.062	0.041
5	qC1	qC8	qC12	E Homo	MR	0.996	0.028	108.976	0.966	0.062	0.041
6	qC1	qC8	qC12	E Homo	V	0.996	0.028	109.496	0.967	0.061	0.040
7	qC1	qC8	qC12	E Homo	SA	0.996	0.029	105.311	0.965	0.062	0.042
8	qC1	qC8	qC12	E Homo	Et	0.994	0.036	68.587	0.936	0.084	0.056
9	qC1	qC8	qC12	E Homo	u	0.980	0.067	19.242	0.571	0.219	0.146
10	qC1	qC8	qC12	E Homo	Hf	0.997	0.024	150.655	0.951	0.074	0.049
11	qC1	qC8	qC12	E Homo	Massa	0.996	0.031	90.317	0.956	0.070	0.046
12	qC1	qC8	qC12	E Lumo	Log P	0.997	0.027	120.340	0.935	0.085	0.057
13	qC1	qC8	qC12	E Lumo	E Hid	0.952	0.102	7.737	Not Pred.	Not Pred.	Not Pred.
14	qC1	qC8	qC12	E Lumo	a	0.951	0.103	7.559	Not Pred.	Not Pred.	Not Pred.
15	qC1	qC8	qC12	E Lumo	MR	0.951	0.103	7.591	Not Pred.	Not Pred.	Not Pred.
16	qC1	qC8	qC12	E Lumo	V	0.950	0.104	7.441	Not Pred.	Not Pred.	Not Pred.
17	qC1	qC8	qC12	E Lumo	SA	0.943	0.111	6.479	Not Pred.	Not Pred.	Not Pred.
18	qC1	qC8	qC12	E Lumo	Et	0.973	0.077	14.402	Not Pred.	Not Pred.	Not Pred.
19	qC1	qC8	qC12	E Lumo	u	0.954	0.100	8.043	Not Pred.	Not Pred.	Not Pred.
20	qC1	qC8	qC12	E Lumo	Hf	0.998	0.020	223.621	0.980	0.047	0.032
21	qC1	qC8	qC12	E Lumo	Massa	0.964	0.088	10.664	Not Pred.	Not Pred.	Not Pred.
22	qC1	qC8	qC12	Log P	E Hid	0.997	0.027	118.872	0.938	0.083	0.055
23	qC1	qC8	qC12	Log P	a	0.997	0.027	118.255	0.938	0.083	0.055
24	qC1	qC8	qC12	Log P	MR	0.997	0.027	118.262	0.938	0.083	0.055
25	qC1	qC8	qC12	Log P	V	0.997	0.027	118.055	0.938	0.083	0.055
26	qC1	qC8	qC12	Log P	SA	0.997	0.027	118.038	0.939	0.083	0.055
27	qC1	qC8	qC12	Log P	Et	0.997	0.027	118.260	0.938	0.083	0.055
28	qC1	qC8	qC12	Log P	u	0.998	0.021	202.147	0.985	0.041	0.027
29	qC1	qC8	qC12	Log P	Massa	0.997	0.027	118.263	0.938	0.083	0.055
30	qC1	qC8	qC12	E Hid	Et	0.997	0.025	140.894	0.930	0.088	0.059
31	qC1	qC8	qC12	E Hid	u	0.954	0.100	8.102	0.057	0.324	0.216

Lampiran 11. Mencari Persamaan dengan *Genetic Algorithm*

The screenshot shows the QMUGSAR software interface. The main window displays a table with columns for ID, Structure, Comment, and various descriptors (qC1 to qC14). A dialog box titled "Build genetic search" is open in the foreground. The dialog box has two tabs: "GA control parameters" and "Biological activity". The "Biological activity" tab is selected, showing a list of descriptors (qC1 to qC14) and their corresponding values. The "Correlation criteria" section shows "Forbidden cross-correlation (Rij) higher than: 0.8". The "Run" button is highlighted.

Lampiran 12. Hasil Persamaan Terbaik dengan *Genetic Algorithm*

Variable selection results

	X-1	X-2	X-3	X-4	X-5	R	s	F	Q ²	SPress	SDep
1	SA		E Home	qC2	HF	0.999	0.011	752.475	0.994	0.026	0.010

Lampiran 13. Pemilihan Persamaan Terbaik dari *Systemic Search* dan Validasi Internal dengan MLR

BulkQSAR - [Data Atomik dan Molekuler Derivat Kurkumin 10 Senyawa.bsq]

File Edit View Dataset QSAR Tools Windows Help

PATH: D:\data terbaru

ID	Structure	Comment	Log 1/C50	qC1	qC2	qC3	qC4	qC5	qC6	qC7	qC8	qC9	qC10	qC11	qC12	qC13	qC14	qC15	qC16	qC17	E Home	E Lumo	Log P	E Hd	a	MR
1	Hu-047		-1.1335	0.11304	-0.17258	-0.07818	-0.15078	0.10815	-0.20524	0.37289	-0.30847	0.16053	-0.15595	-0.06682	0.00826	-0.16639	0.12659	-0.2158	0.12834	-0.20718	-8.9595	-1.055	2.17	-14.35	39.5	104
2	Hu-054		-1.0755	0.12789	-0.18664	-0.06908	-0.15838	0.12332	-0.22216	0.37188	-0.30746	0.16016	-0.15189	-0.07013	0.01891	-0.17432	0.14198	-0.23287	0.1434	-0.22321	-9.0779	-1.1458	2.05	-34.54	32.16	85.5
3	Hu-048		-1.0948	0.12789	-0.18664	-0.06908	-0.15838	0.12332	-0.22216	0.37188	-0.30746	0.16016	-0.15189	-0.07013	0.01891	-0.17432	0.14198	-0.23287	0.1434	-0.22321	-9.0779	-1.1458	2.05	-34.54	32.16	85.5
4	Build MLR model																									
5	Biological activity																									
6	☒ Log 1/C50																									
7																										
8																										
9																										
10																										

Descriptors:

☐ qC3 ☐ qC16 ☐ a ☐ Massa

☐ qC9 ☐ qC15 ☐ MR

☐ qC10 ☐ qC17 ☐ V

☐ qC11 ☐ E Home ☐ SA

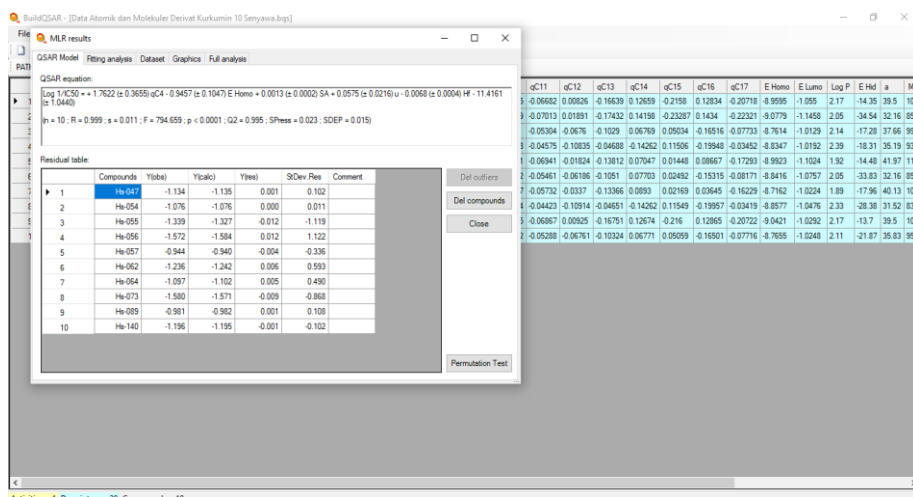
☐ qC12 ☐ E Lumo ☐ Et

☐ qC13 ☐ Log P ☒ H

☐ qC14 ☐ E Hd ☒ HF

Model type: Linear

Lampiran 14. Hasil Persamaan Terbaik dari Systemic Search dan Validasi Internal dengan MLR



QSAR Equation

=====

Log 1/IC50 = + 1.7622 (± 0.3655) qC4 - 0.9457 (± 0.1047) E Homo + 0.0013 (± 0.0002) SA + 0.0575 (± 0.0216) u - 0.0068 (± 0.0004) Hf - 11.4161 (± 1.0440)

(n = 10 ; R = 0.999 ; s = 0.011 ; F = 794.659 ; p < 0.0001 ; Q2 = 0.995 ; SPress = 0.023 ; SDEP = 0.015)

Dataset

=====

No.	Compounds	Log 1/IC50	qC4	E Homo	SA	u	Hf
1	Hs-047	-1.134	-0.151	-8.960	657.850	3.512	-150.023
2	Hs-054	-1.076	-0.158	-9.078	490.230	3.276	-178.479
3	Hs-055	-1.339	-0.151	-8.761	600.480	4.451	-152.376
4	Hs-056	-1.572	-0.151	-8.835	561.400	3.567	-119.332
5	Hs-057	-0.944	-0.155	-8.992	685.950	2.029	-182.385
6	Hs-062	-1.236	-0.158	-8.842	480.890	4.681	-176.754
7	Hs-064	-1.097	-0.151	-8.716	646.400	3.848	-188.164
8	Hs-073	-1.580	-0.159	-8.858	478.180	3.842	-133.652
9	Hs-089	-0.981	-0.098	-9.042	645.030	3.818	-147.169
10	Hs-140	-1.196	-0.065	-8.766	547.420	4.600	-157.956

Coefficient Analysis

=====

Predictor	Coef.	Stdev	95% Conf.	t-ratio	p	Comment
Constant	-11.4161	0.3761	1.0440	-30.3559	0.0000	
qC4	1.7622	0.1317	0.3655	13.3848	0.0000	
E Homo	-0.9457	0.0377	0.1047	-25.0691	0.0000	
SA	0.0013	0.0001	0.0002	22.5791	0.0000	
u	0.0575	0.0078	0.0216	7.3973	0.0007	
Hf	-0.0068	0.0002	0.0004	-42.0706	0.0000	

Correlation Matrix

=====

	qC4	E Homo	SA	u	Hf
qC4	1	0.090	0.113	0.351	0.128
E Homo	0.090	1	0.092	0.597	0.066
SA	0.113	0.092	1	0.472	0.166
u	0.351	0.597	0.472	1	0.187
Hf	0.128	0.066	0.166	0.187	1

Residual table

=====

No.	Compounds	Y(obs)	Y(calc)	Y(res)	StDev.Res	Comment
1	Hs-047	-1.134	-1.135	0.001	0.102	
2	Hs-054	-1.076	-1.076	0.000	0.011	
3	Hs-055	-1.339	-1.327	-0.012	-1.119	
4	Hs-056	-1.572	-1.584	0.012	1.122	
5	Hs-057	-0.944	-0.940	-0.004	-0.336	
6	Hs-062	-1.236	-1.242	0.006	0.593	
7	Hs-064	-1.097	-1.102	0.005	0.490	
8	Hs-073	-1.580	-1.571	-0.009	-0.868	
9	Hs-089	-0.981	-0.982	0.001	0.108	
10	Hs-140	-1.196	-1.195	-0.001	-0.102	

Analysis of Variance

=====

Source	DF	SS	MS	F	p
Regression	5	0.4447	0.0889	794.6590	0.0000
Error	4	0.0004	0.0001		
Total	9	0.4451			

Fitting Parameters

=====

Property Value

n 10

k 5

R² 0.9990R²-Adj. 0.9977

s 0.0106

F 794.6590

p 0.0000

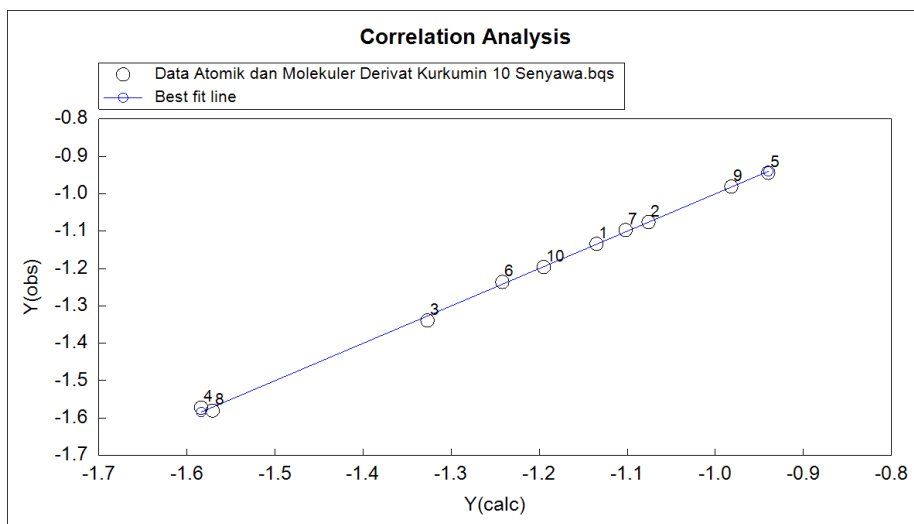
Q2 0.9952

SPress 0.0232

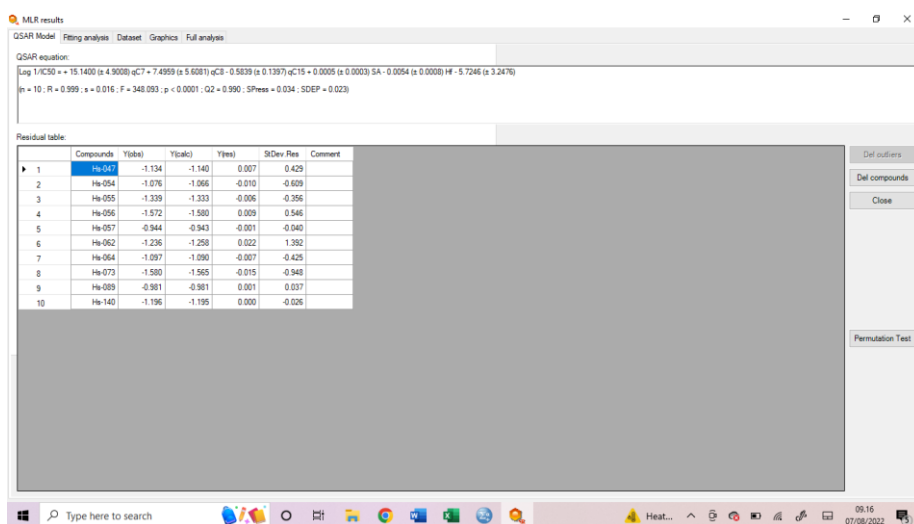
SDEP 0.0155

C.V. -0.8706

Lampiran 15. Analisis Penuh Persamaan HKSA Model 1



Lampiran 16. Hasil Persamaan Terbaik dari *Genetic Algorithm* dan Validasi Internal dengan MLR



QSAR Equation

=====

Log 1/IC50 = + 15.1400 ($\pm$ 4.9008) qC7 + 7.4959 ($\pm$ 5.6081) qC8 -
 0.5839 ($\pm$ 0.1397) qC15 + 0.0005 ($\pm$ 0.0003) SA - 0.0054 ($\pm$ 0.0008) Hf
 - 5.7246 ($\pm$ 3.2476)

(n = 10 ; R = 0.999 ; s = 0.016 ; F = 348.093 ; p < 0.0001 ; Q2 = 0.990 ;
 SPress = 0.034 ; SDEP = 0.023)

Dataset

=====

No.	Compounds	Log 1/IC50	qC7	qC8	qC15	SA	Hf
1	Hs-047	-1.134	0.373	-0.308	-0.216	657.850	-150.023
2	Hs-054	-1.076	0.372	-0.307	-0.233	490.230	-178.479
3	Hs-055	-1.339	0.373	-0.313	0.050	600.480	-152.376
4	Hs-056	-1.572	0.374	-0.315	0.115	561.400	-119.332
5	Hs-057	-0.944	0.378	-0.299	0.014	685.950	-182.385
6	Hs-062	-1.236	0.373	-0.313	0.025	480.890	-176.754
7	Hs-064	-1.097	0.373	-0.311	0.022	646.400	-188.164
8	Hs-073	-1.580	0.373	-0.316	0.115	478.180	-133.652
9	Hs-089	-0.981	0.382	-0.302	-0.216	645.030	-147.169
10	Hs-140	-1.196	0.382	-0.312	0.051	547.420	-157.956

Coefficient Analysis

=====

Predictor	Coef.	Stdev	95% Conf.	t-ratio	p	Comment
Constant	-5.7246	1.1699	3.2476	-4.8934	0.0045	
qC7	15.1400	1.7654	4.9008	8.5759	0.0004	
qC8	7.4959	2.0202	5.6081	3.7105	0.0138	
qC15	-0.5839	0.0503	0.1397	-11.6007	0.0001	
SA	0.0005	0.0001	0.0003	5.2416	0.0033	
Hf	-0.0054	0.0003	0.0008	-18.6129	0.0000	

Correlation Matrix

=====

	qC7	qC8	qC15	SA	Hf
qC7	1	0.475	0.082	0.352	0.052
qC8	0.475	1	0.575	0.645	0.449
qC15	0.082	0.575	1	0.245	0.235
SA	0.352	0.645	0.245	1	0.166
Hf	0.052	0.449	0.235	0.166	1

Residual table

=====

No.	Compounds	Y(obs)	Y(calc)	Y(res)	StDev.Res	Comment
1	Hs-047	-1.134	-1.140	0.007	0.429	
2	Hs-054	-1.076	-1.066	-0.010	-0.609	
3	Hs-055	-1.339	-1.333	-0.006	-0.356	
4	Hs-056	-1.572	-1.580	0.009	0.546	
5	Hs-057	-0.944	-0.943	-0.001	-0.040	
6	Hs-062	-1.236	-1.258	0.022	1.392	
7	Hs-064	-1.097	-1.090	-0.007	-0.425	
8	Hs-073	-1.580	-1.565	-0.015	-0.948	
9	Hs-089	-0.981	-0.981	0.001	0.037	
10	Hs-140	-1.196	-1.195	0.000	-0.026	

Analysis of Variance

=====

Source	DF	SS	MS	F	p
Regression	5	0.4441	0.0888	348.0932	0.0000
Error	4	0.0010	0.0003		
Total	9	0.4451			

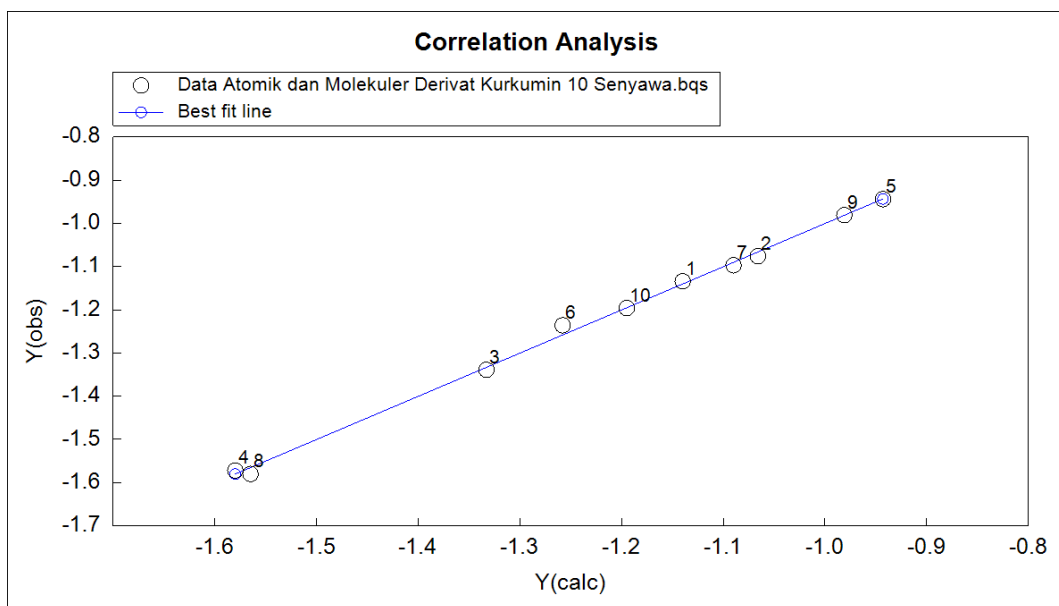
Fitting Parameters

=====

Property Value

n 10
 k 5
 R^2 0.9977
 R^2 -Adj. 0.9948
 s 0.0160
 F 348.0932
 p 0.0000
 Q^2 0.9895
 SPress 0.0341
 SDEP 0.0228
 C.V. -1.3145

Lampiran 17. Analisis Penuh Persamaan HKSA Model 6



Lampiran 18. Hasil SPSS Validasi Eksternal

Validasi Eksternal Persamaan HKSA Model 1

Variables Entered/Removed^a

Model	Variables Entered	Variables Removed	Method
1	Log 1/IC50 Pred ^b	.	Enter

a. Dependent Variable: Log 1/IC50 Eks

b. All requested variables entered.

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	,737 ^a	,543	,087	,3084640

a. Predictors: (Constant), Log 1/IC50 Pred

ANOVA^a

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	,113	1	,113	1,191	,472 ^b
	Residual	,095	1	,095		
	Total	,208	2			

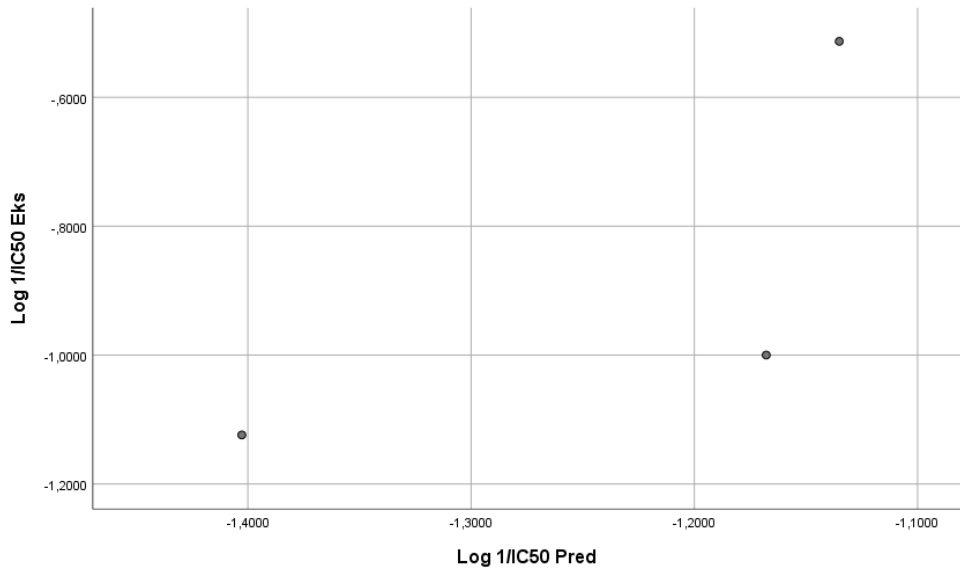
a. Dependent Variable: Log 1/IC50 Eks

b. Predictors: (Constant), Log 1/IC50 Pred

Coefficients^a

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.
		B	Std. Error	Beta		
1	(Constant)	1,135	1,854		,612	,650
	Log 1/IC50 Pred	1,630	1,494	,737	1,091	,472

a. Dependent Variable: Log 1/IC50 Eks



Validasi Eksternal Persamaan HKSA Model 1

Variables Entered/Removed^a

Model	Variables Entered	Variables Removed	Method
1	Log 1/IC50 Pred ^b	.	Enter

a. Dependent Variable: Log 1/IC50 Eks

b. All requested variables entered.

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	,870 ^a	,757	,513	,2251760

a. Predictors: (Constant), Log 1/IC50 Pred

ANOVA^a

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	,158	1	,158	3,111	,328 ^b
	Residual	,051	1	,051		
	Total	,208	2			

a. Dependent Variable: Log 1/IC50 Eks

b. Predictors: (Constant), Log 1/IC50 Pred

Coefficients^a

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.
		B	Std. Error	Beta		
1	(Constant)	2,093	1,690		1,238	,432
	Log 1/IC50 Pred	2,393	1,357	,870	1,764	,328

a. Dependent Variable: Log 1/IC50 Eks

