Appendix I

Dataset S1: Structure of 1,7-naphthyridine Analogues and Their Corresponding pIC50

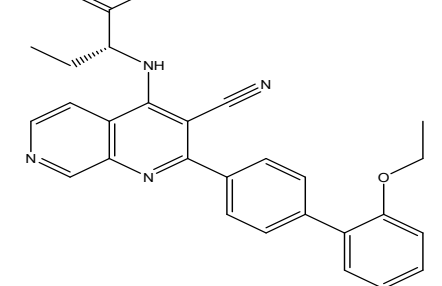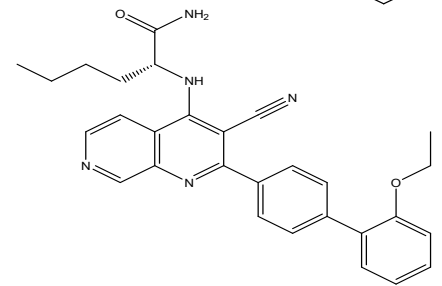| S/N	Structures of 1,7-Naphthyridine Analogs	IC50
1		0.61
2		3.000
3		7.45
4		0.089
5		0.65
6		0.82

7

0.740

8

0.490

9

0.300

10

0.040

11

0.030
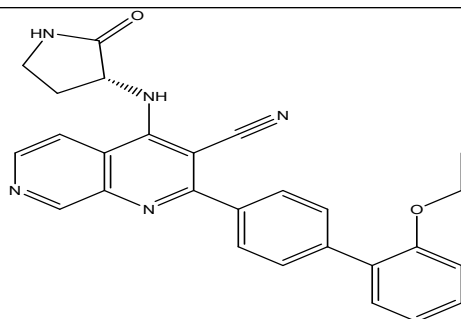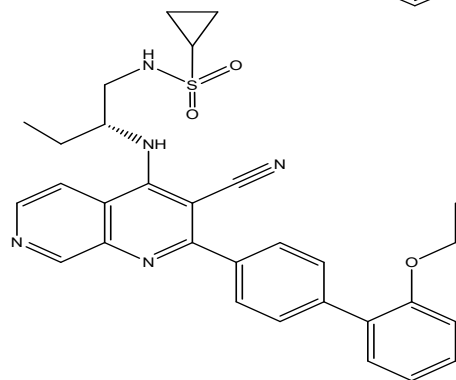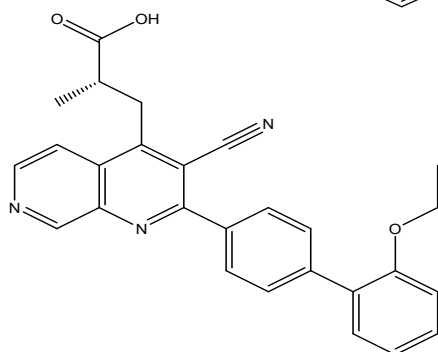
12		0.560
13		0.910
14		0.200
15		3.240
16		0.63
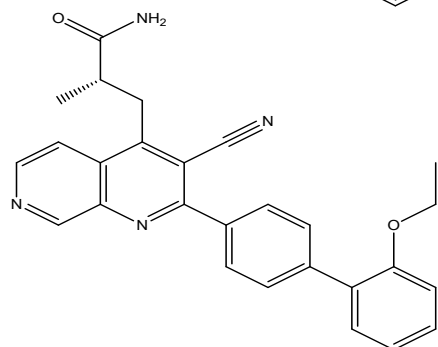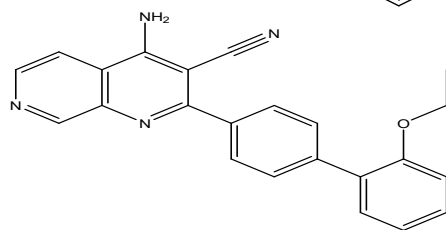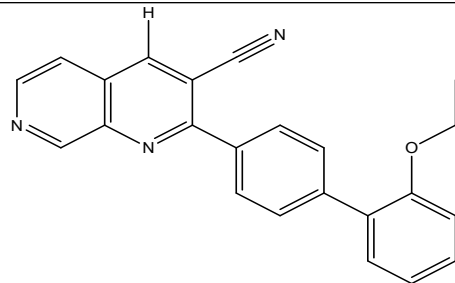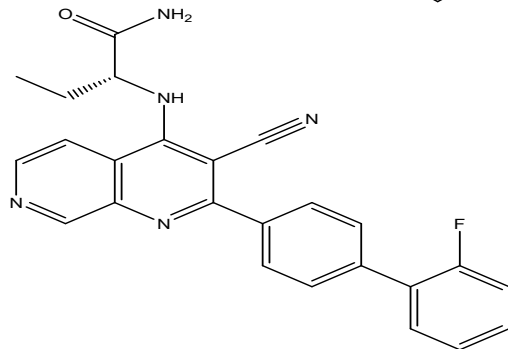
17		10.20
18		0.037
19		0.160
20		0.11
21		0.042
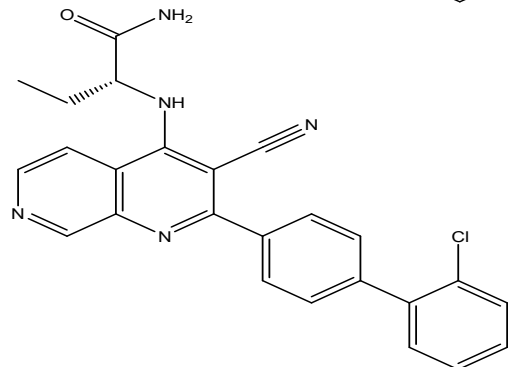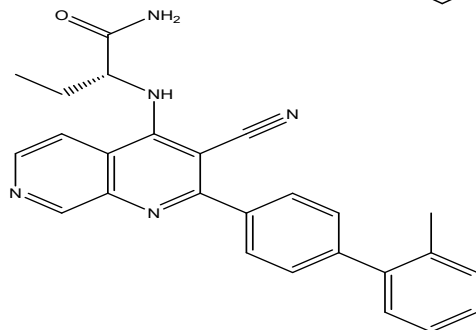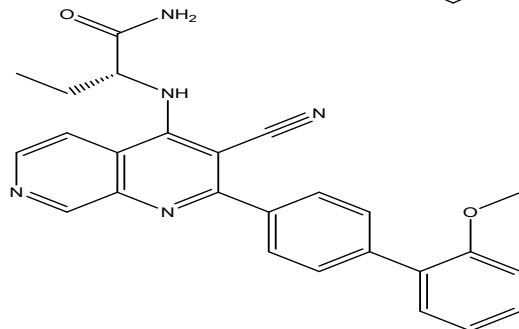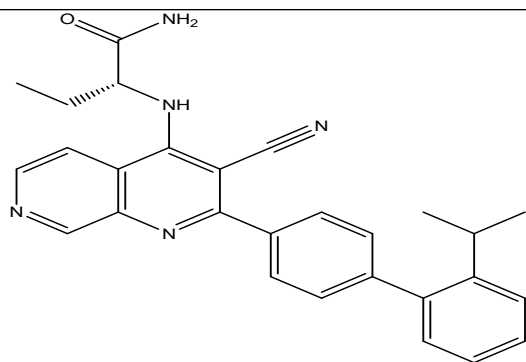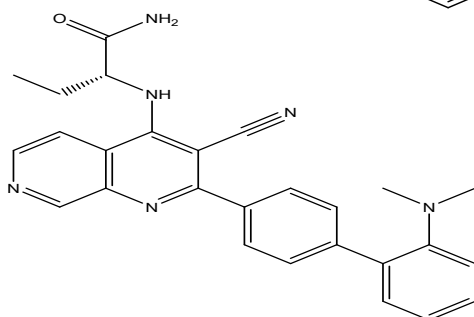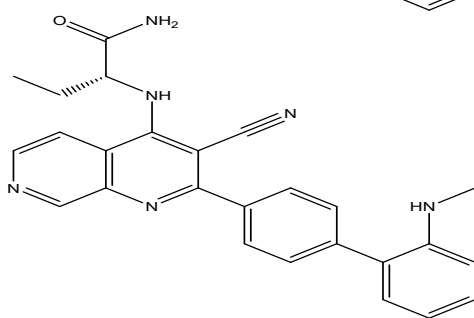
22		1.520
23		2.480
24		0.240
25		1.92
26		1.02
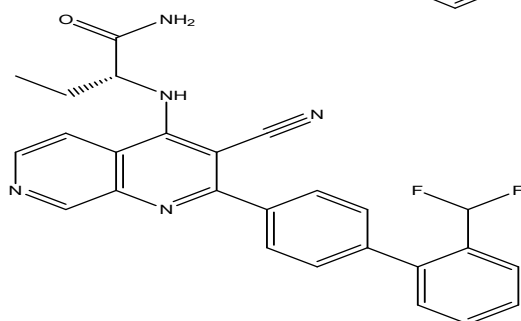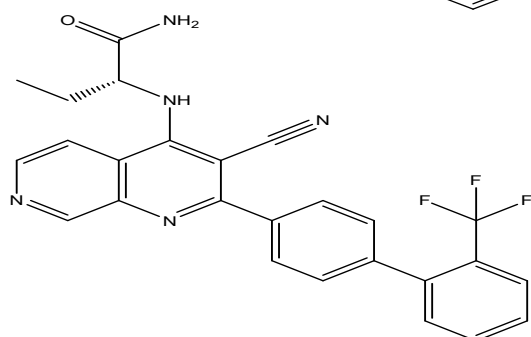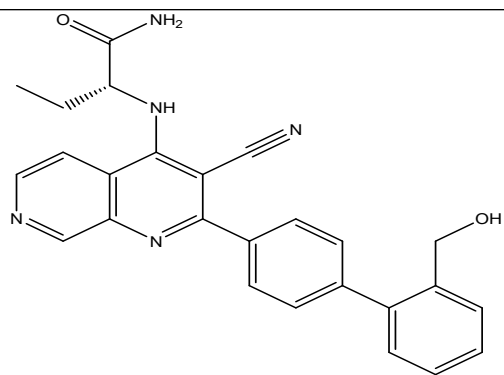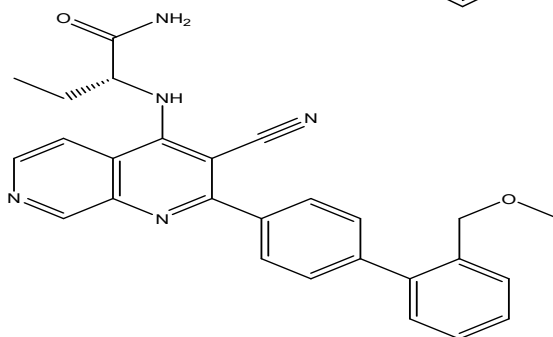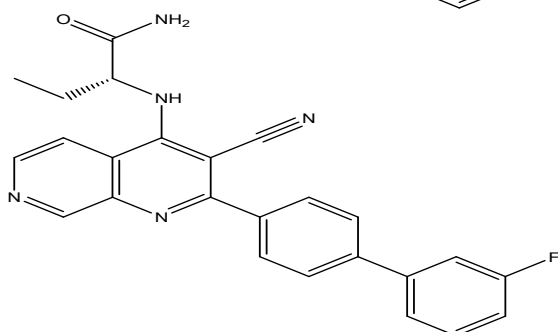
| 27 | | 0.52 |

| 28 | | 2.19 |

| 29 | | 0.18 |

| 30 | | 0.074 |

| 31 | | 0.061 |
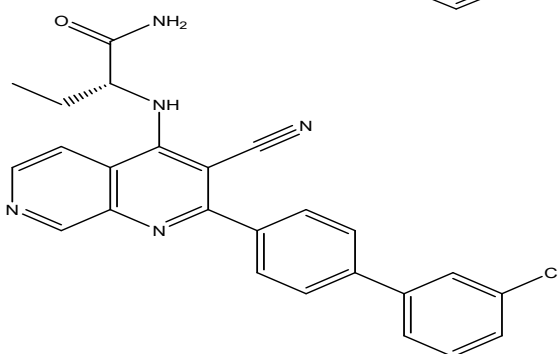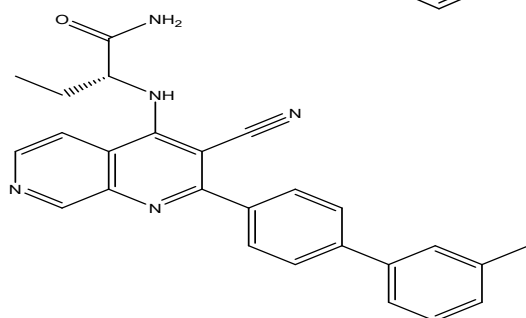
32		0.200
33		0.284
34		0.088
35		0.30
36		0.66
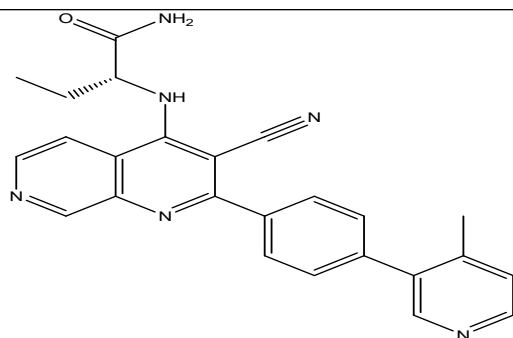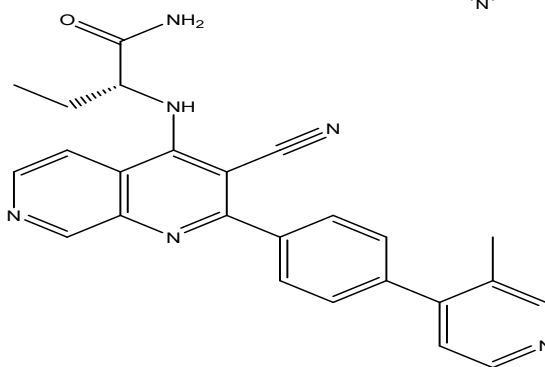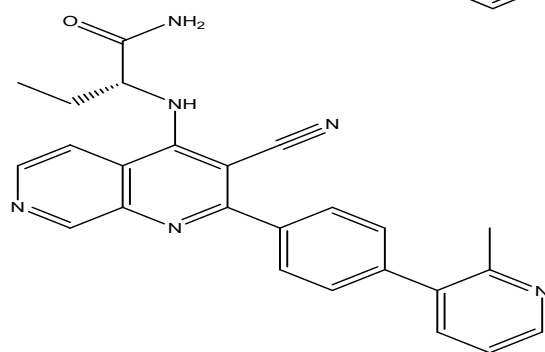
37		10.2
38		7.34
39		18.0
40		0.047
41		0.32
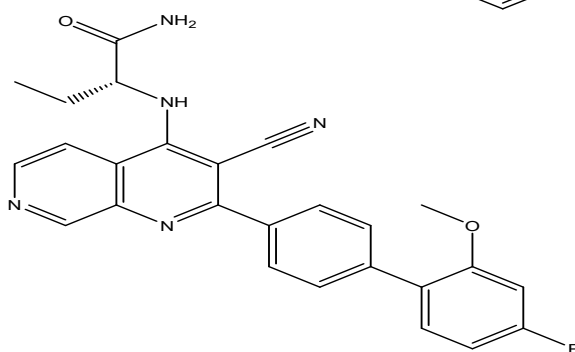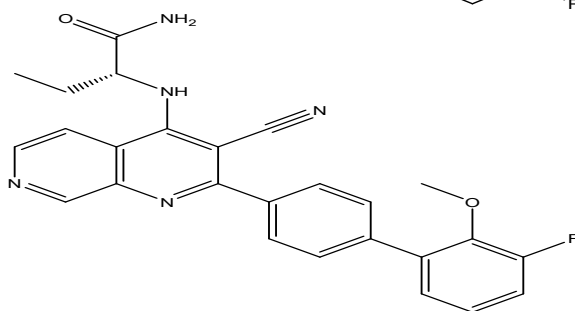
42
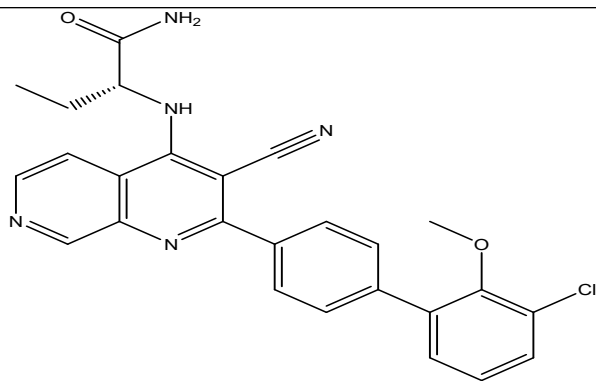
1.04

43
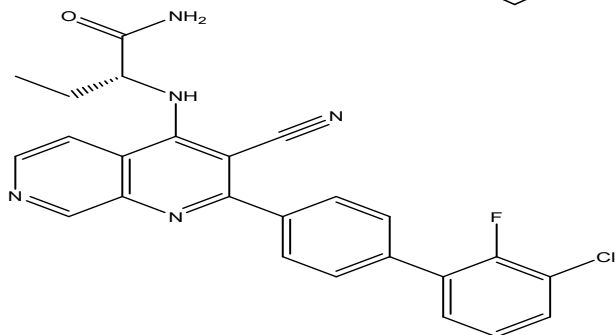
0.013

44
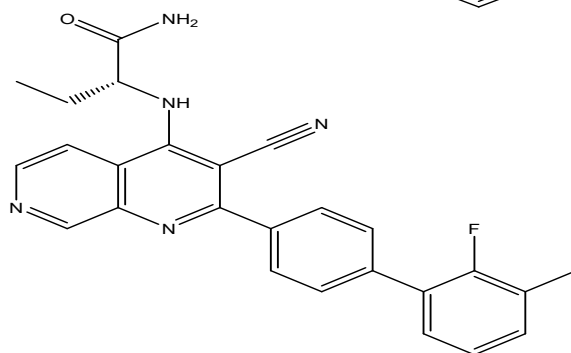
0.019

Appendix II

ANN and SVM Hyperparameter optimization
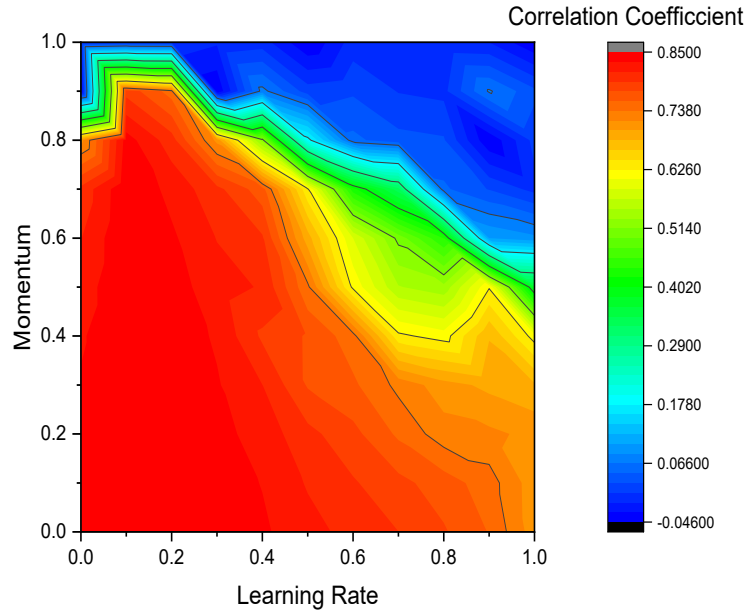
Figure 1: Contour Plot of Optimization of Learning rate and Momentum 2D.
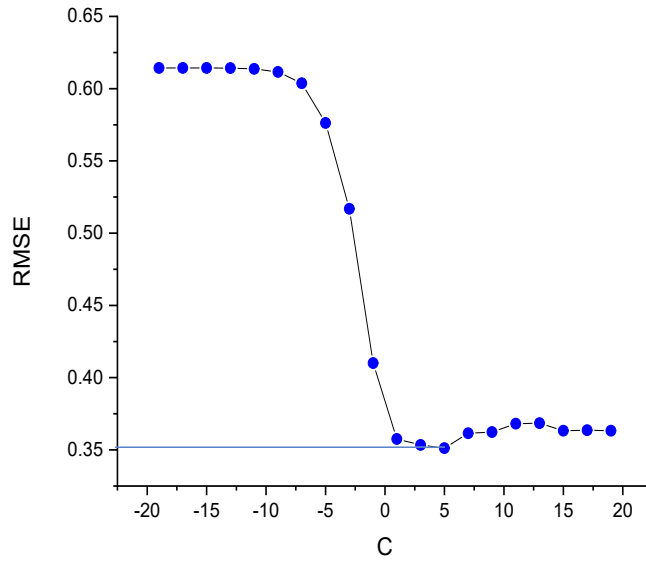
Figure 2: Optimization of Complexity Parameter as a function of RMSE for SVM model development
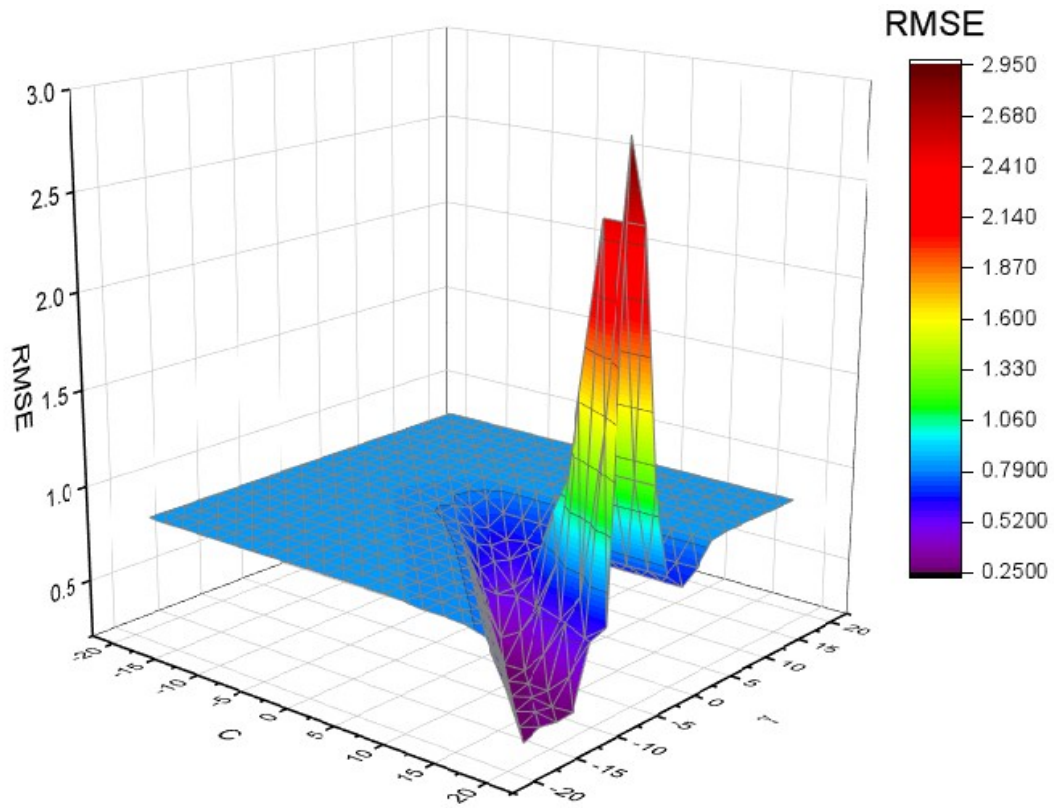
Figure3 : 3D Response Surface Plot for Optimization of Complexity Parameter and Gamma
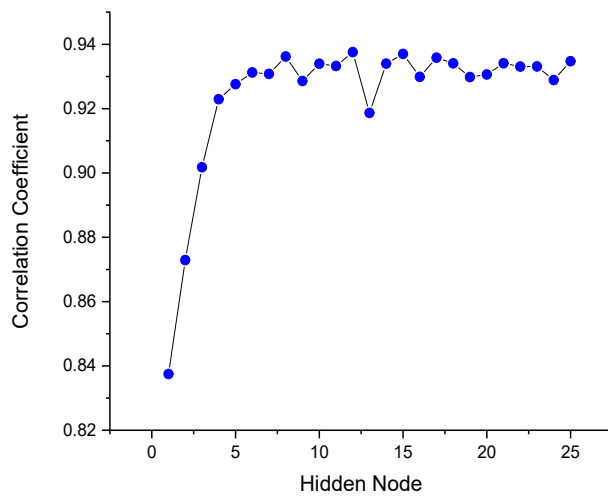
Figure 4: Optimization number of Nodes in the Hidden Layer

Table 1: Summary of Hyperparameter values for Global optimization

Kernel			Optimal Parameters			Training Set		LOO-CV Set	
	σ	ω	E	C	γ	R_{TR}	$RMSE_{TR}$	Q_{CV}	$RMSE_{CV}$
Polynomial	--	--	32.0	5.0	--	0.9410	0.3518	0.6310	0.3564
PUK	1.0	1.0	--	--	--	0.9559	0.2765	0.6653	0.5385
RBF	--	--	--	10	-14	0.9737	0.2774	0.6793	0.5045

Appendix III

Molecular Descriptors

Table 1: List of Molecular Descriptors

Compounds	ATSC7p	MATS8c	MATS6i	SpMin2_Bhv	SpMin5_Bhe	SpMax8_Bhi	Kier3
1	-3.95020	-0.04155	-0.16174	1.926035	1.180851	2.8922	4.716269
2	-3.80767	0.048379	-0.25845	1.896522	1.094336	2.838079	4.716269
3	-3.14083	-0.05434	-0.22777	1.925811	1.153203	2.841426	4.465975
4	-1.93283	-0.04922	-0.18782	1.925112	1.14442	2.838079	4.411458
5	-5.72512	-0.03381	-0.15233	2.048158	1.463167	3.258753	6.297163
6	-3.17196	0.053682	-0.16565	2.032161	1.413584	3.139477	7.158566
7	-5.5976	-0.03571	-0.12193	2.047613	1.442135	3.314672	6.027701
8	-3.55278	0.002363	-0.15931	2.047952	1.449371	3.259178	6.716049
9	-2.81149	0.044699	-0.08466	2.032097	1.399019	3.172670	7.853186
10	-0.38008	0.114342	-0.18244	2.032189	1.396213	3.144387	6.781867
11	2.369722	0.0001155	-0.15941	2.033125	1.517697	3.203577	7.506173
12	1.505188	-0.00278	-0.13892	2.032897	1.513502	3.397291	7.130864
13	-4.4786	-0.02114	-0.17131	2.047466	1.433013	3.193821	5.64337

							8
14	-1.82201	-0.06844	-0.19096	2.032683	1.511198	3.386397	7.324212
15	-4.53702	-0.02509	-0.19042	2.045349	1.447604	3.140539	6.049149
16	-5.20679	-0.03431	-0.23451	2.045644	1.447398	3.136040	6.049149
17	-1.02352	0.05207	-0.10169	2.045766	1.319193	2.958045	4.54179
18	-1.06878	0.061436	-0.17716	2.042989	1.318933	2.955129	4.609418
19	-4.71081	-0.04778	-0.10722	2.046918	1.461972	3.177501	5.644464
20	-3.61538	-0.05888	-0.14333	2.042578	1.46212	3.177500	5.644464
21	-3.58517	-0.07887	-0.13466	2.055893	1.464189	3.177524	5.644464
22	-3.65806	-0.07471	-0.15681	2.064214	1.475226	3.258753	6.123457
23	-4.15352	-0.04259	-0.15083	2.058152	1.465346	3.258753	6.123457
24	-4.10078	-0.04437	-0.14094	2.054638	1.463604	3.258753	5.877551
25	-3.52711	-0.08786	-0.09773	2.056829	1.464181	3.258752	6.123457
26	-3.53764	-0.06853	-0.13936	2.055827	1.464209	3.187472	5.877551
27	-4.8505	-0.07001	-0.14291	2.056505	1.464581	3.258753	6.297163
28	-4.60756	-0.09537	-0.12422	2.046544	1.461953	3.177681	5.814213
29	-5.12309	-0.0947	-0.14002	2.043529	1.462612	3.177562	5.814213
30	-5.26967	-0.08415	-0.14542	2.052993	1.471692	3.179297	5.814213
31	-5.51165	-0.08406	-0.14185	2.0469	1.464074	3.187821	6.049149
32	-4.66608	-0.09464	-0.14404	2.046439	1.461943	3.177881	5.814213
33	-3.82882	-0.04824	-0.12863	2.089072	1.468597	3.255969	5.644464
34	-4.22443	-0.04728	-0.13133	2.094364	1.472362	3.180344	5.644464
35	-4.44549	-0.04341	-0.12222	2.048186	1.462417	3.197044	6.123457
36	-5.1157	0.022455	-0.21499	2.028963	1.390646	3.136933	5.95684

37	-6.00225	0.015323	-0.15575	2.028308	1.390342	3.01493	5.713152
38	-4.35888	-0.09383	-0.13558	2.043795	1.462886	3.177633	5.814213
39	-4.82362	-0.09894	-0.12357	2.046752	1.464969	3.187385	6.049149
40	-3.71992	-0.06653	-0.1415	2.086564	1.472871	3.214962	5.644464
41	-5.33839	-0.04621	-0.11078	2.054323	1.471689	3.179299	5.713152
42	-4.99965	-0.07626	-0.12628	2.080494	1.510711	3.229736	5.887109
43	-5.06222	-0.07824	-0.12505	2.082599	1.515043	3.233094	5.88526
44	-5.1248	-0.08022	-0.12381	2.084704	1.519375	3.236451	5.88341

Table 2: Description of Molecular Descriptors

Descriptor	Class	Type	Description
ATSC7p	2D	Autocorrelation	Centered Broto-Moreau Autocorrelation descriptor of lag 7 weighed by polarizabilities
MATS8c	2D	Autocorrelation	Moran Autocorrelation descriptor of lag 7 weighed by charges
MATS6i	2D	Autocorrelation	Moran Autocorrelation descriptor of lag 6 weighed by ionization potential
SpMin2_Bhv	2D	Burden Modifiied Eigenvalue	Burden Matrix of the H-filled molecular graph weighted by volume
SpMin5_Bhe	2D	Burden Modified Eigenvalue	Burden Matrix of the H-filled molecular graph weighted by electronegativities
SpMax8_Bhi	2D	Burden Modifiied Eigenvalue	Burden Matrix of the H-filled molecular graph weighted by first ionization potentials
Kier3	2D	Kappa Shape Indices	Kappa shape index descriptor; describes the importance of molecular topology