

Monte Carlo Based QSGFEAR: Prediction of Gibb's Free Energy of Activation at Different Temperatures Using SMILES Based Descriptors

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Table S1: The Gibbs free energy of activation (ΔG^\ddagger) values of 2-aryliminothiazolidin-4-one derivatives at different temperatures.

Compound	SMILES	ΔG_{298}^\ddagger	ΔG_{318}^\ddagger	ΔG_{328}^\ddagger	ΔG_{338}^\ddagger	ΔG_{348}^\ddagger	ΔG_{358}^\ddagger	ΔG_{378}^\ddagger
1.	<chem>COc1ccc(cc1)/N=C/I\SCC(=O)N1</chem>	14.72	15.17	15.36	15.56	15.7	15.93	16.34
2.	<chem>O=C1N/C(=N/c2ccccc2)/S/C/I=C\C=C\c1cccc1</chem>	16.08	16.41	16.64	16.71	16.81	16.98	17.28
3.	<chem>Clc1ccc(cc1)/N=C\I/NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	14.48	14.94	15.17	15.43	15.58	15.75	16.18
4.	<chem>Cc1ccc(cc1)/N=C\I/NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	15.13	15.39	15.54	15.7	15.87	15.92	16.18
5.	<chem>COc1ccc(cc1)/N=C\I/NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	16.08	16.41	16.64	16.71	16.81	16.98	17.28
6.	<chem>COc1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccccc2)/NC1=O</chem>	15.67	16.11	16.33	16.53	16.72	16.94	17.33
7.	<chem>COc1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccc(cc2)Cl)/NC1=O</chem>	14.97	15.34	15.52	15.69	15.9	16.07	16.4
8.	<chem>COc1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccc(cc2)C)/NC1=O</chem>	14.97	15.34	15.52	15.69	15.87	16.07	16.4
9.	<chem>COc1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccc(cc2)OC)/NC1=O</chem>	14.07	14.73		15.42		16.07	16.72
10.	<chem>O=C1N/C(=N/c2ccccc2)/S/C/I=C\C=C\c1ccc(cc1)[N+](=O)[O-]</chem>	16.08	16.25	16.42	16.5	16.49	16.56	16.81
11.	<chem>Clc1ccc(cc1)/N=C\I/NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1</chem>	16.08	16.25	16.42	16.5	16.49	16.56	16.81
12.	<chem>Cc1ccc(cc1)/N=C\I/NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1</chem>	13.8	14.42	14.73	15.05	15.35	15.64	16.24
13.	<chem>COc1ccc(cc1)/N=C/I\S/C(=C\C=C\c2ccc(cc2)[N+](=O)[O-])/C(=O)N1</chem>	16.49	16.76	16.86	17.05	17.11	17.19	17.34
14.	<chem>CN(c1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccccc2)/NC1=O)C</chem>	15.67	16.11	16.33	16.53	16.72	16.94	17.33

15.	<chem>Cle1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1</chem>	16.08	16.18	16.19	16.31	16.33	16.33	16.43
16.	<chem>Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1</chem>	13.93	14.52	14.81	15.11	15.39	15.66	16.27
17.	<chem>COc1ccc(cc1)/N=C\1/S/C(=C\C=C/c2ccc(cc2)N(C)C)/C(=O)N1</chem>	14.17	14.73	14.96	15.23	15.52	15.79	16.29

Table S2: Split distribution with SMILES notation at different temperatures, experimental, calculated ΔG^\ddagger values with applicability domain (AD) and DCW's using TF₁

TF1																			
Split				ID	SMILES	T (K)	$\Delta G^\ddagger_{(Expt)}$	$\Delta G^\ddagger_{(Calc)}$				DCWs(T*,N*)				Applicability Domain			
1	2	3	4					Split 1	Split 2	Split 3	Split 4	DCW(1,8)	DCW(2,5)	DCW(2,13)	DCW(1,23)	YES	YES	YES	NO
V	C	A	P	TH001	<chem>COc1ccc(cc1)/N=C/1\SCC(=O)N1</chem>	298	14.72	14.4568	14.5604	14.9474	14.8297	34.34822	32.94961	52.06421	62.05937	YES	YES	YES	NO
C	V	P	A	TH002	<chem>O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccccc1</chem>	298	16.08	15.749	15.8295	16.0288	16.0033	37.41577	36.07755	55.6778	65.15171	YES	YES	YES	YES
P	A	C	V	TH003	<chem>Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	298	14.48	14.421	14.5067	14.8196	14.719	34.26322	32.8172	51.63741	61.76762	YES	YES	YES	YES
C	V	P	A	TH004	<chem>Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	298	15.13	14.3771	14.4936	14.9993	14.9481	34.15912	32.78488	52.23776	62.37119	YES	YES	YES	YES
V	C	A	P	TH005	<chem>COc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	298	16.08	15.6256	15.7162	16.018	16.0114	37.12271	35.79837	55.64198	65.17299	YES	YES	YES	YES
C	V	P	A	TH006	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O</chem>	298	15.67	15.5919	15.6911	15.824	15.791	37.04282	35.73645	54.99361	64.59214	YES	YES	YES	YES
C	V	P	A	TH007	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)Cl)/NC1=O</chem>	298	14.97	14.7747	14.801	15.0252	14.9639	35.10303	33.54256	52.32433	62.4129	YES	YES	YES	YES
V	C	A	P	TH008	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)C)/NC1=O</chem>	298	14.97	14.6444	14.7229	14.9757	14.8741	34.79363	33.35015	52.15903	62.17637	NO	YES	YES	YES
C	V	P	A	TH009	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)OC)/NC1=O</chem>	298	14.07	14.4635	14.5495	14.759	14.6947	34.3642	32.92278	51.43486	61.70348	YES	YES	YES	YES
A	P	V	C	TH010	<chem>O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccc(cc1)[N+](=O)[O-]</chem>	298	16.08	15.6876	15.8048	15.6601	15.6248	37.27011	36.01668	54.44589	64.15424	YES	YES	YES	YES
P	A	C	V	TH011	<chem>Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1~</chem>	298	16.08	15.6077	15.6961	15.6557	15.6068	37.08043	35.74881	54.43126	64.10697	YES	YES	YES	YES
A	P	V	C	TH012	<chem>Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1</chem>	298	13.8	14.1977	14.2311	14.3413	14.2481	33.73314	32.13796	50.03909	60.52683	YES	YES	YES	YES
V	C	A	P	TH013	<chem>COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)[N+](=O)[O-])/C(=O)N1</chem>	298	16.49	15.918	15.9964	16.3261	16.3154	37.81701	36.48902	56.67144	65.97401	YES	YES	YES	YES
V	C	A	P	TH014	<chem>CN(c1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O)C</chem>	298	15.67	15.5663	15.6426	15.9019	15.8531	36.98202	35.61706	55.25401	64.75572	YES	YES	YES	YES
C	V	P	A	TH015	<chem>Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1</chem>	298	16.08	15.3999	15.4356	15.5253	15.5041	36.58711	35.10685	53.99553	63.83627	YES	YES	YES	YES
P	A	C	V	TH016	<chem>Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1</chem>	298	13.93	14.2033	14.268	14.3317	14.2357	33.74666	32.22889	50.0069	60.49408	YES	YES	YES	YES
V	C	A	P	TH017	<chem>COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)N(C)C)/C(=O)N1</chem>	298	14.17	14.2871	14.3309	14.1409	13.9696	33.94551	32.38401	49.36937	59.79302	NO	YES	YES	YES
V	C	A	P	TH018	<chem>COc1ccc(cc1)/N=C/1\SCC(=O)N1</chem>	318	15.17	14.9114	15.03	15.341	15.2487	35.42755	34.10708	53.37946	63.16339	YES	YES	YES	NO
C	V	P	A	TH019	<chem>O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccccc1</chem>	318	16.41	16.2037	16.2991	16.4223	16.4223	38.49511	37.23502	56.99305	66.25573	YES	YES	YES	YES
A	P	V	C	TH020	<chem>Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	318	14.94	14.8756	14.9763	15.2132	15.138	35.34256	33.97468	52.95266	62.87164	YES	YES	YES	YES
C	V	P	A	TH021	<chem>Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	318	15.39	14.8318	14.9632	15.3929	15.3671	35.23846	33.94235	53.553	63.4752	YES	YES	YES	YES
V	C	A	P	TH022	<chem>COc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	318	16.41	16.0802	16.1858	16.4116	16.4304	38.20205	36.95584	56.95722	66.277	YES	YES	YES	YES
V	C	A	P	TH023	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O</chem>	318	16.11	16.0466	16.1607	16.2176	16.21	38.12216	36.89393	56.30886	65.69616	YES	YES	YES	YES
C	V	P	A	TH024	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)Cl)/NC1=O</chem>	318	15.34	15.2294	15.2706	15.4188	15.3829	36.18237	34.70003	53.63958	63.51692	YES	YES	YES	YES
V	C	A	P	TH025	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)C)/NC1=O</chem>	318	15.34	15.0991	15.1925	15.3693	15.2931	35.87297	34.50762	53.47428	63.28039	NO	YES	YES	YES
A	P	V	C	TH026	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)OC)/NC1=O</chem>	318	14.73	14.9182	15.0191	15.1526	15.1137	35.44354	34.08025	52.75011	62.8075	YES	YES	YES	YES
C	V	P	A	TH027	<chem>O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccc(cc1)[N+](=O)[O-]</chem>	318	16.25	16.1423	16.2744	16.0537	16.0438	38.34945	37.17415	55.76113	65.25826	YES	YES	YES	YES
V	C	A	P	TH028	<chem>Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1</chem>	318	16.25	16.0624	16.1657	16.0493	16.0258	38.15977	36.90628	55.7465	65.21099	YES	YES	YES	YES
A	P	V	C	TH029	<chem>Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1</chem>	318	14.42	14.6523	14.7007	14.7349	14.6671	34.81248	33.29543	51.35434	61.63085	YES	YES	YES	YES
V	C	A	P	TH030	<chem>COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)[N+](=O)[O-])/C(=O)N1</chem>	318	16.76	16.3727	16.466	16.7197	16.7344	38.89634	37.6465	57.98669	67.07803	YES	YES	YES	YES
A	P	V	C	TH031	<chem>CN(c1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O)C</chem>	318	16.11	16.021	16.1123	16.2955	16.2721	38.06136	36.77453	56.56926	65.85974	YES	YES	YES	YES
P	A	C	V	TH032	<chem>Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1</chem>	318	16.18	15.8546	15.9052	15.9189	15.9231	37.66645	36.26432	55.31077	64.94029	YES	YES	YES	YES
C	V	P	A	TH033	<chem>Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1</chem>	318	14.52	14.658	14.7376	14.7253	14.6547	34.826	33.38636	51.32215	61.5981	YES	YES	YES	YES
P	A	C	V	TH034	<chem>COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)N(C)C)/C(=O)N1</chem>	318	14.73	14.7418	14.8005	14.5345	14.3886	35.02485	33.54148	50.68462	60.89704	NO	YES	YES	YES
P	A	C	V	TH035	<chem>COc1ccc(cc1)/N=C/1\SCC(=O)N1</chem>	328	15.36	15.2812	15.3902	15.4626	15.3679	36.30532	34.99492	53.78607	63.47735	YES	YES	YES	NO
A	P	V	C	TH036	<chem>O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccccc1</chem>	328	16.64	16.5735	16.6593	16.544	16.5415	39.37287	38.12286	57.39966	66.5697	YES	YES	YES	YES
A	P	V	C	TH037	<chem>Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	328	15.17	15.2454	15.3365	15.3349	15.2572	36.22032	34.86252	53.35928	63.1856	YES	YES	YES	YES

P	A	C	V	TH038	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	328	15.54	15.2016	15.3234	15.5146	15.4862	36.11622	34.83019	53.95962	63.78917	YES	YES	YES	YES
P	A	C	V	TH039	COc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	328	16.64	16.45	16.546	16.5333	16.5496	39.07982	37.84368	57.36384	66.59097	YES	YES	YES	YES
V	C	A	P	TH040	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O	328	16.33	16.4164	16.5209	16.3393	16.3291	38.99993	37.78177	56.71547	66.01012	YES	YES	YES	YES
C	V	P	A	TH041	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)Cl)/NC1=O	328	15.52	15.5992	15.6308	15.5405	15.5021	37.06014	35.58787	54.0462	63.83089	YES	YES	YES	YES
V	C	A	P	TH042	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)C)/NC1=O	328	15.52	15.4689	15.5527	15.491	15.4123	36.75074	35.39546	53.8809	63.59436	NO	YES	YES	YES
A	P	V	C	TH044	O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccc(cc1)[N+](=O)[O-]	328	16.42	16.5121	16.6346	16.1754	16.1629	39.22721	38.062	56.16775	65.57222	YES	YES	YES	YES
P	A	C	V	TH045	Clc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1~	328	16.42	16.4322	16.5259	16.171	16.145	39.03753	37.79412	56.15312	65.52496	YES	YES	YES	YES
C	V	P	A	TH046	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1	328	14.73	15.0221	15.0609	14.8566	14.7863	35.69024	34.18327	51.76096	61.94481	YES	YES	YES	YES
A	P	V	C	TH047	COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)[N+](=O)[O-])/C(=O)N1~	328	16.86	16.7425	16.8263	16.8414	16.8536	39.77411	38.53434	58.39331	67.39199	YES	YES	YES	YES
A	P	V	C	TH048	CN(c1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O)C	328	16.33	16.3907	16.4725	16.4172	16.3912	38.93913	37.66237	56.97588	66.17371	YES	YES	YES	YES
A	P	V	C	TH049	Clc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	328	16.19	16.2244	16.2655	16.0406	16.0423	38.54421	37.15216	55.71739	65.25425	YES	YES	YES	YES
V	C	A	P	TH050	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	328	14.81	15.0278	15.0978	14.847	14.7738	35.70376	34.2742	51.72876	61.91207	YES	YES	YES	YES
P	A	C	V	TH051	COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)N(C)C)/C(=O)N1	328	14.96	15.1116	15.1607	14.6562	14.5078	35.90261	34.42932	51.09124	61.211	NO	YES	YES	YES
C	V	P	A	TH052	COc1ccc(cc1)/N=C/1\SCC(=O)N1	338	15.56	15.3481	15.4806	15.7116	15.6209	36.464	35.21763	54.61787	64.14394	YES	YES	YES	NO
C	V	P	A	TH053	O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccccc1	338	16.71	16.6403	16.7497	16.793	16.7945	39.53155	38.34557	58.23147	67.23628	YES	YES	YES	YES
P	A	C	V	TH054	Clc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	338	15.43	15.3123	15.4269	15.5838	15.5101	36.379	35.08523	54.19108	63.85219	YES	YES	YES	YES
C	V	P	A	TH055	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	338	15.7	15.2684	15.4137	15.7635	15.7392	36.2749	35.0529	54.79142	64.45576	YES	YES	YES	YES
V	C	A	P	TH056	COc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	338	16.71	16.5169	16.6364	16.7822	16.8026	39.2385	38.06639	58.19564	67.25756	YES	YES	YES	YES
A	P	V	C	TH057	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O	338	16.53	16.4832	16.6113	16.5882	16.5821	39.15861	38.00448	57.54728	66.67671	YES	YES	YES	YES
A	P	V	C	TH058	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)Cl)/NC1=O	338	15.69	15.666	15.7212	15.7894	15.755	37.21882	35.81058	54.878	64.49747	YES	YES	YES	YES
P	A	C	V	TH059	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)C)/NC1=O	338	15.69	15.5357	15.6431	15.7399	15.6653	36.90942	35.61817	54.7127	64.26095	NO	YES	YES	YES
A	P	V	C	TH060	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)OC)/NC1=O	338	15.42	15.3548	15.4697	15.5232	15.4858	36.47999	35.1908	53.98853	63.78805	YES	YES	YES	YES
C	V	P	A	TH061	O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccc(cc1)[N+](=O)[O-]	338	16.5	16.5789	16.725	16.4243	16.4159	39.38589	38.28471	56.99955	66.23881	YES	YES	YES	YES
V	C	A	P	TH062	Clc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1	338	16.5	16.499	16.6163	16.4199	16.398	39.19621	38.01683	56.98492	66.19154	YES	YES	YES	YES
A	P	V	C	TH063	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1	338	15.05	15.089	15.1513	15.1055	15.0392	35.84892	34.40598	52.59276	62.6114	YES	YES	YES	YES
P	A	C	V	TH064	COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)[N+](=O)[O-])/C(=O)N1~	338	17.05	16.8093	16.9166	17.0903	17.1066	39.93279	38.75705	59.22511	68.05858	YES	YES	YES	YES
P	A	C	V	TH065	CN(c1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O)C	338	16.53	16.4576	16.5628	16.6661	16.6442	39.09781	37.88508	57.80768	66.84029	YES	YES	YES	YES
C	V	P	A	TH066	Clc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	338	16.31	16.2912	16.3558	16.2895	16.2953	38.70289	37.37487	56.54919	65.92084	YES	YES	YES	YES
P	A	C	V	TH067	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	338	15.11	15.0946	15.1882	15.0959	15.0268	35.86244	34.49691	52.56057	62.57865	YES	YES	YES	YES
P	A	C	V	TH068	COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)N(C)C)/C(=O)N1	338	15.23	15.1784	15.2511	14.9051	14.7607	36.06129	34.65203	51.92304	61.87759	NO	YES	YES	YES
V	C	A	P	TH069	COc1ccc(cc1)/N=C/1\SCC(=O)N1	348	15.7	15.4648	15.6167	15.7977	15.7485	36.74113	35.55317	54.90583	64.48014	YES	YES	YES	NO
A	P	V	C	TH070	O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccccc1	348	16.81	16.7571	16.8858	16.8791	16.9221	39.80868	38.68111	58.51942	67.57249	YES	YES	YES	YES
V	C	A	P	TH071	Clc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	348	15.58	15.429	15.563	15.67	15.6377	36.65613	35.42076	54.47903	64.18839	YES	YES	YES	YES
C	V	P	A	TH072	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	348	15.87	15.3851	15.5499	15.8497	15.8668	36.55203	35.38844	55.07937	64.79196	YES	YES	YES	YES
P	A	C	V	TH073	COc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	348	16.81	16.6336	16.7725	16.8684	16.9302	39.51562	38.40193	58.48359	67.59376	YES	YES	YES	YES
A	P	V	C	TH074	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O	348	16.72	16.5999	16.7474	16.6744	16.7097	39.43574	38.34001	57.83523	67.01292	YES	YES	YES	YES
A	P	V	C	TH075	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)Cl)/NC1=O	348	15.9	15.7828	15.8573	15.8756	15.8826	37.49595	36.14611	55.16595	64.83368	YES	YES	YES	YES
V	C	A	P	TH076	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)C)/NC1=O	348	15.87	15.6524	15.7792	15.8261	15.7929	37.18654	35.95371	55.00065	64.59715	NO	YES	YES	YES
A	P	V	C	TH078	O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccc(cc1)[N+](=O)[O-]	348	16.49	16.6957	16.8611	16.5105	16.5435	39.66302	38.62024	57.2875	66.57501	YES	YES	YES	YES
P	A	C	V	TH079	Clc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1~	348	16.49	16.6158	16.7524	16.5061	16.5256	39.47334	38.35236	57.27287	66.52775	YES	YES	YES	YES
A	P	V	C	TH080	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1	348	15.35	15.2057	15.2874	15.1917	15.1668	36.12605	34.74152	52.88071	62.9476	YES	YES	YES	YES

C	V	P	A	TH081	COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)[N+](=O)[O-])/C(=O)N1~	348	17.11	16.9261	17.0527	17.1765	17.2342	40.20992	39.09258	59.51306	68.39479	YES	YES	YES	YES
P	A	C	V	TH082	CN(c1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O)C	348	16.72	16.5743	16.699	16.7523	16.7718	39.37494	38.22062	58.09563	67.1765	YES	YES	YES	YES
P	A	C	V	TH083	Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	348	16.33	16.408	16.492	16.3757	16.4228	38.98002	37.71041	56.83715	66.25704	YES	YES	YES	YES
V	C	A	P	TH084	Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	348	15.39	15.2114	15.3243	15.1821	15.1544	36.13957	34.83245	52.84852	62.91486	YES	YES	YES	YES
A	P	V	C	TH085	COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)N(C)C)/C(=O)N1	348	15.52	15.2952	15.3872	14.9913	14.8883	36.33842	34.98757	52.21099	62.21379	NO	YES	YES	YES
C	V	P	A	TH086	COc1ccc(cc1)/N=C/1\SCC(=O)N1	358	15.93	15.8534	15.9672	15.8648	15.8391	37.66347	36.41708	55.13006	64.7189	YES	YES	YES	NO
V	C	A	P	TH087	O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccccc1	358	16.98	17.1456	17.2363	16.9462	17.0127	40.73102	39.54502	58.74365	67.81124	YES	YES	YES	YES
A	P	V	C	TH088	Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1	358	15.75	15.8175	15.9135	15.7371	15.7284	37.57847	36.28468	54.70327	64.42715	YES	YES	YES	YES
P	A	C	V	TH089	Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1	358	15.92	15.7737	15.9004	15.9168	15.9574	37.47437	36.25235	55.30361	65.03072	YES	YES	YES	YES
A	P	V	C	TH090	COc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1	358	16.98	17.0221	17.123	16.9355	17.0208	40.43796	39.26584	58.70783	67.83252	YES	YES	YES	YES
P	A	C	V	TH091	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O	358	16.94	16.9885	17.0979	16.7415	16.8003	40.35808	39.20393	58.05946	67.25167	YES	YES	YES	YES
V	C	A	P	TH092	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)Cl)/NC1=O	358	16.07	16.1713	16.2078	15.9427	15.9733	38.41829	37.01003	55.39019	65.07244	YES	YES	YES	YES
A	P	V	C	TH093	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)C)/NC1=O	358	16.07	16.041	16.1297	15.8932	15.8835	38.10888	36.81762	55.22489	64.83591	NO	YES	YES	YES
P	A	C	V	TH094	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)OC)/NC1=O	358	16.07	15.8601	15.9563	15.6765	15.704	37.67946	36.39025	54.50071	64.36301	YES	YES	YES	YES
C	V	P	A	TH095	O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccc(cc1)[N+](=O)[O-]	358	16.56	17.0842	17.2116	16.5776	16.6341	40.58536	39.48416	57.51174	66.81377	YES	YES	YES	YES
V	C	A	P	TH096	Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1	358	16.56	17.0043	17.1029	16.5732	16.6162	40.39568	39.21628	57.49711	66.7665	YES	YES	YES	YES
A	P	V	C	TH097	Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1	358	15.64	15.5942	15.6379	15.2588	15.2574	37.04839	35.60543	53.10494	63.18636	YES	YES	YES	YES
V	C	A	P	TH098	COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)[N+](=O)[O-])/C(=O)N1	358	17.19	17.3146	17.4033	17.2436	17.3248	41.13226	39.9565	59.7373	68.63354	YES	YES	YES	YES
C	V	P	A	TH099	CN(c1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O)C	358	16.94	16.9629	17.0495	16.8194	16.8624	40.29728	39.08453	58.31987	67.41526	YES	YES	YES	YES
C	V	P	A	TH100	Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	358	16.33	16.7965	16.8425	16.4428	16.5135	39.90236	38.57432	57.06138	66.4958	YES	YES	YES	YES
P	A	C	V	TH101	Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	358	15.66	15.5999	15.6748	15.2492	15.245	37.06191	35.69636	53.07275	63.15361	YES	YES	YES	YES
P	A	C	V	TH102	COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)N(C)C)/C(=O)N1	358	15.79	15.6837	15.7378	15.0584	14.9789	37.26076	35.85148	52.43522	62.45255	NO	YES	YES	YES
V	C	A	P	TH103	COc1ccc(cc1)/N=C/1\SCC(=O)N1	378	16.34	15.1064	15.297	15.8912	15.9238	35.89033	34.76503	55.21803	64.94223	YES	YES	YES	NO
A	P	V	C	TH104	O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccccc1	378	17.28	17.4514	17.6055	17.3895	17.3906	41.45699	40.45506	60.2249	68.80701	YES	YES	YES	YES
C	V	P	A	TH105	Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1	378	16.18	16.1234	16.2827	16.1804	16.1063	38.30444	37.19472	56.18451	65.42292	YES	YES	YES	YES
V	C	A	P	TH106	Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1	378	16.18	16.0795	16.2696	16.36	16.3353	38.20034	37.16239	56.78485	66.02649	YES	YES	YES	YES
P	A	C	V	TH107	COc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1	378	17.28	17.328	17.4923	17.3788	17.3987	41.16393	40.17588	60.18907	68.82829	YES	YES	YES	YES
C	V	P	A	TH108	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O	378	17.33	17.2943	17.4671	17.1848	17.1783	41.08404	40.11397	59.54071	68.24744	YES	YES	YES	YES
A	P	V	C	TH109	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)Cl)/NC1=O	378	16.4	16.4772	16.577	16.386	16.3512	39.14425	37.92007	56.87143	66.06821	YES	YES	YES	YES
P	A	C	V	TH110	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)C)/NC1=O	378	16.4	16.3468	16.499	16.3365	16.2614	38.83485	37.72766	56.70613	65.83168	NO	YES	YES	YES
C	V	P	A	TH111	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)OC)/NC1=O	378	16.72	16.1659	16.3256	16.1198	16.0819	38.40542	37.30029	55.98196	65.35878	YES	YES	YES	YES
C	V	P	A	TH112	O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccc(cc1)[N+](=O)[O-]	378	16.81	17.3901	17.5808	17.0208	17.0121	41.31133	40.3942	58.99298	67.80954	YES	YES	YES	YES
V	C	A	P	TH113	Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1	378	16.81	17.3102	17.4722	17.0165	16.9941	41.12165	40.12632	58.97835	67.76227	YES	YES	YES	YES
P	A	C	V	TH114	Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1	378	16.24	15.9001	16.0071	15.7021	15.6354	37.77436	36.51547	54.58619	64.18213	YES	YES	YES	YES
A	P	V	C	TH115	COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)[N+](=O)[O-])/C(=O)N1~	378	17.34	17.6204	17.7725	17.6869	17.7027	41.85823	40.86654	61.21854	69.62931	YES	YES	YES	YES
V	C	A	P	TH116	CN(c1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O)C	378	17.33	17.2687	17.4187	17.2627	17.2403	41.02324	39.99457	59.80111	68.41103	YES	YES	YES	YES
C	V	P	A	TH117	Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	378	16.43	17.1023	17.2117	16.8861	16.8914	40.62833	39.48436	58.54262	67.49157	YES	YES	YES	YES
A	P	V	C	TH118	Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	378	16.27	15.9058	16.044	15.6924	15.6229	37.78788	36.6064	54.554	64.14938	YES	YES	YES	YES
P	A	C	V	TH119	COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)N(C)C)/C(=O)N1	378	16.29	15.9895	16.107	15.5017	15.3569	37.98673	36.76152	53.91647	63.44832	NO	YES	YES	YES

A = Active training set, P = Passive training set, C = Calibration set, V = Validation set

Table S3: Split distribution with SMILES notation at different temperatures, experimental, calculated ΔG^\ddagger values with applicability domain (AD) and DCWs using TF₂

				TF ₂															
Split				ID	SMILES	T (K)	$\Delta G^\ddagger_{(Exp)}$				DCWs(T*,N*)				Applicability Domain				
1	2	3	4				$\Delta G^\ddagger_{(Exp)}$	Split 1	Split 2	Split 3	Split 4	DCW(3,14)	DCW(2,9)	DCW(2,20)					DCW(1,18)
V	C	A	P	TH001	<chem>COc1ccc(cc1)/N=C/1\SCC(=O)N1</chem>	298	14.72	14.4835	14.7899	14.9168	14.9215	56.27885	57.3131	47.11404	49.29291	YES	YES	YES	NO
C	V	P	A	TH002	<chem>O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\Cc1ccccc1</chem>	298	16.08	15.7902	15.9483	15.989	16.0307	59.5549	61.08181	49.88841	52.20742	YES	YES	YES	YES
P	A	C	V	TH003	<chem>Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	298	14.48	14.4582	14.5334	14.759	14.7025	56.21557	56.47841	46.70579	48.71742	YES	YES	YES	YES
C	V	P	A	TH004	<chem>Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	298	15.13	14.5435	14.5759	14.8938	14.9627	56.42942	56.61677	47.05463	49.4013	YES	YES	YES	YES
V	C	A	P	TH005	<chem>COc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	298	16.08	15.6035	15.8116	15.9794	15.9887	59.08673	60.63714	49.86354	52.09711	YES	YES	YES	YES
C	V	P	A	TH006	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O</chem>	298	15.67	15.5804	15.7528	15.8311	15.8295	59.02877	60.44582	49.47978	51.6786	YES	YES	YES	YES
C	V	P	A	TH007	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)Cl)/NC1=O</chem>	298	14.97	14.7563	14.8561	14.9623	14.9642	56.96277	57.52834	47.23186	49.40521	YES	YES	YES	YES
V	C	A	P	TH008	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)C)/NC1=O</chem>	298	14.97	14.6293	14.6945	14.9529	14.9386	56.64435	57.00274	47.20747	49.33781	YES	YES	YES	YES
C	V	P	A	TH009	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)OC)/NC1=O</chem>	298	14.07	14.5141	14.575	14.7401	14.6149	56.35552	56.61393	46.65689	48.48744	YES	YES	YES	YES
A	P	V	C	TH010	<chem>O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\Cc1ccc(cc1)[N+](=O)[O-]</chem>	298	16.08	15.6782	15.8735	15.6023	15.6868	59.27403	60.83871	48.88778	51.3039	YES	YES	YES	YES
P	A	C	V	TH011	<chem>Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1</chem>	298	16.08	15.6402	15.6492	15.6744	15.6443	59.17881	60.10867	49.07437	51.19199	YES	YES	YES	YES
A	P	V	C	TH012	<chem>Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1</chem>	298	13.8	14.1763	14.2548	14.4354	14.2629	55.50863	55.57215	45.86855	47.5624	YES	YES	YES	YES
V	C	A	P	TH013	<chem>COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)[N+](=O)[O-])/C(=O)N1~</chem>	298	16.49	15.9219	16.1861	16.318	16.2729	59.88507	61.85557	50.73957	52.84372	YES	YES	YES	YES
V	C	A	P	TH014	<chem>CN(c1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O)C</chem>	298	15.67	15.5278	15.7114	15.8076	15.8269	58.89707	60.31129	49.41896	51.67187	YES	YES	YES	YES
C	V	P	A	TH015	<chem>Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1</chem>	298	16.08	15.3615	15.5177	15.4739	15.5194	58.48018	59.6811	48.55551	50.86406	YES	YES	YES	YES
P	A	C	V	TH016	<chem>Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1</chem>	298	13.93	14.2808	14.2816	14.3407	14.3526	55.77074	55.65919	45.6234	47.79805	YES	YES	YES	YES
V	C	A	P	TH017	<chem>COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)N(C)C)/C(=O)N1</chem>	298	14.17	14.3042	14.3844	14.3456	14.2432	55.82941	55.9939	45.63599	47.51076	YES	YES	YES	YES
V	C	A	P	TH018	<chem>COc1ccc(cc1)/N=C/1\SCC(=O)N1</chem>	318	15.17	14.9376	15.2315	15.3298	15.3124	57.41739	58.74968	48.18278	50.32014	YES	YES	YES	NO
C	V	P	A	TH019	<chem>O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\Cc1ccccc1</chem>	318	16.41	16.2444	16.3898	16.4021	16.4217	60.69345	62.51839	50.95715	53.23465	YES	YES	YES	YES
A	P	V	C	TH020	<chem>Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	318	14.94	14.9124	14.9749	15.172	15.0934	57.35412	57.915	47.77453	49.74465	YES	YES	YES	YES
C	V	P	A	TH021	<chem>Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	318	15.39	14.9977	15.0174	15.3069	15.3537	57.56797	58.05336	48.12337	50.42853	YES	YES	YES	YES
V	C	A	P	TH022	<chem>COc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	318	16.41	16.0576	16.2531	16.3924	16.3797	60.22527	62.07372	50.93228	53.12434	YES	YES	YES	YES
V	C	A	P	TH023	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O</chem>	318	16.11	16.0345	16.1943	16.2441	16.2204	60.16732	61.88241	50.54852	52.70583	YES	YES	YES	YES
C	V	P	A	TH024	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)Cl)/NC1=O</chem>	318	15.34	15.2104	15.2976	15.3754	15.3552	58.10132	58.96493	48.3006	50.43244	YES	YES	YES	YES
V	C	A	P	TH025	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)C)/NC1=O</chem>	318	15.34	15.0834	15.1361	15.3659	15.3295	57.7829	58.43932	48.27621	50.36504	YES	YES	YES	YES
A	P	V	C	TH026	<chem>COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)OC)/NC1=O</chem>	318	14.73	14.9682	15.0166	15.1531	15.0059	57.49407	58.05051	47.72563	49.51467	YES	YES	YES	YES
C	V	P	A	TH027	<chem>O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\Cc1ccc(cc1)[N+](=O)[O-]</chem>	318	16.25	16.1323	16.3151	16.0153	16.0778	60.41257	62.2753	49.95652	52.33113	YES	YES	YES	YES
V	C	A	P	TH028	<chem>Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1~</chem>	318	16.25	16.0944	16.0907	16.0874	16.0352	60.31735	61.54525	50.14311	52.21922	YES	YES	YES	YES
A	P	V	C	TH029	<chem>Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1</chem>	318	14.42	14.6304	14.6964	14.8485	14.6538	56.64718	57.00874	46.93729	48.58963	YES	YES	YES	YES
V	C	A	P	TH030	<chem>COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)[N+](=O)[O-])/C(=O)N1~</chem>	318	16.76	16.3761	16.6276	16.731	16.6638	61.02361	63.29215	51.80831	53.87095	YES	YES	YES	YES
A	P	V	C	TH031	<chem>CN(c1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O)C</chem>	318	16.11	15.982	16.153	16.2206	16.2178	60.03561	61.74787	50.4877	52.6991	YES	YES	YES	YES
P	A	C	V	TH032	<chem>Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1</chem>	318	16.18	15.8157	15.9593	15.8869	15.9104	59.61873	61.11769	49.62425	51.89129	YES	YES	YES	YES
C	V	P	A	TH033	<chem>Cc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1</chem>	318	14.52	14.7349	14.7231	14.7537	14.7435	56.90929	57.09578	46.69214	48.82528	YES	YES	YES	YES
P	A	C	V	TH034	<chem>COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)N(C)C)/C(=O)N1</chem>	318	14.73	14.7583	14.826	14.7586	14.6342	56.96795	57.43049	46.70473	48.53799	YES	YES	YES	YES
P	A	C	V	TH035	<chem>COc1ccc(cc1)/N=C/1\SCC(=O)N1</chem>	328	15.36	15.2979	15.5432	15.3953	15.4459	58.32057	59.76404	48.3521	50.67072	YES	YES	YES	NO
A	P	V	C	TH036	<chem>O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\Cc1ccccc1</chem>	328	16.64	16.6046	16.7016	16.4675	16.5551	61.59663	63.53275	51.12647	53.58523	YES	YES	YES	YES
A	P	V	C	TH037	<chem>Clc1ccc(cc1)/N=C\1\NC(=O)/C(=C/C=C/c2ccccc2)/S1</chem>	328	15.17	15.2726	15.2867	15.2375	15.2268	58.2573	58.92935	47.94385	50.09523	YES	YES	YES	YES

P	A	C	V	TH038	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	328	15.54	15.3579	15.3292	15.3723	15.4871	58.47115	59.06771	48.29269	50.77911	YES	YES	YES	YES
P	A	C	V	TH039	COc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	328	16.64	16.4179	16.5649	16.4579	16.5131	61.12845	63.08808	51.1016	53.47492	YES	YES	YES	YES
V	C	A	P	TH040	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O	328	16.33	16.3948	16.5061	16.3096	16.3538	61.0705	62.89676	50.71784	53.05641	YES	YES	YES	YES
C	V	P	A	TH041	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)Cl)/NC1=O	328	15.52	15.5707	15.6094	15.4408	15.4886	59.0045	59.97928	48.46993	50.78303	YES	YES	YES	YES
V	C	A	P	TH042	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)C)/NC1=O	328	15.52	15.4437	15.4478	15.4314	15.463	58.68608	59.45368	48.44553	50.71562	YES	YES	YES	YES
A	P	V	C	TH044	O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccc(cc1)[N+](=O)[O-]	328	16.42	16.4926	16.6269	16.0808	16.2112	61.31576	63.28965	50.12584	52.68171	YES	YES	YES	YES
P	A	C	V	TH045	Clc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1	328	16.42	16.4546	16.4025	16.1529	16.1686	61.22053	62.55961	50.31243	52.5698	YES	YES	YES	YES
C	V	P	A	TH046	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1	328	14.73	14.9907	15.0081	14.9139	14.7873	57.55036	58.0231	47.10661	48.94021	YES	YES	YES	YES
A	P	V	C	TH047	COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)[N+](=O)[O-])/C(=O)N1~	328	16.86	16.7363	16.9394	16.7964	16.7973	61.9268	64.30651	51.97763	54.22153	YES	YES	YES	YES
A	P	V	C	TH048	CN(c1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O)C	328	16.33	16.3422	16.4647	16.2861	16.3513	60.93879	62.76223	50.65702	53.04968	YES	YES	YES	YES
A	P	V	C	TH049	Clc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	328	16.19	16.176	16.2711	15.9524	16.0438	60.52191	62.13205	49.79358	52.24187	YES	YES	YES	YES
V	C	A	P	TH050	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	328	14.81	15.0952	15.0349	14.8192	14.8769	57.81247	58.11014	46.86146	49.17586	YES	YES	YES	YES
P	A	C	V	TH051	COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)N(C)C)/C(=O)N1	328	14.96	15.1186	15.1378	14.824	14.7676	57.87113	58.44484	46.87406	48.88857	YES	YES	YES	YES
C	V	P	A	TH052	COc1ccc(cc1)/N=C/1\SCC(=O)N1	338	15.56	15.3898	15.6698	15.665	15.6542	58.55091	60.17571	49.04997	51.21821	YES	YES	YES	NO
C	V	P	A	TH053	O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccccc1	338	16.71	16.6965	16.8281	16.7372	16.7635	61.82697	63.94442	51.82434	54.13272	YES	YES	YES	YES
P	A	C	V	TH054	Clc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	338	15.43	15.3645	15.4132	15.5072	15.4352	58.48764	59.34102	48.64172	50.64272	YES	YES	YES	YES
C	V	P	A	TH055	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	338	15.7	15.4498	15.4557	15.642	15.6955	58.70149	59.47938	48.99056	51.3266	YES	YES	YES	YES
V	C	A	P	TH056	COc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	338	16.71	16.5098	16.6914	16.7276	16.7215	61.35879	63.49975	51.79947	54.02241	YES	YES	YES	YES
A	P	V	C	TH057	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O	338	16.53	16.4866	16.6326	16.5793	16.5622	61.30083	63.30843	51.41571	53.6039	YES	YES	YES	YES
A	P	V	C	TH058	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)Cl)/NC1=O	338	15.69	15.6626	15.7359	15.7105	15.697	59.23484	60.39095	49.1678	51.33051	YES	YES	YES	YES
P	A	C	V	TH059	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)C)/NC1=O	338	15.69	15.5356	15.5744	15.7011	15.6713	58.91642	59.86535	49.1434	51.2631	YES	YES	YES	YES
A	P	V	C	TH060	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)OC)/NC1=O	338	15.42	15.4203	15.4549	15.4883	15.3477	58.62759	59.47654	48.59282	50.41274	YES	YES	YES	YES
C	V	P	A	TH061	O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccc(cc1)[N+](=O)[O-]	338	16.5	16.5845	16.7534	16.3505	16.4196	61.54609	63.70132	50.82371	53.2292	YES	YES	YES	YES
V	C	A	P	TH062	Clc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1~	338	16.5	16.5465	16.529	16.4226	16.377	61.45087	62.97128	51.0103	53.11729	YES	YES	YES	YES
A	P	V	C	TH063	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1	338	15.05	15.0825	15.1347	15.1836	14.9956	57.7807	58.43477	47.80448	49.4877	YES	YES	YES	YES
P	A	C	V	TH064	COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)[N+](=O)[O-])/C(=O)N1	338	17.05	16.8282	17.0659	17.0662	17.0056	62.15713	64.71818	52.6755	54.76902	YES	YES	YES	YES
P	A	C	V	TH065	CN(c1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O)C	338	16.53	16.4341	16.5913	16.5558	16.5596	61.16913	63.1739	51.35489	53.59716	YES	YES	YES	YES
C	V	P	A	TH066	Clc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	338	16.31	16.2678	16.3976	16.2221	16.2522	60.75225	62.54372	50.49145	52.78936	YES	YES	YES	YES
P	A	C	V	TH067	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	338	15.11	15.1871	15.1614	15.0889	15.0853	58.04281	58.52181	47.55933	49.72335	YES	YES	YES	YES
P	A	C	V	TH068	COc1ccc(cc1)/N=C/1\S/C(=C\C=C\c2ccc(cc2)N(C)C)/C(=O)N1	338	15.23	15.2105	15.2643	15.0937	14.976	58.10147	58.85651	47.57193	49.43606	YES	YES	YES	YES
V	C	A	P	TH069	COc1ccc(cc1)/N=C/1\SCC(=O)N1	348	15.7	15.4989	15.7803	15.7911	15.8155	58.82465	60.53529	49.37633	51.64204	YES	YES	YES	NO
A	P	V	C	TH070	O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccccc1	348	16.81	16.8057	16.9386	16.8633	16.9248	62.10071	64.304	52.1507	54.55655	YES	YES	YES	YES
V	C	A	P	TH071	Clc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	348	15.58	15.4737	15.5237	15.6333	15.5965	58.76138	59.7006	48.96808	51.06655	YES	YES	YES	YES
C	V	P	A	TH072	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	348	15.87	15.559	15.5663	15.7681	15.8568	58.97523	59.83896	49.31692	51.75043	YES	YES	YES	YES
P	A	C	V	TH073	COc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccccc2)/S1	348	16.81	16.619	16.8019	16.8537	16.8828	61.63254	63.85933	52.12583	54.44624	YES	YES	YES	YES
A	P	V	C	TH074	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccccc2)/NC1=O	348	16.72	16.5958	16.7431	16.7054	16.7235	61.57458	63.66801	51.74206	54.02773	YES	YES	YES	YES
A	P	V	C	TH075	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)Cl)/NC1=O	348	15.9	15.7718	15.8464	15.8366	15.8583	59.50858	60.75053	49.49415	51.75434	YES	YES	YES	YES
V	C	A	P	TH076	COc1ccc(cc1)/C=C/C=C/1\S/C(=N\c2ccc(cc2)C)/NC1=O	348	15.87	15.6447	15.6849	15.8272	15.8326	59.19016	60.22493	49.46976	51.68693	YES	YES	YES	YES
A	P	V	C	TH078	O=C1N/C(=N/c2ccccc2)/S/C/1=C\C=C\c1ccc(cc1)[N+](=O)[O-]	348	16.49	16.6937	16.8639	16.4766	16.5809	61.81984	64.0609	51.15007	53.65303	YES	YES	YES	YES
P	A	C	V	TH079	Clc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1	348	16.49	16.6557	16.6395	16.5487	16.5383	61.72461	63.33086	51.33666	53.54112	YES	YES	YES	YES
A	P	V	C	TH080	Cc1ccc(cc1)/N=C\1/NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1	348	15.35	15.1917	15.2452	15.3097	15.1569	58.05444	58.79435	48.13083	49.91153	YES	YES	YES	YES

C	V	P	A	TH081	COc1ccc(cc1)/N=C/I\S/C(=C\C=C\c2ccc(cc2)[N+](=O)[O-])/C(=O)N1~	348	17.11	16.9374	17.1764	17.1923	17.1669	62.43088	65.07776	53.00186	55.19285	YES	YES	YES	YES
P	A	C	V	TH082	CN(c1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccc(cc2)/NC1=O)C	348	16.72	16.5433	16.7018	16.6819	16.7209	61.44288	63.53348	51.68124	54.02099	YES	YES	YES	YES
P	A	C	V	TH083	Clc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	348	16.33	16.377	16.5081	16.3482	16.4135	61.02599	62.9033	50.8178	53.21319	YES	YES	YES	YES
V	C	A	P	TH084	Cc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	348	15.39	15.2963	15.2719	15.215	15.2466	58.31655	58.88139	47.88569	50.14718	YES	YES	YES	YES
A	P	V	C	TH085	COc1ccc(cc1)/N=C/I\S/C(=C\C=C\c2ccc(cc2)N(C)C)/C(=O)N1	348	15.52	15.3197	15.3748	15.2199	15.1373	58.37522	59.21609	47.89828	49.85989	YES	YES	YES	YES
C	V	P	A	TH086	COc1ccc(cc1)/N=C/I\SCC(=O)N1	358	15.93	15.8354	16.1544	15.9217	15.9079	59.66823	61.75248	49.71421	51.88483	YES	YES	YES	NO
V	C	A	P	TH087	O=C1N/C(=N/c2ccccc2)/S/C/I=C\C=C\Cc1ccccc1	358	16.98	17.1422	17.3127	16.9939	17.0172	62.94429	65.52119	52.48858	54.79934	YES	YES	YES	YES
A	P	V	C	TH088	Clc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccc(cc2)/S1	358	15.75	15.8102	15.8978	15.7639	15.6889	59.60496	60.9178	49.30596	51.30933	YES	YES	YES	YES
P	A	C	V	TH089	Cc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccc(cc2)/S1	358	15.92	15.8955	15.9404	15.8987	15.9492	59.81881	61.05616	49.6548	51.99322	YES	YES	YES	YES
A	P	V	C	TH090	COc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccccc2)/S1	358	16.98	16.9554	17.1761	16.9843	16.9752	62.47611	65.07652	52.46371	54.68903	YES	YES	YES	YES
P	A	C	V	TH091	COc1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccccc2)/NC1=O	358	16.94	16.9323	17.1173	16.836	16.8159	62.41816	64.88521	52.07995	54.27052	YES	YES	YES	YES
V	C	A	P	TH092	COc1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccc(cc2)Cl)/NC1=O	358	16.07	16.1082	16.2205	15.9672	15.9507	60.35216	61.96773	49.83203	51.99713	YES	YES	YES	YES
A	P	V	C	TH093	COc1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccc(cc2)C)/NC1=O	358	16.07	15.9812	16.059	15.9578	15.925	60.03374	61.44212	49.80764	51.92972	YES	YES	YES	YES
P	A	C	V	TH094	COc1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccc(cc2)OC)/NC1=O	358	16.07	15.866	15.9395	15.745	15.6014	59.74491	61.05331	49.25706	51.07936	YES	YES	YES	YES
C	V	P	A	TH095	O=C1N/C(=N/c2ccccc2)/S/C/I=C\C=C\Cc1ccccc1	358	16.56	17.0302	17.238	16.6072	16.6733	62.66342	65.27809	51.48795	53.89582	YES	YES	YES	YES
V	C	A	P	TH096	Clc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1~	358	16.56	16.9922	17.0136	16.6793	16.6307	62.56819	64.54805	51.67454	53.78391	YES	YES	YES	YES
A	P	V	C	TH097	Cc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1	358	15.64	15.5282	15.6193	15.4403	15.2493	58.89802	60.01154	48.46872	50.15432	YES	YES	YES	YES
V	C	A	P	TH098	COc1ccc(cc1)/N=C/I\S/C(=C\C=C\c2ccc(cc2)[N+](=O)[O-])/C(=O)N1~	358	17.19	17.2739	17.5506	17.3229	17.2593	63.27446	66.29495	53.33974	55.43564	YES	YES	YES	YES
C	V	P	A	TH099	CN(c1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccc(cc2)/NC1=O)C	358	16.94	16.8798	17.0759	16.8125	16.8133	62.28645	64.75067	52.01913	54.26378	YES	YES	YES	YES
C	V	P	A	TH100	Clc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	358	16.33	16.7135	16.8822	16.4788	16.5059	61.86957	64.12049	51.15568	53.45598	YES	YES	YES	YES
P	A	C	V	TH101	Cc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	358	15.66	15.6328	15.6461	15.3456	15.339	59.16013	60.09858	48.22357	50.38997	YES	YES	YES	YES
P	A	C	V	TH102	COc1ccc(cc1)/N=C/I\S/C(=C\C=C\c2ccc(cc2)N(C)C)/C(=O)N1	358	15.79	15.6562	15.7489	15.3505	15.2297	59.21879	60.43329	48.23616	50.10268	YES	YES	YES	YES
V	C	A	P	TH103	COc1ccc(cc1)/N=C/I\SCC(=O)N1	378	16.34	15.2267	15.5963	15.7972	15.6882	58.14206	59.93673	49.39203	51.3074	YES	YES	YES	NO
A	P	V	C	TH104	O=C1N/C(=N/c2ccccc2)/S/C/I=C\C=C\Cc1ccccc1	378	17.28	17.5086	17.6517	17.3976	17.4184	63.8629	66.624	53.53313	55.85362	YES	YES	YES	YES
C	V	P	A	TH105	Clc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccc(cc2)/S1	378	16.18	16.1766	16.2368	16.1676	16.0902	60.52356	62.02061	50.35051	52.36361	YES	YES	YES	YES
V	C	A	P	TH106	Cc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccc(cc2)/S1	378	16.18	16.2619	16.2793	16.3024	16.3504	60.73741	62.15897	50.69935	53.0475	YES	YES	YES	YES
P	A	C	V	TH107	COc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccccc2)/S1	378	17.28	17.3219	17.515	17.388	17.3764	63.39472	66.17933	53.50826	55.74331	YES	YES	YES	YES
C	V	P	A	TH108	COc1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccccc2)/NC1=O	378	17.33	17.2987	17.4562	17.2397	17.2172	63.33676	65.98802	53.1245	55.3248	YES	YES	YES	YES
A	P	V	C	TH109	COc1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccc(cc2)Cl)/NC1=O	378	16.4	16.4747	16.5595	16.3709	16.3519	61.27077	63.07054	50.87658	53.05141	YES	YES	YES	YES
P	A	C	V	TH110	COc1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccc(cc2)C)/NC1=O	378	16.4	16.3476	16.398	16.3615	16.3263	60.95234	62.54493	50.85219	52.984	YES	YES	YES	YES
C	V	P	A	TH111	COc1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccc(cc2)OC)/NC1=O	378	16.72	16.2324	16.2785	16.1487	16.0026	60.66352	62.15612	50.30161	52.13364	YES	YES	YES	YES
C	V	P	A	TH112	O=C1N/C(=N/c2ccccc2)/S/C/I=C\C=C\Cc1ccccc1	378	16.81	17.3966	17.577	17.0109	17.0745	63.58202	66.38091	52.5325	54.9501	YES	YES	YES	YES
V	C	A	P	TH113	Clc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1~	378	16.81	17.3586	17.3526	17.083	17.032	63.4868	65.65086	52.71909	54.83819	YES	YES	YES	YES
P	A	C	V	TH114	Cc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccc(cc2)[N+](=O)[O-])/S1	378	16.24	15.8946	15.9583	15.844	15.6506	59.81662	61.11435	49.51327	51.2086	YES	YES	YES	YES
A	P	V	C	TH115	COc1ccc(cc1)/N=C/I\S/C(=C\C=C\c2ccc(cc2)[N+](=O)[O-])/C(=O)N1~	378	17.34	17.6403	17.8895	17.7266	17.6606	64.19306	67.39776	54.38429	56.48992	YES	YES	YES	YES
V	C	A	P	TH116	CN(c1ccc(cc1)/C=C/C=C/I\S/C(=N\c2ccc(cc2)/NC1=O)C	378	17.33	17.2462	17.4149	17.2162	17.2146	63.20506	65.85349	53.06368	55.31806	YES	YES	YES	YES
C	V	P	A	TH117	Clc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	378	16.43	17.0799	17.2212	16.8825	16.9071	62.78818	65.2233	52.20024	54.51026	YES	YES	YES	YES
A	P	V	C	TH118	Cc1ccc(cc1)/N=C/I\NC(=O)/C(=C/C=C/c2ccc(cc2)N(C)C)/S1	378	16.27	15.9992	15.985	15.7493	15.7403	60.07873	61.20139	49.26812	51.44425	YES	YES	YES	YES
P	A	C	V	TH119	COc1ccc(cc1)/N=C/I\S/C(=C\C=C\c2ccc(cc2)N(C)C)/C(=O)N1	378	16.29	16.0226	16.0879	15.7542	15.6309	60.1374	61.5361	49.28072	51.15695	YES	YES	YES	YES

A = Active training set, P = Passive training set, C = Calibration set, V = Validation set