Converting SMILES to Stacking Interaction Energies

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Predicting the strength of stacking interactions involving heterocycles is vital for several fields, including structure-based drug design. While quantum chemical computations can provide accurate stacking interaction energies, these come at a steep computational cost. To address this challenge, we recently developed quantitative predictive models of stacking interactions between drug-like heterocycles and the aromatic amino acids Phe, Tyr, and Trp (DOI: 10.26434/chemrxiv.7628939.v4). These models depend on heterocycle descriptors derived from electrostatic potentials (ESPs) computed using density functional theory and provide accurate stacking interactions without the need for expensive computations on stacked dimers. Herein, we show that these ESP-based descriptors can be reliably evaluated directly from the atom connectivity of the heterocycle, providing a means of predicting both the descriptors and the potential for a given heterocycle to engage in stacking interactions without resorting to any quantum chemical computations. This enables the conversion of simple molecular representations (e.g. SMILES) directly into accurate stacking interaction energies using a freely-available online tool, thereby providing a way to rapidly rank the stacking abilities of large sets of heterocycles.

File list (2)

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Supporting Information

Converting SMILES to Stacking Interaction Energies

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Trends in Error for ESP_{mean}

Figure S1. Trends in ESP_{mean} based on the number of heteroatoms in the heterocycle (C=O is considered a single heteroatom). In general, ESP_{mean} increases with the amount of substitution on the ring, and a very large amount of substitution is required to achieve a high value of ESP_{mean} .

Figure S2. Trends in the error of equation 2 based on the number of heteroatoms in the heterocycle. In general, increasing amounts of substitution lead to increased errors. This is likely a result of a breakdown in the additivity assumed by equation (2) at high levels of substitution. This fact, combined with the trend seen in Figure S1, result in increased errors for large values of ESP_{mean} .

Subset Trends

Figure S3. Scatter plots of DFT-computed ESP_{mean} values vs values predicted using equation 2, split into subcategories: A) 5-membered monocycles; B) 6-membered monocycles; C) 5-5 bicycles; D) 5-6 bicycles; E) 6-6 bicycles; F) heterocycles with 0 or 1 heteroatoms; G) heterocycles with 2 or 3 heteroatoms; H) heterocycles with 4 or more heteroatoms.

Figure S4. Scatter plots of DFT-computed ESP_{max} values vs values predicted using equation (3), split into subcategories: A) 5-membered monocycles; B) 6-membered monocycles; C) 5-5 bicycles; D) 5-6 bicycles; E) 6-6 bicycles; F) heterocycles with 0 or 1 heteroatoms; G) heterocycles with 2 or 3 heteroatoms; H) heterocycles with 4 or more heteroatoms.

Fitting Other Descriptors

ESP_{range} can be predicted using the same functional form as ESP_{max} since it is similarly dependent on the number and arrangement of heteroatoms

$$ESP_{\text{range}}^{\text{pred}} = e_0 + \sum_i^{\text{hetatm}} e_i + \sum_{i < j}^{\text{hetatm}} \frac{\cos(\alpha_{ij})}{R_{ij}} f_i f_j + g \quad (4)$$

Atom types	e_i	f_i
C=O	3.08	2.97
N: (imino)	0.65	2.12
O	-0.29	0.37
S	-0.92	0.12
NH (amino)	3.00	-1.67
N (ring fusion)	1.67	-0.60
$e_0 = 11.22$		$g = -2.15$

Figure S5. Scatter plot of DFT-computed ESP_{range} values for known (blue) and unknown (red) heterocycles vs. those predicted using equation (4)

F_{mean} can be predicted using a similar functional form that incorporates a constant shift to the geometry-based scaling factor.

$$F_{\text{mean}}^{\text{pred}} = h_0 + \sum_i^{\text{hetatm}} h_i + \sum_{i < j}^{\text{hetatm}} \left(\frac{\cos(\alpha_{ij})}{R_{ij}} + j \right) k_i k_j + l \quad (5)$$

Atom types	h_i	k_i
C=O	-0.015	0.45
N: (imino)	-0.038	0.37
O	-0.004	0.13
S	-0.026	0.05
NH (amino)	0.17	-0.25
N (ring fusion)	0.099	-0.12
	$h_0 = 0.41$	$l = -0.07$
	$j = 0.29$

Figure S6. Scatter plot of DFT-computed F_{mean} values for known (blue) and unknown (red) heterocycles vs. those predicted using equation (5)

Table S1. Values for distances and angles used in equation (3)-(5). Distances are based on a side length of 1, angles in degrees

5 membered rings			6 membered rings			5-5 bicycles		
pair	distance	angle	pair	distance	angle	pair	distance	angle
A-B	1	72	A-B	1	60	A-C	2.60	108
A-C	1.62	144	A-C	1.73	120	A-D	3.07	180
			A-D	2	180	B-C	1.87	36
						B-E	2.50	180

5-6 bicycles			6-6 bicycles		
pair	distance	angle	pair	distance	angle
A-C	2.60	90	A-D	3.48	120
A-D	3.30	150	A-E	3.62	180
B-C	1.81	18	B-C	1.78	0
B-D	2.69	78	B-D	2.68	60
B-E	2.98	138	B-E	3.03	120
B-F	2.57	162	B-F	2.69	180

Alternate Energy Predictors

Chart S1. Heterocycles considered when comparing the use of DFT and SMILES-based descriptors for predicting stacking interaction energies.

These atom connectivity based descriptors can be incorporated into other predictors of stacking energy.

$$\Delta E_{pred} = N_{HA}^{AA}(-0.032ESP_{max}^{Het} - 0.087N_{HA}^{Het}) - 1.46 \quad (6)$$

Figure S7. Scatter plot of computed DLPNO-CCSD(T)/cc-pVQZ interaction energies vs predicted interaction energies from equation (6) incorporating descriptors obtained from equation (3) for global minimum energy stacked dimers of heterocycles **1-42** and **47-58** with Phe, Tyr, and Trp side chains.

$$\Delta E_{pred} = N_{HA}^{AA}(-0.036ESP_{mean}^{Het} - 0.013ESP_{range}^{Het} - 0.095N_{HA}^{Het}) - 1.36 \quad (7)$$

Figure S8. Scatter plot of computed DLPNO-CCSD(T)/cc-pVQZ interaction energies vs predicted interaction energies from equation (7) incorporating descriptors obtained from equations (2) and (4) for global minimum energy stacked dimers of heterocycles **1-42** and **47-58** with Phe, Tyr, and Trp side chains.

$$\Delta E_{\text{pred}} = N_{\text{HA}}^{\text{AA}}(-0.46F_{\text{mean}}^{\text{Het}} - 0.042\text{ESP}_{\text{mean}}^{\text{Het}} - 0.098N_{\text{HA}}^{\text{Het}}) - 0.67 \quad (8)$$

Figure S9. Scatter plot of computed DLPNO-CCSD(T)/cc-pVQZ interaction energies vs predicted interaction energies from equation (8) incorporating descriptors obtained from equations (2) and (5) for global minimum energy stacked dimers of heterocycles **1-42** and **47-58** with Phe, Tyr, and Trp side chains.

Checking Against Random Data

Equations (2) and (3) were checked for overfitting by comparing both fits where the true ESP values were fit with random numbers of heteroatoms and heteroatom pairs, and where the true heteroatom and pair counts were used to fit random data. This was done using three different sets of random data

Figure S10. A representative example of random ESP_{mean} values predicted using real heteroatom counts, and the R^2 and RMSE values for the three trials

Figure S11. A representative example of real ESP_{mean} values predicted using random heteroatom counts, and the R^2 and RMSE values for the three trials

	R^2	RMSE
Trial 1	0.01	3.33
Trial 2	0.01	3.28
Trial 3	0.01	3.25

Figure S12. A representative example of random $ESP_{\max}$ values predicted using real heteroatom counts, and the R^2 and RMSE values for the three trials

	R^2	RMSE
Trial 1	0.01	3.27
Trial 2	0.01	3.27
Trial 3	0.00	3.27

Figure S13. A representative example of real $ESP_{\max}$ values predicted using random heteroatom and heteroatom pair counts, and the R^2 and RMSE values for the three trials

Table S2. DLPNO-CCSD(T)/cc-pVQZ interaction energies for heterocycles stacked with amino acids and interaction energies predicted by multivariate fits (1), (6)-(7) using both QM descriptors and those obtained from SMILES via equations (2)-(5)

AA	Het	Equation (1)			Equation (6)		Equation (7)		Equation (8)	
		E _{int}	QM	SMILES	QM	SMILES	QM	SMILES	QM	SMILES
Phe	2	-4.2	-4.3	-4.7	-4.3	-4.8	-4.3	-4.8	-4.3	-4.3
Phe	3	-4.5	-4.2	-4.4	-4.3	-4.7	-4.2	-4.5	-4.3	-4.1
Phe	4	-5.1	-5.2	-5.2	-5.3	-5.2	-5.3	-5.3	-5.1	-4.8
Phe	5	-5.1	-5.1	-5.1	-5.0	-5.1	-5.0	-5.2	-4.8	-4.7
Phe	6	-5.5	-5.0	-5.0	-5.1	-5.1	-5.0	-5.1	-4.7	-4.5
Phe	7	-5.5	-4.9	-4.9	-4.9	-5.0	-4.8	-5.0	-4.6	-4.5
Phe	8	-3.6	-4.9	-5.0	-5.2	-5.3	-4.8	-5.1	-4.8	-4.7
Phe	10	-4.3	-5.8	-5.5	-6.0	-5.6	-5.5	-5.6	-5.3	-5.0
Phe	12	-4.8	-5.1	-5.2	-5.1	-5.2	-4.8	-5.3	-4.6	-4.8
Phe	13	-5.2	-6.0	-5.9	-6.0	-5.8	-5.9	-5.9	-5.6	-5.4
Phe	14	-6.1	-5.6	-5.5	-5.4	-5.4	-5.7	-5.7	-5.6	-5.1
Phe	15	-4.5	-4.7	-5.0	-4.8	-5.3	-4.8	-5.2	-5.0	-4.7
Phe	16	-5.6	-5.6	-5.5	-5.6	-5.6	-5.6	-5.7	-5.3	-5.1
Phe	17	-6.0	-5.8	-5.9	-5.5	-5.8	-5.6	-6.0	-5.5	-5.4
Phe	18	-6.1	-6.2	-6.0	-6.0	-5.9	-5.9	-6.1	-5.6	-5.5
Phe	19	-6.5	-6.4	-6.2	-6.3	-6.2	-6.6	-6.4	-6.3	-5.8
Phe	20	-5.9	-6.2	-6.3	-5.7	-6.0	-6.0	-6.3	-5.9	-5.9
Phe	21	-7.0	-6.8	-6.5	-6.5	-6.2	-6.7	-6.6	-6.5	-6.2
Phe	22	-7.3	-7.2	-6.8	-7.0	-6.7	-7.3	-7.0	-7.2	-6.6
Phe	23	-6.8	-7.0	-6.9	-6.4	-6.5	-6.7	-7.0	-7.1	-6.8
Phe	24	-7.1	-7.1	-7.0	-6.6	-6.5	-7.1	-7.1	-7.3	-6.9
Phe	25	-8.0	-7.8	-7.3	-7.5	-6.9	-7.7	-7.4	-7.9	-7.3
Phe	26	-7.3	-7.8	-7.4	-7.8	-7.4	-8.1	-7.7	-7.7	-7.2
Phe	27	-7.3	-7.2	-7.1	-7.7	-7.5	-7.2	-7.1	-7.1	-6.9
Phe	28	-7.1	-7.3	-7.1	-7.9	-7.5	-7.3	-7.1	-7.1	-6.9

Phe	29	-7.6	-7.0	-7.8	-7.2	-8.0	-7.1	-7.8	-7.0	-7.6
Phe	30	-6.4	-7.9	-8.5	-8.4	-8.7	-7.7	-8.4	-7.5	-8.1
Phe	31	-9.4	-9.3	-8.9	-9.5	-9.0	-9.2	-8.9	-8.8	-8.5
Phe	32	-7.9	-8.7	-8.6	-8.8	-8.4	-8.4	-8.5	-7.9	-8.1
Phe	33	-7.6	-7.9	-7.4	-8.0	-7.4	-7.7	-7.4	-7.4	-7.1
Phe	34	-9.4	-9.2	-9.3	-8.9	-9.3	-9.3	-9.1	-9.3	-8.7
Phe	35	-9.2	-9.3	-9.8	-9.2	-9.6	-9.6	-9.8	-9.3	-9.4
Phe	36	-9.4	-10.5	-9.7	-10.2	-9.4	-10.4	-9.6	-10.0	-9.4
Phe	37	-8.8	-11.4	-10.5	-11.5	-10.6	-11.4	-10.5	-11.0	-10.2
Phe	38	-8.1	-8.0	-8.7	-7.9	-8.7	-8.0	-8.8	-7.7	-8.2
Phe	39	-8.9	-8.6	-9.4	-8.5	-9.3	-8.9	-9.5	-8.5	-9.0
Phe	40	-8.6	-8.5	-7.8	-8.2	-7.7	-8.4	-7.8	-8.0	-7.3
Phe	41	-7.7	-8.2	-8.5	-8.3	-8.5	-8.1	-8.5	-7.9	-8.1
Phe	42	-9.1	-9.8	-8.9	-10.1	-9.1	-10.0	-9.0	-9.3	-8.5
Phe	48	-5.7	-5.7	-5.7	-5.6	-5.5	-5.9	-5.9	-6.0	-5.3
Phe	49	-7.3	-7.2	-7.4	-7.4	-7.6	-7.1	-7.4	-7.1	-7.1
Phe	50	-8.3	-7.7	-7.7	-7.8	-7.8	-7.8	-7.7	-7.6	-7.3
Phe	51	-7.4	-7.3	-7.5	-7.5	-7.7	-7.2	-7.5	-7.3	-7.1
Phe	52	-7.8	-7.2	-7.4	-7.1	-7.4	-7.1	-7.5	-7.1	-6.9
Phe	53	-7.3	-7.3	-7.5	-7.3	-7.7	-7.4	-7.6	-7.7	-7.2
Phe	54	-8.5	-8.6	-8.5	-8.4	-8.4	-8.5	-8.6	-8.2	-8.0
Phe	55	-9.1	-9.1	-9.0	-8.7	-8.6	-8.9	-9.0	-8.7	-8.6
Phe	56	-8.7	-9.1	-9.1	-8.8	-9.1	-9.5	-9.2	-9.2	-8.8
Phe	57	-8.6	-9.2	-9.4	-9.0	-9.1	-9.5	-9.5	-9.1	-9.0
Phe	58	-8.9	-9.6	-9.7	-9.6	-9.6	-9.8	-9.8	-9.3	-9.3
Tyr	2	-4.3	-4.6	-5.1	-4.8	-5.3	-4.7	-5.3	-4.8	-4.9
Tyr	3	-5.2	-4.5	-4.8	-4.7	-5.1	-4.6	-5.0	-4.8	-4.5
Tyr	4	-5.1	-5.7	-5.7	-5.8	-5.8	-5.9	-5.9	-5.8	-5.4
Tyr	5	-5.1	-5.6	-5.6	-5.5	-5.6	-5.6	-5.8	-5.3	-5.3
Tyr	6	-5.8	-5.5	-5.5	-5.6	-5.6	-5.5	-5.6	-5.3	-5.0
Tyr	7	-5.5	-5.4	-5.4	-5.4	-5.4	-5.3	-5.6	-5.2	-5.0

Tyr	8	-4.5	-5.3	-5.5	-5.8	-5.8	-5.3	-5.6	-5.4	-5.2
Tyr	10	-4.3	-6.4	-6.1	-6.7	-6.2	-6.1	-6.1	-6.0	-5.7
Tyr	12	-5.1	-5.6	-5.8	-5.6	-5.8	-5.3	-5.9	-5.2	-5.4
Tyr	13	-4.8	-6.6	-6.5	-6.6	-6.4	-6.5	-6.5	-6.3	-6.1
Tyr	14	-6.3	-6.1	-6.0	-6.0	-5.9	-6.4	-6.3	-6.3	-5.7
Tyr	15	-4.9	-5.1	-5.5	-5.3	-5.8	-5.3	-5.7	-5.6	-5.2
Tyr	16	-5.8	-6.1	-6.1	-6.2	-6.2	-6.2	-6.3	-6.0	-5.7
Tyr	17	-6.4	-6.4	-6.5	-6.1	-6.4	-6.2	-6.6	-6.1	-6.1
Tyr	18	-6.4	-6.8	-6.6	-6.7	-6.5	-6.6	-6.7	-6.3	-6.2
Tyr	19	-6.7	-7.1	-6.9	-7.0	-6.9	-7.3	-7.1	-7.1	-6.6
Tyr	20	-6.6	-6.9	-7.0	-6.3	-6.6	-6.6	-7.1	-6.6	-6.7
Tyr	21	-7.6	-7.5	-7.2	-7.2	-6.9	-7.5	-7.3	-7.3	-6.9
Tyr	22	-8.6	-7.9	-7.6	-7.8	-7.4	-8.1	-7.8	-8.1	-7.4
Tyr	23	-7.2	-7.7	-7.7	-7.1	-7.2	-7.5	-7.8	-8.0	-7.7
Tyr	24	-7.8	-7.9	-7.8	-7.3	-7.3	-7.9	-7.9	-8.2	-7.8
Tyr	25	-8.7	-8.6	-8.1	-8.3	-7.7	-8.6	-8.2	-9.0	-8.2
Tyr	26	-7.3	-8.6	-8.2	-8.7	-8.3	-9.0	-8.6	-8.7	-8.1
Tyr	27	-8.6	-8.0	-7.9	-8.6	-8.3	-8.0	-7.9	-8.0	-7.8
Tyr	28	-7.8	-8.1	-7.9	-8.9	-8.3	-8.1	-7.9	-8.0	-7.8
Tyr	29	-8.1	-7.8	-8.7	-8.0	-8.9	-7.9	-8.8	-7.9	-8.6
Tyr	30	-9.3	-8.8	-9.4	-9.4	-9.7	-8.7	-9.5	-8.5	-9.1
Tyr	31	-11.2	-10.4	-10.0	-10.6	-10.0	-10.3	-10.0	-9.9	-9.6
Tyr	32	-9.1	-9.8	-9.6	-9.8	-9.4	-9.4	-9.5	-8.9	-9.1
Tyr	33	-8.3	-8.8	-8.2	-8.9	-8.2	-8.6	-8.3	-8.4	-8.0
Tyr	34	-11.7	-10.3	-10.4	-10.0	-10.4	-10.5	-10.2	-10.6	-9.9
Tyr	35	-10.5	-10.4	-10.9	-10.3	-10.8	-10.8	-11.0	-10.6	-10.7
Tyr	36	-11.5	-11.8	-10.8	-11.4	-10.5	-11.7	-10.8	-11.3	-10.7
Tyr	37	-11.2	-12.8	-11.8	-12.9	-11.9	-12.8	-11.9	-12.5	-11.6
Tyr	38	-8.5	-8.9	-9.7	-8.8	-9.7	-8.9	-9.8	-8.8	-9.3
Tyr	39	-9.2	-9.6	-10.5	-9.5	-10.4	-10.0	-10.7	-9.6	-10.2
Tyr	40	-9.3	-9.5	-8.7	-9.2	-8.6	-9.4	-8.8	-9.1	-8.2

Tyr	41	-9.1	-9.1	-9.4	-9.3	-9.5	-9.1	-9.5	-8.9	-9.2
Tyr	42	-10.1	-11.0	-9.9	-11.3	-10.1	-11.2	-10.1	-10.5	-9.6
Tyr	47	-5.6	-6.3	-6.1	-6.1	-5.8	-6.2	-6.2	-6.1	-5.8
Tyr	48	-5.7	-6.3	-6.3	-6.2	-6.1	-6.6	-6.5	-6.8	-6.0
Tyr	49	-7.6	-8.0	-8.3	-8.2	-8.5	-7.9	-8.3	-8.0	-8.0
Tyr	50	-8.9	-8.5	-8.6	-8.7	-8.7	-8.8	-8.7	-8.6	-8.3
Tyr	51	-7.9	-8.2	-8.3	-8.3	-8.6	-8.1	-8.4	-8.2	-8.1
Tyr	52	-8.1	-8.0	-8.3	-7.9	-8.2	-8.0	-8.4	-8.0	-7.8
Tyr	53	-8.0	-8.1	-8.4	-8.1	-8.6	-8.3	-8.5	-8.7	-8.1
Tyr	54	-9.8	-9.6	-9.5	-9.4	-9.3	-9.5	-9.6	-9.3	-9.1
Tyr	55	-10.3	-10.1	-10.1	-9.8	-9.6	-10.0	-10.1	-9.8	-9.7
Tyr	56	-11.0	-10.2	-10.2	-9.9	-10.2	-10.6	-10.4	-10.4	-10.0
Tyr	57	-9.3	-10.3	-10.5	-10.1	-10.1	-10.6	-10.7	-10.3	-10.2
Tyr	58	-9.6	-10.8	-10.9	-10.8	-10.7	-11.1	-11.0	-10.5	-10.5
Trp	1	-4.5	-5.8	-5.8	-6.8	-6.6	-5.9	-6.1	-6.3	-6.0
Trp	2	-5.3	-5.4	-5.9	-5.6	-6.3	-5.5	-6.2	-5.9	-5.9
Trp	3	-5.8	-5.2	-5.6	-5.5	-6.0	-5.4	-5.9	-5.8	-5.5
Trp	4	-7.2	-6.8	-6.7	-6.9	-6.9	-7.0	-7.0	-7.0	-6.6
Trp	5	-6.7	-6.5	-6.6	-6.5	-6.7	-6.6	-6.9	-6.5	-6.4
Trp	6	-7.2	-6.5	-6.4	-6.7	-6.6	-6.5	-6.6	-6.5	-6.1
Trp	7	-7.3	-6.3	-6.3	-6.4	-6.4	-6.3	-6.6	-6.3	-6.1
Trp	8	-5.1	-6.3	-6.4	-6.8	-6.9	-6.3	-6.7	-6.5	-6.4
Trp	9	-8.4	-7.0	-6.8	-7.8	-7.5	-7.1	-7.0	-7.3	-6.7
Trp	11	-6.0	-7.5	-7.5	-8.0	-8.0	-7.8	-7.8	-8.0	-7.4
Trp	12	-6.2	-6.5	-6.8	-6.7	-6.8	-6.3	-7.0	-6.3	-6.6
Trp	14	-9.1	-7.2	-7.1	-7.1	-7.1	-7.6	-7.5	-7.8	-7.0
Trp	15	-6.0	-6.0	-6.5	-6.2	-6.9	-6.3	-6.8	-6.9	-6.4
Trp	16	-7.7	-7.2	-7.2	-7.4	-7.4	-7.4	-7.5	-7.3	-7.0
Trp	17	-8.1	-7.5	-7.7	-7.2	-7.6	-7.4	-8.0	-7.5	-7.4
Trp	18	-8.4	-8.1	-7.8	-8.0	-7.7	-7.9	-8.1	-7.7	-7.6
Trp	19	-9.5	-8.4	-8.2	-8.4	-8.3	-8.8	-8.5	-8.8	-8.0

Trp 20	-8.4	-8.2	-8.3	-7.5	-7.9	-7.9	-8.5	-8.1	-8.1
Trp 21	-9.9	-9.0	-8.6	-8.7	-8.3	-9.0	-8.8	-9.0	-8.5
Trp 22	-10.3	-9.5	-9.0	-9.4	-8.9	-9.8	-9.4	-10.0	-9.1
Trp 23	-9.8	-9.2	-9.2	-8.5	-8.6	-9.0	-9.4	-9.8	-9.5
Trp 24	-9.9	-9.4	-9.3	-8.7	-8.7	-9.6	-9.5	-10.1	-9.6
Trp 25	-10.8	-10.4	-9.7	-10.1	-9.2	-10.3	-10.0	-11.1	-10.1
Trp 26	-10.4	-10.4	-9.9	-10.5	-10.0	-11.0	-10.4	-10.7	-9.9
Trp 27	-11.2	-9.6	-9.4	-10.4	-10.1	-9.7	-9.6	-9.8	-9.6
Trp 28	-10.4	-9.7	-9.4	-10.7	-10.1	-9.8	-9.6	-9.8	-9.6
Trp 29	-11.0	-9.3	-10.4	-9.6	-10.7	-9.5	-10.6	-9.7	-10.6
Trp 30	-11.8	-10.6	-11.4	-11.3	-11.8	-10.5	-11.5	-10.4	-11.2
Trp 31	-13.6	-12.5	-12.1	-12.9	-12.2	-12.5	-12.1	-12.2	-11.8
Trp 32	-12.4	-11.8	-11.5	-11.9	-11.4	-11.5	-11.5	-11.0	-11.2
Trp 33	-10.2	-10.6	-9.9	-10.8	-9.9	-10.4	-10.0	-10.3	-9.8
Trp 34	-14.0	-12.4	-12.5	-12.1	-12.6	-12.7	-12.4	-13.1	-12.2
Trp 35	-14.4	-12.5	-13.2	-12.5	-13.1	-13.1	-13.4	-13.1	-13.2
Trp 36	-14.2	-14.3	-13.1	-13.9	-12.8	-14.3	-13.2	-14.0	-13.2
Trp 37	-15.8	-15.6	-14.3	-15.8	-14.5	-15.7	-14.5	-15.4	-14.3
Trp 38	-10.5	-10.7	-11.8	-10.7	-11.8	-10.8	-11.9	-10.8	-11.5
Trp 39	-11.8	-11.6	-12.8	-11.5	-12.6	-12.1	-13.0	-11.9	-12.6
Trp 40	-10.7	-11.4	-10.5	-11.1	-10.4	-11.4	-10.6	-11.2	-10.1
Trp 41	-10.9	-11.0	-11.4	-11.2	-11.5	-11.0	-11.5	-11.0	-11.3
Trp 42	-13.3	-13.3	-12.0	-13.8	-12.3	-13.6	-12.3	-13.0	-11.8
Trp 47	-7.2	-7.4	-7.2	-7.3	-6.9	-7.4	-7.4	-7.5	-7.0
Trp 48	-8.0	-7.5	-7.4	-7.4	-7.2	-7.9	-7.8	-8.3	-7.4
Trp 49	-9.0	-9.6	-9.9	-9.9	-10.2	-9.6	-10.1	-9.9	-9.8
Trp 50	-11.3	-10.3	-10.3	-10.5	-10.5	-10.6	-10.5	-10.6	-10.2
Trp 51	-10.6	-9.8	-10.0	-10.0	-10.4	-9.7	-10.2	-10.1	-9.9
Trp 52	-9.9	-9.6	-9.9	-9.5	-9.9	-9.6	-10.1	-9.9	-9.6
Trp 53	-10.0	-9.7	-10.1	-9.8	-10.4	-10.0	-10.3	-10.7	-9.9
Trp 54	-11.3	-11.5	-11.5	-11.4	-11.3	-11.5	-11.6	-11.4	-11.2

Trp 55	-11.5	-12.3	-12.2	-11.8	-11.7	-12.1	-12.2	-12.1	-12.0
Trp 56	-11.9	-12.3	-12.4	-12.0	-12.4	-13.0	-12.6	-12.8	-12.3
Trp 57	-11.9	-12.5	-12.7	-12.3	-12.3	-12.9	-13.0	-12.7	-12.5
Trp 58	-13.2	-13.1	-13.2	-13.1	-13.0	-13.5	-13.4	-13.0	-13.0
R²	--	0.91	0.90	0.89	0.89	0.91	0.90	0.92	0.91
ρ²	--	0.91	0.90	0.89	0.88	0.92	0.91	0.92	0.91
τ	--	0.83	0.82	0.81	0.80	0.84	0.82	0.84	0.82
RMSE	--	0.7	0.8	0.8	0.8	0.7	0.8	0.7	0.8

Table S3. DFT-computed (Comp.) and Predicted (Pred.; from equations 2-5) values of ESP_{mean}, ESP_{max}, ESP_{range}, F_{mean} for the set of 1854 heterocycles. IDs are from the VEHICLE database.

ID	SMILES	ESP _{mean}		ESP _{max}		ESP _{range}		F _{mean}	
		Comp.	Pred.	Comp.	Pred.	Comp.	Pred.	Comp.	Pred.
S1	<chem>c1ccc[nH]1</chem>	-5.93	-5.23	2.98	2.46	14.71	14.22	0.35	0.35
S10	<chem>c1cnn[nH]1</chem>	-1.80	-1.57	6.91	6.77	17.80	17.59	0.40	0.42
S10016	<chem>O=c1[nH]ncc2c1c[nH]c2</chem>	-2.63	-1.76	9.04	5.73	20.96	15.08	0.64	0.62
S10017	<chem>O=c1[nH]ncc2c1coc2</chem>	-0.45	-0.16	5.33	4.83	13.98	11.55	0.70	0.68
S10018	<chem>O=c1[nH]ncc2c1csc2</chem>	-0.99	-0.85	4.96	4.07	13.95	10.95	0.49	0.49
S10019	<chem>O=c1[nH]ncc2c1c[nH]n2</chem>	-0.89	0.07	8.53	6.54	17.17	13.53	0.45	0.43
S10020	<chem>O=c1[nH]ncc2c1n[nH]c2</chem>	-1.02	0.07	9.34	7.14	21.98	16.55	0.50	0.54
S10021	<chem>O=c1[nH]ncc2c1con2</chem>	1.61	1.67	4.42	6.59	9.38	11.34	0.35	0.36
S10022	<chem>O=c1[nH]ncc2c1noc2</chem>	1.48	1.67	8.97	7.19	18.56	14.36	0.40	0.38
S10025	<chem>O=c1[nH]ncc2c1n[nH]n2</chem>	0.77	1.90	7.47	6.93	16.60	12.76	0.42	0.40
S10026	<chem>O=c1[nH]ncc2c1non2</chem>	3.57	3.50	8.67	7.93	14.07	11.90	0.41	0.45
S10027	<chem>O=c1[nH]ncc2c1nsn2</chem>	2.23	2.81	6.00	7.05	13.70	10.98	0.63	0.63
S10028	<chem>O=c1[nH]cc2c(c1)cn[nH]c2=O</chem>	1.63	1.22	7.33	7.34	14.25	14.14	0.39	0.39
S10029	<chem>O=c1[nH]cc2c(c1)c(=O)[nH]nc2</chem>	1.44	1.22	11.42	7.82	19.71	16.66	0.66	0.66
S10034	<chem>O=c1[nH]ncc2c1c(=O)[nH]nc2</chem>	1.98	3.05	8.61	7.72	20.05	14.48	0.41	0.41
S10035	<chem>O=c1[nH]ncc2c1cn[nH]c2=O</chem>	2.66	3.05	6.67	7.55	10.74	12.26	0.45	0.46
S1006	<chem>c1cn2c([nH]1)ccn2</chem>	-4.54	-3.99	6.29	5.29	18.97	17.06	0.42	0.45
S10062	<chem>O=c1[nH]c2cn[nH]c(=O)c2c(=O)[nH]1</chem>	3.39	3.82	12.28	10.04	22.77	18.11	0.60	0.61
S10063	<chem>O=c1[nH]c(=O)c2c([nH]1)c(=O)[nH]nc2</chem>	4.08	3.82	9.43	9.25	12.99	13.94	0.75	0.72
S1007	<chem>[nH]1cc2c(c1)cn[nH]2</chem>	-5.51	-4.74	4.58	5.55	16.35	17.60	0.48	0.47
S10077	<chem>O=c1[nH]ncc2c1nccn2</chem>	1.27	2.28	6.36	6.71	15.74	12.15	0.47	0.45
S1008	<chem>c1cc2n(n1)occ2</chem>	-2.82	-2.39	4.31	4.13	13.70	13.13	0.47	0.45
S1009	<chem>c1cn2c(o1)ccn2</chem>	-2.79	-2.39	3.99	3.76	12.72	12.65	0.33	0.33
S1010	<chem>o1cc2c(c1)cn[nH]2</chem>	-3.39	-3.14	2.24	3.95	9.23	13.30	0.51	0.51
S10113	<chem>O=c1cn[nH]c2c1cn[nH]c2=O</chem>	2.89	3.05	7.67	9.47	13.53	14.98	0.49	0.49

S1012	c1cn2c(s1)ccn2	-3.37	-3.08	3.03	3.05	11.44	12.16	0.41	0.35
S1013	s1cc2c(c1)cn[nH]2	-3.81	-3.83	2.14	3.24	9.48	12.80	0.48	0.47
S1014	n1cc2c([nH]1)[nH]nc2	-2.99	-2.91	6.02	7.00	13.03	16.91	0.48	0.54
S10148	O=c1nccc2n1[nH]cc2	-0.90	-1.01	9.62	7.93	23.91	19.67	0.41	0.42
S1015	n1cc2c([nH]1)cn[nH]2	-3.13	-2.91	2.68	4.87	9.27	14.59	0.60	0.62
S10156	O=c1ncc2c([nH]1)csc2	0.21	-0.85	6.14	7.30	18.88	18.56	0.69	0.70
S10157	O=c1nccc2n1[nH]nc2	1.06	0.82	7.43	8.78	18.83	18.68	0.37	0.37
S1016	c1nn2c(c1)cn[nH]2	-2.61	-2.16	3.53	5.38	10.22	14.58	0.46	0.38
S10160	O=c1ncc2c([nH]1)n[nH]c2	0.07	0.07	10.97	10.01	25.03	21.93	0.48	0.51
S10169	O=c1nccc2n1[nH]cn2	0.76	0.82	11.78	9.83	23.42	19.27	0.51	0.46
S1017	c1nn2c(c1)[nH]nc2	-2.45	-2.16	5.31	6.43	13.72	16.72	0.35	0.33
S10175	O=c1nccc2n1[nH]nn2	2.82	2.65	9.80	11.31	18.06	19.68	0.46	0.43
S10177	O=c1ncc2c([nH]1)n[nH]n2	1.71	1.90	9.24	10.35	20.30	19.33	0.55	0.54
S1018	n1cc2c([nH]1)n[nH]c2	-3.67	-2.91	4.81	5.22	13.50	15.09	0.50	0.54
S1019	n1cc2c([nH]1)c[nH]n2	-3.72	-2.91	5.00	7.13	13.92	18.04	0.53	0.52
S1020	n1oc2c(c1)cn[nH]2	-1.00	-1.31	4.62	5.09	10.99	12.97	0.33	0.32
S10202	O=c1[nH]cc2c(c1)cnc(=O)[nH]2	3.10	1.22	11.67	12.04	20.97	22.93	0.44	0.48
S10203	O=c1[nH]cc2c(c1)[nH]c(=O)nc2	2.88	1.22	12.99	10.32	23.01	20.73	0.36	0.32
S1021	n1cc2c(o1)cn[nH]2	-1.06	-1.31	6.91	5.84	13.91	13.49	0.50	0.48
S1023	c1nn2c(c1)onc2	-0.45	-0.56	3.86	5.86	7.79	13.65	0.44	0.44
S1024	n1cc2c([nH]1)noc2	-1.22	-1.31	4.05	4.58	11.09	12.13	0.47	0.58
S1025	n1cc2c([nH]1)con2	-1.29	-1.31	6.54	6.49	14.60	15.08	0.37	0.38
S10254	O=c1ncc2c([nH]1)ncc(=O)[nH]2	4.79	3.05	11.87	10.52	21.59	18.89	0.57	0.55
S10255	O=c1ncc2c([nH]1)[nH]c(=O)cn2	4.76	3.05	14.57	14.04	22.98	22.25	0.46	0.46
S1026	n1sc2c(c1)cn[nH]2	-1.75	-2.00	5.20	4.40	11.40	12.42	0.51	0.49
S10262	O=c1ncc2c([nH]1)c(=O)[nH]c(=O)[nH]2	5.50	3.82	13.12	11.82	22.43	20.12	0.46	0.45
S10263	O=c1ncc2c([nH]1)[nH]c(=O)[nH]c2=O	5.42	3.82	15.82	14.68	23.68	23.77	0.43	0.46
S1027	n1cc2c(s1)cn[nH]2	-1.73	-2.00	5.97	4.96	12.08	12.59	0.48	0.52
S1029	c1nn2c(c1)snc2	-1.30	-1.25	1.79	5.08	6.50	12.99	0.41	0.39
S10292	O=c1ncc2c([nH]1)nccn2	2.63	2.28	7.94	9.53	18.34	18.26	0.40	0.41
S10294	O=c1ncc2c([nH]1)ncnn2	4.72	4.11	11.00	11.04	17.51	18.06	0.60	0.63

S10295	O=c1ncc2c([nH]1)nncn2	4.69	4.11	10.97	10.26	18.02	17.05	0.51	0.50
S1030	n1cc2c([nH]1)nsc2	-2.01	-2.00	3.45	3.81	8.86	11.46	0.70	0.68
S1032	c1nc2c([nH]1)[nH]nc2	-3.18	-2.91	9.31	9.92	19.72	21.71	0.39	0.39
S1033	c1[nH]c2c(n1)[nH]nc2	-3.30	-2.91	6.78	5.88	15.68	16.43	0.79	0.81
S1034	c1nn2c(c1)nc[nH]2	-2.82	-2.16	8.48	6.65	17.03	16.18	0.51	0.54
S1035	c1cc2n(n1)nc[nH]2	-2.71	-2.16	9.99	8.64	23.01	21.04	0.71	0.68
S1036	c1nc2c(o1)[nH]nc2	-1.45	-1.31	5.18	5.51	11.37	14.27	0.39	0.37
S1037	c1oc2c(n1)[nH]nc2	-1.50	-1.31	2.84	4.35	8.82	11.83	0.59	0.56
S1039	c1cc2n(n1)nco2	-0.99	-0.56	6.06	5.58	14.98	14.46	0.39	0.39
S104	O=c1ccscn1	0.64	0.49	7.14	5.99	18.42	16.93	0.55	0.55
S1040	c1nc2c(s1)[nH]nc2	-2.20	-2.00	4.92	4.98	11.37	14.15	0.59	0.62
S1041	c1sc2c(n1)[nH]nc2	-2.19	-2.00	2.18	3.64	8.38	11.36	0.81	0.74
S1043	c1cc2n(n1)ncs2	-1.80	-1.25	4.83	4.96	14.36	14.24	0.35	0.36
S1044	n1[nH]c2c(c1)nn[nH]2	-1.11	-1.08	9.32	11.07	18.86	21.61	0.31	0.30
S1045	n1[nH]c2c(c1)[nH]nn2	-1.22	-1.08	6.32	7.03	14.32	16.33	0.36	0.35
S1046	c1nn2c(c1)nn[nH]2	-0.76	-0.33	7.33	8.42	13.23	17.23	0.42	0.41
S1047	c1nn2c(c1)[nH]nn2	-0.69	-0.33	9.26	10.42	18.29	22.08	0.42	0.43
S1048	[nH]1nc2c(n1)cn[nH]2	-1.89	-1.08	3.83	5.79	9.25	13.28	0.49	0.49
S1050	n1oc2c(n1)[nH]nc2	0.69	0.52	6.45	6.46	11.66	13.07	0.53	0.51
S1052	c1nn2c(c1)onn2	1.20	1.27	4.31	8.30	8.51	16.85	0.49	0.50
S1053	n1nc2c(s1)[nH]nc2	-0.14	-0.17	7.84	7.03	14.49	15.22	0.45	0.47
S1054	n1sc2c(n1)[nH]nc2	-0.08	-0.17	4.54	5.68	10.34	12.43	0.40	0.41
S10558	O=c1ncc2c(o1)csc2	1.24	0.75	8.13	7.10	19.61	17.05	0.60	0.57
S1056	c1nn2c(c1)snn2	0.21	0.58	4.63	7.63	10.80	16.46	0.47	0.50
S1057	O=c1c(=O)c2c(c1=O)[nH]nc2	4.79	5.54	11.19	11.73	16.63	20.94	0.82	0.80
S1059	o1nc2c(n1)cn[nH]2	0.87	0.52	6.48	6.10	11.63	11.66	0.41	0.41
S1060	s1nc2c(n1)cn[nH]2	-0.24	-0.17	4.24	5.27	7.33	10.82	0.45	0.47
S1061	O=c1[nH]c2c([nH]1)cn[nH]2	-1.32	-2.14	6.88	7.23	15.75	17.86	0.55	0.52
S1067	O=c1[nH]c2c(s1)[nH]nc2	-0.69	-1.23	5.19	6.34	12.71	15.34	0.35	0.37
S1068	O=c1sc2c([nH]1)[nH]nc2	-0.53	-1.23	9.40	9.03	16.86	17.83	0.58	0.58
S1071	c1ccc2c(c1)[nH]nc2	-4.06	-4.36	2.49	3.37	10.23	13.78	0.60	0.59

S1072	<chem>c1ccc2n(c1)ncc2</chem>	-3.67	-3.61	1.79	3.17	10.61	13.15	0.63	0.67
S1073	<chem>c1ncc2c(c1)[nH]nc2</chem>	-2.09	-2.53	5.30	5.03	12.69	14.13	0.56	0.56
S1074	<chem>c1ncc2c(c1)cn[nH]2</chem>	-2.13	-2.53	4.70	4.28	11.47	12.97	0.43	0.43
S1075	<chem>c1cnc2c(c1)cn[nH]2</chem>	-2.54	-2.53	2.26	3.79	8.37	12.56	0.48	0.52
S1076	<chem>c1cnc2c(c1)[nH]nc2</chem>	-2.51	-2.53	5.23	5.84	13.27	15.74	0.51	0.51
S1077	<chem>n1ccn2c(c1)ccn2</chem>	-1.74	-1.78	1.53	4.75	6.63	13.31	0.42	0.42
S1078	<chem>c1ncn2c(c1)ccn2</chem>	-1.71	-1.78	2.88	5.22	8.47	14.51	0.40	0.39
S1079	<chem>c1cnn2c(c1)ccn2</chem>	-2.16	-1.78	4.65	5.39	15.42	15.53	0.47	0.45
S1080	<chem>c1ccn2c(n1)ccn2</chem>	-2.18	-1.78	4.21	4.30	10.43	12.50	0.56	0.57
S1081	<chem>c1nnc2c(c1)[nH]nc2</chem>	-0.45	-0.70	8.46	8.52	18.23	18.34	0.56	0.57
S1082	<chem>c1nnc2c(c1)cn[nH]2</chem>	-0.52	-0.70	4.86	5.72	13.05	14.01	0.42	0.40
S1083	<chem>n1ccn2c(n1)ccn2</chem>	-0.20	0.05	5.35	6.91	12.19	14.91	0.34	0.33
S1085	<chem>n1ncc2c(c1)[nH]nc2</chem>	0.04	-0.70	8.01	6.96	18.01	15.57	0.47	0.38
S1086	<chem>n1ncc2n(c1)ncc2</chem>	0.47	0.05	4.90	7.82	12.40	16.92	0.74	0.70
S1087	<chem>O=c1[nH]ccc2c1cn[nH]2</chem>	-1.84	-1.76	6.62	7.78	17.73	19.45	0.51	0.51
S1088	<chem>O=c1[nH]ccc2c1[nH]nc2</chem>	-1.67	-1.76	5.53	6.36	13.30	15.91	0.52	0.54
S1089	<chem>O=c1ccc2c([nH]1)[nH]nc2</chem>	-0.67	-1.76	8.08	7.45	17.45	16.81	0.72	0.61
S1090	<chem>O=c1ccc2c([nH]1)cn[nH]2</chem>	-0.76	-1.76	7.25	5.98	17.87	15.93	0.61	0.57
S1091	<chem>O=c1[nH]ccn2c1ccn2</chem>	-1.59	-1.01	7.06	6.19	15.58	15.31	0.38	0.37
S1092	<chem>O=c1[nH]ccc2n1ncc2</chem>	-1.72	-1.01	7.70	6.86	20.22	18.61	0.48	0.43
S1094	<chem>O=c1ccn2c([nH]1)ccn2</chem>	-0.34	-1.01	4.29	7.18	12.15	17.09	0.57	0.56
S1097	<chem>O=c1occc2c1cn[nH]2</chem>	-0.20	-0.16	8.51	8.53	18.76	18.90	0.65	0.67
S1098	<chem>O=c1occc2c1[nH]nc2</chem>	-0.06	-0.16	4.49	5.98	12.02	14.25	0.57	0.55
S10999	<chem>O=c1cnc2c([nH]1)coc2</chem>	0.16	-0.16	5.33	6.86	12.58	14.84	0.79	0.83
S11	<chem>c1cn[nH]n1</chem>	-2.10	-1.57	2.67	3.26	7.05	11.08	0.50	0.50
S11002	<chem>O=c1cnc2c([nH]1)csc2</chem>	-0.32	-0.85	5.29	6.17	12.94	14.41	0.45	0.44
S11005	<chem>O=c1cnc2c([nH]1)n[nH]c2</chem>	-0.39	0.07	8.23	7.87	17.28	16.24	0.54	0.51
S11029	<chem>O=c1cnc2c([nH]1)non2</chem>	4.44	3.50	10.55	9.15	13.46	13.45	0.65	0.61
S11030	<chem>O=c1cnc2c([nH]1)nsn2</chem>	3.09	2.81	7.73	8.33	11.49	12.68	0.47	0.46
S11036	<chem>O=c1cncc2n1cccc2</chem>	-0.27	-0.63	6.73	5.81	15.98	14.55	0.80	0.83
S11038	<chem>O=c1cncc2n1cncc2</chem>	1.63	1.20	6.82	7.55	13.50	15.50	0.66	0.66

S11048	<chem>O=c1[nH]cc2c(c1)[nH]c(=O)cn2</chem>	2.14	1.22	8.34	8.52	15.94	16.04	0.36	0.36
S11049	<chem>O=c1[nH]cc2c(c1)ncc(=O)[nH]2</chem>	2.36	1.22	11.36	11.24	20.38	20.40	0.61	0.57
S11072	<chem>O=c1[nH]cc2c(n1)ncc(=O)[nH]2</chem>	3.85	3.05	14.91	16.28	26.21	28.03	0.51	0.48
S11073	<chem>O=c1[nH]cc2c(n1)[nH]c(=O)cn2</chem>	3.29	3.05	11.31	10.30	20.25	18.37	0.73	0.67
S1109	<chem>O=c1ccc2c(s1)[nH]nc2</chem>	-0.38	-0.85	5.35	5.59	13.23	13.97	0.34	0.36
S11091	<chem>O=c1cnc2c([nH]1)ncc(=O)[nH]2</chem>	4.02	3.05	9.06	8.69	14.17	14.49	0.44	0.45
S11098	<chem>O=c1cnc2c([nH]1)[nH]c(=O)[nH]c2=O</chem>	4.68	3.82	15.44	14.20	23.21	22.17	0.33	0.31
S11099	<chem>O=c1cnc2c([nH]1)c(=O)[nH]c(=O)[nH]2</chem>	4.74	3.82	10.32	9.70	15.35	14.96	0.33	0.34
S11102	<chem>O=c1cnc2c([nH]1)[nH]c(=O)c(=O)[nH]2</chem>	5.18	3.82	14.75	13.75	22.60	24.58	0.45	0.46
S11112	<chem>O=c1cnc2c([nH]1)[nH]c(=O)sc2=O</chem>	5.16	4.73	16.39	16.75	23.06	24.17	0.50	0.49
S11113	<chem>O=c1cnc2c([nH]1)c(=O)sc(=O)[nH]2</chem>	5.18	4.73	11.39	10.51	15.46	15.27	0.38	0.38
S11120	<chem>O=c1cnc2c([nH]1)c(=O)cc[nH]2</chem>	1.42	1.22	10.89	8.78	19.63	18.29	0.47	0.51
S11121	<chem>O=c1cnc2c([nH]1)[nH]ccc2=O</chem>	1.54	1.22	16.23	16.00	30.08	29.87	0.46	0.46
S11124	<chem>O=c1cnc2c([nH]1)c(=O)nc[nH]2</chem>	3.32	3.05	12.72	11.09	21.96	20.80	0.63	0.62
S11125	<chem>O=c1cnc2c([nH]1)[nH]cnc2=O</chem>	3.44	3.05	18.69	19.54	32.53	34.38	0.59	0.59
S11128	<chem>O=c1cnc2c([nH]1)ncn2</chem>	2.14	2.28	5.93	8.58	11.55	14.79	0.41	0.40
S11130	<chem>O=c1cnc2c([nH]1)nnn2</chem>	4.30	4.11	10.15	9.55	12.56	14.09	0.46	0.46
S11131	<chem>O=c1cnc2c([nH]1)ncnn2</chem>	4.37	4.11	10.60	10.77	15.64	16.08	0.59	0.57
S11134	<chem>O=c1cnc2c([nH]1)c(=O)[nH]cn2</chem>	2.81	3.05	11.42	12.09	18.85	18.69	0.46	0.44
S11135	<chem>O=c1cnc2c([nH]1)nc[nH]c2=O</chem>	2.36	3.05	12.03	11.04	20.33	19.24	0.44	0.44
S11151	<chem>O=c1cnc2c([nH]1)ncsc2=O</chem>	3.17	3.96	9.17	10.24	16.04	16.62	0.62	0.63
S11154	<chem>O=c1cnc2c([nH]1)nnnn2</chem>	6.65	5.94	14.81	12.76	19.62	17.62	0.62	0.60
S1117	<chem>c1ncc2c(n1)cn[nH]2</chem>	-0.56	-0.70	7.53	6.16	13.00	13.64	0.50	0.51
S1118	<chem>c1ncc2c(n1)[nH]nc2</chem>	-0.54	-0.70	2.97	4.85	7.27	11.62	0.55	0.58
S1119	<chem>c1ncn2c(n1)ccn2</chem>	-0.18	0.05	2.85	5.76	5.97	12.57	0.52	0.47
S1120	<chem>n1cnn2c(c1)ccn2</chem>	-0.20	0.05	5.01	6.38	12.33	14.39	0.72	0.69
S1121	<chem>n1nnc2c(c1)[nH]nc2</chem>	1.63	1.13	11.09	9.86	20.78	18.49	0.45	0.48
S1122	<chem>n1nnc2c(c1)cn[nH]2</chem>	1.61	1.13	6.36	7.80	15.06	15.31	0.38	0.41
S1123	<chem>n1ncn2c(n1)ccn2</chem>	1.98	1.88	6.02	9.39	12.70	17.23	0.49	0.49
S1125	<chem>O=c1[nH]ncc2c1cn[nH]2</chem>	0.00	0.07	8.85	6.89	18.12	15.05	0.38	0.39
S1126	<chem>O=c1[nH]ncc2c1[nH]nc2</chem>	0.22	0.07	3.78	6.23	10.03	12.68	0.36	0.36

S11269	<chem>O=c1nnc2c([nH]1)coc2</chem>	1.93	1.67	8.28	11.07	18.29	21.71	0.47	0.48
S1127	<chem>O=c1[nH]ncn2c1ccn2</chem>	0.35	0.82	3.62	6.45	10.39	13.09	0.42	0.43
S11271	<chem>O=c1[n]ncc2n1ccs2</chem>	2.18	1.73	10.75	9.61	22.90	19.90	0.46	0.46
S11272	<chem>O=c1nnc2c([nH]1)csc2</chem>	1.47	0.98	8.15	10.43	18.72	21.41	0.48	0.48
S11275	<chem>O=c1nnc2c([nH]1)n[nH]c2</chem>	1.45	1.90	11.83	12.39	23.43	23.12	0.69	0.69
S1128	<chem>O=c1[nH]ncc2n1ncc2</chem>	0.16	0.82	5.65	6.65	15.61	15.18	0.44	0.43
S11290	<chem>O=c1[n]ncc2n1ncs2</chem>	3.17	3.56	13.23	11.47	25.66	22.57	0.44	0.46
S113	<chem>O=c1cnsnc1</chem>	2.58	2.32	6.27	5.37	11.13	9.82	0.47	0.46
S1131	<chem>O=c1ncc2c([nH]1)cn[nH]2</chem>	1.03	0.07	9.49	8.67	21.97	19.30	0.47	0.43
S1132	<chem>O=c1ncc2c([nH]1)[nH]nc2</chem>	1.21	0.07	10.91	10.89	22.50	21.33	0.54	0.53
S1133	<chem>O=c1ncn2c([nH]1)ccn2</chem>	1.55	0.82	6.98	11.02	16.56	22.62	0.42	0.41
S11396	<chem>O=c1nnc2c([nH]1)nccn2</chem>	4.04	4.11	9.54	13.05	17.53	21.96	0.61	0.60
S11398	<chem>O=c1nnc2c([nH]1)nncn2</chem>	6.08	5.94	13.21	13.45	17.64	20.01	0.41	0.47
S11399	<chem>O=c1nnc2c([nH]1)ncnn2</chem>	6.18	5.94	13.87	14.95	17.93	22.60	0.40	0.39
S114	<chem>O=c1ncscn1</chem>	2.29	2.32	8.66	7.97	19.74	19.35	0.39	0.42
S11594	<chem>O=c1[nH]c(=O)c2c([nH]1)c[nH]c2</chem>	-1.19	-0.99	9.65	8.02	19.10	18.64	0.46	0.45
S11597	<chem>O=c1[nH]c(=O)c2c([nH]1)coc2</chem>	1.02	0.61	6.71	7.04	13.11	14.65	0.34	0.34
S11600	<chem>O=c1[nH]c(=O)c2c([nH]1)csc2</chem>	0.52	-0.08	6.52	6.29	13.14	14.11	0.34	0.33
S11603	<chem>O=c1[nH]c(=O)c2c([nH]1)n[nH]c2</chem>	0.51	0.84	9.40	7.65	16.89	15.37	0.62	0.54
S11604	<chem>O=c1[nH]c(=O)c2c([nH]1)c[nH]n2</chem>	0.43	0.84	10.29	10.23	20.70	20.97	0.45	0.48
S1161	<chem>O=c1cnc2c([nH]1)[nH]nc2</chem>	0.81	0.07	10.62	10.41	17.05	18.72	0.62	0.60
S11613	<chem>O=c1cc2nc[nH]n2c(=O)[nH]1</chem>	1.63	1.59	12.95	10.83	24.07	18.50	0.59	0.70
S1162	<chem>O=c1cnc2c([nH]1)cn[nH]2</chem>	0.67	0.07	5.42	6.89	12.94	14.67	0.45	0.46
S11638	<chem>O=c1cc2ncccn2c(=O)[nH]1</chem>	1.90	1.97	8.35	7.97	18.00	14.69	0.47	0.43
S1164	<chem>O=c1cnn2c([nH]1)ccn2</chem>	1.14	0.82	7.69	9.90	14.38	19.42	0.64	0.67
S1165	<chem>O=c1nnc2c([nH]1)[nH]nc2</chem>	2.72	1.90	14.12	14.87	23.62	25.49	0.39	0.43
S1166	<chem>O=c1nnc2c([nH]1)cn[nH]2</chem>	2.48	1.90	8.66	10.60	18.73	20.28	0.61	0.60
S11660	<chem>O=c1cc2ncnncn2c(=O)[nH]1</chem>	3.89	3.80	10.57	9.41	17.17	14.35	0.84	0.81
S11668	<chem>O=c1ncn2c([nH]1)cc(=O)[nH]c2=O</chem>	5.72	4.57	13.25	13.63	18.56	22.70	0.63	0.60
S11670	<chem>O=c1[nH]cc2c(n1)c(=O)[nH]c(=O)[nH]2</chem>	4.15	3.82	15.73	15.64	26.26	28.67	0.40	0.41
S11671	<chem>O=c1[nH]cc2c(n1)[nH]c(=O)[nH]c2=O</chem>	4.23	3.82	11.45	10.80	18.99	18.22	0.47	0.46

S1169	O=c1[nH]c(=O)c2c([nH]1)[nH]nc2	1.59	0.84	11.97	10.41	19.57	19.13	0.55	0.54
S1170	O=c1[nH]c(=O)c2c([nH]1)cn[nH]2	1.60	0.84	6.78	7.52	12.24	14.71	0.36	0.36
S11714	O=c1[nH]c(=O)c2c([nH]1)c(=O)cc[nH]2	2.44	1.99	9.88	9.41	17.07	17.54	0.52	0.52
S11715	O=c1[nH]c2[nH]ccc(=O)c2c(=O)[nH]1	1.65	1.99	17.00	15.26	32.44	30.08	0.55	0.55
S11718	O=c1[nH]c(=O)c2c([nH]1)c(=O)nc[nH]2	4.35	3.82	11.62	12.32	19.64	20.73	0.45	0.46
S11719	O=c1[nH]c2[nH]cnc(=O)c2c(=O)[nH]1	3.51	3.82	19.49	19.17	34.56	35.43	0.47	0.49
S1172	O=c1[nH]c(=O)n2c([nH]1)ccn2	1.78	1.59	8.73	9.43	17.12	19.20	0.51	0.52
S11720	O=c1cc2[nH]cnc(=O)n2c(=O)[nH]1	3.78	4.57	17.01	15.68	27.39	29.80	0.42	0.41
S11722	O=c1[nH]c2nccnc2c(=O)[nH]1	2.66	3.05	7.33	8.52	14.83	14.70	0.48	0.48
S11724	O=c1[nH]c2nncnc2c(=O)[nH]1	4.87	4.88	11.54	10.08	15.49	14.68	0.56	0.61
S11725	O=c1[nH]c2ncnnc2c(=O)[nH]1	4.84	4.88	11.90	11.07	18.10	16.83	0.42	0.43
S11728	O=c1[nH]c(=O)c2c([nH]1)c(=O)[nH]cn2	3.27	3.82	12.26	11.39	19.70	18.02	0.60	0.58
S11729	O=c1[nH]c2nc[nH]c(=O)c2c(=O)[nH]1	2.53	3.82	12.92	10.53	23.97	18.62	0.39	0.39
S1173	O=c1[nH]c2[nH]ncc2[nH]c1=O	1.57	0.84	10.81	11.46	21.66	24.84	0.54	0.54
S11744	O=c1[nH]c(=O)c2c([nH]1)c(=O)scn2	4.03	4.73	9.73	9.70	15.65	14.29	0.40	0.38
S11745	O=c1[nH]c2ncsc(=O)c2c(=O)[nH]1	3.40	4.73	10.07	10.25	19.17	16.71	0.39	0.38
S11788	O=c1[nH]c(=O)c2c([nH]1)c(=O)cn[nH]2	4.27	3.82	10.23	9.74	14.80	15.13	0.46	0.46
S11789	O=c1[nH]c2[nH]ncc(=O)c2c(=O)[nH]1	3.45	3.82	16.11	14.60	28.14	25.51	0.55	0.56
S1179	O=c1[nH]c2[nH]ncc2oc1=O	2.73	2.44	12.99	14.18	21.69	25.80	0.49	0.50
S1180	O=c1[nH]c2cn[nH]c2oc1=O	2.64	2.44	7.80	11.08	15.49	22.74	0.50	0.55
S11860	O=c1[nH]c2c[nH]cc2[nH]c1=O	-1.10	-0.99	9.67	12.21	24.33	29.90	0.43	0.43
S11866	O=c1[nH]c2csc2[nH]c1=O	0.80	-0.08	6.23	8.79	17.30	23.19	0.83	0.82
S11869	O=c1[nH]c2n[nH]cc2[nH]c1=O	0.50	0.84	9.84	12.38	22.36	27.82	0.52	0.53
S1191	O=c1cc[nH]c2c1[nH]nc2	-1.71	-1.76	9.65	7.13	21.36	18.69	0.51	0.48
S1192	O=c1cc[nH]c2c1cn[nH]2	-1.79	-1.76	12.98	11.68	27.32	25.64	0.50	0.51
S1193	O=c1cc[nH]c2n1ncc2	-1.65	-1.01	11.46	10.40	26.39	25.15	0.50	0.49
S1195	O=c1nc[nH]c2c1[nH]nc2	0.16	0.07	11.65	9.82	24.26	22.06	0.45	0.48
S1196	O=c1nc[nH]c2c1cn[nH]2	0.05	0.07	15.28	15.11	30.08	30.16	0.43	0.43
S11968	O=c1[nH]c2nccnc2[nH]c1=O	3.03	3.05	8.35	10.61	17.14	22.29	0.38	0.39
S11970	O=c1[nH]c2nncnc2[nH]c1=O	5.22	4.88	12.70	11.67	18.21	21.17	0.41	0.40
S1199	c1cnc2c(n1)[nH]nc2	-0.99	-0.70	2.81	5.23	7.16	12.28	0.45	0.46

S1200	c1cnc2n(n1)ncc2	-0.72	0.05	5.48	5.51	13.15	12.63	0.55	0.57
S1201	c1nnc2c(n1)cn[nH]2	1.08	1.13	5.36	6.57	10.39	12.42	0.52	0.50
S1202	c1nnc2c(n1)[nH]nc2	1.13	1.13	6.34	7.32	12.60	13.58	0.43	0.43
S1203	c1nnn2c(n1)ccn2	1.29	1.88	4.55	7.99	9.49	14.95	0.42	0.43
S1205	O=c1[nH]cnc2c1[nH]nc2	-0.13	0.07	7.46	8.37	12.42	15.75	0.73	0.76
S1206	O=c1[nH]cnc2c1cn[nH]2	-0.34	0.07	8.11	7.73	16.08	16.11	0.40	0.42
S1207	O=c1[nH]cnc2n1ncc2	-0.22	0.82	9.67	7.54	19.20	15.83	0.79	0.76
S12077	O=c1oc(=O)c2c([nH]1)coc2	2.48	2.21	9.07	10.11	17.03	18.21	0.48	0.44
S1208	O=c1[nH]cnn2c1ccn2	-0.06	0.82	9.41	7.95	16.88	15.56	0.43	0.45
S12080	O=c1oc(=O)c2c([nH]1)csc2	1.99	1.52	8.77	9.44	17.08	17.80	0.52	0.48
S12087	O=c1oc(=O)c2c([nH]1)noc2	4.47	4.04	9.87	9.92	15.15	15.20	0.80	0.71
S1213	O=c1ocnc2c1[nH]nc2	1.47	1.67	4.54	7.10	9.26	12.84	0.42	0.40
S1214	O=c1ocnc2c1cn[nH]2	1.26	1.67	5.76	7.59	12.94	14.31	0.39	0.36
S1222	O=c1scnc2c1cn[nH]2	0.43	0.98	5.13	6.78	11.87	13.50	0.50	0.51
S1223	O=c1scnc2n1ncc2	0.45	1.73	6.26	7.15	14.53	14.08	0.74	0.75
S1225	n1nnc2c(n1)[nH]nc2	3.30	2.96	9.29	9.68	16.30	15.97	0.40	0.44
S1226	n1nnc2n(n1)ncc2	3.45	3.71	7.69	11.02	11.67	18.31	0.42	0.42
S1227	O=c1[nH][n]c2c([n]1)[nH]nc2	1.97	1.90	6.20	7.92	16.37	14.66	0.62	0.69
S1228	O=c1[nH][n]c2c([n]1)cn[nH]2	1.95	1.90	8.66	9.57	19.73	17.19	0.63	0.60
S1233	O=c1[nH]nnc2c1cn[nH]2	1.46	1.90	5.78	7.87	11.58	13.96	0.43	0.43
S1234	O=c1[nH]nnc2c1[nH]nc2	1.72	1.90	4.93	9.25	8.25	14.76	0.47	0.47
S12343	O=c1[nH]c2csc2oc1=O	1.77	1.52	8.17	10.24	17.47	22.89	0.47	0.44
S1236	O=c1[nH]nnc2n1ncc2	1.61	2.65	6.17	8.35	12.71	14.66	0.37	0.42
S124	n1ncnnc1	2.87	2.47	5.58	6.03	6.95	11.23	0.40	0.39
S1253	O=c1ccoc2c1[nH]nc2	-0.27	-0.16	5.10	5.71	12.68	13.64	0.62	0.57
S1254	O=c1ccoc2c1cn[nH]2	-0.42	-0.16	7.34	7.16	17.70	17.53	0.62	0.64
S1255	O=c1ccoc2n1ncc2	-0.27	0.59	7.53	6.97	18.67	17.58	0.39	0.38
S1257	O=c1ncoc2c1[nH]nc2	1.53	1.67	6.19	7.51	14.67	15.75	0.61	0.61
S1258	O=c1ncoc2c1cn[nH]2	1.35	1.67	9.79	9.71	20.47	20.80	0.46	0.41
S1261	O=c1ccsc2c1cn[nH]2	-1.00	-0.85	7.01	6.64	17.33	17.49	0.49	0.49
S1264	O=c1ccsc2n1ncc2	-0.90	-0.10	6.53	6.38	18.14	17.48	0.56	0.60

S1265	<chem>O=c1cn[nH]c2c1[nH]nc2</chem>	0.08	0.07	8.11	6.99	16.86	15.46	0.57	0.58
S1266	<chem>O=c1cn[nH]c2c1cn[nH]2</chem>	-0.02	0.07	12.00	10.79	22.94	21.25	0.47	0.47
S1267	<chem>O=c1cn[nH]c2n1ncc2</chem>	0.16	0.82	9.47	10.19	20.58	21.73	0.54	0.53
S12742	<chem>O=c1sc(=O)c2c([nH]1)coc2</chem>	1.51	1.52	8.38	9.10	15.02	16.74	0.61	0.57
S1275	<chem>O=c1cnscc2n1ncc2</chem>	0.91	1.73	5.12	7.61	13.51	15.95	0.54	0.52
S1278	<chem>O=c1ncsc2c1cn[nH]2</chem>	0.63	0.98	9.38	9.24	20.39	20.92	0.39	0.37
S1281	<chem>O=c1nn[nH]c2c1[nH]nc2</chem>	1.92	1.90	10.72	10.70	21.11	21.07	0.38	0.37
S1282	<chem>O=c1nn[nH]c2c1cn[nH]2</chem>	1.73	1.90	14.57	15.25	26.49	28.02	0.53	0.50
S12860	<chem>O=c1sc(=O)c2c([nH]1)ncn2</chem>	3.02	3.96	8.54	10.93	15.03	17.05	0.45	0.43
S12862	<chem>O=c1sc(=O)c2c([nH]1)nnn2</chem>	5.18	5.79	12.20	11.70	15.25	15.97	0.41	0.36
S12863	<chem>O=c1sc(=O)c2c([nH]1)ncnn2</chem>	5.16	5.79	12.68	13.08	17.86	18.63	0.44	0.40
S1297	<chem>O=c1oc2ccnn2c(=O)[nH]1</chem>	2.96	3.19	9.24	8.69	14.80	15.64	0.52	0.48
S1299	<chem>O=c1sc2cn[nH]c2c(=O)[nH]1</chem>	2.02	1.75	5.69	7.90	10.44	12.76	0.49	0.54
S1300	<chem>O=c1[nH]c(=O)c2c(s1)[nH]nc2</chem>	1.86	1.75	8.81	7.89	14.05	14.50	0.48	0.48
S1312	<chem>O=c1oc(=O)c2c(o1)[nH]nc2</chem>	4.19	4.04	10.93	10.68	15.80	17.29	0.79	0.80
S13256	<chem>O=c1ncc2n1cc[nH]c2</chem>	-1.04	-1.01	12.55	9.77	29.57	23.32	0.56	0.52
S13259	<chem>O=c1cnc2n1cc[nH]c2</chem>	-1.49	-1.01	10.99	7.18	24.30	17.02	0.42	0.42
S1335	<chem>[nH]1cc2c(c1)cno2</chem>	-3.42	-3.14	7.12	5.91	18.63	16.05	0.50	0.51
S1336	<chem>o1cc2c(c1)cno2</chem>	-1.33	-1.54	3.87	3.76	11.21	11.26	0.50	0.49
S13367	<chem>O=c1ccc2n1ccoc2</chem>	-1.39	-1.24	5.13	5.26	16.33	14.97	0.45	0.43
S1337	<chem>s1cc2c(c1)cno2</chem>	-1.84	-2.23	3.64	3.08	11.45	10.81	0.65	0.65
S1338	<chem>n1cc2c(o1)n[nH]c2</chem>	-1.40	-1.31	7.84	6.93	17.38	15.41	0.63	0.73
S1339	<chem>n1cc2c(o1)c[nH]n2</chem>	-1.66	-1.31	7.10	6.26	15.37	14.76	0.47	0.45
S1340	<chem>n1cc2c(o1)onc2</chem>	1.22	0.29	6.59	5.20	10.71	10.83	0.43	0.44
S1342	<chem>n1cc2c(o1)noc2</chem>	1.02	0.29	8.21	5.73	14.85	11.96	0.55	0.51
S1344	<chem>n1oc2c(c1)cns2</chem>	0.27	-0.40	5.18	4.38	9.84	10.06	0.59	0.59
S1346	<chem>n1cc2c(o1)nsc2</chem>	0.17	-0.40	7.28	4.99	14.13	11.35	0.59	0.59
S1348	<chem>c1nc2c([nH]1)onc2</chem>	-1.18	-1.31	9.04	7.14	17.03	16.55	0.49	0.62
S1349	<chem>c1nc2c([nH]1)cno2</chem>	-1.00	-1.31	10.51	8.56	20.43	17.72	0.47	0.44
S1350	<chem>c1nc2c(o1)onc2</chem>	0.75	0.29	5.16	4.75	10.77	10.91	0.46	0.49
S13507	<chem>O=c1cc[nH]c2c1c[nH]c2</chem>	-4.56	-3.59	6.47	8.49	23.26	22.78	0.76	0.71

S1351	<chem>c1oc2c(n1)onc2</chem>	0.76	0.29	5.83	5.16	12.35	11.45	0.64	0.63
S13510	<chem>O=c1cc[nH]c2c1coc2</chem>	-2.33	-1.99	8.96	7.49	22.18	19.49	0.61	0.59
S13513	<chem>O=c1cc[nH]c2c1csc2</chem>	-2.80	-2.68	8.65	6.74	22.12	18.86	0.36	0.37
S13516	<chem>O=c1cc[nH]c2c1n[nH]c2</chem>	-2.93	-1.76	9.54	11.43	27.11	26.96	0.41	0.35
S13517	<chem>O=c1cc[nH]c2c1c[nH]n2</chem>	-2.82	-1.76	5.73	7.36	19.26	18.14	0.35	0.33
S1352	<chem>c1nc2c(s1)onc2</chem>	-0.17	-0.40	4.71	4.09	10.91	10.57	0.39	0.37
S13521	<chem>O=c1cc[nH]c2c1con2</chem>	-0.25	-0.16	8.58	7.32	18.01	16.19	0.44	0.43
S13526	<chem>O=c1ccn2c(c1)nc[nH]2</chem>	-0.86	-1.01	16.08	11.49	34.21	24.95	0.46	0.51
S1353	<chem>c1nc2c(s1)cno2</chem>	0.00	-0.40	5.00	4.57	12.16	11.18	0.63	0.61
S13534	<chem>O=c1cc[nH]c2c1n[nH]n2</chem>	-1.14	0.07	8.68	9.28	22.65	20.07	0.62	0.65
S1354	<chem>n1cc2c(o1)[nH]nn2</chem>	0.87	0.52	8.12	7.92	13.95	15.93	0.52	0.49
S13540	<chem>O=c1cc[nH]c2c1non2</chem>	1.76	1.67	12.38	10.19	22.37	19.46	0.42	0.41
S13541	<chem>O=c1cc[nH]c2c1nsn2</chem>	0.39	0.98	10.11	9.32	22.27	18.50	0.51	0.49
S13547	<chem>O=c1ccn2c(c1)cccc2</chem>	-1.16	-2.46	7.86	5.40	23.89	16.86	0.49	0.45
S13548	<chem>O=c1ccn2c(c1)cncc2</chem>	0.78	-0.63	9.66	7.17	22.64	17.24	0.82	0.79
S13549	<chem>O=c1ccn2c(c1)ccnc2</chem>	0.67	-0.63	8.65	6.67	21.45	16.14	0.40	0.36
S1355	<chem>n1oc2c(c1)[nH]nn2</chem>	1.08	0.52	10.66	9.34	17.91	17.10	0.44	0.48
S13558	<chem>O=c1ccn2c(c1)[nH]c(=O)cc2</chem>	2.06	0.14	11.43	8.30	22.95	18.87	0.30	0.31
S13559	<chem>O=c1[nH]cc2c(c1)c(=O)cc[nH]2</chem>	-0.33	-0.61	13.28	12.04	25.61	27.18	0.34	0.31
S1356	<chem>[nH]1nc2c(n1)cno2</chem>	0.34	0.52	6.34	6.25	12.13	11.87	0.57	0.54
S13560	<chem>O=c1[nH]cc2c(c1)[nH]ccc2=O</chem>	-0.04	-0.61	9.62	8.50	19.00	19.61	0.43	0.41
S13562	<chem>O=c1ccn2c(c1)ccoc2=O</chem>	2.07	1.74	8.91	8.55	19.40	17.62	0.54	0.57
S13568	<chem>O=c1ccn2c(c1)ccsc2=O</chem>	1.42	1.05	8.25	7.72	19.04	16.78	0.52	0.53
S13570	<chem>O=c1ccn2c(c1)sc(=O)cc2</chem>	2.34	1.05	12.44	9.11	22.61	18.91	0.45	0.46
S13579	<chem>O=c1[nH]nc2c(c1)c(=O)cc[nH]2</chem>	1.08	1.22	10.95	9.74	20.81	19.91	0.42	0.44
S13580	<chem>O=c1[nH]nc2c(c1)[nH]ccc2=O</chem>	1.26	1.22	12.41	10.44	22.58	21.53	0.45	0.46
S1361	<chem>O=c1c(=O)c2c(c1=O)onc2</chem>	6.73	7.14	14.45	11.40	17.22	18.46	0.52	0.55
S1362	<chem>o1nc2c(n1)cno2</chem>	3.04	2.12	8.15	6.01	11.01	9.76	0.65	0.63
S13624	<chem>O=c1cc[nH]c2c1nccn2</chem>	-0.59	0.45	8.49	8.97	22.52	19.35	0.52	0.52
S13626	<chem>O=c1cc[nH]c2c1nncn2</chem>	1.59	2.28	12.04	11.81	24.42	22.71	0.60	0.59
S13627	<chem>O=c1cc[nH]c2c1ncnn2</chem>	1.62	2.28	10.81	10.22	21.28	19.26	0.47	0.43

S1363	<chem>s1nc2c(n1)cno2</chem>	1.91	1.43	4.84	5.21	8.26	8.98	0.32	0.34
S13630	<chem>O=c1cc[nH]c2c1c(=O)[nH]cn2</chem>	-0.81	1.22	9.20	10.74	26.44	22.99	0.43	0.45
S13631	<chem>O=c1cc[nH]c2c1nc[nH]c2=O</chem>	0.27	1.22	8.98	12.10	23.15	22.03	0.40	0.42
S13635	<chem>O=c1cnc2c(o1)[nH]ccc2=O</chem>	2.26	2.82	13.03	11.94	24.93	23.28	0.52	0.51
S13689	<chem>O=c1ccn2c(c1)scce2=O</chem>	1.33	1.05	9.39	7.37	21.01	16.59	0.30	0.30
S1369	<chem>c1ccc2c(c1)onc2</chem>	-2.18	-2.76	2.62	3.33	10.74	11.82	0.47	0.48
S1370	<chem>c1ncc2c(c1)onc2</chem>	-0.23	-0.93	4.13	4.21	9.18	11.10	0.34	0.34
S1371	<chem>c1ncc2c(c1)cno2</chem>	-0.23	-0.93	5.05	4.47	10.02	11.35	0.47	0.38
S1372	<chem>c1cnc2c(c1)cno2</chem>	-0.39	-0.93	6.14	5.37	14.13	12.89	0.38	0.41
S1373	<chem>c1cnc2c(c1)onc2</chem>	-0.65	-0.93	4.44	4.65	10.78	12.18	0.49	0.45
S1375	<chem>c1nnc2c(c1)cno2</chem>	1.70	0.90	9.27	7.54	17.02	14.66	0.55	0.53
S1376	<chem>n1ncc2c(c1)onc2</chem>	1.91	0.90	7.65	6.38	14.49	12.88	0.65	0.71
S13769	<chem>O=c1[n]nc2n1ccsc2</chem>	2.08	1.73	7.58	8.79	17.26	17.16	0.33	0.31
S1377	<chem>O=c1[nH]ccc2c1cno2</chem>	0.14	-0.16	8.92	7.34	16.29	16.10	0.62	0.59
S1380	<chem>O=c1ccc2c([nH]1)cno2</chem>	1.12	-0.16	6.91	6.37	14.65	13.73	0.51	0.47
S1384	<chem>O=c1occc2c1onc2</chem>	1.76	1.44	8.29	7.81	17.00	15.54	0.43	0.41
S1395	<chem>c1ncc2c(n1)cno2</chem>	1.32	0.90	3.75	5.21	6.77	10.42	0.51	0.47
S1396	<chem>c1ncc2c(n1)onc2</chem>	1.58	0.90	7.22	5.66	11.87	10.86	0.67	0.65
S1398	<chem>n1nnc2c(c1)cno2</chem>	3.77	2.73	11.45	8.85	18.02	14.89	0.57	0.48
S1399	<chem>O=c1[nH]ncc2c1cno2</chem>	1.97	1.67	5.57	6.69	11.08	12.04	0.48	0.51
S1400	<chem>O=c1[nH]ncc2c1onc2</chem>	2.03	1.67	8.11	6.93	16.11	12.57	0.46	0.42
S1403	<chem>O=c1ncc2c([nH]1)cno2</chem>	2.96	1.67	10.27	9.29	19.97	17.43	0.34	0.35
S142	<chem>O=c1cnscl</chem>	2.43	2.32	7.68	6.24	15.82	13.64	0.36	0.33
S1428	<chem>O=c1[nH]c(=O)c2c([nH]1)cno2</chem>	3.45	2.44	11.42	9.42	17.73	15.43	0.29	0.29
S1439	<chem>O=c1cc[nH]c2c1cno2</chem>	0.08	-0.16	11.33	8.56	21.92	19.65	0.57	0.55
S14395	<chem>O=c1ccn2c(n1)[nH]cc2</chem>	-0.83	-1.01	9.12	8.22	27.27	21.28	0.57	0.56
S14397	<chem>O=c1nc[nH]c2c1c[nH]c2</chem>	-2.62	-1.76	8.62	12.49	26.31	28.53	0.40	0.37
S14400	<chem>O=c1ccn2c(n1)occ2</chem>	0.92	0.59	11.90	9.82	28.02	21.35	0.57	0.64
S14402	<chem>O=c1nc[nH]c2c1coc2</chem>	-0.44	-0.16	11.13	10.68	25.22	24.10	0.50	0.51
S14407	<chem>O=c1nc[nH]c2c1csc2</chem>	-0.93	-0.85	10.77	9.98	25.16	23.61	0.50	0.50
S1441	<chem>O=c1nc[nH]c2c1cno2</chem>	1.92	1.67	13.54	11.22	24.77	23.10	0.53	0.55

S14410	<chem>O=c1ccn2c(n1)[nH]nc2</chem>	1.23	0.82	11.41	9.01	26.39	19.82	0.45	0.43
S14412	<chem>O=c1nc[nH]c2c1n[nH]c2</chem>	-1.00	0.07	11.78	15.59	29.33	33.06	0.39	0.38
S14413	<chem>O=c1nc[nH]c2c1c[nH]n2</chem>	-0.91	0.07	7.92	10.86	22.49	22.77	0.58	0.61
S14419	<chem>O=c1nc[nH]c2c1con2</chem>	1.62	1.67	10.77	10.00	21.20	19.68	0.53	0.52
S1442	<chem>c1cnc2c(n1)onc2</chem>	1.12	0.90	5.20	5.67	10.47	11.00	0.69	0.62
S14422	<chem>O=c1ccn2c(n1)snc2</chem>	2.42	1.73	13.08	10.59	25.81	20.02	0.46	0.45
S14426	<chem>O=c1ccn2c(n1)nc[nH]2</chem>	0.87	0.82	18.19	16.43	37.10	32.79	0.37	0.42
S14436	<chem>O=c1ccn2c(n1)scn2</chem>	1.38	1.73	9.64	8.61	23.59	17.20	0.62	0.64
S14442	<chem>O=c1nc[nH]c2c1n[nH]n2</chem>	0.77	1.90	10.84	12.93	24.91	25.05	0.63	0.63
S1445	<chem>O=c1[nH]cnc2c1onc2</chem>	1.69	1.67	10.15	8.70	17.12	15.11	0.42	0.47
S14453	<chem>O=c1nc[nH]c2c1non2</chem>	3.60	3.50	14.70	13.03	24.43	23.30	0.54	0.61
S14454	<chem>O=c1nc[nH]c2c1nsn2</chem>	2.29	2.81	12.23	12.21	24.41	22.48	0.38	0.38
S1446	<chem>O=c1[nH]cnc2c1cno2</chem>	1.87	1.67	10.92	8.92	17.29	15.03	0.41	0.46
S14465	<chem>O=c1ccn2c(n1)cccc2</chem>	0.07	-0.63	10.10	8.41	27.00	21.03	0.59	0.62
S14469	<chem>O=c1ccn2c(n1)ccnc2</chem>	1.93	1.20	11.33	9.35	25.05	19.57	0.63	0.62
S14471	<chem>O=c1ccn2c(n1)cccn2</chem>	0.92	1.20	9.61	8.43	25.00	18.33	0.70	0.67
S14473	<chem>O=c1ccn2c(n1)nccc2</chem>	1.51	1.20	13.39	11.87	30.30	25.74	0.71	0.65
S1448	<chem>O=c1cnc2c(o1)cno2</chem>	3.91	3.27	9.08	7.61	12.23	12.04	0.57	0.55
S14481	<chem>O=c1ccn2c(n1)c(=O)[nH]cc2</chem>	1.52	1.97	11.98	13.35	28.40	29.88	0.29	0.30
S14482	<chem>O=c1ncn2c(c1)c(=O)[nH]cc2</chem>	2.29	1.97	12.66	12.78	27.46	26.94	0.38	0.38
S14483	<chem>O=c1ccn2c(n1)cc[nH]c2=O</chem>	1.63	1.97	12.90	10.93	27.30	21.60	0.45	0.45
S14487	<chem>O=c1ccn2c(n1)[nH]c(=O)cc2</chem>	3.20	1.97	13.79	10.45	25.98	22.22	0.50	0.47
S14488	<chem>O=c1ncn2c(c1)[nH]c(=O)cc2</chem>	3.90	1.97	13.10	11.07	25.48	21.88	0.35	0.36
S14493	<chem>O=c1ccn2c(n1)ccoc2=O</chem>	3.30	3.57	10.91	10.59	22.21	19.31	0.35	0.36
S1450	<chem>O=c1ocnc2c1cno2</chem>	3.45	3.27	8.76	7.61	12.32	12.20	0.52	0.53
S14507	<chem>O=c1ccn2c(n1)sc(=O)cc2</chem>	3.53	2.88	14.76	12.89	26.14	24.39	0.56	0.53
S14511	<chem>O=c1ccn2c(n1)ncnc2</chem>	3.46	3.03	14.75	12.22	28.26	22.99	0.55	0.44
S14519	<chem>O=c1ccn2c(n1)c(=O)[nH]nc2</chem>	3.44	3.80	14.16	12.50	27.01	24.83	0.52	0.45
S14521	<chem>O=c1ccn2c(n1)cn[nH]c2=O</chem>	3.60	3.80	11.32	11.29	22.33	19.23	0.48	0.50
S14529	<chem>O=c1[nH]cc2c(n1)[nH]cnc2=O</chem>	3.07	3.05	10.05	12.56	18.14	22.95	0.43	0.43
S1454	<chem>O=c1scnc2c1cno2</chem>	2.57	2.58	7.43	6.88	11.66	11.52	0.75	0.84

S14565	<chem>O=c1ccn2c(n1)[nH]c(=O)[nH]c2=O</chem>	5.04	4.57	14.00	11.52	23.88	19.44	0.39	0.34
S14585	<chem>O=c1ccn2c(n1)[nH]ccc2=O</chem>	1.89	1.97	12.28	10.62	25.34	21.69	0.53	0.51
S14595	<chem>O=c1nc[nH]c2c1nccn2</chem>	1.36	2.28	10.50	12.41	24.55	24.27	0.53	0.53
S14598	<chem>O=c1nc[nH]c2c1nnccn2</chem>	3.49	4.11	14.24	14.97	26.17	26.99	0.44	0.44
S14599	<chem>O=c1nc[nH]c2c1nccnn2</chem>	3.55	4.11	12.91	13.10	23.29	22.93	0.40	0.42
S14604	<chem>O=c1nc[nH]c2c1c(=O)[nH]cn2</chem>	1.15	3.05	11.75	14.55	28.68	28.75	0.45	0.38
S14605	<chem>O=c1nc[nH]c2c1nc[nH]c2=O</chem>	2.30	3.05	11.46	16.15	25.78	27.63	0.50	0.54
S14611	<chem>O=c1cnc2c(o1)[nH]cnc2=O</chem>	4.15	4.65	15.34	14.98	27.40	27.07	0.59	0.63
S1462	<chem>O=c1[nH]nnc2c1cno2</chem>	3.70	3.50	8.38	9.29	10.66	13.23	0.49	0.51
S1463	<chem>O=c1[nH]nnc2c1onc2</chem>	3.52	3.50	7.92	8.81	12.36	13.05	0.41	0.41
S14647	<chem>O=c1ccn2c(n1)nn[nH]c2=O</chem>	4.98	5.63	14.33	15.31	25.28	24.07	0.62	0.60
S14675	<chem>O=c1ccn2c(n1)occc2=O</chem>	3.22	3.57	10.87	10.70	23.06	19.29	0.44	0.42
S1468	<chem>O=c1sn[n]c2c1cno2</chem>	4.45	4.41	9.41	8.70	10.53	11.61	0.44	0.45
S14689	<chem>O=c1ccn2c(n1)scce2=O</chem>	2.53	2.88	9.98	9.88	22.10	18.55	0.60	0.58
S14693	<chem>O=c1ccn2c(n1)[nH]ncc2=O</chem>	3.68	3.80	11.47	10.98	22.39	19.33	0.52	0.52
S14705	<chem>O=c1ccn2c(n1)sncc2=O</chem>	4.35	4.71	12.64	11.69	22.74	18.08	0.42	0.40
S14717	<chem>O=c1ccn2c(n1)[nH]nnc2=O</chem>	5.49	5.63	14.09	14.72	21.99	24.28	0.32	0.34
S1472	<chem>O=c1ccoc2c1onc2</chem>	1.53	1.44	8.01	7.00	17.22	14.59	0.62	0.64
S1479	<chem>O=c1cn[nH]c2c1cno2</chem>	1.90	1.67	8.93	7.91	16.22	15.59	0.51	0.54
S14797	<chem>O=c1ccc2n1cns2</chem>	0.13	-0.10	6.84	6.88	14.79	16.08	0.40	0.39
S1487	<chem>O=c1nn[nH]c2c1cno2</chem>	3.62	3.50	11.69	11.60	19.95	21.29	0.47	0.51
S15162	<chem>O=c1ncn2c(n1)scc2</chem>	2.31	1.73	12.74	11.17	28.33	23.11	0.37	0.40
S15188	<chem>O=c1ncn2c(n1)cncc2</chem>	3.98	3.03	14.13	12.42	27.86	23.88	0.47	0.48
S15191	<chem>O=c1ncn2c(n1)nccc2</chem>	3.51	3.03	15.49	13.96	31.75	27.87	0.41	0.38
S15195	<chem>O=c1[nH]ccn2c1nc(=O)nc2</chem>	3.53	3.80	14.28	16.04	29.81	32.68	0.60	0.50
S15198	<chem>O=c1ncn2c(n1)[nH]c(=O)cc2</chem>	5.11	3.80	15.89	12.63	28.32	23.94	0.48	0.47
S15207	<chem>O=c1ncn2c(n1)ncnc2</chem>	5.38	4.86	17.47	14.01	30.44	24.47	0.43	0.41
S15271	<chem>O=c1ncn2c(n1)scce2=O</chem>	4.54	4.71	12.66	12.63	25.23	22.55	0.62	0.61
S15307	<chem>O=c1ccc2n1cnsn2</chem>	1.61	1.73	6.09	7.65	10.59	13.59	0.61	0.61
S15384	<chem>c1cnc2c(n1)c[nH]c2</chem>	-3.72	-2.53	6.54	4.68	14.50	13.27	0.45	0.55
S15386	<chem>c1cnc2c(n1)csc2</chem>	-2.18	-1.62	1.60	2.93	6.39	9.35	0.83	0.82

S15387	<chem>c1cnc2c(n1)n[nH]c2</chem>	-1.83	-0.70	6.58	5.91	15.64	13.53	0.40	0.39
S15390	<chem>c1cnc2c(n1)n[nH]n2</chem>	0.11	1.13	5.32	6.12	10.01	11.54	0.45	0.44
S15391	<chem>c1cnc2c(n1)non2</chem>	2.98	2.73	10.02	7.03	14.28	10.92	0.72	0.73
S15392	<chem>c1cnc2c(n1)nsn2</chem>	1.54	2.04	5.87	6.15	9.37	9.96	0.52	0.47
S15402	<chem>c1cnc2c(n1)ncn2</chem>	0.35	1.51	4.07	5.94	9.17	11.03	0.44	0.48
S15404	<chem>O=c1[nH]cnc2c1nccn2</chem>	0.74	2.28	8.39	8.38	16.70	14.36	0.47	0.49
S15406	<chem>O=c1ocnc2c1nccn2</chem>	2.49	3.88	6.36	8.25	13.37	12.95	0.39	0.38
S15408	<chem>O=c1scnc2c1nccn2</chem>	1.39	3.19	5.26	7.45	12.21	12.09	0.54	0.53
S15441	<chem>c1nnc2c(n1)c[nH]c2</chem>	-1.58	-0.70	10.16	7.33	20.24	15.80	0.62	0.60
S15443	<chem>c1nnc2c(n1)csc2</chem>	-0.13	0.21	4.10	4.82	10.94	10.89	0.51	0.47
S15444	<chem>c1nnc2c(n1)c[nH]n2</chem>	0.30	1.13	10.31	8.72	19.31	16.41	0.57	0.56
S15445	<chem>c1nnc2c(n1)n[nH]c2</chem>	0.28	1.13	10.41	8.05	17.22	14.94	0.36	0.35
S15450	<chem>c1nnc2c(n1)n[nH]n2</chem>	2.16	2.96	9.11	8.42	14.15	13.29	0.90	0.87
S15473	<chem>O=c1[nH]cnc2c1nncn2</chem>	2.95	4.11	12.31	10.84	19.24	16.91	0.52	0.48
S15474	<chem>O=c1[nH]cnc2c1ncnn2</chem>	3.07	4.11	11.95	11.08	18.00	16.74	0.49	0.50
S15481	<chem>O=c1scnc2c1nncn2</chem>	3.56	5.02	8.92	9.49	14.56	14.09	0.44	0.42
S15482	<chem>O=c1scnc2c1ncnn2</chem>	3.67	5.02	8.95	9.35	13.03	13.42	0.48	0.51
S15520	<chem>O=c1ccc(=O)n2n1cnc2</chem>	2.35	2.72	7.22	8.53	11.35	15.55	0.37	0.36
S15602	<chem>O=c1ccnc2n1cc[nH]2</chem>	-1.59	-1.01	8.53	6.06	19.79	15.42	0.52	0.51
S15603	<chem>O=c1[nH]cnc2c1c[nH]c2</chem>	-3.07	-1.76	6.41	6.46	16.53	15.61	0.62	0.63
S15605	<chem>O=c1ccnc2n1cco2</chem>	0.31	0.59	6.65	6.14	14.33	12.77	0.51	0.50
S15606	<chem>O=c1[nH]cnc2c1coc2</chem>	-0.80	-0.16	5.91	6.37	12.75	13.22	0.60	0.54
S15609	<chem>O=c1[nH]cnc2c1csc2</chem>	-1.50	-0.85	5.60	5.56	12.86	12.48	0.50	0.56
S15611	<chem>O=c1ccnc2n1cn[nH]2</chem>	0.62	0.82	6.33	7.45	14.14	15.61	0.39	0.44
S15612	<chem>O=c1[nH]cnc2c1n[nH]c2</chem>	-1.42	0.07	6.13	7.62	17.50	16.54	0.47	0.47
S15613	<chem>O=c1[nH]cnc2c1c[nH]n2</chem>	-1.06	0.07	6.19	8.19	14.59	16.08	0.57	0.56
S15616	<chem>O=c1[nH]cnc2c1noc2</chem>	1.17	1.67	9.10	8.48	17.39	15.48	0.81	0.87
S15617	<chem>O=c1[nH]cnc2c1con2</chem>	1.56	1.67	9.40	9.05	17.27	15.02	0.39	0.34
S15619	<chem>O=c1ccnc2n1cns2</chem>	1.72	1.73	6.07	7.60	11.27	13.43	0.49	0.47
S15622	<chem>O=c1ccnc2n1[nH]cn2</chem>	0.63	0.82	10.85	10.19	18.34	18.05	0.52	0.58
S15627	<chem>O=c1ccnc2n1ncs2</chem>	0.59	1.73	7.72	6.77	18.04	13.84	0.45	0.43

S15630	<chem>O=c1[nH]cnc2c1n[nH]n2</chem>	0.66	1.90	7.77	8.33	15.56	14.77	0.47	0.46
S15636	<chem>O=c1[nH]cnc2c1non2</chem>	3.58	3.50	12.92	10.14	17.53	15.04	0.46	0.44
S15637	<chem>O=c1[nH]cnc2c1nsn2</chem>	2.05	2.81	9.90	9.21	16.33	13.98	0.56	0.53
S15643	<chem>O=c1ccnc2n1cccc2</chem>	-0.94	-0.63	5.41	5.13	14.05	12.95	0.53	0.48
S15644	<chem>O=c1ccnc2n1ccnc2</chem>	1.10	1.20	4.93	7.24	10.83	14.04	0.50	0.52
S15645	<chem>O=c1ccnc2n1cncc2</chem>	1.01	1.20	4.81	7.11	11.21	14.40	0.53	0.51
S15646	<chem>O=c1ccnc2n1nccc2</chem>	-0.09	1.20	8.01	6.78	19.70	14.82	0.43	0.41
S15647	<chem>O=c1ccnc2n1cccn2</chem>	0.60	1.20	7.22	7.34	14.16	14.14	0.47	0.44
S15651	<chem>O=c1ccnc2n1cc[nH]c2=O</chem>	0.84	1.97	9.04	8.75	17.46	16.97	0.36	0.39
S15652	<chem>O=c1ccnc2n1c(=O)[nH]cc2</chem>	0.07	1.97	10.16	8.28	22.69	17.63	0.36	0.38
S15654	<chem>O=c1ccn2c([nH]1)nccc2=O</chem>	2.32	1.97	7.36	8.52	12.57	16.73	0.57	0.56
S15666	<chem>O=c1ccn2c(s1)nccc2=O</chem>	2.55	2.88	7.50	9.18	12.45	15.93	0.44	0.45
S15669	<chem>O=c1ccnc2n1cncn2</chem>	2.63	3.03	8.16	8.72	12.04	14.30	0.59	0.63
S15673	<chem>O=c1ccnc2n1cn[nH]c2=O</chem>	2.87	3.80	8.55	8.93	15.25	14.83	0.50	0.48
S15675	<chem>O=c1[nH]nc2c(c1)c(=O)[nH]cn2</chem>	2.40	3.05	10.99	9.17	19.36	15.48	0.59	0.58
S15676	<chem>O=c1[nH]nc2c(c1)nc[nH]c2=O</chem>	2.14	3.05	11.00	9.06	19.34	15.55	0.68	0.67
S15679	<chem>O=c1[nH]cc2c(n1)nc[nH]c2=O</chem>	2.45	3.05	10.56	13.25	22.93	22.87	0.68	0.69
S15702	<chem>O=c1[nH]c2nccc(=O)n2c(=O)[nH]1</chem>	3.56	4.57	10.96	10.22	19.29	18.07	0.55	0.71
S15712	<chem>O=c1ccnc2n1c(=O)cc[nH]2</chem>	0.17	1.97	11.24	10.53	25.07	22.80	0.40	0.35
S15718	<chem>O=c1ccnc2n1ncnn2</chem>	3.45	4.86	9.45	10.50	15.47	15.81	0.45	0.49
S15719	<chem>O=c1[nH]cnc2c1c(=O)[nH]cn2</chem>	0.64	3.05	8.03	10.38	19.72	17.17	0.53	0.49
S15720	<chem>O=c1[nH]cnc2c1nc[nH]c2=O</chem>	1.02	3.05	7.81	10.18	16.23	17.12	0.41	0.39
S15724	<chem>O=c1cnc2c(o1)nc[nH]c2=O</chem>	3.43	4.65	12.70	11.23	18.93	17.55	0.50	0.49
S15850	<chem>O=c1cnc2c(o1)coc2</chem>	1.28	1.44	3.93	6.01	10.25	12.42	0.53	0.45
S15851	<chem>O=c1cnc2c(o1)csc2</chem>	0.67	0.75	3.33	5.32	10.21	11.99	0.45	0.51
S15861	<chem>O=c1[nH]cc2c(c1)oc(=O)cn2</chem>	2.98	2.82	10.18	8.88	17.22	15.31	0.68	0.66
S15862	<chem>O=c1[nH]cc2c(c1)ncc(=O)o2</chem>	3.15	2.82	9.13	9.19	16.83	16.34	0.52	0.51
S15869	<chem>O=c1[nH]cc2c(n1)ncc(=O)o2</chem>	4.61	4.65	12.72	13.07	22.52	22.36	0.52	0.51
S15870	<chem>O=c1[nH]cc2c(n1)oc(=O)cn2</chem>	4.37	4.65	13.41	12.39	22.23	20.07	0.62	0.61
S1596	<chem>[nH]1cc2c(c1)cns2</chem>	-4.17	-3.83	7.31	5.07	18.97	15.21	0.41	0.41
S1597	<chem>o1cc2c(c1)cns2</chem>	-2.10	-2.23	3.33	2.96	10.49	10.48	0.37	0.34

S1598	s1cc2c(c1)cns2	-2.50	-2.92	3.01	2.28	10.62	10.02	0.33	0.34
S1599	n1cc2c(s1)n[nH]c2	-2.40	-2.00	7.44	6.00	16.18	14.34	0.58	0.47
S16	c1cnsn1	-0.44	-0.66	3.50	3.30	6.81	9.51	0.47	0.46
S1600	n1cc2c(s1)c[nH]n2	-2.51	-2.00	7.15	5.50	15.59	14.13	0.58	0.58
S1603	n1cc2c(s1)snc2	-0.42	-1.09	3.61	3.57	7.40	9.32	0.52	0.57
S1604	n1cc2c(s1)cns2	-0.43	-1.09	2.85	3.42	6.58	9.30	0.35	0.38
S1605	n1cc2c(s1)nsc2	-0.78	-1.09	6.31	4.10	11.85	10.33	0.32	0.33
S1607	c1nc2c([nH]1)snc2	-2.05	-2.00	9.14	6.51	17.39	16.15	0.56	0.57
S1608	c1nc2c([nH]1)cns2	-1.91	-2.00	9.57	7.57	17.95	16.53	0.69	0.60
S1609	c1nc2c(o1)snc2	-0.30	-0.40	4.55	3.99	9.71	10.29	0.64	0.57
S161	O=c1occoc1=O	3.25	3.55	8.74	9.72	15.44	21.61	0.69	0.65
S1610	c1oc2c(n1)snc2	-0.23	-0.40	4.87	4.29	10.13	10.46	0.48	0.44
S1611	c1nc2c(s1)snc2	-0.99	-1.09	4.04	3.34	9.74	9.97	0.43	0.45
S1612	c1sc2c(n1)snc2	-0.90	-1.09	4.18	3.69	9.92	10.17	0.59	0.63
S1613	n1cc2c(s1)[nH]nn2	0.01	-0.17	8.54	7.31	15.17	15.60	0.41	0.40
S1614	n1sc2c(c1)[nH]nn2	0.14	-0.17	9.36	8.37	16.41	15.97	0.48	0.49
S1615	[nH]1nc2c(n1)cns2	-0.73	-0.17	6.06	5.41	11.31	11.01	0.67	0.68
S1628	c1ccc2c(c1)snc2	-2.73	-3.45	1.83	2.52	9.45	11.03	0.48	0.45
S1629	c1ncc2c(c1)snc2	-0.80	-1.62	3.02	3.45	7.46	10.44	0.49	0.46
S1630	c1ncc2c(c1)cns2	-0.82	-1.62	3.87	3.65	8.48	10.52	0.63	0.60
S1631	c1cnc2c(c1)cns2	-1.23	-1.62	4.99	4.45	11.36	11.81	0.37	0.34
S1632	c1cnc2c(c1)snc2	-1.33	-1.62	4.39	3.91	10.71	11.58	0.50	0.57
S16332	O=c1ncnc2n1[nH]cc2	0.78	0.82	11.46	8.96	22.47	17.55	0.52	0.47
S16338	O=c1ncnc2n1[nH]nc2	2.74	2.65	9.13	9.81	17.13	16.57	0.51	0.59
S16344	O=c1ncnc2n1[nH]cn2	2.66	2.65	14.17	11.93	22.39	19.52	0.52	0.51
S1635	n1ncc2c(c1)snc2	1.32	0.21	5.75	5.60	13.27	12.17	0.45	0.48
S1636	O=c1[nH]ccc2c1cns2	-0.64	-0.85	8.24	6.55	16.55	15.48	0.50	0.47
S16518	s1cc2c(c1)nnnn2	2.04	2.04	7.78	7.74	16.08	14.67	0.64	0.60
S1654	c1ncc2c(n1)cns2	0.61	0.21	4.36	4.45	7.23	9.78	0.66	0.68
S1655	c1ncc2c(n1)snc2	0.72	0.21	5.57	4.80	8.60	9.92	0.62	0.60
S1658	O=c1[nH]ncc2c1cns2	1.21	0.98	5.84	5.89	12.47	11.38	0.44	0.42

S1659	O=c1[nH]ncc2c1snc2	1.28	0.98	6.30	6.07	13.29	11.55	0.47	0.49
S16626	O=c1[nH]nnc2c1c[nH]c2	-1.17	0.07	10.10	7.91	18.81	15.85	0.49	0.54
S16627	O=c1[nH]nnc2c1coc2	1.01	1.67	4.06	7.01	9.53	12.32	0.43	0.40
S16628	O=c1[nH]nnc2c1csc2	0.35	0.98	3.89	6.25	9.83	11.72	0.43	0.46
S16629	O=c1[nH]nnc2c1c[nH]n2	0.80	1.90	9.99	9.80	17.11	16.67	0.42	0.41
S16630	O=c1[nH]nnc2c1n[nH]c2	0.46	1.90	10.02	8.56	19.28	15.66	0.67	0.68
S16632	O=c1[nH]nnc2c1noc2	2.93	3.50	7.27	8.61	13.34	13.47	0.44	0.41
S16639	O=c1[nH]cc2c(c1)c(=O)[nH]nn2	2.59	3.05	10.26	9.21	16.91	15.73	0.45	0.47
S1687	O=c1[nH]c(=O)c2c([nH]1)cns2	2.71	1.75	9.53	8.48	14.79	14.31	0.38	0.40
S16920	O=c1nnc2c(o1)csc2	2.50	2.58	6.91	8.69	15.70	17.74	0.53	0.51
S1701	c1cnc2c(n1)snc2	0.15	0.21	4.75	4.83	9.35	10.12	0.53	0.53
S1702	c1nnc2c(n1)cns2	2.21	2.04	5.68	6.39	9.35	10.56	0.40	0.41
S1703	c1nnc2c(n1)snc2	2.22	2.04	5.52	6.19	8.97	10.48	0.52	0.53
S1704	O=c1[nH]cnc2c1snc2	0.79	0.98	9.31	7.86	15.19	14.16	0.42	0.43
S1705	O=c1[nH]cnc2c1cns2	0.83	0.98	9.93	8.03	15.54	14.13	0.47	0.48
S1707	O=c1cnc2c(o1)cns2	2.94	2.58	7.51	6.77	11.83	11.19	0.51	0.46
S1709	O=c1ocnc2c1cns2	2.43	2.58	7.29	6.79	12.09	11.43	0.35	0.37
S1713	O=c1scnc2c1cns2	1.57	1.89	6.43	6.06	10.83	10.73	0.37	0.38
S1721	O=c1[nH]nnc2c1cns2	2.64	2.81	6.62	8.39	10.03	12.28	0.42	0.46
S1722	O=c1[nH]nnc2c1snc2	2.64	2.81	6.42	8.02	10.16	12.23	0.60	0.58
S1727	O=c1sn[n]c2c1cns2	3.42	3.72	7.61	7.86	10.31	10.77	0.84	0.84
S17553	O=c1ccoc2c1c(=O)cco2	0.69	2.59	7.54	8.30	21.72	19.91	0.42	0.40
S17554	O=c1ccoc2c1occc2=O	1.63	2.59	5.56	7.34	12.31	13.60	0.77	0.77
S1772	c1cn2c(n1)cc[nH]2	-4.29	-3.99	8.44	6.90	23.17	18.90	0.48	0.41
S1773	c1[nH]n2c(c1)cnc2	-3.98	-3.99	8.17	6.26	22.24	17.91	0.66	0.58
S1774	c1nc2n(c1)cc[nH]2	-4.28	-3.99	4.31	4.14	16.81	15.14	0.35	0.37
S1775	c1cn2c([nH]1)cnc2	-3.94	-3.99	6.08	5.41	20.45	17.10	0.44	0.46
S1776	[nH]1cc2c(c1)nc[nH]2	-5.76	-4.74	3.48	6.92	17.31	19.73	0.40	0.40
S1777	c1cn2c(n1)cco2	-2.76	-2.39	4.55	4.23	15.28	13.50	0.50	0.50
S1778	c1on2c(c1)cnc2	-2.45	-2.39	4.96	4.45	15.84	13.72	0.37	0.40
S1781	o1cc2c(c1)nc[nH]2	-3.55	-3.14	6.66	5.97	16.42	16.33	0.61	0.56

S1784	c1nc2n(c1)ccs2	-2.98	-3.08	5.06	4.31	16.02	13.40	0.41	0.43
S1785	c1cn2c(s1)cnc2	-2.66	-3.08	5.08	3.98	15.75	13.26	0.56	0.61
S1786	s1cc2c(c1)nc[nH]2	-4.10	-3.83	6.56	5.21	16.57	15.71	0.69	0.63
S1787	c1cn2c(n1)cn[nH]2	-2.30	-2.16	8.00	8.05	18.57	18.56	0.53	0.49
S1788	n1cc2n(c1)[nH]nc2	-2.05	-2.16	7.35	6.98	17.30	16.63	0.55	0.49
S1789	c1cn2c(n1)[nH]nc2	-2.19	-2.16	4.06	5.29	12.91	14.80	0.42	0.44
S1790	n1cc2n(c1)cn[nH]2	-1.94	-2.16	4.68	6.12	15.04	15.82	0.51	0.53
S1791	c1nc2c([nH]1)n[nH]c2	-3.88	-2.91	3.76	6.03	13.70	15.95	0.86	0.83
S1792	c1nc2c([nH]1)c[nH]n2	-3.71	-2.91	6.70	9.64	20.91	22.65	0.55	0.52
S1797	c1nc2c([nH]1)noc2	-1.37	-1.31	7.68	6.02	15.38	13.89	0.56	0.60
S1798	c1nc2c([nH]1)con2	-1.16	-1.31	10.60	9.63	23.02	20.59	0.53	0.53
S18	O=c1occ[nH]1	-0.70	-1.03	6.95	6.17	17.98	16.13	0.56	0.58
S1801	c1cn2c(n1)snc2	-0.91	-1.25	6.61	6.35	14.23	14.23	0.57	0.62
S18017	O=c1cn[nH]c2c1c[nH]c2	-2.73	-1.76	8.75	8.91	22.13	20.77	0.43	0.48
S1802	n1cc2n(c1)cns2	-0.65	-1.25	6.59	5.59	13.72	13.16	0.51	0.47
S18020	O=c1cn[nH]c2c1coc2	-0.55	-0.16	7.19	7.10	16.86	16.35	0.49	0.52
S18023	O=c1cn[nH]c2c1csc2	-1.05	-0.85	6.81	6.41	16.92	15.86	0.46	0.55
S18026	O=c1cn[nH]c2c1n[nH]c2	-1.13	0.07	10.01	11.35	23.96	23.83	0.55	0.57
S18027	O=c1cn[nH]c2c1c[nH]n2	-0.95	0.07	8.43	7.95	18.58	16.48	0.37	0.34
S1803	c1nc2c([nH]1)nsc2	-2.28	-2.00	6.39	5.21	12.99	13.11	0.63	0.60
S18031	O=c1cn[nH]c2c1con2	1.56	1.67	5.26	7.09	11.16	13.39	0.59	0.56
S1804	c1nc2c([nH]1)csn2	-2.05	-2.00	9.41	8.82	21.63	19.81	0.58	0.52
S18044	O=c1cn[nH]c2c1n[nH]n2	0.68	1.90	7.52	9.36	17.87	17.29	0.47	0.49
S1805	c1nc2c([nH]1)[nH]cn2	-3.22	-2.91	9.30	13.54	24.82	28.05	0.67	0.68
S1806	c1nc2c([nH]1)nc[nH]2	-3.53	-2.91	3.23	5.89	11.34	16.08	0.63	0.59
S18069	O=c1[nH]cc2c(c1)c(=O)cn[nH]2	1.47	1.22	13.01	11.57	22.61	23.02	0.63	0.61
S1807	c1nc2n(c1)[nH]cn2	-2.29	-2.16	11.71	11.03	26.46	23.91	0.62	0.61
S18070	O=c1[nH]cc2c(c1)[nH]ncc2=O	1.70	1.22	7.00	8.64	14.44	16.75	0.60	0.59
S1808	c1[nH]n2c(n1)cnc2	-2.19	-2.16	11.43	9.25	23.58	20.43	0.37	0.36
S1809	c1cn2c(n1)[nH]cn2	-2.71	-2.16	7.67	5.80	17.36	15.37	0.60	0.56
S1810	c1nn2c([nH]1)cnc2	-2.40	-2.16	9.78	7.64	22.18	18.59	0.39	0.41

S1811	c1oc2c(n1)nc[nH]2	-1.45	-1.31	8.82	8.27	19.99	19.39	0.58	0.54
S1812	c1nc2c(o1)nc[nH]2	-1.50	-1.31	6.65	6.07	14.46	13.86	0.49	0.52
S1814	c1on2c(n1)cnc2	-0.69	-0.56	6.83	5.90	15.50	14.08	0.34	0.36
S1815	c1cn2c(n1)ocn2	-0.76	-0.56	5.86	5.30	14.03	12.40	0.39	0.42
S1816	c1nn2c(o1)cnc2	-0.67	-0.56	6.88	5.44	15.96	13.23	0.64	0.60
S1817	c1sc2c(n1)nc[nH]2	-2.34	-2.00	8.48	7.79	20.28	19.42	0.55	0.56
S1818	c1nc2c(s1)nc[nH]2	-2.44	-2.00	5.96	5.24	13.79	13.10	0.58	0.57
S1821	c1cn2c(n1)scn2	-1.69	-1.25	5.06	4.52	13.38	11.73	0.48	0.50
S1822	c1nn2c(s1)cnc2	-1.36	-1.25	5.82	4.76	15.09	12.86	0.42	0.46
S1823	c1nc2c([nH]1)[nH]nn2	-1.01	-1.08	12.28	15.12	25.69	28.88	0.45	0.43
S1824	c1[nH]c2c(n1)[nH]nn2	-1.31	-1.08	7.20	7.47	16.70	16.91	0.59	0.53
S1825	c1cn2c(n1)nn[nH]2	-0.24	-0.33	11.74	12.80	22.51	24.95	0.48	0.47
S1826	n1cn2c(c1)nn[nH]2	-0.25	-0.33	11.08	10.60	18.58	20.54	0.47	0.44
S1827	c1cn2c(n1)[nH]nn2	-0.68	-0.33	5.88	7.57	11.41	16.42	0.44	0.46
S1828	n1cn2c(c1)[nH]nn2	-0.49	-0.33	8.66	8.98	16.70	18.70	0.75	0.77
S1829	[nH]1nc2c(n1)nc[nH]2	-1.81	-1.08	7.39	7.72	17.22	16.63	0.38	0.42
S1831	c1nc2c([nH]1)nno2	0.85	0.52	11.24	8.60	18.81	16.03	0.61	0.51
S1834	c1cn2c(n1)onn2	1.49	1.27	5.23	8.03	10.13	14.79	0.53	0.48
S1835	n1cn2c(c1)onn2	1.44	1.27	5.33	7.74	9.86	14.69	0.71	0.70
S18354	O=c1[nH]cc2c(c1)c(=O)cns2	2.15	2.13	10.86	8.56	18.84	16.90	0.46	0.42
S1836	c1nc2c([nH]1)snn2	-0.15	-0.17	11.69	10.26	21.85	21.42	0.46	0.44
S1837	c1nc2c([nH]1)nns2	-0.23	-0.17	9.47	7.71	17.03	15.10	0.47	0.53
S1840	c1cn2c(n1)snn2	0.31	0.58	3.25	7.19	7.88	13.95	0.64	0.64
S1841	n1cn2c(c1)snn2	0.56	0.58	3.39	7.01	8.81	14.15	0.56	0.48
S18429	O=c1[nH]cc2c(n1)scnc2=O	3.54	3.96	10.81	11.14	18.21	18.90	0.49	0.48
S1845	o1nc2c(n1)nc[nH]2	1.05	0.52	12.13	8.67	20.47	15.90	0.40	0.43
S1846	s1nc2c(n1)nc[nH]2	-0.21	-0.17	9.59	7.79	17.69	14.95	0.45	0.53
S1847	O=c1[nH]c2c([nH]1)nc[nH]2	-1.64	-2.14	9.93	8.93	20.80	21.08	0.47	0.44
S18476	O=c1nn[nH]c2c1c[nH]c2	-0.81	0.07	11.25	13.94	26.54	28.77	0.58	0.61
S18479	O=c1nn[nH]c2c1coc2	1.28	1.67	9.93	11.32	21.34	23.21	0.59	0.58
S18482	O=c1nn[nH]c2c1csc2	0.81	0.98	9.51	10.67	21.46	22.86	0.45	0.41

S18485	O=c1nn[nH]c2c1n[nH]c2	0.78	1.90	12.67	16.53	27.24	32.17	0.69	0.70
S18486	O=c1nn[nH]c2c1c[nH]n2	0.92	1.90	10.93	12.47	22.95	23.36	0.37	0.34
S18490	O=c1nn[nH]c2c1con2	3.34	3.50	8.11	10.80	15.61	19.13	0.62	0.69
S1862	c1ccc2c(c1)[nH]cn2	-4.54	-4.36	6.44	5.22	16.99	16.64	0.38	0.34
S1863	c1ccc2n(c1)ccn2	-3.35	-3.61	3.94	3.93	15.12	14.18	0.50	0.53
S1864	c1ccc2n(c1)cnc2	-2.88	-3.61	3.60	3.93	14.38	14.18	0.60	0.62
S1865	c1ncc2c(c1)[nH]cn2	-2.47	-2.53	9.24	7.57	19.21	18.52	0.48	0.55
S1866	c1ncc2c(c1)nc[nH]2	-2.55	-2.53	8.76	6.16	17.24	15.90	0.56	0.51
S1867	c1cnc2c(c1)nc[nH]2	-3.02	-2.53	5.11	4.88	12.67	13.76	0.52	0.63
S1868	c1cnc2c(c1)[nH]cn2	-2.72	-2.53	8.82	8.77	22.36	20.97	0.41	0.37
S1869	n1ccn2c(c1)ncc2	-1.37	-1.78	6.08	6.18	13.96	15.81	0.51	0.46
S1870	n1ccn2c(c1)cnc2	-0.96	-1.78	5.47	5.49	12.55	14.28	0.54	0.53
S1871	c1ncn2c(c1)ncc2	-1.42	-1.78	4.78	5.31	12.60	14.07	0.55	0.58
S1872	c1ncn2c(c1)cnc2	-0.99	-1.78	4.40	5.29	11.86	14.01	0.56	0.61
S1873	c1cnn2c(c1)ncc2	-2.16	-1.78	3.86	4.32	12.39	12.53	0.38	0.42
S1874	c1cnn2c(c1)cnc2	-1.65	-1.78	4.79	5.08	14.35	14.19	0.67	0.65
S1875	c1ccn2c(n1)ncc2	-1.58	-1.78	7.35	6.90	20.30	17.56	0.34	0.38
S1876	c1ccn2c(n1)cnc2	-1.35	-1.78	7.02	5.82	16.66	15.19	0.48	0.53
S1877	c1nnc2c(c1)[nH]cn2	-0.52	-0.70	12.19	12.14	26.13	25.09	0.71	0.72
S1878	c1nnc2c(c1)nc[nH]2	-0.91	-0.70	7.94	6.84	17.29	15.27	0.37	0.38
S1879	n1ccn2c(n1)ncc2	0.46	0.05	9.98	10.17	20.71	21.44	0.41	0.43
S1880	n1ccn2c(n1)cnc2	0.59	0.05	9.22	8.40	16.21	17.55	0.49	0.52
S1882	c1nnn2c(c1)cnc2	0.18	0.05	6.14	7.46	12.29	16.28	0.36	0.37
S1883	n1ncc2c(c1)[nH]cn2	-0.29	-0.70	12.03	9.53	23.96	20.02	0.46	0.47
S1884	n1ncc2n(c1)ccn2	0.80	0.05	7.93	8.59	15.51	17.95	0.64	0.65
S1885	n1ncc2n(c1)cnc2	1.18	0.05	7.24	7.87	14.22	16.37	0.51	0.51
S1886	O=c1[nH]ccc2c1nc[nH]2	-2.36	-1.76	9.04	10.03	25.45	24.42	0.71	0.70
S1887	O=c1[nH]ccc2c1[nH]cn2	-2.11	-1.76	3.94	7.35	12.06	16.40	0.59	0.58
S1888	O=c1ccc2c([nH]1)[nH]cn2	-1.12	-1.76	11.59	10.18	22.52	21.06	0.39	0.41
S1889	O=c1ccc2c([nH]1)nc[nH]2	-1.32	-1.76	10.84	7.39	24.09	19.07	0.89	0.95
S1890	O=c1[nH]ccn2c1ncc2	-1.35	-1.01	7.96	8.22	21.97	20.83	0.51	0.51

S1891	<chem>O=c1[nH]ccn2c1cnc2</chem>	-0.83	-1.01	8.21	7.82	17.64	18.72	0.57	0.50
S1892	<chem>O=c1[nH]ccc2n1ccn2</chem>	-1.29	-1.01	7.82	6.36	15.97	15.15	0.64	0.63
S1893	<chem>O=c1[nH]ccc2n1cnc2</chem>	-0.83	-1.01	8.08	7.22	17.44	17.52	0.62	0.58
S1896	<chem>O=c1ccn2c([nH]1)ncc2</chem>	-0.06	-1.01	7.82	6.63	16.37	17.00	0.53	0.50
S1897	<chem>O=c1ccn2c([nH]1)cnc2</chem>	0.43	-1.01	7.60	7.07	14.95	16.73	0.34	0.37
S19238	<chem>O=c1oc2cocc2c(=O)[nH]1</chem>	2.27	2.21	5.67	7.04	11.57	12.35	0.55	0.54
S19239	<chem>O=c1oc2cscc2c(=O)[nH]1</chem>	1.63	1.52	4.89	6.29	11.26	11.80	0.51	0.50
S19243	<chem>O=c1oc2nocc2c(=O)[nH]1</chem>	4.51	4.04	9.97	9.24	14.08	12.69	0.59	0.55
S1928	<chem>c1ncc2c(n1)nc[nH]2</chem>	-0.70	-0.70	11.29	9.11	21.82	18.92	0.83	0.84
S1929	<chem>c1ncc2c(n1)[nH]cn2</chem>	-0.93	-0.70	8.23	6.64	14.85	14.35	0.38	0.41
S19294	<chem>O=c1sc2cocc2c(=O)[nH]1</chem>	1.36	1.52	5.44	6.22	11.18	11.60	0.48	0.50
S1930	<chem>c1ncn2c(n1)ncc2</chem>	0.40	0.05	8.31	7.69	17.90	16.16	0.45	0.41
S1931	<chem>c1ncn2c(n1)cnc2</chem>	0.58	0.05	7.95	6.59	14.10	13.73	0.70	0.72
S1932	<chem>n1cnn2c(c1)ncc2</chem>	-0.15	0.05	2.60	5.98	7.67	12.86	0.30	0.29
S1933	<chem>n1cnn2c(c1)cnc2</chem>	0.30	0.05	4.19	6.05	9.89	13.00	0.67	0.69
S1934	<chem>c1nc2c([nH]1)cnnn2</chem>	1.62	1.13	14.88	13.50	27.24	25.30	0.79	0.84
S1935	<chem>c1nc2c([nH]1)nnnc2</chem>	1.29	1.13	11.47	9.62	21.64	18.10	0.59	0.58
S1936	<chem>n1ncn2c(n1)ncc2</chem>	2.59	1.88	11.59	11.99	19.61	22.28	0.43	0.51
S19363	<chem>O=c1ccc2n1ncsc2</chem>	-0.70	-0.10	6.52	6.67	18.86	17.70	0.42	0.45
S1937	<chem>n1ncn2c(n1)cnc2</chem>	2.71	1.88	10.95	10.19	17.54	18.34	0.51	0.55
S19383	<chem>O=c1nc2c(n1)scn[nH]2</chem>	3.19	2.81	10.33	8.52	21.72	15.29	0.54	0.56
S1939	<chem>n1nnn2c(c1)cnc2</chem>	2.33	1.88	6.95	9.45	11.98	17.33	0.49	0.52
S1940	<chem>O=c1[nH]ncc2c1nc[nH]2</chem>	-0.46	0.07	12.10	9.17	26.08	20.09	0.27	0.28
S1941	<chem>O=c1[nH]ncc2c1[nH]cn2</chem>	-0.15	0.07	7.53	7.91	14.08	14.69	0.34	0.37
S1942	<chem>O=c1[nH]ncn2c1ncc2</chem>	0.58	0.82	8.96	7.81	20.47	17.14	0.83	0.79
S1943	<chem>O=c1[nH]ncn2c1cnc2</chem>	1.03	0.82	8.65	7.38	16.29	14.97	0.47	0.48
S1944	<chem>O=c1[nH]ncc2n1ccn2</chem>	0.62	0.82	4.28	6.82	8.47	13.19	0.53	0.50
S1945	<chem>O=c1[nH]ncc2n1cnc2</chem>	1.03	0.82	4.77	6.99	10.05	14.04	0.66	0.68
S1948	<chem>O=c1ncc2c([nH]1)nc[nH]2</chem>	0.56	0.07	13.28	10.10	28.10	22.49	0.92	0.91
S1949	<chem>O=c1ncc2c([nH]1)[nH]cn2</chem>	0.85	0.07	14.47	14.31	27.77	27.12	0.74	0.75
S1950	<chem>O=c1ncn2c([nH]1)ncc2</chem>	1.78	0.82	9.14	9.79	18.86	21.07	0.56	0.66

S1951	<chem>O=c1ncn2c([nH]1)cnc2</chem>	2.22	0.82	9.03	10.21	17.87	20.73	0.43	0.50
S19590	<chem>O=c1[nH]nc2n(c1=O)cccc2</chem>	1.31	1.97	6.71	8.58	17.64	17.80	0.49	0.49
S19591	<chem>O=c1[nH]nc2n(c1=O)ccnc2</chem>	3.31	3.80	9.14	10.40	17.15	17.66	0.87	0.82
S19592	<chem>O=c1[nH]nc2n(c1=O)cncc2</chem>	3.27	3.80	9.09	10.87	17.30	19.32	0.47	0.45
S19593	<chem>O=c1[nH]nc2n(c1=O)nccc2</chem>	2.09	3.80	9.60	11.03	21.00	21.43	0.78	0.80
S19611	<chem>O=c1[nH]nc2n(c1=O)ncnc2</chem>	4.12	5.63	11.13	12.25	19.73	19.99	0.76	0.76
S19645	<chem>O=c1[nH]nc2n(c1=O)ncen2</chem>	3.51	5.63	11.93	11.41	21.50	18.68	0.57	0.58
S19848	<chem>O=c1ccc2n1nc[nH]n2</chem>	-0.51	0.82	8.43	8.27	21.28	18.17	0.37	0.33
S19850	<chem>O=c1ncc2n1nc[nH]n2</chem>	1.67	2.65	11.55	11.66	24.27	22.33	0.56	0.60
S19852	<chem>O=c1cnc2n1nc[nH]n2</chem>	1.43	2.65	10.56	9.38	20.49	16.74	0.52	0.56
S1988	<chem>O=c1cnc2c([nH]1)[nH]cn2</chem>	0.61	0.07	13.82	14.22	22.92	25.34	0.95	0.95
S1989	<chem>O=c1cnc2c([nH]1)nc[nH]2</chem>	0.14	0.07	9.24	7.54	19.26	16.14	0.50	0.52
S1992	<chem>O=c1cnn2c([nH]1)ncc2</chem>	1.13	0.82	5.49	7.52	10.58	15.30	0.58	0.59
S1993	<chem>O=c1cnn2c([nH]1)cnc2</chem>	1.63	0.82	6.32	8.71	12.30	16.69	0.80	0.81
S1994	<chem>O=c1nnc2c([nH]1)[nH]cn2</chem>	2.65	1.90	17.43	19.37	29.26	33.64	0.34	0.38
S1995	<chem>O=c1nnc2c([nH]1)nc[nH]2</chem>	2.08	1.90	12.64	11.28	25.19	21.82	0.71	0.66
S2000	<chem>O=c1[nH]c(=O)c2c([nH]1)[nH]cn2</chem>	1.06	0.84	14.85	13.54	27.13	25.49	0.47	0.50
S2001	<chem>O=c1[nH]c(=O)c2c([nH]1)nc[nH]2</chem>	1.09	0.84	8.90	8.07	16.34	15.48	0.41	0.44
S2004	<chem>O=c1[nH]c(=O)n2c([nH]1)ncc2</chem>	2.14	1.59	7.61	7.61	11.03	14.62	0.65	0.63
S2005	<chem>O=c1[nH]c(=O)n2c([nH]1)cnc2</chem>	2.62	1.59	8.12	8.91	13.12	16.72	0.52	0.52
S2006	<chem>O=c1[nH]c2[nH]cnc2[nH]c1=O</chem>	0.99	0.84	13.82	13.74	26.74	29.37	0.69	0.70
S2009	<chem>O=c1oc(=O)c2c([nH]1)[nH]cn2</chem>	2.54	2.44	17.17	18.03	28.86	30.43	0.66	0.61
S2010	<chem>O=c1oc(=O)c2c([nH]1)nc[nH]2</chem>	2.52	2.44	11.37	10.42	20.28	17.89	0.36	0.37
S20299	<chem>O=c1cnn2c(n1)sc2=O</chem>	3.43	4.71	10.76	10.40	20.02	17.94	0.76	0.72
S2033	<chem>O=c1cc[nH]c2c1[nH]cn2</chem>	-2.19	-1.76	5.66	6.95	17.97	17.36	0.70	0.66
S2034	<chem>O=c1cc[nH]c2c1nc[nH]2</chem>	-2.31	-1.76	13.79	15.56	33.07	33.13	0.48	0.48
S2035	<chem>O=c1cc[nH]c2n1ccn2</chem>	-1.30	-1.01	8.82	7.10	17.82	17.36	0.49	0.49
S2036	<chem>O=c1cc[nH]c2n1cnc2</chem>	-0.83	-1.01	11.14	9.13	20.65	21.56	0.41	0.44
S2039	<chem>O=c1nc[nH]c2c1[nH]cn2</chem>	-0.28	0.07	7.64	9.66	21.14	20.79	0.39	0.40
S2040	<chem>O=c1nc[nH]c2c1nc[nH]2</chem>	-0.40	0.07	16.09	19.69	35.02	39.18	0.72	0.60
S2041	<chem>O=c1nc[nH]c2n1ccn2</chem>	0.54	0.82	10.93	10.27	20.70	21.43	0.77	0.76

S2045	c1cnc2c(n1)[nH]cn2	-1.19	-0.70	7.87	7.40	17.60	15.84	0.47	0.44
S2046	c1cnc2n(n1)ccn2	-0.42	0.05	5.82	6.27	15.63	13.66	0.52	0.58
S2047	c1cnc2n(n1)cnc2	-0.16	0.05	6.64	5.95	14.60	12.96	0.33	0.36
S2048	c1nnc2c(n1)nc[nH]2	0.98	1.13	11.08	8.77	17.55	16.05	0.51	0.49
S2049	c1nnc2c(n1)[nH]cn2	1.07	1.13	11.66	10.18	21.81	18.67	0.38	0.41
S20516	O=c1ccc2n1ncsn2	0.68	1.73	4.94	7.01	13.92	14.27	0.42	0.49
S2052	n1cnn2c(n1)ncc2	1.67	1.88	6.06	8.95	12.93	16.24	0.60	0.64
S2053	n1cnn2c(n1)cnc2	1.85	1.88	5.72	7.94	9.12	14.02	0.48	0.43
S2054	O=c1[nH]cnc2c1[nH]cn2	-0.36	0.07	6.01	10.43	15.36	18.60	0.42	0.39
S2055	O=c1[nH]cnc2c1nc[nH]2	-0.90	0.07	7.18	9.23	20.37	19.42	0.43	0.42
S2056	O=c1[nH]cnc2n1ccn2	0.48	0.82	10.39	8.87	19.92	16.40	0.82	0.75
S2057	O=c1[nH]cnc2n1cnc2	0.74	0.82	10.51	8.65	18.67	16.42	0.51	0.59
S2058	O=c1[nH]cnn2c1ncc2	-0.09	0.82	9.86	8.15	20.74	17.05	0.86	0.80
S2059	O=c1[nH]cnn2c1cnc2	0.46	0.82	10.20	8.50	17.99	16.61	0.44	0.52
S2084	n1nnc2c(n1)[nH]cn2	3.30	2.96	15.02	12.57	24.34	21.12	0.39	0.44
S2085	n1nnc2n(n1)ccn2	3.73	3.71	9.12	11.79	13.94	19.34	0.52	0.49
S2086	n1nnc2n(n1)cnc2	3.83	3.71	8.89	10.75	12.35	17.05	0.41	0.46
S2093	O=c1[nH]nnc2c1nc[nH]2	0.98	1.90	10.53	9.39	20.87	17.33	0.51	0.54
S2094	O=c1[nH]nnc2c1[nH]cn2	1.58	1.90	10.03	12.01	17.53	19.14	0.61	0.64
S2097	O=c1[nH]nnc2n1ccn2	2.32	2.65	7.70	10.35	13.82	16.70	0.57	0.55
S2098	O=c1[nH]nnc2n1cnc2	2.52	2.65	7.71	9.44	11.39	15.18	0.43	0.38
S2126	O=c1ccoc2n1cnc2	0.64	0.59	8.02	6.85	15.58	15.59	0.48	0.46
S2139	O=c1ccsc2n1ccn2	-0.42	-0.10	6.36	5.67	12.24	13.09	0.51	0.46
S2140	O=c1ccsc2n1cnc2	0.05	-0.10	7.10	6.18	14.62	15.29	0.71	0.65
S2141	O=c1cn[nH]c2c1[nH]cn2	-0.28	0.07	7.43	7.50	16.90	15.66	0.70	0.64
S2142	O=c1cn[nH]c2c1nc[nH]2	-0.48	0.07	14.77	14.70	30.56	28.79	0.63	0.66
S2143	O=c1cn[nH]c2n1ccn2	0.56	0.82	5.12	7.56	10.80	15.41	0.29	0.31
S2144	O=c1cn[nH]c2n1cnc2	0.94	0.82	8.68	8.90	14.96	18.07	0.55	0.49
S2155	O=c1cnc2n1ccn2	1.43	1.73	6.09	7.57	9.79	13.03	0.38	0.41
S2156	O=c1cnc2n1cnc2	1.84	1.73	6.57	7.39	11.42	13.70	0.58	0.53
S2165	O=c1nn[nH]c2c1[nH]cn2	1.61	1.90	10.13	11.24	21.53	21.33	0.35	0.37

S2166	<chem>O=c1nn[nH]c2c1nc[nH]2</chem>	1.33	1.90	17.35	19.85	33.13	37.09	0.42	0.41
S21724	<chem>O=c1cnnc2n1nc[nH]2</chem>	1.90	2.65	14.06	10.74	23.44	19.42	0.49	0.49
S21726	<chem>O=c1cnnc2n1nco2</chem>	3.81	4.25	11.96	9.51	17.64	14.94	0.49	0.45
S21728	<chem>O=c1cnnc2n1ncs2</chem>	2.75	3.56	10.53	8.78	17.37	14.46	0.44	0.40
S21744	<chem>O=c1cnnc2n1nccc2</chem>	2.08	3.03	10.42	8.91	18.74	15.80	0.44	0.37
S21762	<chem>O=c1cnnc2n1ncnc2</chem>	4.12	4.86	10.84	10.13	16.45	14.94	0.68	0.65
S21778	<chem>O=c1cnn2c([nH]1)nncc2=O</chem>	5.24	5.63	13.00	12.05	17.23	17.97	0.39	0.45
S21798	<chem>O=c1cnnc2n1ncnn2</chem>	5.64	6.69	13.23	12.72	17.03	16.98	0.40	0.43
S218	<chem>c1cc2c([nH]1)[nH]cc2</chem>	-7.18	-6.57	3.98	5.30	18.47	18.43	0.39	0.41
S21806	<chem>O=c1cnn2c(s1)nncc2=O</chem>	5.38	6.54	12.48	11.80	15.46	15.98	0.42	0.42
S2189	<chem>O=c1oc2cnnc2c(=O)[nH]1</chem>	3.87	3.19	10.92	9.32	14.63	14.77	0.52	0.65
S219	<chem>c1cc2c([nH]1)cc[nH]2</chem>	-7.26	-6.57	0.32	3.16	13.20	16.10	0.51	0.45
S2194	<chem>O=c1sc2nccn2c(=O)[nH]1</chem>	2.51	2.50	8.48	8.70	11.73	13.87	0.77	0.73
S220	<chem>c1cc2n(c1)[nH]cc2</chem>	-6.29	-5.82	5.62	3.90	20.02	16.20	0.47	0.44
S221	<chem>c1cc2n(c1)cc[nH]2</chem>	-6.28	-5.82	3.54	3.04	17.61	15.39	0.48	0.47
S222	<chem>[nH]1cc2c(c1)cc[nH]2</chem>	-7.63	-6.57	1.22	3.89	15.76	16.89	0.47	0.48
S223	<chem>c1oc2c(c1)cc[nH]2</chem>	-5.43	-4.97	3.08	2.80	13.33	13.66	0.56	0.50
S224	<chem>c1cc2c(o1)cc[nH]2</chem>	-5.43	-4.97	3.48	3.55	13.63	14.18	0.37	0.34
S2246	<chem>[nH]1cc2c(c1)nco2</chem>	-3.92	-3.14	5.02	4.79	14.45	14.68	0.61	0.56
S2248	<chem>s1cc2c(c1)nco2</chem>	-2.38	-2.23	2.07	2.56	7.89	10.23	0.59	0.55
S2249	<chem>c1nc2c(o1)n[nH]c2</chem>	-1.89	-1.31	5.23	5.23	11.41	12.78	0.49	0.51
S225	<chem>c1cc2n(c1)occ2</chem>	-4.77	-4.22	2.37	2.46	13.01	12.53	0.44	0.48
S2250	<chem>c1nc2c(o1)c[nH]n2</chem>	-1.90	-1.31	5.31	6.27	14.92	15.87	0.50	0.46
S2251	<chem>c1nc2c(o1)noc2</chem>	0.59	0.29	5.15	4.67	11.54	10.22	0.44	0.53
S2252	<chem>c1nc2c(o1)con2</chem>	0.57	0.29	6.02	5.71	14.48	13.31	0.54	0.50
S2256	<chem>c1nc2c(o1)nco2</chem>	0.51	0.29	3.23	4.38	6.61	9.98	0.33	0.36
S2257	<chem>c1oc2c(n1)ncs2</chem>	-0.55	-0.40	3.16	4.41	10.72	12.34	0.34	0.34
S2258	<chem>c1nc2c(o1)ncs2</chem>	-0.51	-0.40	2.73	3.67	6.89	9.42	0.43	0.39
S2259	<chem>c1nc2c(o1)[nH]nn2</chem>	0.70	0.52	8.73	9.47	18.42	19.71	0.47	0.46
S2260	<chem>c1oc2c(n1)[nH]nn2</chem>	0.68	0.52	5.87	7.28	13.85	14.18	0.67	0.74
S2261	<chem>[nH]1nc2c(n1)nco2</chem>	0.13	0.52	4.28	5.68	9.49	11.72	0.38	0.39

S2263	c1oc2c(n1)onn2	2.74	2.12	8.27	6.54	12.89	11.63	0.45	0.41
S2267	o1nc2c(n1)nco2	2.91	2.12	9.70	6.08	14.25	10.50	0.39	0.44
S2268	s1nc2c(n1)nco2	1.66	1.43	6.38	5.24	10.30	9.61	0.67	0.55
S227	o1cc2c(c1)cc[nH]2	-5.41	-4.97	3.52	3.30	13.70	14.00	0.43	0.39
S2274	c1ccc2c(c1)ocn2	-2.88	-2.76	1.61	2.68	8.09	11.19	0.40	0.42
S2275	c1ncc2c(c1)ocn2	-0.85	-0.93	4.37	4.26	10.95	11.99	0.58	0.64
S2276	c1ncc2c(c1)nco2	-0.89	-0.93	4.46	3.85	10.41	10.78	0.44	0.47
S2277	c1cnc2c(c1)nco2	-1.11	-0.93	2.39	3.96	8.05	10.59	0.44	0.39
S2278	c1cnc2c(c1)ocn2	-1.08	-0.93	4.06	5.08	13.51	13.91	0.46	0.49
S2279	c1nnc2c(c1)ocn2	1.07	0.90	6.80	7.68	16.99	16.96	0.75	0.66
S228	c1sc2c(c1)cc[nH]2	-5.92	-5.66	3.31	2.15	14.02	13.21	0.50	0.47
S2280	c1nnc2c(c1)nco2	1.04	0.90	5.87	6.16	13.83	12.42	0.57	0.53
S2281	n1ncc2c(c1)ocn2	1.33	0.90	7.83	6.45	16.64	13.83	0.33	0.35
S2282	O=c1[nH]ccc2c1nco2	-0.62	-0.16	7.26	7.10	20.10	17.57	0.46	0.43
S2283	O=c1[nH]ccc2c1ocn2	-0.48	-0.16	6.48	6.33	16.18	13.87	0.39	0.41
S2285	O=c1ccc2c([nH]1)nco2	0.31	-0.16	6.04	5.28	16.49	13.37	0.75	0.75
S229	c1cc2c(s1)cc[nH]2	-5.85	-5.66	3.83	2.71	14.97	13.38	0.50	0.56
S23	[nH]1cnnc1	-1.37	-1.57	10.04	8.62	23.00	20.45	0.47	0.48
S2300	c1ncc2c(n1)nco2	0.93	0.90	6.40	5.66	12.83	12.20	0.45	0.45
S2301	c1ncc2c(n1)ocn2	0.93	0.90	5.31	4.95	8.65	10.09	0.42	0.42
S2302	c1nc2c(o1)cnnn2	3.19	2.73	10.49	9.28	19.35	17.50	0.67	0.67
S2303	c1nc2c(o1)nnnc2	3.18	2.73	9.47	8.17	17.22	14.17	0.63	0.56
S2304	O=c1[nH]ncc2c1nco2	1.25	1.67	6.46	6.48	16.86	13.58	0.41	0.45
S2305	O=c1[nH]ncc2c1ocn2	1.45	1.67	5.69	6.11	13.31	11.08	0.47	0.58
S2308	O=c1ncc2c([nH]1)nco2	2.20	1.67	9.44	8.23	21.57	17.13	0.73	0.79
S231	c1cc2n(c1)ccs2	-4.93	-4.91	2.47	1.96	12.78	12.01	0.38	0.46
S232	s1cc2c(c1)cc[nH]2	-5.84	-5.66	3.51	2.52	14.38	13.32	0.71	0.65
S2329	O=c1cnc2c([nH]1)nco2	2.04	1.67	6.50	7.06	13.78	12.72	0.43	0.45
S233	c1cc2c([nH]1)[nH]nc2	-5.04	-4.74	6.37	6.48	17.67	18.40	0.60	0.58
S2331	O=c1nnc2c([nH]1)nco2	3.98	3.50	11.08	11.03	20.91	18.73	0.40	0.35
S2333	O=c1[nH]c(=O)c2c([nH]1)nco2	2.70	2.44	7.44	7.47	13.70	12.70	0.55	0.50

S234	c1[nH]c2c(c1)[nH]nc2	-5.13	-4.74	3.58	4.35	14.63	16.08	0.80	0.73
S2340	O=c1sc(=O)c2c([nH]1)nco2	3.03	3.35	9.05	9.19	14.75	14.06	0.70	0.68
S2343	O=c1cc[nH]c2c1ocn2	-0.56	-0.16	8.74	7.46	21.95	16.36	0.57	0.51
S2344	O=c1cc[nH]c2c1nco2	-0.67	-0.16	11.59	9.94	27.30	23.64	0.46	0.42
S2345	O=c1nc[nH]c2c1ocn2	1.35	1.67	10.83	10.42	24.36	20.12	0.55	0.54
S2346	O=c1nc[nH]c2c1nco2	1.21	1.67	13.80	13.30	29.28	28.61	0.51	0.50
S2347	c1cnc2c(n1)ocn2	0.69	0.90	4.41	5.34	9.92	11.06	0.50	0.55
S2348	c1nnc2c(n1)nco2	2.87	2.73	8.66	6.94	13.26	11.60	0.75	0.70
S2349	c1nnc2c(n1)ocn2	2.88	2.73	8.54	7.35	14.78	12.82	0.42	0.47
S235	c1cn2c(c1)cn[nH]2	-4.27	-3.99	4.89	5.28	14.60	16.39	0.43	0.45
S2350	O=c1[nH]cnc2c1ocn2	1.27	1.67	8.46	8.26	14.99	14.47	0.43	0.48
S2351	O=c1[nH]cnc2c1nco2	1.08	1.67	9.06	7.92	18.59	14.85	0.52	0.58
S236	c1cn2c(c1)[nH]nc2	-4.19	-3.99	2.22	4.43	11.75	15.58	0.54	0.54
S2360	n1nnc2c(n1)ocn2	5.12	4.56	13.10	9.98	18.89	15.60	0.67	0.62
S2367	O=c1[nH]nnc2c1nco2	2.96	3.50	7.14	8.32	13.82	13.09	0.51	0.51
S237	c1cc2c([nH]1)n[nH]c2	-5.78	-4.74	1.25	3.81	11.68	14.91	0.39	0.34
S23721	O=c1sc(=O)n2c(n1)scc2	2.80	3.41	9.76	9.84	18.98	16.05	0.48	0.49
S238	c1cc2c([nH]1)c[nH]n2	-5.79	-4.74	3.57	5.72	16.58	17.86	0.37	0.37
S2384	O=c1cn[nH]c2c1nco2	1.18	1.67	10.25	9.32	22.49	19.64	0.53	0.47
S23868	O=c1oc2c(o1)csc2	0.85	0.14	4.10	5.33	11.47	13.28	0.44	0.48
S239	c1cc2c([nH]1)onc2	-3.04	-3.14	5.72	4.94	15.77	14.98	0.47	0.47
S2392	O=c1nn[nH]c2c1nco2	2.95	3.50	12.99	13.70	25.34	26.86	0.41	0.44
S23950	O=c1oc2cscc2oc1=O	2.80	3.12	8.02	9.35	14.63	20.50	0.32	0.33
S24	c1ncn[nH]1	-1.71	-1.57	6.75	5.11	13.81	13.95	0.41	0.36
S240	c1cc2c([nH]1)cno2	-3.03	-3.14	7.29	5.69	18.47	15.49	0.50	0.45
S24119	O=c1sc2c(s1)con2	1.46	1.28	7.07	6.06	11.02	12.17	0.70	0.66
S24120	O=c1sc2c(s1)csn2	0.63	0.59	6.71	5.33	12.28	11.62	0.44	0.44
S243	c1cc2c([nH]1)noc2	-3.22	-3.14	4.15	4.17	14.34	13.36	0.38	0.39
S244	c1cc2c([nH]1)con2	-3.22	-3.14	7.37	6.08	19.70	16.31	0.45	0.49
S245	c1cc2c([nH]1)snc2	-3.77	-3.83	6.10	4.23	16.25	14.36	0.69	0.59
S246	c1cc2c([nH]1)cns2	-3.70	-3.83	6.65	4.79	17.07	14.53	0.57	0.59

S248	c1cn2c(c1)snc2	-2.85	-3.08	3.76	4.24	9.94	13.37	0.43	0.39
S249	c1cc2c([nH]1)nsc2	-4.06	-3.83	3.08	3.33	11.92	12.52	0.66	0.71
S2499	[nH]1cc2c(c1)ncs2	-4.72	-3.83	5.36	4.11	15.26	14.27	0.47	0.50
S2500	o1cc2c(c1)ncs2	-2.56	-2.23	1.34	2.64	7.18	10.43	0.54	0.49
S2501	s1cc2c(c1)ncs2	-3.10	-2.92	1.21	1.92	7.56	9.87	0.55	0.48
S2502	c1nc2c(s1)n[nH]c2	-2.91	-2.00	5.25	4.47	11.55	12.13	0.55	0.58
S2503	c1nc2c(s1)c[nH]n2	-2.79	-2.00	5.40	5.67	15.78	15.67	0.42	0.43
S2504	c1nc2c(s1)noc2	-0.43	-0.40	4.44	3.95	10.89	9.64	0.66	0.61
S2505	c1nc2c(s1)con2	-0.28	-0.40	5.06	5.15	14.05	13.17	0.34	0.37
S2506	c1nc2c(s1)nsc2	-1.35	-1.09	2.78	3.16	7.95	8.91	0.74	0.72
S2507	c1nc2c(s1)csn2	-1.20	-1.09	4.63	4.37	13.38	12.44	0.53	0.57
S2508	c1nc2c(s1)scn2	-1.40	-1.09	2.35	3.81	10.76	12.17	0.45	0.45
S2509	c1nc2c(s1)ncs2	-1.43	-1.09	2.21	2.96	6.41	8.84	0.54	0.47
S251	c1[nH]c2c(c1)nc[nH]2	-5.30	-4.74	6.94	8.98	21.39	22.27	0.54	0.57
S2510	c1nc2c(s1)[nH]nn2	-0.16	-0.17	8.31	9.02	18.68	19.80	0.59	0.59
S2511	c1sc2c(n1)[nH]nn2	-0.25	-0.17	4.88	6.47	13.10	13.48	0.75	0.83
S2512	[nH]1nc2c(n1)ncs2	-0.95	-0.17	4.13	5.00	10.43	11.29	0.41	0.42
S2513	c1nc2c(s1)onn2	1.60	1.43	6.95	6.59	11.94	14.06	0.56	0.59
S2514	c1nc2c(s1)nno2	1.79	1.43	7.40	5.86	12.83	11.14	0.50	0.46
S2515	c1nc2c(s1)snn2	0.79	0.74	6.20	5.93	13.82	13.73	0.46	0.50
S2516	c1sc2c(n1)snn2	0.75	0.74	6.10	5.08	12.18	10.39	0.68	0.66
S2518	o1nc2c(n1)ncs2	1.87	1.43	8.38	5.44	13.75	10.13	0.42	0.44
S2519	s1nc2c(n1)ncs2	0.60	0.74	5.24	4.59	10.10	9.24	0.50	0.50
S252	c1[nH]c2c(c1)[nH]cn2	-5.42	-4.74	3.39	4.94	14.33	16.99	0.85	0.79
S2520	O=c1[nH]c2c([nH]1)ncs2	-0.57	-1.23	4.77	5.26	13.92	14.53	0.45	0.45
S2522	O=c1oc2c([nH]1)scn2	1.09	0.37	8.32	8.01	17.15	16.59	0.55	0.56
S2525	c1ccc2c(c1)scn2	-3.50	-3.45	0.74	2.03	7.71	10.82	0.40	0.44
S2526	c1ncc2c(c1)scn2	-1.47	-1.62	3.57	3.66	10.54	11.76	0.32	0.33
S2527	c1ncc2c(c1)ncs2	-1.53	-1.62	3.71	3.19	9.87	10.37	0.73	0.77
S2528	c1cnc2c(c1)ncs2	-2.01	-1.62	2.08	3.21	7.55	9.94	0.37	0.44
S2529	c1cnc2c(c1)scn2	-1.83	-1.62	3.97	4.50	14.01	13.74	0.64	0.58

S253	c1cn2c(c1)nc[nH]2	-4.54	-3.99	8.84	7.13	21.39	19.26	0.64	0.58
S2530	c1nnc2c(c1)scn2	0.31	0.21	6.71	7.15	17.50	16.92	0.62	0.67
S2531	c1nnc2c(c1)ncs2	0.08	0.21	5.23	5.39	13.37	11.74	0.37	0.37
S2532	n1ncc2c(c1)scn2	0.70	0.21	7.07	5.84	16.51	13.55	0.64	0.58
S2533	O=c1[nH]ccc2c1ncs2	-1.43	-0.85	6.68	6.47	20.04	17.38	0.76	0.73
S2534	O=c1[nH]ccc2c1scn2	-1.36	-0.85	6.00	5.58	15.29	13.15	0.52	0.56
S2535	O=c1ccc2c([nH]1)scn2	-0.18	-0.85	5.09	5.53	14.53	14.09	0.58	0.54
S2536	O=c1ccc2c([nH]1)ncs2	-0.24	-0.85	5.30	4.60	16.08	13.03	0.54	0.53
S254	c1cn2c(c1)[nH]cn2	-4.75	-3.99	7.15	5.51	19.01	17.42	0.61	0.74
S2540	O=c1occc2c1scn2	0.30	0.75	4.70	5.57	13.36	11.83	0.39	0.42
S255	c1nc2c(o1)[nH]cc2	-3.57	-3.14	5.60	4.94	15.46	15.34	0.57	0.55
S2551	c1ncc2c(n1)ncs2	0.18	0.21	5.24	5.07	12.42	11.99	0.54	0.50
S2552	c1ncc2c(n1)scn2	0.05	0.21	4.76	4.25	8.73	9.58	0.59	0.62
S2553	c1nc2c(s1)cnnn2	2.47	2.04	9.12	8.74	18.70	17.42	0.43	0.47
S2554	c1nc2c(s1)nnnc2	2.27	2.04	8.60	7.45	17.01	13.62	0.82	0.82
S2555	O=c1[nH]ncc2c1ncs2	0.48	0.98	5.90	5.84	17.05	13.34	0.36	0.38
S2556	O=c1[nH]ncc2c1scn2	0.61	0.98	5.39	5.41	12.78	10.49	0.43	0.45
S256	c1oc2c(n1)[nH]cc2	-3.59	-3.14	3.21	3.78	9.89	12.90	0.56	0.58
S2560	O=c1ncc2c([nH]1)scn2	1.77	0.98	8.31	8.94	19.81	19.19	0.40	0.43
S257	c1cn2c(c1)nco2	-2.99	-2.39	4.05	4.15	12.33	13.43	0.53	0.47
S2579	O=c1cnc2c([nH]1)scn2	1.41	0.98	8.20	8.50	14.81	16.96	0.42	0.46
S258	c1cn2c(c1)ocn2	-2.99	-2.39	4.00	3.68	12.03	12.58	0.51	0.49
S2581	O=c1nnc2c([nH]1)scn2	3.37	2.81	11.86	12.93	21.29	24.31	0.66	0.69
S2583	O=c1[nH]c(=O)c2c([nH]1)scn2	1.90	1.75	9.37	8.52	18.87	17.29	0.67	0.74
S2585	O=c1[nH]c2scnc2[nH]c1=O	2.00	1.75	8.21	9.50	19.21	22.18	0.45	0.49
S2586	O=c1oc(=O)c2c([nH]1)scn2	3.37	3.35	11.93	11.92	21.19	21.32	0.79	0.70
S2588	O=c1[nH]c2scnc2oc1=O	3.22	3.35	10.77	12.23	19.83	24.05	0.51	0.49
S259	c1nc2c(s1)[nH]cc2	-4.31	-3.83	5.40	4.38	15.70	15.15	0.57	0.56
S2590	O=c1sc(=O)c2c([nH]1)scn2	2.32	2.66	10.54	10.89	18.91	19.79	0.58	0.66
S2594	O=c1cc[nH]c2c1scn2	-1.34	-0.85	7.80	6.62	20.53	15.45	0.46	0.56
S2595	O=c1cc[nH]c2c1ncs2	-1.41	-0.85	11.19	9.49	27.38	23.77	0.57	0.52

S2596	O=c1nc[nH]c2c1scn2	0.56	0.98	9.74	9.56	23.10	19.17	0.54	0.47
S2597	O=c1nc[nH]c2c1ncs2	0.49	0.98	13.33	12.90	29.39	28.87	0.50	0.46
S2598	c1cnc2c(n1)scn2	-0.35	0.21	3.44	4.66	10.06	10.62	0.36	0.37
S2599	c1nnc2c(n1)ncs2	1.81	2.04	7.38	6.25	12.36	11.11	0.51	0.45
S260	c1sc2c(n1)[nH]cc2	-4.29	-3.83	2.81	3.04	10.31	12.37	0.40	0.42
S2600	c1nnc2c(n1)scn2	1.85	2.04	7.26	6.72	14.41	12.50	0.51	0.57
S2601	O=c1[nH]cnc2c1scn2	0.27	0.98	7.85	7.59	14.24	13.94	0.67	0.61
S2602	O=c1[nH]cnc2c1ncs2	0.02	0.98	8.23	7.19	18.59	14.37	0.35	0.42
S2605	O=c1ocnc2c1scn2	1.95	2.58	5.85	6.69	11.59	11.37	0.65	0.67
S2611	n1nnc2c(n1)scn2	4.11	3.87	11.43	9.33	18.24	15.25	0.63	0.56
S2618	O=c1[nH]nnc2c1ncs2	1.90	2.81	6.51	7.57	14.31	12.58	0.78	0.78
S2619	O=c1[nH]nnc2c1scn2	2.21	2.81	6.73	8.45	11.72	13.53	0.49	0.43
S262	c1cn2c(c1)scn2	-3.66	-3.08	2.87	2.99	11.20	12.14	0.51	0.45
S2628	O=c1ccoc2c1scn2	0.19	0.75	4.66	5.21	13.33	11.32	0.57	0.60
S263	c1cc2c([nH]1)[nH]nn2	-3.10	-2.91	9.12	10.80	22.69	23.63	0.58	0.54
S2630	O=c1ncoc2c1scn2	2.05	2.58	6.72	7.26	16.03	13.79	0.54	0.49
S2634	O=c1cn[nH]c2c1scn2	0.54	0.98	5.86	6.45	15.48	12.80	0.51	0.48
S2635	O=c1cn[nH]c2c1ncs2	0.41	0.98	9.84	8.85	22.66	19.73	0.47	0.43
S264	c1cc2c([nH]1)nn[nH]2	-3.19	-2.91	3.66	6.75	15.45	18.36	0.44	0.54
S2642	O=c1nn[nH]c2c1scn2	2.40	2.81	8.56	10.41	19.47	18.76	0.47	0.51
S2643	O=c1nn[nH]c2c1ncs2	2.25	2.81	12.55	13.28	25.65	27.08	0.40	0.42
S265	c1cn2c(c1)nn[nH]2	-2.44	-2.16	8.51	9.15	17.54	20.84	0.32	0.32
S266	c1cn2c(c1)[nH]nn2	-2.71	-2.16	6.08	7.53	12.88	19.00	1.06	1.05
S267	[nH]1nc2c(n1)cc[nH]2	-3.89	-2.91	3.99	4.61	12.48	13.64	0.56	0.50
S2672	c1on2c(c1)cnn2	-0.40	-0.56	7.51	6.76	18.84	15.71	0.56	0.52
S2674	o1cc2c(c1)nn[nH]2	-1.54	-1.31	5.79	7.25	14.68	17.02	0.60	0.53
S2677	s1cc2c(c1)nn[nH]2	-2.05	-2.00	5.52	6.56	15.00	16.58	0.56	0.48
S2684	n1nc2c([nH]1)noc2	0.58	0.52	5.74	7.06	10.64	14.05	0.44	0.37
S269	c1cc2c([nH]1)nno2	-1.22	-1.31	7.74	6.55	17.10	15.60	0.47	0.46
S2690	c1[nH]n2c(n1)cnn2	-0.39	-0.33	11.64	9.40	22.94	18.74	0.47	0.47
S2691	c1nn2c([nH]1)cnn2	-0.30	-0.33	13.20	11.40	26.86	23.60	0.39	0.41

S2692	c1on2c(n1)cnn2	1.37	1.27	9.30	7.39	18.04	14.27	0.29	0.32
S2695	c1nn2c(s1)cnn2	0.57	0.58	8.47	7.37	18.96	16.35	0.64	0.56
S271	c1cn2c(c1)onn2	-0.73	-0.56	2.01	6.65	5.67	15.49	0.49	0.61
S272	c1cc2c([nH]1)snn2	-2.11	-2.00	8.61	7.09	19.23	17.69	0.49	0.45
S273	c1cc2c([nH]1)nns2	-2.07	-2.00	6.19	5.75	15.90	14.91	0.77	0.79
S2740	c1ccc2c(c1)[nH]nn2	-2.37	-2.53	5.70	6.77	15.86	17.59	0.38	0.39
S2741	c1ccc2n(c1)nnc2	-1.29	-1.78	5.00	5.89	16.54	15.82	0.62	0.61
S2742	c1ncc2c(c1)[nH]nn2	-0.38	-0.70	8.63	8.58	15.92	18.29	0.41	0.45
S2743	c1ncc2c(c1)nn[nH]2	-0.46	-0.70	8.10	7.17	15.03	15.66	0.62	0.61
S2744	c1cnc2c(c1)nn[nH]2	-0.82	-0.70	3.38	6.43	11.34	14.71	0.32	0.36
S2745	c1cnc2c(c1)[nH]nn2	-0.56	-0.70	8.56	10.31	20.06	21.91	0.78	0.77
S2746	n1ccn2c(c1)cnn2	0.60	0.05	4.31	6.94	12.47	14.81	0.49	0.53
S2747	c1ncn2c(c1)cnn2	0.60	0.05	5.78	7.41	14.11	16.01	0.81	0.78
S275	c1cn2c(c1)snn2	-1.64	-1.25	1.28	5.90	6.00	14.89	0.38	0.41
S2750	c1nnc2c(c1)[nH]nn2	1.52	1.13	11.98	13.15	21.91	24.86	0.31	0.34
S2751	c1nnc2c(c1)nn[nH]2	1.17	1.13	5.78	7.85	11.07	15.03	0.46	0.52
S2754	n1ncc2c(c1)[nH]nn2	1.73	1.13	11.48	10.00	19.22	18.61	0.47	0.50
S2755	n1ncc2n(c1)nnc2	2.72	1.88	7.36	9.47	11.83	17.24	0.32	0.38
S2756	O=c1[nH]ccc2c1nn[nH]2	-0.09	0.07	8.89	12.18	22.19	26.29	0.32	0.36
S2757	O=c1[nH]ccc2c1[nH]nn2	0.16	0.07	7.45	9.50	15.27	18.27	0.63	0.60
S2758	O=c1ccc2c([nH]1)[nH]nn2	1.00	0.07	11.33	11.13	18.32	20.36	0.54	0.50
S2759	O=c1ccc2c([nH]1)nn[nH]2	0.89	0.07	10.61	8.34	19.71	18.36	0.65	0.65
S276	O=c1c(=O)c2c(c1=O)[nH]cc2	2.73	3.71	12.52	12.09	21.46	24.93	0.60	0.52
S2760	O=c1[nH]ccn2c1cnn2	0.85	0.82	10.35	9.52	19.41	18.92	0.55	0.55
S2761	O=c1[nH]ccc2n1nnc2	0.66	0.82	10.80	10.19	22.79	22.21	0.38	0.35
S2763	O=c1ccn2c([nH]1)cnn2	1.94	0.82	6.93	9.32	13.85	18.11	0.35	0.39
S2766	O=c1occc2c1nn[nH]2	1.50	1.67	11.65	13.17	23.06	26.08	0.40	0.34
S2767	O=c1occc2c1[nH]nn2	1.76	1.67	5.28	8.35	10.22	15.53	0.96	0.90
S2778	O=c1ccc2c(s1)[nH]nn2	1.19	0.98	8.49	8.20	14.03	16.12	0.41	0.44
S278	o1nc2c(n1)cc[nH]2	-0.99	-1.31	8.53	5.93	17.86	13.43	0.54	0.48
S2786	c1ncc2c(n1)nn[nH]2	1.37	1.13	11.06	10.12	19.21	18.69	0.57	0.51

S2787	<chem>c1ncc2c(n1)[nH]nn2</chem>	1.18	1.13	6.38	7.65	11.29	14.11	0.61	0.56
S279	<chem>s1nc2c(n1)cc[nH]2</chem>	-2.20	-2.00	6.30	5.03	13.72	12.42	0.55	0.51
S2790	<chem>n1nnc2c(c1)[nH]nn2</chem>	3.60	2.96	14.82	13.98	22.95	23.89	0.46	0.43
S2791	<chem>n1nnc2c(c1)nn[nH]2</chem>	3.30	2.96	9.46	10.09	15.45	16.68	0.44	0.40
S2794	<chem>O=c1[nH]ncc2c1nn[nH]2</chem>	1.70	1.90	12.07	10.78	22.95	20.78	0.32	0.35
S2795	<chem>O=c1[nH]ncc2c1[nH]nn2</chem>	2.04	1.90	5.86	9.52	10.04	15.39	0.41	0.47
S2796	<chem>O=c1[nH]ncn2c1cnn2</chem>	2.69	2.65	7.93	9.24	13.12	15.51	0.44	0.39
S2797	<chem>O=c1[nH]ncc2n1nnc2</chem>	2.49	2.65	8.40	9.44	16.65	17.61	0.31	0.32
S28	<chem>s1cnncl</chem>	-0.45	-0.66	4.08	3.98	12.71	12.73	0.72	0.64
S2800	<chem>O=c1ncc2c([nH]1)nn[nH]2</chem>	2.65	1.90	13.03	10.52	23.65	20.61	0.34	0.37
S2801	<chem>O=c1ncc2c([nH]1)[nH]nn2</chem>	2.88	1.90	14.27	14.73	23.55	25.23	0.55	0.50
S2802	<chem>O=c1ncn2c([nH]1)cnn2</chem>	3.73	2.65	9.67	12.62	15.94	22.47	0.48	0.55
S281	<chem>O=c1[nH]n2c([nH]1)ccc2</chem>	-2.44	-3.22	4.62	5.82	12.94	18.21	0.51	0.48
S2831	<chem>O=c1cnc2c([nH]1)nn[nH]2</chem>	2.38	1.90	7.71	8.50	13.53	15.44	0.39	0.44
S2833	<chem>O=c1cnn2c([nH]1)cnn2</chem>	3.47	2.65	10.48	12.04	18.00	20.44	0.58	0.53
S285	<chem>O=c1[nH]n2c(o1)ccc2</chem>	-0.94	-1.62	8.09	8.31	15.98	19.11	0.57	0.52
S2860	<chem>O=c1cc[nH]c2c1[nH]nn2</chem>	0.06	0.07	8.80	8.49	17.57	18.31	0.55	0.51
S2861	<chem>O=c1cc[nH]c2c1nn[nH]2</chem>	-0.10	0.07	15.73	17.10	31.69	34.07	0.76	0.75
S2862	<chem>O=c1cc[nH]c2n1nnc2</chem>	0.70	0.82	14.19	13.12	27.33	27.83	0.46	0.54
S2864	<chem>O=c1nc[nH]c2c1[nH]nn2</chem>	1.93	1.90	10.83	10.67	20.59	20.55	0.31	0.31
S2865	<chem>O=c1nc[nH]c2c1nn[nH]2</chem>	1.76	1.90	18.14	20.70	33.54	38.94	0.42	0.46
S2868	<chem>c1cnc2c(n1)[nH]nn2</chem>	0.98	1.13	6.28	8.95	14.74	16.79	0.36	0.41
S2869	<chem>c1cnc2n(n1)nnc2</chem>	1.73	1.88	9.69	8.23	18.98	15.31	0.38	0.42
S2870	<chem>c1nnc2c(n1)nn[nH]2</chem>	2.98	2.96	9.19	9.78	13.51	15.81	0.47	0.48
S2871	<chem>c1nnc2c(n1)[nH]nn2</chem>	3.07	2.96	10.08	11.19	15.92	18.44	0.57	0.51
S2874	<chem>O=c1[nH]cnc2c1[nH]nn2</chem>	1.96	1.90	9.88	12.58	18.63	20.47	0.44	0.49
S2875	<chem>O=c1[nH]cnc2c1nn[nH]2</chem>	1.43	1.90	10.43	11.38	20.69	21.29	0.39	0.42
S2876	<chem>O=c1[nH]cnc2n1nnc2</chem>	2.20	2.65	13.22	10.86	23.05	19.44	0.43	0.41
S2877	<chem>O=c1[nH]cnn2c1cnn2</chem>	2.44	2.65	13.00	11.28	21.99	19.17	0.60	0.70
S2883	<chem>O=c1ocnc2c1nn[nH]2</chem>	2.99	3.50	9.03	11.47	17.02	19.83	0.63	0.66
S289	<chem>O=c1[nH]n2c(s1)ccc2</chem>	-1.69	-2.31	6.73	7.34	14.13	17.96	0.83	0.82

S290	<chem>c1ccc2c(c1)[nH]cc2</chem>	-6.17	-6.19	3.51	2.46	15.45	14.22	0.58	0.52
S291	<chem>c1ccc2n(c1)ccc2</chem>	-5.15	-5.44	1.12	1.84	11.47	12.89	0.56	0.52
S292	<chem>c1ncc2c(c1)[nH]cc2</chem>	-4.14	-4.36	6.31	4.65	17.77	15.75	0.57	0.53
S2925	<chem>O=c1ccoc2c1nn[nH]2</chem>	1.28	1.67	10.62	11.44	22.57	24.36	0.37	0.35
S2926	<chem>O=c1ccoc2n1nnc2</chem>	2.11	2.42	10.76	9.70	20.78	20.26	0.43	0.50
S2929	<chem>O=c1ncoc2c1nn[nH]2</chem>	3.06	3.50	13.18	14.15	24.39	27.98	0.46	0.47
S293	<chem>c1ncc2c(c1)cc[nH]2</chem>	-4.18	-4.36	5.84	3.90	16.64	14.60	0.46	0.44
S2935	<chem>O=c1ccsc2n1nnc2</chem>	1.42	1.73	9.57	9.10	19.98	20.15	0.39	0.42
S2936	<chem>O=c1cn[nH]c2c1[nH]nn2</chem>	1.87	1.90	5.87	8.51	11.69	15.42	0.47	0.50
S2937	<chem>O=c1cn[nH]c2c1nn[nH]2</chem>	1.66	1.90	15.03	15.70	27.28	28.56	0.56	0.51
S2938	<chem>O=c1cn[nH]c2n1nnc2</chem>	2.43	2.65	12.02	12.38	21.46	23.22	0.48	0.54
S294	<chem>c1cnc2c(c1)cc[nH]2</chem>	-4.69	-4.36	2.07	2.88	10.73	13.01	0.51	0.44
S2946	<chem>O=c1cnc2c1nnc2</chem>	3.18	3.56	9.13	9.80	16.35	17.45	0.36	0.38
S295	<chem>c1cnc2c(c1)[nH]cc2</chem>	-4.62	-4.36	5.93	4.93	17.94	16.18	0.35	0.37
S296	<chem>n1ccn2c(c1)ccc2</chem>	-3.17	-3.61	3.07	3.93	10.79	14.18	0.42	0.47
S297	<chem>c1ncn2c(c1)ccc2</chem>	-3.21	-3.61	1.75	3.73	8.16	13.91	0.43	0.41
S298	<chem>c1cnn2c(c1)ccc2</chem>	-3.96	-3.61	1.85	2.99	10.17	12.90	0.71	0.63
S299	<chem>c1ccn2c(n1)ccc2</chem>	-3.66	-3.61	4.37	3.73	14.03	13.91	0.69	0.61
S3	<chem>c1cccs1</chem>	-4.49	-4.32	-0.85	0.71	6.99	10.30	0.70	0.65
S300	<chem>c1nnc2c(c1)[nH]cc2</chem>	-2.47	-2.53	9.10	8.14	22.86	19.96	0.62	0.58
S301	<chem>c1nnc2c(c1)cc[nH]2</chem>	-2.57	-2.53	5.39	5.34	17.12	15.63	0.59	0.62
S302	<chem>n1ccn2c(n1)ccc2</chem>	-1.63	-1.78	6.69	6.85	16.92	17.44	0.48	0.52
S303	<chem>c1nnn2c(c1)ccc2</chem>	-2.05	-1.78	3.54	5.90	10.91	16.17	0.50	0.52
S304	<chem>n1ncc2c(c1)[nH]cc2</chem>	-1.95	-2.53	9.02	7.12	22.80	18.38	0.63	0.54
S305	<chem>n1ncc2n(c1)ccc2</chem>	-0.98	-1.78	4.99	6.85	15.17	17.44	0.32	0.33
S306	<chem>O=c1[nH]ccc2c1cc[nH]2</chem>	-4.03	-3.59	6.32	6.27	20.67	18.96	0.45	0.47
S3066	<chem>s1cc2c(c1)nno2</chem>	-0.23	-0.40	3.84	4.86	9.90	12.43	0.53	0.49
S307	<chem>O=c1[nH]ccc2c1[nH]cc2</chem>	-3.85	-3.59	2.47	4.85	12.98	15.43	0.37	0.38
S309	<chem>O=c1ccc2c([nH]1)cc[nH]2</chem>	-2.83	-3.59	7.97	5.65	22.35	18.02	0.64	0.64
S310	<chem>O=c1[nH]ccn2c1ccc2</chem>	-3.16	-2.84	5.56	5.13	17.35	16.50	0.36	0.38
S3103	<chem>c1ccc2c(c1)onn2</chem>	-0.58	-0.93	4.00	5.18	10.79	13.47	0.36	0.34

S3104	c1ncc2c(c1)onn2	1.34	0.90	4.81	6.22	8.48	13.09	0.62	0.66
S3105	c1ncc2c(c1)nno2	1.33	0.90	4.15	5.81	7.68	11.88	0.38	0.36
S3106	c1cnc2c(c1)nno2	1.24	0.90	6.48	6.46	11.99	12.87	0.61	0.65
S3107	c1cnc2c(c1)onn2	1.15	0.90	6.81	7.58	12.88	16.19	0.78	0.79
S311	O=c1[nH]ccc2n1ccc2	-3.16	-2.84	5.40	4.53	14.10	15.31	0.58	0.64
S312	O=c1ccc2n([nH]1)ccc2	-1.82	-2.84	4.33	6.18	14.23	17.51	0.56	0.57
S3129	c1ncc2c(n1)nno2	3.08	2.73	7.22	7.62	9.80	13.31	0.57	0.51
S313	O=c1ccn2c([nH]1)ccc2	-1.78	-2.84	5.03	5.57	15.11	17.09	0.64	0.57
S3130	c1ncc2c(n1)onn2	3.16	2.73	6.93	6.91	9.14	11.19	0.48	0.43
S316	O=c1occc2c1cc[nH]2	-2.36	-1.99	8.89	7.82	22.36	19.55	0.70	0.66
S317	O=c1occc2c1[nH]cc2	-2.17	-1.99	4.44	5.28	14.98	14.90	0.56	0.52
S3176	c1cnc2c(n1)onn2	2.94	2.73	7.66	7.84	11.28	13.34	0.42	0.45
S328	O=c1ccc2c(s1)[nH]cc2	-2.44	-2.68	6.80	5.26	17.92	16.07	0.67	0.62
S3348	O=c1ccn2n1cccc2	-1.88	-2.09	7.09	4.86	21.27	16.12	0.61	0.60
S3359	O=c1ccn2n1cc[nH]c2=O	0.13	0.51	8.08	7.04	18.66	16.52	0.59	0.52
S336	c1ncc2c(n1)cc[nH]2	-2.59	-2.53	8.29	5.78	17.62	15.26	0.29	0.31
S337	c1ncc2c(n1)[nH]cc2	-2.62	-2.53	5.01	4.48	13.27	13.24	0.57	0.51
S3373	O=c1ccn2n1ccnc2	0.06	-0.26	8.71	6.67	19.92	16.20	0.79	0.75
S3374	O=c1ccn2n1cncc2	0.09	-0.26	9.04	7.40	20.39	18.26	0.51	0.51
S338	c1ncn2c(n1)ccc2	-1.67	-1.78	5.05	5.03	11.68	13.63	0.41	0.37
S3388	O=c1ccn2n1ccoc2=O	1.88	2.11	6.45	8.01	13.90	15.71	0.38	0.42
S339	n1cnn2c(c1)ccc2	-1.94	-1.78	1.47	4.49	6.11	12.89	0.34	0.39
S340	c1cc2c([nH]1)cnnn2	-0.32	-0.70	11.74	10.02	25.28	21.29	0.40	0.46
S341	c1cc2c([nH]1)nnnc2	-0.39	-0.70	8.51	7.96	20.93	18.11	0.39	0.43
S342	n1ncn2c(n1)ccc2	0.54	0.05	8.12	9.17	17.98	19.41	0.66	0.61
S343	n1nnn2c(c1)ccc2	0.17	0.05	4.57	8.43	13.05	18.40	0.32	0.36
S3432	O=c1ccn2n1cn[nH]c2=O	2.13	2.34	6.89	7.78	14.04	15.07	0.47	0.43
S344	O=c1[nH]ncc2c1cc[nH]2	-2.13	-1.76	9.30	5.92	21.80	15.75	0.45	0.47
S345	O=c1[nH]ncc2c1[nH]cc2	-1.88	-1.76	5.03	5.25	13.97	13.37	0.33	0.34
S3451	O=c1ccn2n1cns2=O	2.99	3.25	8.35	9.32	13.10	15.23	0.52	0.49
S346	O=c1[nH]ncn2c1ccc2	-1.19	-1.01	6.06	5.23	16.05	13.93	0.42	0.52

S347	<chem>O=c1[nH]ncc2n1ccc2</chem>	-1.23	-1.01	2.56	4.83	9.56	13.01	0.59	0.56
S350	<chem>O=c1ncc2c([nH]1)cc[nH]2</chem>	-0.93	-1.76	10.37	8.88	26.68	22.57	0.69	0.61
S352	<chem>O=c1ncn2c([nH]1)ccc2</chem>	0.09	-1.01	5.95	9.24	17.59	22.28	0.63	0.63
S353	<chem>O=c1ncc2n([nH]1)ccc2</chem>	0.07	-1.01	7.34	10.06	19.58	22.96	0.71	0.65
S3534	<chem>s1cc2c(c1)nns2</chem>	-1.05	-1.09	4.06	4.16	11.36	11.91	0.51	0.57
S3567	<chem>c1ccc2c(c1)snn2</chem>	-1.33	-1.62	3.77	4.47	11.70	12.94	0.69	0.64
S3568	<chem>c1ncc2c(c1)snn2</chem>	0.63	0.21	5.66	5.56	10.64	12.70	0.42	0.43
S3569	<chem>c1ncc2c(c1)nns2</chem>	0.57	0.21	3.92	5.09	8.52	11.31	0.40	0.47
S3571	<chem>c1cnc2c(c1)snn2</chem>	0.34	0.21	6.95	6.94	15.61	15.86	0.58	0.58
S3575	<chem>O=c1[nH]ccc2c1nns2</chem>	0.81	0.98	10.06	9.51	21.14	20.43	0.62	0.68
S3576	<chem>O=c1[nH]ccc2c1snn2</chem>	0.94	0.98	9.00	8.62	15.09	16.19	0.53	0.45
S3578	<chem>O=c1ccc2c([nH]1)nns2</chem>	1.95	0.98	7.80	6.45	15.13	13.50	0.91	0.91
S3593	<chem>c1ncc2c(n1)nns2</chem>	2.26	2.04	7.63	6.97	12.96	12.93	0.39	0.43
S3597	<chem>O=c1[nH]ncc2c1nns2</chem>	2.64	2.81	8.95	8.34	17.68	15.21	0.51	0.49
S3598	<chem>O=c1[nH]ncc2c1snn2</chem>	2.82	2.81	6.57	7.92	10.81	12.36	0.31	0.36
S3622	<chem>O=c1cnc2c([nH]1)nns2</chem>	3.41	2.81	7.84	8.12	12.11	12.57	0.46	0.49
S3643	<chem>O=c1[nH]cnc2c1snn2</chem>	2.61	2.81	11.35	10.63	17.79	16.99	0.52	0.43
S3644	<chem>O=c1[nH]cnc2c1nns2</chem>	2.29	2.81	11.89	10.23	20.00	17.42	0.49	0.42
S382	<chem>O=c1cnc2n([nH]1)ccc2</chem>	-0.41	-1.01	7.06	8.57	14.06	18.48	0.54	0.49
S383	<chem>O=c1cnn2c([nH]1)ccc2</chem>	-0.61	-1.01	4.20	7.21	10.96	17.06	0.62	0.67
S386	<chem>O=c1nnc2n([nH]1)ccc2</chem>	1.48	0.82	10.58	13.47	20.90	26.18	0.33	0.37
S390	<chem>O=c1[nH]c(=O)c2n([nH]1)ccc2</chem>	0.35	-0.24	8.39	8.02	16.04	17.77	0.84	0.87
S391	<chem>O=c1[nH]c(=O)n2c([nH]1)ccc2</chem>	0.36	-0.24	5.52	6.81	10.65	16.16	0.37	0.35
S393	<chem>O=c1[nH]n2cccc2[nH]c1=O</chem>	0.64	-0.24	7.17	11.31	17.39	27.59	0.56	0.55
S396	<chem>O=c1oc(=O)c2n([nH]1)ccc2</chem>	1.85	1.36	10.85	12.12	19.08	22.13	0.45	0.42
S4	<chem>c1ccn[nH]1</chem>	-3.96	-3.40	3.23	3.37	12.23	13.78	0.39	0.48
S400	<chem>O=c1[nH]n2cccc2oc1=O</chem>	1.72	1.36	9.74	13.17	17.90	27.63	0.44	0.49
S404	<chem>O=c1sc(=O)c2n([nH]1)ccc2</chem>	0.92	0.67	9.76	11.04	16.73	20.56	0.49	0.52
S408	<chem>O=c1[nH]n2cccc2sc1=O</chem>	0.96	0.67	8.27	12.23	16.57	26.60	0.64	0.54
S410	<chem>O=c1cc[nH]c2c1[nH]cc2</chem>	-3.84	-3.59	6.90	6.22	21.60	19.14	0.58	0.52
S4100	<chem>O=c1c(=O)c2c(c1=O)cccc2</chem>	3.14	4.09	8.40	10.14	15.75	21.50	0.52	0.58

S4102	<chem>O=c1c(=O)c(=O)c2c1nccc2</chem>	4.50	5.92	10.70	12.11	17.14	23.13	0.47	0.49
S411	<chem>O=c1cc[nH]c2c1cc[nH]2</chem>	-3.98	-3.59	11.35	10.76	29.13	26.08	0.43	0.55
S412	<chem>O=c1cc[nH]c2n1ccc2</chem>	-3.12	-2.84	8.94	7.04	20.82	20.27	0.51	0.49
S413	<chem>O=c1cc[nH]n2c1ccc2</chem>	-3.09	-2.84	10.95	8.69	25.64	22.47	0.57	0.52
S4138	<chem>O=c1c(=O)c2c(c1=O)ncn2</chem>	5.83	7.75	12.65	13.06	17.56	22.52	0.49	0.46
S4139	<chem>O=c1c(=O)c2c(c1=O)nnn2</chem>	7.96	9.58	17.23	14.14	19.18	21.38	0.60	0.61
S414	<chem>O=c1nc[nH]c2c1[nH]cc2</chem>	-1.93	-1.76	8.89	9.44	24.67	23.68	0.28	0.30
S415	<chem>O=c1nc[nH]c2c1cc[nH]2</chem>	-2.10	-1.76	13.55	14.74	31.75	31.79	0.56	0.49
S416	<chem>O=c1nc[nH]c2n1ccc2</chem>	-1.28	-1.01	11.20	10.72	23.79	25.46	0.49	0.42
S417	<chem>O=c1nc[nH]n2c1ccc2</chem>	-1.20	-1.01	13.14	12.57	28.15	27.92	0.49	0.56
S418	<chem>c1cnc2c(n1)[nH]cc2</chem>	-3.11	-2.53	4.73	4.32	12.86	12.72	0.35	0.40
S419	<chem>c1cnc2n(n1)ccc2</chem>	-2.49	-1.78	3.07	3.86	9.52	11.67	0.73	0.65
S420	<chem>c1nnc2c(n1)cc[nH]2</chem>	-0.92	-0.70	7.88	6.20	16.82	14.05	0.53	0.49
S421	<chem>c1nnc2c(n1)[nH]cc2</chem>	-0.88	-0.70	8.39	6.94	18.82	15.20	0.61	0.67
S423	<chem>n1cnn2c(n1)ccc2</chem>	-0.36	0.05	3.46	6.38	10.25	13.91	0.62	0.55
S424	<chem>O=c1[nH]cnc2c1[nH]cc2</chem>	-2.34	-1.76	4.04	6.86	11.62	15.26	0.75	0.72
S425	<chem>O=c1[nH]cnc2c1cc[nH]2</chem>	-2.60	-1.76	4.79	6.22	16.00	15.62	0.42	0.45
S426	<chem>O=c1[nH]cnc2n1ccc2</chem>	-1.66	-1.01	7.53	5.96	13.90	14.20	0.71	0.65
S427	<chem>O=c1[nH]cnn2c1ccc2</chem>	-1.90	-1.01	7.27	5.81	15.88	14.39	0.58	0.65
S4290	<chem>O=c1[nH]cc2n1cc[nH]2</chem>	-3.62	-3.22	6.93	6.89	21.34	20.54	0.28	0.33
S4297	<chem>O=c1[nH]c2c([nH]1)csc2</chem>	-2.09	-3.06	2.87	4.32	11.73	14.85	0.57	0.48
S4300	<chem>O=c1[nH]c2c([nH]1)c[nH]n2</chem>	-2.07	-2.14	5.56	6.91	15.86	18.49	0.81	0.86
S432	<chem>O=c1ocnc2c1[nH]cc2</chem>	-0.66	-0.16	5.88	6.39	13.70	13.49	0.59	0.51
S433	<chem>O=c1ocnc2c1cc[nH]2</chem>	-0.93	-0.16	7.10	6.89	17.50	14.96	0.67	0.59
S4331	<chem>O=c1[nH]c2c([nH]1)cccc2</chem>	-2.30	-3.59	2.43	4.40	12.29	15.84	0.55	0.49
S4332	<chem>O=c1[nH]cc2n1cccc2</chem>	-2.86	-2.84	3.21	4.99	14.38	16.39	0.42	0.35
S4333	<chem>O=c1[nH]c2c([nH]1)ccnc2</chem>	-0.34	-1.76	5.52	5.82	12.66	15.45	0.37	0.41
S4334	<chem>O=c1[nH]c2c([nH]1)ccn2</chem>	-0.85	-1.76	5.46	5.66	13.97	15.94	0.45	0.52
S4336	<chem>O=c1[nH]cc2n1cncc2</chem>	-0.87	-1.01	5.79	7.65	14.45	18.82	0.33	0.36
S4344	<chem>O=c1[nH]c2c([nH]1)cc[nH]c2=O</chem>	-0.11	-0.99	8.00	7.74	17.84	19.49	0.36	0.42
S4345	<chem>O=c1ccc2c([nH]1)[nH]c(=O)[nH]2</chem>	1.13	-0.99	8.79	8.10	18.38	18.41	0.31	0.33

S4346	<chem>O=c1[nH]cc2n1cc[nH]c2=O</chem>	-0.74	-0.24	5.34	7.31	13.72	17.24	0.48	0.40
S4353	<chem>O=c1[nH]cc2n1ccoc2=O</chem>	0.98	1.36	7.72	8.78	14.58	16.97	0.39	0.43
S4365	<chem>O=c1[nH]c2c([nH]1)cn[nH]c2=O</chem>	1.14	0.07	7.14	6.50	12.83	14.25	0.58	0.68
S4371	<chem>O=c1[nH]c2c([nH]1)cn[nH]c2=O</chem>	1.80	0.84	8.78	7.37	15.28	15.51	0.34	0.35
S4378	<chem>O=c1[nH]cc2c(n1)[nH]c(=O)[nH]2</chem>	2.02	0.84	11.81	10.96	23.84	23.07	0.35	0.36
S4395	<chem>O=c1cnc2c([nH]1)[nH]c(=O)[nH]2</chem>	2.52	0.84	11.69	9.86	18.73	18.47	0.40	0.38
S441	<chem>O=c1scnc2c1cc[nH]2</chem>	-1.78	-0.85	6.48	6.03	16.31	14.01	0.53	0.56
S4418	<chem>O=c1[nH]c2c([nH]1)[nH]ccc2=O</chem>	-0.06	-0.99	14.07	10.43	26.23	24.06	0.48	0.43
S4421	<chem>O=c1[nH]c2c([nH]1)[nH]cnc2=O</chem>	1.79	0.84	16.30	13.64	29.20	27.84	0.58	0.53
S4424	<chem>O=c1[nH]c2c([nH]1)ncn2</chem>	0.65	0.07	3.52	5.90	10.01	13.79	0.66	0.60
S4426	<chem>O=c1[nH]c2c([nH]1)ncnn2</chem>	2.84	1.90	8.09	7.76	13.77	14.35	0.29	0.31
S4429	<chem>O=c1[nH]c2c([nH]1)nc[nH]c2=O</chem>	1.30	0.84	9.63	8.54	18.47	17.46	0.66	0.59
S444	<chem>n1nnc2c(n1)[nH]cc2</chem>	1.41	1.13	11.60	9.84	22.70	18.78	0.63	0.55
S445	<chem>n1nnc2n(n1)ccc2</chem>	1.74	1.88	6.34	9.73	13.53	18.12	0.38	0.43
S4473	<chem>O=c1[nH]c2c([nH]1)[nH]ncc2=O</chem>	1.78	0.84	13.40	10.06	22.87	20.08	0.69	0.75
S452	<chem>O=c1[nH]nnc2c1cc[nH]2</chem>	-0.70	0.07	7.58	6.89	16.64	14.66	0.79	0.91
S453	<chem>O=c1[nH]nnc2c1[nH]cc2</chem>	-0.39	0.07	6.74	8.28	13.40	15.45	0.42	0.36
S4536	<chem>O=c1[nH]c2c(o1)csc2</chem>	-0.64	-1.46	6.10	5.99	14.73	15.11	0.49	0.46
S455	<chem>O=c1[nH]nnc2n1ccc2</chem>	0.23	0.82	3.56	7.28	7.73	14.15	0.44	0.39
S4575	<chem>O=c1occ2n1cccc2</chem>	-0.77	-1.24	4.43	5.75	14.85	15.58	0.64	0.60
S4579	<chem>O=c1oc2c([nH]1)cccc2</chem>	0.52	-0.16	4.05	6.29	12.05	14.62	0.37	0.42
S4581	<chem>O=c1occ2n1cncc2</chem>	1.17	0.59	5.95	7.60	13.69	16.88	0.47	0.46
S4620	<chem>O=c1oc2c([nH]1)ncnc2</chem>	2.53	1.67	7.03	7.37	12.25	13.27	0.59	0.58
S472	<chem>O=c1ccoc2c1[nH]cc2</chem>	-2.41	-1.99	3.85	4.80	14.44	14.08	0.61	0.55
S473	<chem>O=c1ccoc2c1cc[nH]2</chem>	-2.65	-1.99	7.85	6.25	21.53	17.97	0.45	0.36
S474	<chem>O=c1ccoc2n1ccc2</chem>	-1.72	-1.24	5.45	4.76	13.52	14.30	0.27	0.29
S476	<chem>O=c1ncoc2c1[nH]cc2</chem>	-0.57	-0.16	6.04	7.13	17.81	17.38	0.38	0.44
S477	<chem>O=c1ncoc2c1cc[nH]2</chem>	-0.83	-0.16	10.12	9.33	24.13	22.43	0.41	0.46
S48	<chem>c1ccccc1</chem>	-4.74	-4.85	-1.41	0.73	7.36	11.22	0.37	0.40
S480	<chem>O=c1ccsc2c1cc[nH]2</chem>	-3.18	-2.68	7.61	5.73	20.98	17.93	0.55	0.47
S483	<chem>O=c1ccsc2n1ccc2</chem>	-2.26	-1.93	4.57	4.09	12.72	14.00	0.50	0.46

S484	O=c1cn[nH]c2c1[nH]cc2	-1.97	-1.76	5.38	6.61	17.23	17.08	0.42	0.36
S4845	O=c1sc2n1ccs2	-1.32	-1.40	4.57	4.72	13.41	13.62	0.52	0.47
S485	O=c1cn[nH]c2c1cc[nH]2	-2.14	-1.76	11.87	10.41	26.38	22.87	0.46	0.52
S486	O=c1cn[nH]c2n1ccc2	-1.31	-1.01	6.69	7.34	15.24	17.97	0.67	0.60
S4884	O=c1sc2c([nH]1)cncc2	0.35	-0.85	6.17	5.95	12.61	13.72	0.66	0.60
S4885	O=c1sc2c([nH]1)ccnc2	0.36	-0.85	7.59	6.89	13.92	14.96	0.60	0.60
S4887	O=c1sc2c([nH]1)necc2	-0.29	-0.85	4.35	5.44	12.33	13.75	0.76	0.67
S49	c1ccnc1	-2.78	-3.02	2.18	2.35	10.04	11.87	0.63	0.62
S4928	O=c1sc2c([nH]1)ncnc2	1.69	0.98	5.12	6.50	10.20	12.35	0.49	0.49
S494	O=c1cncs2n1ccc2	-0.42	-0.10	2.52	5.84	7.90	13.60	0.51	0.55
S497	O=c1ncsc2c1cc[nH]2	-1.53	-0.85	9.76	8.87	23.82	22.54	0.52	0.56
S50	c1ccnnc1	-0.74	-1.19	5.49	4.99	15.44	14.77	0.43	0.45
S500	O=c1nn[nH]c2c1[nH]cc2	-0.08	0.07	7.91	10.86	21.71	23.88	0.56	0.50
S501	O=c1nn[nH]c2c1cc[nH]2	-0.30	0.07	14.45	15.41	29.98	30.82	0.42	0.44
S51	O=c1cccc[nH]1	-1.77	-2.25	5.75	4.24	17.36	14.82	0.51	0.56
S516	O=c1oc2cccn2c(=O)[nH]1	1.56	1.36	6.97	7.22	11.97	14.21	0.50	0.46
S5176	O=c1[nH]nc2n1cccc2	-0.92	-1.01	4.25	5.25	13.03	13.43	0.41	0.44
S5177	O=c1[nH]nc2n1ccnc2	1.03	0.82	4.08	7.54	10.29	14.42	0.52	0.47
S5178	O=c1[nH]nc2n1cncc2	1.03	0.82	4.15	7.40	10.48	14.74	0.47	0.54
S5179	O=c1[nH]nc2n1necc2	0.23	0.82	7.36	6.82	19.12	15.09	0.61	0.57
S5197	O=c1[nH]nc2n1ncnc2	2.19	2.65	7.09	8.52	16.09	14.79	0.58	0.49
S52	O=c1ccccol	-0.31	-0.65	5.51	4.94	16.04	14.56	0.41	0.48
S5231	O=c1[nH]nc2n1ncn2	1.91	2.65	9.39	7.93	18.42	13.89	0.40	0.42
S54	c1ccnnc1	-0.83	-1.19	4.15	3.38	8.84	11.22	0.44	0.50
S55	c1cnnnc1	1.23	0.64	8.49	7.04	17.64	16.37	0.26	0.32
S5528	C1C=[S]c2n1c(=O)sn2	0.50	0.43	6.83	6.13	13.21	11.94	0.66	0.60
S554	[nH]1cc2c(c1)cco2	-5.81	-4.97	3.32	3.30	13.99	14.00	0.61	0.52
S555	c1cc2c(o1)occ2	-3.48	-3.37	0.03	2.33	5.81	10.70	0.49	0.57
S557	o1cc2c(c1)cco2	-3.61	-3.37	0.97	2.15	7.30	10.62	0.61	0.65
S558	c1oc2c(c1)ccs2	-4.15	-4.06	0.16	1.54	7.23	10.03	0.36	0.39
S559	c1cc2c(o1)ccs2	-4.16	-4.06	0.25	1.35	7.40	9.99	0.48	0.50

S56	O=c1cccn[nH]1	-0.03	-0.42	5.66	4.07	14.84	11.88	0.60	0.54
S560	s1cc2c(c1)cco2	-4.13	-4.06	0.79	1.41	8.08	10.00	0.46	0.54
S561	c1cc2c(o1)[nH]nc2	-3.30	-3.14	2.34	3.62	10.55	13.13	0.46	0.49
S562	c1oc2c(c1)[nH]nc2	-3.32	-3.14	2.92	4.37	11.31	13.64	0.47	0.54
S563	c1cc2c(o1)n[nH]c2	-3.80	-3.14	3.57	4.56	13.04	13.90	0.40	0.46
S564	c1cc2c(o1)c[nH]n2	-3.98	-3.14	3.28	3.89	12.07	13.25	0.41	0.45
S565	c1cc2c(o1)onc2	-1.07	-1.54	3.81	4.10	11.71	11.50	0.31	0.38
S567	c1cc2c(o1)noc2	-1.25	-1.54	4.32	4.37	13.52	11.86	0.37	0.43
S5673	c1[nH]n2c(c1)nnc2	-1.78	-2.16	11.60	9.90	27.86	22.00	0.72	0.66
S5674	c1cn2c([nH]1)nnc2	-1.72	-2.16	7.57	7.14	22.74	18.24	0.41	0.46
S5678	c1cn2c(s1)nnc2	-0.46	-1.25	8.24	6.96	21.17	16.05	0.66	0.60
S5679	n1cn2c(n1)cn[nH]2	0.12	-0.33	11.19	10.37	23.45	20.19	0.60	0.56
S5680	n1nc2n(c1)cn[nH]2	0.28	-0.33	7.67	7.61	19.29	16.43	0.50	0.57
S5684	n1nc2n(c1)cns2	1.53	0.58	10.24	8.33	19.87	15.41	0.58	0.53
S5685	c1[nH]n2c(n1)nnc2	0.25	-0.33	14.95	13.78	30.41	26.47	0.60	0.65
S5686	c1nn2c([nH]1)nnc2	-0.15	-0.33	10.90	8.55	23.79	17.93	0.53	0.47
S5687	c1on2c(n1)nnc2	1.71	1.27	10.35	9.19	21.89	18.39	0.65	0.73
S5688	c1nn2c(o1)nnc2	1.78	1.27	9.57	7.69	20.00	14.45	0.33	0.34
S569	c1cc2c(o1)snc2	-2.02	-2.23	3.04	3.25	10.25	10.66	0.37	0.41
S5690	c1nn2c(s1)nnc2	0.84	0.58	8.59	6.93	19.53	13.84	0.42	0.45
S57	O=c1nccc[nH]1	0.09	-0.42	9.33	7.65	22.41	19.64	0.50	0.53
S5703	c1ccc2n(c1)cnn2	-0.82	-1.78	7.00	6.66	20.29	16.85	0.99	0.94
S5704	n1ccn2c(c1)nnc2	1.09	0.05	9.10	8.37	18.95	17.31	0.54	0.48
S5705	c1ncn2c(c1)nnc2	1.04	0.05	8.18	7.50	18.25	15.57	0.41	0.44
S5706	c1cnn2c(c1)nnc2	0.39	0.05	7.55	7.05	19.05	15.20	0.45	0.47
S5707	c1ccn2c(n1)nnc2	1.00	0.05	10.65	9.62	24.42	20.23	0.51	0.44
S5708	n1ccn2c(n1)nnc2	2.92	1.88	13.33	12.36	23.82	22.93	0.73	0.68
S571	c1cc2c(o1)nsc2	-2.14	-2.23	3.06	3.56	11.34	11.07	0.62	0.54
S5711	O=c1[nH]ccn2c1nnc2	1.19	0.82	11.03	11.55	24.61	24.43	0.77	0.75
S5712	O=c1[nH]ccc2n1cnn2	1.33	0.82	11.09	9.69	22.29	18.75	0.26	0.32
S5713	O=c1ccc2n([nH]1)cnn2	2.36	0.82	10.09	10.70	18.40	19.56	0.50	0.49

S5714	O=c1ccn2c([nH]1)nnc2	2.40	0.82	11.10	8.76	19.74	18.03	0.59	0.63
S5723	c1ncn2c(n1)nnc2	2.88	1.88	12.10	9.88	22.52	17.65	0.88	0.80
S5724	n1cnn2c(c1)nnc2	2.32	1.88	6.71	8.17	14.52	14.36	0.64	0.60
S5725	n1ncn2c(n1)nnc2	4.96	3.71	15.37	13.64	22.05	22.60	0.57	0.67
S5727	O=c1[nH]ncn2c1nnc2	3.02	2.65	12.24	10.60	22.21	19.56	0.28	0.34
S5728	O=c1[nH]ncc2n1cnn2	3.16	2.65	8.89	9.61	16.06	15.62	0.32	0.37
S5729	O=c1ncn2c([nH]1)nnc2	4.15	2.65	13.07	11.39	19.62	20.91	0.83	0.77
S573	c1cc2c(o1)[nH]cn2	-3.54	-3.14	6.24	5.25	16.78	15.77	0.58	0.57
S5730	O=c1ncc2n([nH]1)cnn2	4.15	2.65	12.99	14.19	19.17	24.18	0.46	0.50
S5739	O=c1cnc2n([nH]1)cnn2	4.12	2.65	13.53	14.16	22.66	22.89	0.42	0.36
S574	c1oc2c(c1)[nH]cn2	-3.38	-3.14	6.62	6.66	17.55	16.94	0.45	0.51
S5740	O=c1cnn2c([nH]1)nnc2	3.62	2.65	9.95	9.65	17.49	16.33	0.67	0.61
S5754	O=c1cc[nH]c2n1cnn2	1.30	0.82	11.72	9.82	21.82	20.04	0.35	0.43
S5755	O=c1cc[nH]n2c1nnc2	1.16	0.82	16.35	15.54	30.74	31.05	0.41	0.44
S5757	O=c1nc[nH]n2c1nnc2	3.02	2.65	18.82	19.03	31.94	35.68	0.33	0.38
S5758	c1cnc2n(n1)cnn2	2.15	1.88	10.27	8.99	21.53	16.34	0.49	0.54
S576	c1oc2c(c1)ocn2	-1.58	-1.54	2.17	3.63	8.70	11.18	0.62	0.54
S5760	n1cnn2c(n1)nnc2	4.08	3.71	10.42	11.14	17.80	17.74	0.38	0.44
S5761	O=c1[nH]cnc2n1cnn2	3.15	2.65	13.96	12.19	25.10	20.01	0.64	0.67
S5762	O=c1[nH]cnn2c1nnc2	2.50	2.65	13.40	11.47	24.80	20.66	0.93	0.88
S577	c1cc2c(o1)scn2	-2.53	-2.23	1.44	2.54	7.93	10.24	0.66	0.59
S578	c1oc2c(c1)scn2	-2.38	-2.23	1.99	3.01	9.15	10.85	0.52	0.60
S5787	O=c1ccsc2n1cnn2	2.16	1.73	9.45	8.39	18.62	15.76	0.54	0.59
S5788	O=c1cn[nH]c2n1cnn2	3.10	2.65	8.92	9.75	16.23	16.90	0.33	0.36
S5792	O=c1cns2n1cnn2	3.96	3.56	10.71	9.76	17.41	14.53	0.39	0.38
S581	[nH]1nc2c(n1)cco2	-1.93	-1.31	2.44	4.13	7.62	10.89	0.34	0.39
S5823	c1nn2c(n1)cc[nH]2	-2.50	-2.16	8.10	6.22	19.09	15.38	0.53	0.57
S5824	c1cn2c([nH]1)ncn2	-2.42	-2.16	6.79	5.37	15.98	14.57	0.70	0.64
S5826	c1cn2c(o1)ncn2	-0.50	-0.56	6.28	5.18	13.73	12.03	0.73	0.76
S5828	c1cn2c(s1)ncn2	-1.31	-1.25	5.40	4.38	12.73	11.31	0.60	0.50
S5829	c1nn2c(n1)cn[nH]2	-0.52	-0.33	6.81	7.12	13.77	14.50	0.32	0.36

S5830	c1nn2c(n1)[nH]nc2	-0.37	-0.33	5.10	6.26	10.18	13.69	0.24	0.29
S5832	c1nn2c(n1)onc2	1.84	1.27	7.46	7.03	11.76	12.49	0.56	0.52
S5834	c1nn2c(n1)snc2	0.74	0.58	4.63	6.17	8.71	11.61	0.54	0.57
S5835	c1nc2n(n1)[nH]cn2	-0.48	-0.33	11.66	9.52	22.53	18.58	0.88	0.86
S5836	c1nc2n(n1)nc[nH]2	-0.60	-0.33	10.78	7.90	20.24	16.74	0.63	0.58
S5838	c1nc2n(n1)nco2	1.31	1.27	8.36	6.17	13.73	12.04	1.05	1.08
S5840	c1nc2n(n1)ncs2	0.27	0.58	7.33	5.47	13.72	11.59	0.64	0.58
S5853	c1ccc2n(c1)ncn2	-1.74	-1.78	4.24	4.24	12.17	12.19	0.58	0.53
S5854	n1ccn2c(c1)ncn2	0.20	0.05	4.54	5.98	9.30	12.70	0.31	0.37
S5855	c1ncn2c(c1)ncn2	0.20	0.05	3.01	5.78	7.58	12.43	0.32	0.35
S5856	c1cnn2c(c1)ncn2	-0.24	0.05	6.66	5.70	14.36	12.90	0.33	0.35
S5857	c1ccn2c(n1)ncn2	0.03	0.05	7.08	6.45	16.60	13.90	0.70	0.73
S5858	n1ccn2c(n1)ncn2	2.01	1.88	8.99	9.21	16.08	16.66	0.61	0.52
S5859	c1nnn2c(c1)ncn2	1.67	1.88	7.16	8.27	12.32	15.39	0.29	0.31
S5860	n1ncc2n(c1)ncn2	2.35	1.88	6.46	8.54	11.10	15.19	0.65	0.72
S5861	O=c1[nH]ccn2c1ncn2	0.32	0.82	9.63	8.27	20.09	17.39	0.60	0.59
S5862	O=c1[nH]ccc2n1ncn2	0.29	0.82	10.22	7.67	19.52	16.20	0.44	0.40
S5864	O=c1ccn2c([nH]1)ncn2	1.48	0.82	5.59	7.22	11.70	14.75	0.31	0.38
S5873	c1ncn2c(n1)ncn2	1.98	1.88	7.05	7.40	13.10	12.85	0.67	0.57
S5874	n1cnn2c(c1)ncn2	1.71	1.88	5.54	6.85	9.68	12.12	0.64	0.60
S5875	n1ncn2c(n1)ncn2	4.12	3.71	10.46	11.18	15.03	17.86	0.45	0.43
S5876	n1nnn2c(c1)ncn2	3.80	3.71	8.94	10.44	12.55	16.85	0.51	0.45
S5877	O=c1[nH]ncn2c1ncn2	2.22	2.65	7.54	8.01	15.52	14.05	0.61	0.64
S5878	O=c1[nH]ncc2n1ncn2	2.12	2.65	7.09	7.62	13.84	13.12	0.51	0.45
S5879	O=c1ncn2c([nH]1)ncn2	3.33	2.65	8.87	10.55	16.28	19.17	0.45	0.43
S5890	O=c1cnn2c([nH]1)ncn2	2.99	2.65	8.62	9.18	12.33	15.42	0.68	0.54
S5904	O=c1cc[nH]c2n1ncn2	0.28	0.82	11.38	9.43	23.10	19.99	0.62	0.70
S5906	O=c1nc[nH]c2n1ncn2	2.12	2.65	13.81	12.76	25.04	24.41	0.45	0.40
S5908	c1cnc2n(n1)ncn2	1.46	1.88	8.43	6.89	14.79	12.37	0.60	0.53
S5909	c1nnn2c(n1)ncn2	3.43	3.71	8.36	8.87	10.77	13.56	0.43	0.48
S5910	n1cnn2c(n1)ncn2	3.47	3.71	8.45	9.07	11.60	13.83	0.37	0.43

S5911	O=c1[nH]cnc2n1ncn2	2.05	2.65	12.73	9.42	19.17	15.79	0.47	0.53
S5912	O=c1[nH]cnn2c1ncn2	1.89	2.65	12.16	9.27	19.31	15.98	0.64	0.58
S5919	O=c1scnc2n1ncn2	2.58	3.56	9.01	8.31	14.19	13.09	0.62	0.54
S5937	O=c1ccsc2n1ncn2	1.01	1.73	8.49	6.93	17.13	14.32	0.39	0.44
S5938	O=c1cn[nH]c2n1ncn2	2.10	2.65	8.24	9.38	16.16	16.92	0.81	0.79
S594	c1ccc2c(c1)occ2	-4.55	-4.59	0.37	1.46	8.80	10.93	0.67	0.63
S5942	O=c1cncsc2n1ncn2	2.84	3.56	8.49	8.33	13.87	13.14	0.27	0.38
S595	c1ncc2c(c1)occ2	-2.55	-2.76	2.95	2.88	11.15	11.38	0.31	0.37
S596	c1ncc2c(c1)cco2	-2.53	-2.76	3.27	3.14	11.71	11.64	0.54	0.62
S597	c1cnc2c(c1)cco2	-2.83	-2.76	2.29	3.50	11.05	11.99	0.69	0.67
S5974	c1cn2c([nH]1)nnn2	0.11	-0.33	10.41	8.99	23.55	19.05	0.51	0.45
S5976	c1cn2c(o1)nnn2	2.04	1.27	10.23	8.44	20.68	16.00	0.54	0.60
S5978	c1cn2c(s1)nnn2	1.19	0.58	9.13	7.66	19.78	15.34	0.33	0.40
S598	c1cnc2c(c1)occ2	-3.01	-2.76	1.68	2.78	9.78	11.29	0.42	0.50
S60	O=c1ccens1	0.84	0.49	7.41	5.35	15.00	12.52	0.41	0.40
S600	c1nnc2c(c1)cco2	-0.66	-0.93	5.70	6.21	16.50	14.95	0.32	0.42
S601	n1ncc2c(c1)occ2	-0.33	-0.93	6.23	5.58	17.15	14.34	0.31	0.34
S6018	c1ccc2n(c1)nnn2	0.80	0.05	7.86	7.59	19.20	16.25	0.44	0.49
S6019	n1ccn2c(c1)nnn2	2.69	1.88	8.15	8.80	16.16	15.58	0.75	0.80
S602	O=c1[nH]ccc2c1cco2	-2.33	-1.99	5.38	4.87	16.36	14.28	0.69	0.61
S6020	c1ncn2c(c1)nnn2	2.67	1.88	7.35	8.60	15.44	15.31	0.67	0.62
S6021	c1cnn2c(c1)nnn2	2.36	1.88	10.66	9.06	20.92	16.96	0.58	0.53
S6022	c1ccn2c(n1)nnn2	2.62	1.88	11.01	9.80	21.62	17.97	0.56	0.56
S6026	O=c1[nH]ccn2c1nnn2	2.91	2.65	13.29	12.22	23.48	22.38	0.68	0.62
S6027	O=c1[nH]ccc2n1nnn2	2.87	2.65	13.83	11.63	23.96	21.19	0.57	0.63
S6029	O=c1ccn2c([nH]1)nnn2	3.93	2.65	9.76	9.99	16.42	17.16	0.46	0.42
S603	O=c1[nH]ccc2c1occ2	-2.23	-1.99	4.92	5.37	17.29	15.06	0.49	0.43
S6038	c1ncn2c(n1)nnn2	4.49	3.71	11.79	10.22	18.81	15.73	0.56	0.56
S6039	n1cnn2c(c1)nnn2	4.23	3.71	10.48	9.67	17.19	15.00	0.42	0.48
S605	O=c1ccc2c([nH]1)cco2	-1.24	-1.99	4.96	5.09	16.73	14.48	0.41	0.45
S6069	O=c1cc[nH]c2n1nnn2	2.81	2.65	14.65	12.79	24.40	24.06	0.57	0.48

S6073	c1cnc2n(n1)nnn2	4.11	3.71	13.40	10.25	22.17	16.43	0.73	0.70
S61	O=c1ncccs1	0.67	0.49	7.71	6.65	18.32	17.28	0.42	0.49
S6104	O=c1ccsc2n1nnn2	3.56	3.56	12.04	10.29	20.29	18.38	0.58	0.55
S62	O=c1cncc[nH]1	0.14	-0.42	8.26	6.36	16.71	15.42	0.48	0.42
S620	c1ncc2c(n1)cco2	-0.96	-0.93	4.72	3.88	10.29	10.70	0.39	0.45
S621	c1ncc2c(n1)occ2	-0.79	-0.93	4.45	4.33	10.45	11.15	0.64	0.61
S623	c1cc2c(o1)nnnc2	1.50	0.90	8.19	8.06	18.51	16.35	0.77	0.76
S624	O=c1[nH]ncc2c1cco2	-0.42	-0.16	4.51	4.76	13.59	11.40	0.50	0.46
S625	O=c1[nH]ncc2c1occ2	-0.29	-0.16	5.56	5.00	15.83	11.93	0.41	0.47
S628	O=c1ncc2c([nH]1)cco2	0.70	-0.16	8.00	8.55	21.83	19.37	0.58	0.49
S653	O=c1[nH]c(=O)c2c([nH]1)cco2	1.08	0.61	8.38	7.54	17.13	15.26	0.35	0.37
S66	O=c1cc[nH]c(=O)o1	2.40	1.95	12.39	9.70	20.96	18.82	0.35	0.41
S664	O=c1cc[nH]c2c1cco2	-2.34	-1.99	9.16	6.69	23.60	18.76	0.58	0.64
S666	O=c1nc[nH]c2c1cco2	-0.48	-0.16	11.26	9.89	26.25	23.38	0.58	0.49
S667	c1cnc2c(n1)occ2	-1.26	-0.93	3.12	3.80	8.21	10.11	0.49	0.43
S668	c1nnc2c(n1)cco2	0.98	0.90	6.98	5.92	14.41	11.77	0.38	0.41
S669	c1nnc2c(n1)occ2	0.93	0.90	6.47	5.65	13.48	11.51	0.54	0.48
S67	O=c1[nH]ccoc1=O	1.73	1.95	10.08	10.61	20.16	23.99	0.30	0.34
S670	O=c1[nH]cnc2c1occ2	-0.72	-0.16	6.41	6.23	15.67	13.29	0.54	0.53
S671	O=c1[nH]cnc2c1cco2	-0.66	-0.16	7.05	6.45	14.85	13.21	0.30	0.38
S673	O=c1cnc2c(o1)cco2	1.46	1.44	5.96	6.33	13.23	12.80	0.35	0.45
S68	O=c1cc[nH]c(=O)s1	1.43	1.26	11.10	8.66	18.23	17.33	0.71	0.67
S687	O=c1[nH]nnc2c1cco2	1.26	1.67	5.46	7.36	11.12	12.58	0.39	0.44
S688	O=c1[nH]nnc2c1occ2	1.17	1.67	5.77	6.88	12.68	12.41	0.76	0.72
S7	c1ncc[nH]1	-3.69	-3.40	6.24	5.22	17.67	16.64	0.44	0.48
S704	O=c1cn[nH]c2c1cco2	-0.47	-0.16	7.41	6.58	18.61	15.88	0.41	0.48
S71	O=c1cc[nH]cn1	-0.36	-0.42	12.77	10.16	28.39	24.60	0.62	0.59
S712	O=c1nn[nH]c2c1cco2	1.33	1.67	9.98	10.80	22.30	22.75	0.38	0.38
S72	O=c1nc[nH]cn1	1.50	1.41	15.43	12.97	30.50	28.12	0.60	0.55
S73	n1ccncc1	-0.91	-1.19	1.62	2.95	5.38	10.27	0.71	0.79
S739	O=c1ccc2=c1ccc2=O	1.10	1.11	2.93	5.82	6.84	13.85	0.45	0.51

S74	<chem>n1ccnnc1</chem>	1.08	0.64	6.20	5.00	12.31	11.87	0.67	0.58
S75	<chem>O=c1ccnc[nH]1</chem>	0.12	-0.42	7.34	5.40	15.54	13.34	0.64	0.71
S76	<chem>O=c1cncco1</chem>	1.55	1.18	6.18	5.51	13.11	13.00	0.41	0.47
S77	<chem>O=c1ccnco1</chem>	1.55	1.18	4.63	5.21	11.87	11.83	0.74	0.75
S79	<chem>O=c1ccnes1</chem>	0.68	0.49	4.42	4.40	11.07	10.99	0.58	0.49
S7949	<chem>c1ccc2c(c1)c[nH]c2</chem>	-6.74	-6.19	4.45	2.46	17.68	14.22	0.87	0.93
S7950	<chem>c1ccc2c(c1)coc2</chem>	-4.55	-4.59	-0.47	1.46	7.84	10.93	0.30	0.36
S7951	<chem>c1ccc2c(c1)csc2</chem>	-4.95	-5.28	-0.61	0.71	8.15	10.30	0.37	0.36
S7952	<chem>c1ccc2c(c1)n[nH]c2</chem>	-5.09	-4.36	4.22	3.37	14.31	13.78	0.49	0.66
S7953	<chem>c1ccc2c(c1)noc2</chem>	-2.55	-2.76	3.17	3.33	12.13	11.82	0.33	0.37
S7954	<chem>c1ccc2c(c1)nsc2</chem>	-3.39	-3.45	2.68	2.52	10.57	11.03	0.40	0.45
S7955	<chem>c1ccc2c(c1)n[nH]n2</chem>	-3.39	-2.53	3.02	3.26	9.11	11.08	0.53	0.47
S7956	<chem>c1ccc2c(c1)non2</chem>	-0.50	-0.93	4.76	4.17	11.18	10.47	0.42	0.47
S7957	<chem>c1ccc2c(c1)nsn2</chem>	-1.78	-1.62	2.00	3.30	6.05	9.51	0.63	0.64
S7958	<chem>c1ccc2c(c1)cccc2</chem>	-5.16	-5.81	-1.20	0.73	7.73	11.22	0.56	0.50
S7959	<chem>c1ccc2c(c1)cncc2</chem>	-3.17	-3.98	1.66	2.35	9.92	11.87	0.51	0.47
S7960	<chem>c1ccc2c(c1)ncec2</chem>	-3.91	-3.98	1.66	2.35	10.24	11.87	0.58	0.51
S7961	<chem>c1ccc2c(c1)nncc2</chem>	-1.85	-2.15	4.01	4.99	14.36	14.77	0.65	0.56
S7962	<chem>c1ccc2c(c1)cnnc2</chem>	-0.90	-2.15	4.71	4.99	16.17	14.77	0.53	0.47
S7963	<chem>O=c1[nH]ccc2c1cccc2</chem>	-3.38	-3.21	4.47	4.24	15.22	14.82	0.53	0.51
S7964	<chem>O=c1ccc2c([nH]1)cccc2</chem>	-1.76	-3.21	3.01	4.24	14.02	14.82	0.64	0.62
S7966	<chem>O=c1occc2c1cccc2</chem>	-1.65	-1.61	3.73	4.94	13.95	14.56	0.39	0.46
S7967	<chem>O=c1ccc2c(o1)cccc2</chem>	-0.93	-1.61	4.83	4.94	15.46	14.56	0.63	0.56
S7970	<chem>O=c1ccc2c(s1)cccc2</chem>	-1.45	-2.30	4.33	4.08	14.40	13.56	0.48	0.41
S7972	<chem>c1ccc2c(c1)ncnc2</chem>	-1.84	-2.15	3.00	3.38	9.09	11.22	0.67	0.59
S7973	<chem>c1ccc2c(c1)nnnc2</chem>	0.40	-0.32	6.41	7.04	17.20	16.37	0.63	0.60
S7974	<chem>O=c1[nH]ncc2c1cccc2</chem>	-1.36	-1.38	4.00	4.07	13.31	11.88	0.68	0.58
S7982	<chem>O=c1sncc2c1cccc2</chem>	-0.33	-0.47	5.59	5.35	13.81	12.52	0.75	0.69
S7984	<chem>O=c1ncc2c(s1)cccc2</chem>	0.31	-0.47	6.14	6.65	17.65	17.28	0.49	0.52
S7986	<chem>O=c1cnc2c([nH]1)cccc2</chem>	-0.59	-1.38	5.25	6.36	13.44	15.42	0.59	0.51
S7987	<chem>O=c1nnc2c([nH]1)cccc2</chem>	1.31	0.45	8.23	10.79	19.18	22.49	0.54	0.47

S7988	<chem>O=c1[nH]c2ccccc2c(=O)[nH]1</chem>	0.14	-0.61	6.39	6.31	13.53	15.07	0.59	0.53
S7990	<chem>O=c1oc(=O)c2c([nH]1)cccc2</chem>	1.67	0.99	8.66	9.70	17.08	18.82	0.62	0.54
S7992	<chem>O=c1sc(=O)c2c([nH]1)cccc2</chem>	0.72	0.30	7.53	8.66	14.42	17.33	0.46	0.59
S7994	<chem>O=c1cc[nH]c2c1cccc2</chem>	-3.16	-3.21	8.61	6.76	22.75	19.78	0.53	0.44
S7995	<chem>O=c1nc[nH]c2c1cccc2</chem>	-1.26	-1.38	10.68	10.16	25.64	24.60	0.34	0.41
S7996	<chem>c1ccc2c(c1)nccn2</chem>	-2.66	-2.15	1.39	2.95	6.32	10.27	0.50	0.43
S7997	<chem>c1ccc2c(c1)nncn2</chem>	-0.52	-0.32	4.31	5.00	11.45	11.87	0.70	0.60
S7998	<chem>O=c1[nH]cnc2c1cccc2</chem>	-2.12	-1.38	5.82	5.40	13.67	13.34	0.33	0.38
S7999	<chem>O=c1cnc2c(o1)cccc2</chem>	0.23	0.22	3.70	5.51	11.11	13.00	0.64	0.71
S80	<chem>n1cncnc1</chem>	1.06	0.64	2.52	3.82	3.82	9.28	0.70	0.60
S8000	<chem>O=c1ocnc2c1cccc2</chem>	-0.39	0.22	3.35	5.21	10.88	11.83	0.36	0.35
S8002	<chem>O=c1scnc2c1cccc2</chem>	-1.25	-0.47	2.69	4.40	9.59	10.99	0.56	0.48
S8003	<chem>c1ccc2c(c1)nnnn2</chem>	1.75	1.51	7.67	8.07	16.07	15.72	0.44	0.55
S8004	<chem>O=c1[nH][n]c2c([n]1)cccc2</chem>	0.44	0.45	5.52	6.45	17.60	14.46	0.62	0.57
S8007	<chem>O=c1[nH]nnc2c1cccc2</chem>	-0.17	0.45	4.09	6.25	10.34	12.65	0.67	0.60
S8010	<chem>O=c1sn[n]c2c1cccc2</chem>	0.66	1.36	5.76	6.70	11.40	12.19	0.54	0.50
S8012	<chem>O=c1ccoc2c1cccc2</chem>	-1.99	-1.61	3.89	4.06	14.31	13.46	0.35	0.42
S8013	<chem>O=c1ncoc2c1cccc2</chem>	-0.12	0.22	4.88	6.57	16.15	17.03	0.62	0.54
S8014	<chem>O=c1ccsc2c1cccc2</chem>	-2.44	-2.30	3.04	3.42	13.14	13.20	0.43	0.40
S8015	<chem>O=c1cn[nH]c2c1cccc2</chem>	-1.34	-1.38	6.96	6.58	17.83	16.84	0.47	0.40
S8017	<chem>O=c1ensc2c1cccc2</chem>	-0.59	-0.47	4.49	4.69	11.81	12.16	0.50	0.46
S8018	<chem>O=c1nsc2c1cccc2</chem>	-0.75	-0.47	4.78	5.99	16.17	16.93	0.32	0.43
S8019	<chem>O=c1nn[nH]c2c1cccc2</chem>	0.54	0.45	9.57	11.01	22.14	23.91	0.64	0.70
S8021	<chem>O=c1nnsc2c1cccc2</chem>	1.06	1.36	6.75	8.28	15.81	18.13	0.50	0.44
S8023	<chem>O=c1oc2ccccc2c(=O)[nH]1</chem>	1.12	0.99	5.00	6.31	11.56	12.76	0.58	0.55
S8024	<chem>O=c1sc2ccccc2c(=O)[nH]1</chem>	0.42	0.30	5.13	5.49	11.62	12.01	0.37	0.37
S8030	<chem>O=c1oc2ccccc2c(=O)s1</chem>	1.51	1.90	6.11	7.40	12.44	13.97	0.78	0.82
S8032	<chem>O=c1oc(=O)c2c(s1)cccc2</chem>	1.79	1.90	7.17	7.62	14.75	14.71	0.39	0.50
S8035	<chem>c1ncc2c(c1)c[nH]c2</chem>	-4.73	-4.36	7.28	4.68	19.58	15.80	0.46	0.45
S8036	<chem>c1cnc2c(c1)c[nH]c2</chem>	-5.24	-4.36	5.40	4.08	17.37	14.87	0.39	0.48
S8037	<chem>c1ncc2c(c1)coc2</chem>	-2.59	-2.76	2.32	2.87	10.22	11.37	0.44	0.50

S8038	c1cnc2c(c1)coc2	-3.03	-2.76	2.34	3.08	10.42	11.58	0.59	0.57
S8039	c1ncc2c(c1)csc2	-2.99	-3.45	1.97	2.17	10.36	10.88	0.77	0.82
S8040	c1cnc2c(c1)csc2	-3.57	-3.45	1.88	2.33	10.44	10.95	0.56	0.61
S8041	c1ncc2c(c1)n[nH]c2	-3.09	-2.53	7.24	5.08	16.33	14.23	0.45	0.41
S8042	c1ncc2c(c1)c[nH]n2	-3.07	-2.53	7.16	5.75	17.03	15.70	0.44	0.50
S8043	c1cnc2c(c1)c[nH]n2	-3.33	-2.53	5.73	6.07	18.49	16.79	0.58	0.53
S8044	c1cnc2c(c1)n[nH]c2	-3.58	-2.53	5.00	4.24	12.99	12.76	0.54	0.55
S8045	c1ncc2c(c1)noc2	-0.62	-0.93	6.04	4.23	12.03	11.15	0.36	0.43
S8046	c1ncc2c(c1)con2	-0.61	-0.93	5.78	4.90	11.49	12.61	0.59	0.54
S8047	c1cnc2c(c1)con2	-0.76	-0.93	6.33	6.02	17.32	14.84	0.67	0.63
S8049	c1ncc2c(c1)nsc2	-1.43	-1.62	5.30	3.47	11.22	10.49	0.47	0.51
S8050	c1ncc2c(c1)csn2	-1.41	-1.62	5.36	4.14	12.30	11.96	0.32	0.40
S8051	c1cnc2c(c1)csn2	-1.72	-1.62	5.11	5.21	15.96	14.04	0.51	0.42
S8053	c1ncc2c(c1)n[nH]n2	-1.42	-0.70	5.92	5.13	12.34	11.89	0.52	0.45
S8054	c1cnc2c(c1)n[nH]n2	-1.64	-0.70	4.05	5.20	12.67	12.43	0.46	0.47
S8055	c1ncc2c(c1)non2	1.37	0.90	4.11	5.23	7.28	10.14	0.57	0.52
S8056	c1cnc2c(c1)non2	1.26	0.90	7.66	6.11	14.65	11.82	0.55	0.51
S8057	c1ncc2c(c1)nsn2	0.17	0.21	2.82	4.41	7.09	9.32	0.34	0.41
S8058	c1cnc2c(c1)nsn2	-0.10	0.21	4.63	5.24	11.68	10.86	0.79	0.73
S8059	n1ccc2c(c1)cncc2	-1.20	-2.15	3.16	3.68	8.25	11.87	0.32	0.36
S8060	c1ncc2c(c1)cncc2	-1.21	-2.15	2.40	3.41	7.29	11.28	0.45	0.55
S8061	c1cnc2c(c1)cncc2	-1.89	-2.15	3.80	3.63	10.33	11.78	0.32	0.40
S8062	c1cnc2c(c1)ccnc2	-1.86	-2.15	4.44	4.35	12.26	13.36	0.73	0.62
S8063	c1cnc2c(c1)cccn2	-2.35	-2.15	4.23	5.12	16.06	15.04	0.40	0.53
S8064	c1cnc2c(c1)ncnc2	-2.67	-2.15	1.54	3.21	7.25	10.85	0.45	0.54
S8065	n1ccc2c(c1)nncc2	0.15	-0.32	6.74	6.70	14.20	15.61	0.49	0.44
S8066	n1ccc2c(c1)ccnn2	0.12	-0.32	6.11	5.71	13.22	13.44	0.69	0.62
S8067	c1cnc2c(c1)nncc2	-0.61	-0.32	4.58	5.51	12.85	13.00	0.66	0.58
S8068	c1cnc2c(c1)ccnn2	-0.23	-0.32	7.39	8.14	19.48	18.78	0.80	0.83
S8069	n1ccc2c(c1)cnnc2	1.02	-0.32	5.59	5.75	13.86	13.53	0.29	0.33
S8070	c1ccc2c(n1)cnnc2	0.42	-0.32	7.24	6.66	17.62	15.52	0.45	0.50

S8071	O=c1[nH]ccc2c1cncc2	-1.34	-1.38	7.38	6.61	16.51	17.16	0.66	0.57
S8072	O=c1[nH]ccc2c1ccnc2	-1.30	-1.38	6.94	6.13	14.76	15.41	0.58	0.53
S8073	O=c1[nH]ccc2c1cccn2	-2.02	-1.38	5.31	5.41	13.53	13.71	0.64	0.52
S8074	O=c1[nH]ccc2c1nccc2	-2.09	-1.38	5.61	6.70	19.71	18.35	0.32	0.44
S8075	O=c1ccc2c([nH]1)ccnc2	0.18	-1.38	5.31	5.62	13.38	14.32	0.38	0.45
S8076	O=c1ccc2c([nH]1)cncc2	0.20	-1.38	5.26	5.11	13.67	13.90	0.71	0.69
S8077	O=c1ccc2c([nH]1)nccc2	-0.57	-1.38	5.73	5.00	16.25	14.66	0.59	0.56
S8078	O=c1ccc2c([nH]1)cccn2	-0.52	-1.38	6.12	6.35	15.50	15.75	0.63	0.62
S8083	O=c1occc2c1cncc2	0.36	0.22	6.53	6.86	14.93	16.27	0.61	0.57
S8084	O=c1occc2c1ccnc2	0.39	0.22	5.37	5.97	12.67	13.96	0.31	0.37
S8085	O=c1occc2c1cccn2	-0.29	0.22	3.71	5.59	11.67	12.74	0.51	0.56
S8086	O=c1occc2c1nccc2	-0.35	0.22	6.71	7.97	19.17	18.89	0.29	0.33
S8087	O=c1ccc2c(o1)ccnc2	1.03	0.22	6.32	5.81	14.12	13.34	0.60	0.59
S8088	O=c1ccc2c(o1)cncc2	1.09	0.22	7.77	6.39	15.94	14.45	0.53	0.59
S8090	O=c1ccc2c(o1)cccn2	0.30	0.22	4.84	5.89	13.64	13.88	0.49	0.55
S81	c1cnenn1	2.97	2.47	6.44	6.46	11.18	12.17	0.65	0.58
S8107	n1cnc2c(c1)ccnc2	0.16	-0.32	5.20	4.82	9.60	11.47	0.45	0.54
S8108	c1ncc2c(c1)ncnc2	0.13	-0.32	4.08	4.37	7.34	10.49	0.56	0.51
S8109	c1cnc2c(c1)ncnc2	-0.56	-0.32	4.66	4.62	9.52	11.04	0.48	0.55
S8110	c1cnc2c(c1)cnnc2	-0.27	-0.32	6.36	5.81	15.37	13.66	0.71	0.64
S8111	c1ncc2c(c1)cnnc2	2.35	1.51	8.51	8.19	16.28	15.97	0.53	0.47
S8112	n1ccc2c(c1)cnnc2	2.31	1.51	7.33	7.47	14.85	14.39	0.80	0.66
S8113	c1cnc2c(c1)nnnc2	1.68	1.51	8.01	7.95	17.11	15.44	0.42	0.48
S8114	c1cnc2c(c1)cnnc2	2.02	1.51	9.81	9.86	20.37	19.64	0.33	0.40
S8115	O=c1[nH]ncc2c1cncc2	0.61	0.45	6.22	5.88	13.75	12.98	0.30	0.34
S8116	O=c1[nH]ncc2c1ccnc2	0.66	0.45	4.62	5.66	11.05	11.83	0.32	0.42
S8117	O=c1[nH]ncc2c1cccn2	0.01	0.45	4.65	5.61	11.52	11.61	0.38	0.38
S8118	O=c1[nH]ncc2c1nccc2	-0.07	0.45	7.12	6.19	19.22	14.67	0.81	0.83
S8123	O=c1ncc2c([nH]1)cncc2	2.08	0.45	6.91	7.95	17.22	17.48	0.53	0.50
S8124	O=c1ncc2c([nH]1)ccnc2	2.08	0.45	7.99	8.73	18.17	18.49	0.44	0.51
S8125	O=c1ncc2c([nH]1)cccn2	1.45	0.45	8.88	10.13	20.58	21.41	0.60	0.53

S8126	<chem>O=c1ncc2c([nH]1)necc2</chem>	1.35	0.45	7.81	8.06	20.00	18.74	0.48	0.52
S8149	<chem>O=c1sncc2c1cccn2</chem>	0.93	1.36	6.37	6.42	12.39	11.62	0.41	0.45
S8150	<chem>O=c1sncc2c1necc2</chem>	0.88	1.36	8.63	8.01	19.01	16.01	0.62	0.66
S8163	<chem>O=c1cnc2c([nH]1)ccnc2</chem>	1.43	0.45	7.96	8.12	13.25	15.76	0.41	0.47
S8164	<chem>O=c1cnc2c([nH]1)cncc2</chem>	1.40	0.45	6.45	6.89	12.02	13.77	0.56	0.63
S8165	<chem>O=c1cnc2c([nH]1)necc2</chem>	0.60	0.45	4.48	6.35	12.10	13.59	0.77	0.74
S8166	<chem>O=c1cnc2c([nH]1)cccn2</chem>	0.97	0.45	8.54	9.61	15.63	18.88	0.53	0.44
S8167	<chem>O=c1nnc2c([nH]1)ccnc2</chem>	3.28	2.28	11.03	12.25	18.98	22.18	0.61	0.55
S8168	<chem>O=c1nnc2c([nH]1)cncc2</chem>	3.20	2.28	9.54	10.75	17.48	19.59	0.57	0.50
S8169	<chem>O=c1nnc2c([nH]1)necc2</chem>	2.48	2.28	7.55	10.44	17.37	19.91	0.45	0.41
S8170	<chem>O=c1nnc2c([nH]1)cccn2</chem>	2.86	2.28	11.68	14.42	21.17	26.78	0.57	0.48
S8171	<chem>O=c1[nH]c2ccncc2c(=O)[nH]1</chem>	2.15	1.22	9.07	8.43	14.82	16.25	0.59	0.53
S8172	<chem>O=c1[nH]c2cnccc2c(=O)[nH]1</chem>	2.16	1.22	7.49	7.44	11.81	14.09	0.60	0.52
S8173	<chem>O=c1[nH]c2ncccc2c(=O)[nH]1</chem>	1.40	1.22	5.10	6.60	11.18	13.15	0.54	0.46
S8174	<chem>O=c1[nH]c2ccncc2c(=O)[nH]1</chem>	1.40	1.22	9.52	9.24	19.63	18.87	0.58	0.52
S8175	<chem>O=c1[nH]c2cnccc2[nH]c1=O</chem>	2.58	1.22	8.51	9.79	17.55	22.23	0.35	0.43
S8176	<chem>O=c1[nH]c2ncccc2[nH]c1=O</chem>	1.82	1.22	8.88	10.40	19.63	24.42	0.58	0.55
S8177	<chem>O=c1oc(=O)c2c([nH]1)ccnc2</chem>	3.64	2.82	11.50	11.38	17.83	19.38	0.58	0.51
S8178	<chem>O=c1oc(=O)c2c([nH]1)cncc2</chem>	3.64	2.82	9.98	9.98	15.90	16.65	0.24	0.29
S8179	<chem>O=c1oc(=O)c2c([nH]1)necc2</chem>	2.91	2.82	7.39	9.48	15.00	16.18	0.71	0.62
S8185	<chem>O=c1sc(=O)c2c([nH]1)ccnc2</chem>	2.69	2.13	10.20	10.37	15.18	17.96	0.54	0.59
S8186	<chem>O=c1sc(=O)c2c([nH]1)cncc2</chem>	2.70	2.13	8.50	9.00	13.03	15.30	0.56	0.61
S8187	<chem>O=c1sc(=O)c2c([nH]1)necc2</chem>	1.87	2.13	6.55	8.48	13.03	14.78	0.57	0.51
S8188	<chem>O=c1sc(=O)c2c([nH]1)cccn2</chem>	1.89	2.13	10.60	12.14	19.41	21.84	0.82	0.75
S8189	<chem>O=c1[nH]c2ccncc2sc1=O</chem>	2.83	2.13	9.52	10.86	16.78	21.64	0.63	0.53
S8190	<chem>O=c1[nH]c2cnccc2sc1=O</chem>	2.80	2.13	7.73	9.85	14.87	20.30	0.68	0.64
S8191	<chem>O=c1[nH]c2ncccc2sc1=O</chem>	1.94	2.13	7.03	9.86	16.01	21.70	0.79	0.74
S8193	<chem>O=c1cc[nH]c2c1cncc2</chem>	-1.15	-1.38	10.48	7.58	21.64	18.73	0.83	0.75
S8194	<chem>O=c1cc[nH]c2c1cncc2</chem>	-1.13	-1.38	11.36	9.17	23.55	22.19	0.65	0.55
S8195	<chem>O=c1cc[nH]c2c1necc2</chem>	-1.86	-1.38	10.85	10.49	27.71	25.28	0.84	0.84
S8196	<chem>O=c1cc[nH]c2c1cccn2</chem>	-1.89	-1.38	6.33	6.25	18.04	16.10	0.30	0.35

S8197	<chem>O=c1nc[nH]c2c1ccnc2</chem>	0.73	0.45	12.43	10.42	24.41	22.31	0.61	0.56
S8198	<chem>O=c1nc[nH]c2c1cncc2</chem>	0.73	0.45	13.46	12.28	26.31	26.36	0.45	0.41
S8199	<chem>O=c1nc[nH]c2c1nccc2</chem>	0.09	0.45	13.00	14.27	29.69	30.94	0.42	0.48
S82	<chem>O=c1cn[nH]1</chem>	1.86	1.41	4.83	5.60	10.72	11.19	0.60	0.67
S8200	<chem>O=c1nc[nH]c2c1cccn2</chem>	0.03	0.45	8.27	9.32	21.04	20.18	0.61	0.53
S8201	<chem>n1ccc2c(c1)ncn2</chem>	-0.61	-0.32	4.62	4.61	10.43	11.02	0.67	0.71
S8202	<chem>c1ccc2c(n1)ncn2</chem>	-1.14	-0.32	3.23	4.95	11.88	11.77	0.77	0.73
S8203	<chem>n1ccc2c(c1)ncnn2</chem>	1.46	1.51	4.15	6.10	7.83	11.38	0.36	0.37
S8204	<chem>n1ccc2c(c1)nnn2</chem>	1.48	1.51	4.15	6.37	8.21	11.98	0.34	0.41
S8207	<chem>O=c1[nH]cnc2c1ccnc2</chem>	0.01	0.45	8.76	7.67	14.68	14.77	0.59	0.59
S8208	<chem>O=c1[nH]cnc2c1cncc2</chem>	-0.06	0.45	8.91	7.43	15.53	14.94	0.49	0.40
S8209	<chem>O=c1[nH]cnc2c1nccc2</chem>	-0.86	0.45	6.98	7.09	18.19	15.20	0.64	0.54
S8210	<chem>O=c1[nH]cnc2c1cccn2</chem>	-0.49	0.45	7.24	7.71	15.45	14.76	0.38	0.41
S8211	<chem>O=c1cnc2c(o1)ccnc2</chem>	2.26	2.05	6.64	6.76	11.19	12.62	0.58	0.65
S8212	<chem>O=c1cnc2c(o1)cncc2</chem>	2.26	2.05	6.88	6.62	11.72	12.15	0.54	0.49
S8215	<chem>O=c1ocnc2c1ccnc2</chem>	1.71	2.05	6.01	6.62	10.56	12.07	0.43	0.54
S8216	<chem>O=c1ocnc2c1cncc2</chem>	1.63	2.05	6.08	6.79	11.74	12.81	0.65	0.60
S8217	<chem>O=c1ocnc2c1nccc2</chem>	0.89	2.05	5.66	7.48	15.33	14.49	0.38	0.46
S8218	<chem>O=c1ocnc2c1cccn2</chem>	1.25	2.05	5.07	7.01	10.31	12.54	0.45	0.51
S8222	<chem>O=c1cnc2c(s1)ccn2</chem>	1.00	1.36	6.36	6.93	12.06	14.31	0.35	0.41
S8226	<chem>O=c1scnc2c1cccn2</chem>	0.26	1.36	4.21	6.24	10.26	11.77	0.73	0.71
S8227	<chem>n1ccc2c(c1)nnnn2</chem>	3.68	3.34	8.02	8.88	13.19	14.58	0.61	0.51
S8228	<chem>c1ccc2c(n1)nnnn2</chem>	3.34	3.34	10.32	10.13	17.99	17.32	0.55	0.47
S8229	<chem>O=c1[nH][n]c2c([n]1)ccnc2</chem>	2.35	2.28	7.57	7.83	16.66	13.98	0.77	0.63
S823	<chem>[nH]1cc2c(c1)ccs2</chem>	-6.33	-5.66	4.23	2.52	16.34	13.32	0.35	0.39
S8230	<chem>O=c1[nH][n]c2c([n]1)cncc2</chem>	2.44	2.28	7.35	8.43	16.39	15.28	0.38	0.46
S824	<chem>o1cc2c(c1)ccs2</chem>	-4.15	-4.06	0.27	1.41	7.60	10.00	0.38	0.39
S8241	<chem>O=c1[nH]nnc2c1cncc2</chem>	1.82	2.28	5.49	7.72	9.88	13.01	0.77	0.70
S8242	<chem>O=c1[nH]nnc2c1ccnc2</chem>	1.91	2.28	5.58	8.22	8.95	13.44	0.36	0.43
S8244	<chem>O=c1[nH]nnc2c1nccc2</chem>	1.10	2.28	6.36	7.61	15.27	13.76	0.68	0.63
S825	<chem>c1cc2c(s1)scc2</chem>	-4.59	-4.75	-0.12	0.77	7.50	9.39	0.55	0.55

S8255	O=c1sn[n]c2c1cccn2	2.21	3.19	7.56	8.91	12.65	13.82	0.51	0.44
S826	c1cc2c(s1)ccs2	-4.58	-4.75	-0.17	0.62	7.36	9.37	0.33	0.43
S8261	O=c1ccoc2c1ccnc2	0.09	0.22	6.21	5.46	13.63	13.22	0.59	0.56
S8262	O=c1ccoc2c1cncc2	0.05	0.22	6.51	5.97	15.15	15.16	0.61	0.61
S8263	O=c1ccoc2c1nccc2	-0.73	0.22	5.64	6.64	18.87	17.35	0.51	0.65
S8264	O=c1ccoc2c1cccn2	-0.45	0.22	3.77	5.29	11.76	12.21	0.61	0.69
S8265	O=c1ncoc2c1ccnc2	1.93	2.05	7.65	7.41	15.87	15.55	0.43	0.48
S8266	O=c1ncoc2c1cncc2	1.89	2.05	8.12	8.19	17.35	18.08	0.78	0.66
S8267	O=c1ncoc2c1nccc2	1.20	2.05	8.04	9.54	20.99	21.77	0.43	0.48
S8268	O=c1ncoc2c1cccn2	1.45	2.05	5.63	7.47	14.69	15.04	0.79	0.67
S827	s1cc2c(c1)ccs2	-4.57	-4.75	0.05	0.67	7.67	9.38	0.71	0.59
S8273	O=c1cn[nH]c2c1ccnc2	0.65	0.45	8.57	7.11	16.51	15.15	0.58	0.53
S8274	O=c1cn[nH]c2c1cncc2	0.64	0.45	9.66	8.44	18.47	18.01	0.58	0.52
S8276	O=c1cn[nH]c2c1cccn2	-0.01	0.45	4.23	6.46	12.70	14.00	0.40	0.48
S828	c1cc2c(s1)[nH]nc2	-3.80	-3.83	2.48	2.99	10.32	12.74	0.81	0.74
S8283	O=c1cns2c1nccc2	0.57	1.36	7.09	7.01	17.18	15.51	0.82	0.77
S8289	O=c1nn[nH]c2c1ccnc2	2.52	2.28	11.24	10.97	20.75	20.97	0.64	0.53
S829	c1sc2c(c1)[nH]nc2	-3.75	-3.83	3.18	3.55	11.18	12.91	0.81	0.78
S8290	O=c1nn[nH]c2c1cncc2	2.50	2.28	12.35	12.57	22.44	24.43	0.73	0.60
S8292	O=c1nn[nH]c2c1cccn2	1.90	2.28	7.00	10.55	17.35	20.33	0.45	0.56
S83	O=c1ncnc[nH]1	2.03	1.41	11.12	8.21	20.61	16.87	0.53	0.45
S830	c1cc2c(s1)n[nH]c2	-4.53	-3.83	4.09	3.69	13.82	12.99	0.35	0.42
S8303	O=c1oc2cnccc2c(=O)[nH]1	3.18	2.82	8.47	8.01	12.77	12.59	0.57	0.51
S8304	O=c1oc2ccncc2c(=O)[nH]1	3.12	2.82	8.29	7.92	12.13	13.23	0.61	0.53
S8305	O=c1oc2cccnc2c(=O)[nH]1	2.36	2.82	7.51	8.09	15.03	14.96	0.32	0.41
S8306	O=c1oc2ncccc2c(=O)[nH]1	2.63	2.82	6.73	8.34	13.56	13.27	0.63	0.51
S8307	O=c1sc2cnccc2c(=O)[nH]1	2.44	2.13	6.74	7.16	10.87	11.74	0.35	0.40
S8308	O=c1sc2ccncc2c(=O)[nH]1	2.40	2.13	6.43	7.14	10.27	12.57	0.35	0.43
S8309	O=c1sc2cccnc2c(=O)[nH]1	1.56	2.13	7.63	7.35	15.68	14.40	0.66	0.57
S831	c1cc2c(s1)c[nH]n2	-4.60	-3.83	3.96	3.19	12.51	12.78	0.44	0.44
S832	c1cc2c(s1)onc2	-1.76	-2.23	3.28	3.34	11.23	10.89	0.58	0.61

S833	c1cc2c(s1)cno2	-1.82	-2.23	3.43	3.14	11.50	10.85	0.39	0.46
S8330	O=c1oc2ncccc2c(=O)s1	2.92	3.73	7.71	8.95	14.26	13.85	0.58	0.51
S8332	O=c1sc2c(s1)cccn2	0.18	0.06	6.01	5.76	13.08	13.36	0.40	0.47
S834	c1cc2c(s1)noc2	-2.02	-2.23	3.78	3.54	12.52	11.01	0.57	0.46
S8343	c1nnc2c(c1)c[nH]c2	-3.17	-2.53	8.66	7.32	22.15	18.70	0.54	0.58
S8344	c1nnc2c(c1)coc2	-1.08	-0.93	4.66	5.51	14.08	14.27	0.53	0.48
S8345	c1nnc2c(c1)csc2	-1.59	-1.62	4.53	4.81	14.72	13.78	0.59	0.68
S8346	c1nnc2c(c1)n[nH]c2	-1.54	-0.70	8.48	6.97	18.73	15.47	0.75	0.64
S8347	c1nnc2c(c1)c[nH]n2	-1.25	-0.70	9.05	9.47	21.97	20.96	0.42	0.49
S8349	c1nnc2c(c1)con2	1.17	0.90	9.04	8.61	18.07	17.88	0.34	0.42
S835	c1cc2c(s1)con2	-2.09	-2.23	3.09	3.04	11.42	10.80	0.58	0.63
S8351	c1nnc2c(c1)csn2	0.30	0.21	8.25	7.85	19.00	17.22	0.65	0.67
S8352	c1nnc2c(c1)n[nH]n2	0.39	1.13	7.45	8.09	16.57	15.49	0.83	0.83
S8355	c1nnc2c(c1)ccnn2	1.81	1.51	10.07	10.87	19.82	21.87	0.33	0.33
S8357	n1ncc2c(c1)nncc2	2.39	1.51	9.53	8.44	16.48	16.53	0.65	0.66
S8358	O=c1[nH]ccc2c1nncc2	-0.01	0.45	8.84	10.09	22.01	22.93	0.56	0.48
S8359	O=c1[nH]ccc2c1ccnn2	0.15	0.45	8.06	8.31	16.21	16.55	0.40	0.50
S836	c1cc2c(s1)snc2	-2.47	-2.92	2.69	2.50	9.84	10.08	0.59	0.49
S8365	O=c1occc2c1ccnn2	1.85	2.05	5.37	7.64	10.69	14.38	0.44	0.44
S8366	O=c1ccc2c(o1)ccnn2	2.35	2.05	6.19	7.78	11.73	14.91	0.24	0.30
S837	c1sc2c(c1)snc2	-2.46	-2.92	3.00	2.35	10.39	10.07	0.62	0.75
S8376	c1nnc2c(c1)cncn2	1.79	1.51	9.14	8.27	17.96	16.15	0.57	0.51
S8377	n1cnc2c(c1)nncc2	1.45	1.51	4.78	6.63	9.96	12.55	0.59	0.47
S8378	c1nnc2c(c1)cnnn2	4.03	3.34	12.73	12.02	20.14	21.49	0.59	0.62
S838	c1cc2c(s1)nsc2	-2.85	-2.92	3.21	2.73	11.03	10.22	0.61	0.51
S8380	O=c1[nH]ncc2c1nncc2	1.95	2.28	9.73	9.01	20.67	18.01	0.62	0.55
S8381	O=c1[nH]ncc2c1ccnn2	2.13	2.28	5.71	8.22	10.18	13.80	0.64	0.55
S839	c1cc2c(s1)csn2	-2.93	-2.92	2.33	2.23	9.52	10.01	0.30	0.30
S840	c1cc2c(s1)[nH]cn2	-4.18	-3.83	6.25	4.67	16.50	15.53	0.43	0.50
S8405	O=c1cnc2c([nH]1)nncc2	2.66	2.28	6.98	7.91	11.76	14.18	0.44	0.53
S8407	O=c1nnc2c([nH]1)nncc2	4.44	4.11	9.87	11.43	16.46	19.26	0.62	0.69

S8409	O=c1[nH]c2nnccc2c(=O)[nH]1	3.54	3.05	8.69	8.76	12.38	14.42	0.42	0.37
S841	c1sc2c(c1)[nH]cn2	-4.05	-3.83	6.75	5.73	17.46	15.91	0.69	0.75
S8416	O=c1sc(=O)c2c([nH]1)nncc2	3.95	3.96	9.31	9.84	13.41	15.00	0.68	0.60
S8419	O=c1cc[nH]c2c1ccnn2	0.25	0.45	8.61	8.10	16.85	17.30	0.77	0.66
S842	c1nc2c(o1)sc2	-2.41	-2.23	1.56	2.52	7.63	10.19	0.48	0.45
S8421	O=c1nc[nH]c2c1ccnn2	2.16	2.28	10.31	10.60	19.59	20.13	0.58	0.47
S8423	c1cnc2c(n1)nncc2	0.96	1.51	6.61	7.64	16.01	14.77	0.68	0.60
S8426	O=c1[nH]cnc2c1ccnn2	1.75	2.28	10.43	11.00	19.91	18.43	0.75	0.77
S8427	O=c1[nH]cnc2c1nncc2	1.25	2.28	10.42	10.15	21.06	19.04	0.32	0.39
S843	c1oc2c(n1)sc2	-2.34	-2.23	1.62	2.83	8.05	10.36	0.51	0.45
S8430	O=c1ocnc2c1ccnn2	3.46	3.88	8.78	9.44	15.25	15.02	0.74	0.68
S844	c1sc2c(c1)ncs2	-3.12	-2.92	0.96	1.85	7.46	9.81	0.32	0.39
S845	c1sc2c(c1)scn2	-3.02	-2.92	1.55	2.20	8.47	10.01	0.46	0.60
S8454	O=c1ccoc2c1ccnn2	1.78	2.05	6.45	7.72	12.41	14.21	0.63	0.61
S8456	O=c1ncoc2c1ccnn2	3.64	3.88	8.81	9.33	14.30	15.80	0.32	0.40
S846	c1cc2c(s1)[nH]nn2	-2.01	-2.00	5.78	6.15	15.85	16.45	0.60	0.59
S8460	O=c1cn[nH]c2c1ccnn2	2.09	2.28	5.91	8.02	10.91	14.55	0.42	0.37
S8468	O=c1nn[nH]c2c1ccnn2	3.99	4.11	9.26	11.54	15.97	19.64	0.35	0.46
S847	c1sc2c(c1)[nH]nn2	-1.86	-2.00	6.39	7.21	16.84	16.83	0.28	0.37
S8472	O=c1ccc(=O)n2n1cccc2	0.36	0.89	3.83	6.12	9.96	13.76	0.52	0.45
S848	[nH]1nc2c(n1)ccs2	-2.76	-2.00	2.87	3.34	8.02	10.20	0.50	0.40
S849	c1cc2c(s1)onn2	-0.15	-0.40	5.01	4.95	11.54	12.44	0.65	0.57
S850	c1cc2c(s1)nno2	-0.05	-0.40	5.71	5.25	12.75	12.61	0.47	0.52
S851	c1cc2c(s1)snn2	-0.94	-1.09	4.30	4.21	11.95	11.89	0.60	0.53
S852	c1cc2c(s1)nns2	-0.83	-1.09	4.95	4.57	13.02	12.09	0.47	0.61
S8528	[nH]1cc2c(c1)cnnc2	-2.47	-2.53	10.45	7.92	25.63	19.62	0.82	0.73
S8529	o1cc2c(c1)cnnc2	-0.38	-0.93	5.18	5.30	16.31	14.07	0.41	0.47
S853	O=c1c(=O)c2c(c1=O)sc2	3.74	4.62	9.85	10.06	16.80	20.55	0.84	0.94
S8530	s1cc2c(c1)cnnc2	-0.77	-1.62	4.96	4.66	16.65	13.71	0.40	0.32
S8531	n1ncc2c(c1)n[nH]c2	-0.85	-0.70	10.52	8.48	22.95	18.41	0.52	0.50
S8532	n1ncc2c(c1)noc2	1.56	0.90	9.06	6.82	16.87	14.18	0.52	0.62

S8533	<chem>n1ncc2c(c1)nsc2</chem>	0.80	0.21	8.40	6.11	18.10	13.67	0.33	0.43
S8534	<chem>n1ncc2c(c1)n[nH]n2</chem>	0.78	1.13	9.15	8.02	18.44	14.94	0.33	0.43
S8537	<chem>n1ncc2c(c1)cnnc2</chem>	3.17	1.51	7.26	7.54	11.78	14.54	0.57	0.49
S8538	<chem>O=c1[nH]ccc2c1cnnc2</chem>	0.97	0.45	10.47	9.52	20.78	19.99	0.47	0.58
S854	<chem>o1nc2c(n1)ccs2</chem>	0.08	-0.40	6.46	4.14	12.80	9.55	0.35	0.35
S8541	<chem>O=c1occc2c1cnnc2</chem>	2.63	2.05	8.84	8.92	16.12	17.92	0.50	0.44
S8542	<chem>O=c1ccc2c(o1)cnnc2</chem>	3.29	2.05	9.85	8.28	16.23	15.48	0.69	0.59
S8547	<chem>c1ncc2c(n1)cnnc2</chem>	2.38	1.51	7.62	6.83	14.61	12.98	0.77	0.80
S8548	<chem>n1ncc2c(c1)nnnc2</chem>	4.52	3.34	11.22	9.64	15.26	16.24	0.48	0.39
S8549	<chem>O=c1[nH]ncc2c1cnnc2</chem>	2.88	2.28	8.21	8.49	14.62	15.17	1.07	0.95
S855	<chem>s1nc2c(n1)ccs2</chem>	-1.13	-1.09	3.80	3.28	7.94	8.60	0.34	0.42
S856	<chem>O=c1[nH]c2c([nH]1)ccs2</chem>	-2.11	-3.06	2.98	4.28	13.38	14.87	0.37	0.44
S8561	<chem>O=c1cnc2c([nH]1)cnnc2</chem>	3.66	2.28	10.32	9.67	16.98	16.35	0.32	0.32
S8562	<chem>O=c1nnc2c([nH]1)cnnc2</chem>	5.43	4.11	13.65	13.24	18.26	21.53	0.59	0.46
S8563	<chem>O=c1[nH]c2cnnc2c(=O)[nH]1</chem>	4.39	3.05	11.43	10.59	17.19	17.52	0.40	0.48
S8567	<chem>O=c1sc(=O)c2c([nH]1)cnnc2</chem>	4.91	3.96	12.48	11.73	16.82	18.19	0.70	0.64
S8569	<chem>O=c1cc[nH]c2c1cnnc2</chem>	1.14	0.45	13.77	11.02	23.52	23.39	0.34	0.44
S857	<chem>O=c1oc2c([nH]1)ccs2</chem>	-0.62	-1.46	5.95	6.45	15.71	15.26	0.34	0.46
S8570	<chem>O=c1nc[nH]c2c1cnnc2</chem>	2.96	2.28	15.90	13.56	25.57	26.32	0.38	0.45
S8571	<chem>c1cnc2c(n1)cnnc2</chem>	1.71	1.51	8.41	7.30	17.20	14.02	0.61	0.61
S8572	<chem>n1cnc2c(n1)cnnc2</chem>	3.72	3.34	8.77	8.49	13.78	13.73	0.54	0.68
S8573	<chem>O=c1[nH]cnc2c1cnnc2</chem>	2.31	2.28	12.45	10.72	21.54	18.61	0.50	0.41
S8574	<chem>O=c1cnc2c(o1)cnnc2</chem>	4.53	3.88	11.28	8.89	16.79	14.02	0.37	0.45
S8575	<chem>O=c1ocnc2c1cnnc2</chem>	3.96	3.88	10.60	9.23	16.55	15.29	0.57	0.48
S858	<chem>O=c1oc2c([nH]1)sc2</chem>	-0.67	-1.46	5.50	5.69	15.22	15.06	0.92	0.85
S8582	<chem>O=c1[nH]nnc2c1cnnc2</chem>	4.14	4.11	10.21	10.71	15.26	16.04	0.62	0.55
S8587	<chem>O=c1ccoc2c1cnnc2</chem>	2.36	2.05	9.53	8.39	17.33	17.16	0.31	0.40
S8588	<chem>O=c1ncoc2c1cnnc2</chem>	4.16	3.88	12.01	10.04	17.88	18.85	0.69	0.63
S859	<chem>O=c1sc2c([nH]1)ccs2</chem>	-1.39	-2.15	5.30	5.49	14.28	14.18	0.64	0.52
S8590	<chem>O=c1cn[nH]c2c1cnnc2</chem>	2.89	2.28	11.90	9.99	18.86	18.56	0.40	0.49
S8594	<chem>O=c1nn[nH]c2c1cnnc2</chem>	4.70	4.11	14.76	13.55	21.55	23.75	0.31	0.40

S8599	O=c1sc2cncc2c(=O)[nH]1	4.66	3.96	10.93	9.83	15.59	14.55	0.32	0.38
S860	O=c1sc2c([nH]1)sc2	-1.41	-2.15	4.49	4.78	13.44	14.00	0.61	0.51
S861	c1ccc2c(c1)sc2	-4.87	-5.28	-0.22	0.71	8.17	10.30	0.42	0.51
S8611	O=c1cccc2n1cc[nH]2	-3.16	-2.84	9.59	6.49	24.24	19.41	0.74	0.83
S8612	O=c1[nH]ccc2c1c[nH]c2	-4.59	-3.59	5.59	5.30	18.78	17.09	0.50	0.66
S8616	O=c1[nH]ccc2c1coc2	-2.35	-1.99	4.32	5.21	14.19	14.69	0.54	0.48
S862	c1ncc2c(c1)sc2	-2.88	-3.45	2.38	2.18	10.27	10.89	0.93	0.97
S8620	O=c1[nH]ccc2c1csc2	-2.91	-2.68	4.18	4.40	14.32	13.95	0.53	0.62
S8621	O=c1ccc2c([nH]1)csc2	-1.63	-2.68	3.70	4.05	14.24	13.81	0.49	0.60
S8623	O=c1cccc2n1cn[nH]2	-1.01	-1.01	8.36	7.88	19.49	19.61	0.67	0.66
S8624	O=c1[nH]ccc2c1c[nH]n2	-2.81	-1.76	5.09	5.95	15.04	15.20	0.57	0.66
S8625	O=c1[nH]ccc2c1n[nH]c2	-2.96	-1.76	5.70	7.22	20.20	19.68	0.32	0.44
S8626	O=c1ccc2c([nH]1)n[nH]c2	-1.83	-1.76	7.84	6.52	20.11	17.30	0.75	0.65
S863	c1ncc2c(c1)ccs2	-2.90	-3.45	2.72	2.38	10.81	10.97	0.42	0.50
S8630	O=c1[nH]ccc2c1con2	-0.23	-0.16	7.22	6.82	13.63	14.14	0.31	0.42
S8631	O=c1[nH]ccc2c1noc2	-0.39	-0.16	7.18	8.08	18.75	18.62	0.53	0.52
S8635	O=c1cccc2n1cns2	0.15	-0.10	4.61	6.51	12.69	15.43	0.97	0.97
S864	c1cnc2c(c1)ccs2	-3.40	-3.45	2.29	2.65	10.66	11.08	0.52	0.38
S8640	O=c1cccc2n1[nH]cn2	-1.24	-1.01	8.58	7.50	17.94	16.50	0.37	0.46
S8645	O=c1cccc2n1ncs2	-0.94	-0.10	6.26	6.45	19.60	17.51	0.73	0.68
S8648	O=c1[nH]ccc2c1n[nH]n2	-1.10	0.07	5.88	6.85	16.87	15.54	0.39	0.43
S8649	O=c1ccc2c([nH]1)n[nH]n2	-0.13	0.07	6.27	6.69	15.43	14.35	0.41	0.49
S865	c1cnc2c(c1)sc2	-3.48	-3.45	1.60	2.11	9.47	10.86	0.75	0.67
S8655	O=c1[nH]ccc2c1non2	1.80	1.67	10.45	8.66	17.86	15.82	0.41	0.53
S8656	O=c1ccc2c([nH]1)non2	2.73	1.67	6.77	6.71	10.95	12.14	0.69	0.69
S8657	O=c1[nH]ccc2c1nsn2	0.38	0.98	7.89	7.73	17.40	14.75	0.73	0.65
S8658	O=c1ccc2c([nH]1)nsn2	1.48	0.98	4.52	5.90	11.24	11.38	0.86	0.73
S866	c1nnc2c(c1)sc2	-1.41	-1.62	4.06	4.60	14.19	13.69	0.76	0.63
S8664	O=c1cccc2n1cccc2	-2.30	-2.46	4.44	4.36	16.04	15.08	0.75	0.74
S8665	O=c1cccc2n1ccnc2	-0.31	-0.63	4.52	6.08	13.37	15.33	0.42	0.54
S8666	O=c1cccc2n1cncc2	-0.37	-0.63	5.40	6.67	14.62	17.27	0.61	0.49

S8667	<chem>O=c1cccc2n1nccc2</chem>	-1.40	-0.63	7.03	6.77	21.71	18.63	0.29	0.30
S8668	<chem>O=c1cccc2n1cccn2</chem>	-1.06	-0.63	5.32	5.42	14.49	13.75	0.66	0.66
S867	<chem>c1nnc2c(c1)ccs2</chem>	-1.31	-1.62	5.02	5.33	15.40	14.00	0.33	0.42
S8672	<chem>O=c1[nH]ccc2c1c(=O)[nH]cc2</chem>	-2.17	-0.61	6.27	7.84	23.51	21.12	0.49	0.62
S8673	<chem>O=c1[nH]ccc2c1cc[nH]c2=O</chem>	-1.43	-0.61	5.11	6.96	13.14	16.00	0.59	0.68
S8676	<chem>O=c1ccc2c([nH]1)[nH]c(=O)cc2</chem>	1.66	-0.61	8.31	7.90	15.33	16.87	0.45	0.54
S8677	<chem>O=c1ccc2c([nH]1)ccc(=O)[nH]2</chem>	1.80	-0.61	7.36	6.95	15.17	16.58	0.52	0.62
S8678	<chem>O=c1cccc2n1cc[nH]c2=O</chem>	-0.50	0.14	7.25	7.14	15.95	16.23	0.67	0.53
S8679	<chem>O=c1cccc2n1c(=O)[nH]cc2</chem>	-1.31	0.14	8.44	7.97	23.55	21.53	0.63	0.52
S868	<chem>n1ncc2c(c1)sc2</chem>	-0.71	-1.62	5.69	4.87	16.58	13.80	0.55	0.45
S8681	<chem>O=c1ccn2c([nH]1)cccc2=O</chem>	1.02	0.14	6.73	8.62	13.81	19.67	0.65	0.66
S8682	<chem>O=c1[nH]cc2c(c1)cc[nH]c2=O</chem>	-0.36	-0.61	7.29	7.21	17.64	17.01	0.42	0.51
S8683	<chem>O=c1[nH]cc2c(c1)c(=O)[nH]cc2</chem>	-0.50	-0.61	8.02	8.29	19.70	20.83	0.32	0.33
S8686	<chem>O=c1occc2c1c(=O)[nH]cc2</chem>	-0.38	0.99	9.08	9.66	24.62	22.48	0.66	0.67
S8687	<chem>O=c1occc2c1cc[nH]c2=O</chem>	0.34	0.99	7.87	8.05	15.57	15.68	0.63	0.55
S869	<chem>O=c1[nH]ccc2c1ccs2</chem>	-2.85	-2.68	5.26	4.15	16.03	13.82	0.41	0.52
S8690	<chem>O=c1ccc2c(o1)cc[nH]c2=O</chem>	0.85	0.99	10.00	8.56	19.13	17.77	0.32	0.41
S87	<chem>O=c1ncncl</chem>	2.38	2.32	7.96	6.38	15.52	13.41	0.62	0.77
S870	<chem>O=c1[nH]ccc2c1sc2</chem>	-2.86	-2.68	4.93	4.52	16.72	14.07	0.59	0.49
S871	<chem>O=c1ccc2c([nH]1)sc2</chem>	-1.52	-2.68	3.45	3.92	14.44	13.82	0.47	0.54
S8718	<chem>O=c1[nH]ccc2c1ncnc2</chem>	0.03	0.45	8.19	7.99	19.36	17.64	0.30	0.40
S8719	<chem>O=c1[nH]ccc2c1cncn2</chem>	0.08	0.45	8.46	7.18	14.94	14.75	0.31	0.41
S872	<chem>O=c1ccc2c([nH]1)ccs2</chem>	-1.53	-2.68	4.46	4.31	15.94	13.89	0.32	0.39
S8720	<chem>O=c1ccc2c([nH]1)cncn2</chem>	1.50	0.45	6.72	6.63	13.40	13.54	0.38	0.49
S8721	<chem>O=c1ccc2c([nH]1)ncnc2</chem>	1.41	0.45	6.55	5.79	13.99	12.86	0.65	0.62
S8722	<chem>O=c1cccc2n1cncn2</chem>	0.96	1.20	4.94	7.14	11.63	14.65	0.63	0.55
S8736	<chem>O=c1[nH]nc2c(c1)cc[nH]c2=O</chem>	0.94	1.22	9.30	7.87	18.09	16.94	0.39	0.43
S8737	<chem>O=c1[nH]nc2c(c1)c(=O)[nH]cc2</chem>	0.93	1.22	8.73	7.66	18.39	16.13	0.98	1.00
S8742	<chem>O=c1ccc2c([nH]1)cnc(=O)[nH]2</chem>	3.68	1.22	10.51	9.61	20.43	19.84	0.44	0.57
S8743	<chem>O=c1ccc2c([nH]1)[nH]c(=O)nc2</chem>	3.53	1.22	11.39	11.06	20.71	20.53	0.77	0.65
S875	<chem>O=c1occc2c1ccs2</chem>	-1.19	-1.08	4.30	4.62	14.49	13.50	0.57	0.51

S876	O=c1occc2c1scc2	-1.18	-1.08	4.72	5.28	15.65	13.83	0.33	0.41
S877	O=c1ccc2c(o1)scc2	-0.57	-1.08	5.23	5.09	15.43	13.69	0.65	0.60
S878	O=c1ccc2c(o1)ccs2	-0.61	-1.08	4.50	4.67	15.14	13.53	0.43	0.54
S8790	O=c1cnc2c([nH]1)cc[nH]c2=O	1.22	1.22	10.52	11.51	21.68	23.20	0.61	0.53
S8791	O=c1cnc2c([nH]1)c(=O)[nH]cc2	1.33	1.22	9.05	9.30	17.79	17.36	0.69	0.58
S8792	O=c1ccc2c([nH]1)[nH]c(=O)cn2	2.84	1.22	11.40	10.50	17.37	17.75	0.37	0.47
S8793	O=c1cnc2c([nH]1)ccc(=O)[nH]2	2.91	1.22	10.08	8.20	18.05	16.37	0.66	0.62
S8798	O=c1ccc2c([nH]1)[nH]c(=O)nn2	4.76	3.05	14.94	14.68	22.53	23.66	0.77	0.69
S88	c1cnnnn1	3.09	2.47	10.60	8.07	16.78	15.72	0.57	0.47
S8802	O=c1[nH]c2cc[nH]c(=O)c2c(=O)[nH]1	1.35	1.99	11.48	10.70	24.94	22.67	0.87	0.76
S8803	O=c1[nH]c(=O)c2c([nH]1)c(=O)[nH]cc2	2.05	1.99	9.60	8.91	16.53	16.35	0.40	0.52
S8804	O=c1ccc2c([nH]1)[nH]c(=O)[nH]c2=O	3.48	1.99	12.65	10.77	18.07	18.42	0.30	0.37
S8805	O=c1ccc2c([nH]1)c(=O)[nH]c(=O)[nH]2	3.55	1.99	11.25	8.90	19.35	16.93	0.35	0.45
S8807	O=c1[nH]c2cccc(=O)n2c(=O)[nH]1	2.27	2.74	9.67	10.77	20.60	22.77	0.57	0.51
S8809	O=c1ccc2c([nH]1)[nH]c(=O)c(=O)[nH]2	4.07	1.99	11.62	12.01	19.65	24.51	0.77	0.66
S8825	O=c1ccc2c([nH]1)[nH]c(=O)sc2=O	4.07	2.90	13.65	12.78	17.70	19.70	0.38	0.39
S8826	O=c1ccc2c([nH]1)c(=O)sc(=O)[nH]2	4.12	2.90	12.43	10.20	19.49	17.86	0.64	0.55
S8839	O=c1cccc2n1c(=O)cc[nH]2	-1.14	0.14	12.42	11.88	29.03	29.26	0.36	0.46
S884	O=c1ccc2c(s1)ccs2	-1.21	-1.77	4.67	3.83	14.64	12.54	0.73	0.62
S8841	O=c1nc[nH]c2c1cc[nH]c2=O	0.98	1.22	8.98	12.50	21.63	23.41	0.33	0.42
S8842	O=c1nc[nH]c2c1c(=O)[nH]cc2	-0.05	1.22	13.30	15.85	32.51	35.30	0.71	0.64
S8843	O=c1ccc2c([nH]1)c(=O)nc[nH]2	2.09	1.22	15.42	11.43	26.45	25.27	0.57	0.45
S8844	O=c1ccc2c([nH]1)[nH]cnc2=O	2.15	1.22	16.57	14.93	28.11	28.08	0.67	0.57
S8847	O=c1[nH]ccc2c1ncn2	-0.76	0.45	6.61	6.84	17.86	14.99	0.30	0.40
S8848	O=c1ccc2c([nH]1)ncn2	0.68	0.45	4.64	6.08	13.12	13.34	0.40	0.53
S8850	O=c1[nH]ccc2c1ncnn2	1.48	2.28	9.64	9.15	17.38	16.53	0.51	0.42
S8851	O=c1[nH]ccc2c1nncn2	1.44	2.28	10.32	9.64	20.24	18.27	0.64	0.52
S8852	O=c1ccc2c([nH]1)nncn2	2.84	2.28	7.24	7.38	12.64	13.37	0.31	0.33
S8853	O=c1ccc2c([nH]1)ncnn2	2.83	2.28	7.33	7.89	12.07	13.79	0.68	0.65
S8856	O=c1[nH]ccc2c1nc[nH]c2=O	-0.19	1.22	7.32	8.95	18.55	17.40	0.37	0.47
S8857	O=c1[nH]ccc2c1c(=O)[nH]cn2	-0.89	1.22	7.27	8.53	21.89	17.88	0.27	0.35

S8858	<chem>O=c1ccc2c([nH]1)c(=O)[nH]cn2</chem>	1.27	1.22	10.53	9.29	20.92	17.32	0.63	0.63
S8859	<chem>O=c1ccc2c([nH]1)nc[nH]c2=O</chem>	1.14	1.22	11.26	8.85	20.88	17.43	0.62	0.50
S8862	<chem>O=c1cnc2c(o1)cc[nH]c2=O</chem>	2.04	2.82	10.77	9.97	19.83	19.08	0.71	0.57
S887	<chem>c1ncc2c(n1)ccs2</chem>	-1.47	-1.62	3.79	3.18	9.13	10.23	0.60	0.48
S888	<chem>c1ncc2c(n1)sc2</chem>	-1.38	-1.62	3.80	3.53	9.37	10.37	0.43	0.50
S8882	<chem>O=c1ccc2c([nH]1)c(=O)scn2</chem>	2.13	2.13	7.24	7.23	16.09	13.64	0.69	0.56
S8883	<chem>O=c1ccc2c([nH]1)ncsc2=O</chem>	2.06	2.13	8.13	7.51	15.90	14.10	0.51	0.59
S8887	<chem>O=c1ccc2c([nH]1)nnnn2</chem>	5.09	4.11	11.43	10.21	16.68	16.07	0.55	0.47
S889	<chem>c1cc2c(s1)cnnn2</chem>	0.76	0.21	7.07	6.70	17.45	15.31	0.50	0.64
S890	<chem>c1cc2c(s1)nnnc2</chem>	0.86	0.21	7.38	7.24	17.76	15.54	0.71	0.60
S891	<chem>O=c1[nH]ncc2c1ccs2</chem>	-0.93	-0.85	3.82	4.02	12.93	10.90	0.52	0.66
S892	<chem>O=c1[nH]ncc2c1sc2</chem>	-0.89	-0.85	4.90	4.20	14.71	11.07	0.67	0.52
S8932	<chem>O=c1ccoc2c1c(=O)[nH]cc2</chem>	-0.77	0.99	8.73	8.31	24.88	20.78	0.60	0.57
S895	<chem>O=c1ncc2c([nH]1)ccs2</chem>	0.38	-0.85	7.32	7.76	20.90	18.73	0.67	0.67
S896	<chem>O=c1ncc2c([nH]1)sc2</chem>	0.39	-0.85	6.07	7.17	18.97	18.58	0.71	0.60
S9	<chem>c1nccs1</chem>	-2.53	-2.49	1.87	2.03	8.82	10.82	0.30	0.40
S9057	<chem>O=c1ccc2c(o1)coc2</chem>	-0.17	-0.39	5.91	5.44	15.68	13.98	0.35	0.46
S9059	<chem>O=c1ccc2c(o1)csc2</chem>	-0.64	-1.08	5.53	4.75	15.69	13.55	0.70	0.61
S9067	<chem>O=c1ccc2c(o1)con2</chem>	1.82	1.44	5.38	6.45	11.63	13.01	0.59	0.63
S9072	<chem>O=c1occc2c1n[nH]n2</chem>	0.52	1.67	6.58	7.92	16.27	15.43	0.59	0.49
S9080	<chem>O=c1[nH]cc2c(c1)oc(=O)cc2</chem>	1.86	0.99	12.10	9.10	20.53	18.57	0.48	0.57
S9081	<chem>O=c1[nH]cc2c(c1)ccc(=O)o2</chem>	2.03	0.99	7.29	7.82	15.04	16.14	0.72	0.64
S9082	<chem>O=c1occc2c1c(=O)occ2</chem>	1.37	2.59	9.27	10.82	22.44	23.24	0.62	0.66
S9083	<chem>O=c1occc2c1ccoc2=O</chem>	2.09	2.59	5.20	7.86	10.54	14.21	0.36	0.46
S91	<chem>O=c1nccns1</chem>	2.46	2.32	9.53	6.90	17.58	14.00	0.33	0.44
S9104	<chem>O=c1occc2c1ncnc2</chem>	1.72	2.05	7.85	8.41	17.36	16.99	0.30	0.41
S9105	<chem>O=c1occc2c1cnnc2</chem>	1.77	2.05	6.04	6.93	11.97	13.15	0.76	0.65
S9106	<chem>O=c1ccc2c(o1)cnnc2</chem>	2.37	2.05	6.17	6.75	12.37	12.47	0.86	0.82
S9110	<chem>O=c1ccc2c(o1)cnnn2</chem>	4.59	3.88	10.49	9.66	16.25	15.75	0.61	0.50
S9127	<chem>O=c1[nH]cc2c(n1)oc(=O)cc2</chem>	3.26	2.82	15.16	13.38	25.71	25.00	0.55	0.47
S915	<chem>O=c1cnc2c([nH]1)sc2</chem>	-0.20	-0.85	5.16	5.81	13.28	14.33	0.51	0.41

S916	O=c1cnc2c([nH]1)ccs2	-0.12	-0.85	6.50	6.74	15.14	14.62	0.52	0.67
S917	O=c1nnc2c([nH]1)scc2	1.72	0.98	8.55	10.09	19.42	21.33	0.38	0.46
S918	O=c1nnc2c([nH]1)ccs2	1.83	0.98	9.93	11.21	21.63	21.71	0.72	0.84
S919	O=c1[nH]c(=O)c2c([nH]1)scc2	0.53	-0.08	6.47	5.91	13.74	13.99	0.56	0.44
S9190	O=c1cc[nH]c2c1ccoc2=O	0.76	0.99	7.86	8.32	17.03	16.75	0.55	0.48
S9191	O=c1cc[nH]c2c1c(=O)occ2	-0.20	0.99	13.81	13.60	31.13	30.23	0.44	0.59
S9193	O=c1ccc2c(o1)[nH]ccc2=O	1.06	0.99	11.31	9.26	20.20	19.98	0.41	0.52
S9197	O=c1ccc2c(o1)[nH]cnc2=O	2.90	2.82	13.42	11.91	23.40	22.94	0.32	0.41
S9198	O=c1occc2c1ncn2	0.98	2.05	5.26	7.60	15.11	14.82	0.52	0.67
S920	O=c1[nH]c(=O)c2c([nH]1)ccs2	0.54	-0.08	7.68	6.67	15.84	14.31	0.32	0.35
S9207	O=c1ccc2c(o1)nc[nH]c2=O	2.24	2.82	11.93	10.59	21.30	17.91	0.70	0.56
S921	O=c1[nH]c2sccc2[nH]c1=O	0.73	-0.08	6.64	8.92	18.56	23.29	0.67	0.62
S922	O=c1oc(=O)c2c([nH]1)scc2	2.00	1.52	8.92	9.07	17.15	17.68	0.63	0.52
S923	O=c1oc(=O)c2c([nH]1)ccs2	2.03	1.52	10.02	10.13	19.01	18.08	0.76	0.60
S924	O=c1[nH]c2sccc2oc1=O	1.70	1.52	7.52	10.03	17.21	22.89	1.04	1.10
S925	O=c1[nH]c2ccsc2oc1=O	1.74	1.52	8.40	10.84	17.98	23.11	0.42	0.57
S9258	O=c1ccoc2c1ccoc2=O	1.88	2.59	6.14	7.76	12.63	13.98	0.48	0.41
S9259	O=c1ccoc2c1c(=O)occ2	1.00	2.59	8.03	9.44	21.72	21.53	0.35	0.46
S926	O=c1sc(=O)c2c([nH]1)scc2	1.07	0.83	7.57	8.05	14.19	16.19	0.27	0.39
S927	O=c1sc(=O)c2c([nH]1)ccs2	1.06	0.83	9.04	9.09	16.56	16.58	0.49	0.64
S928	O=c1[nH]c2sccc2sc1=O	1.04	0.83	6.24	9.14	15.80	21.91	0.30	0.42
S929	O=c1[nH]c2ccsc2sc1=O	1.04	0.83	7.68	9.91	17.20	22.10	0.45	0.60
S930	O=c1cc[nH]c2c1scc2	-2.75	-2.68	9.63	7.33	24.84	19.12	0.51	0.64
S931	O=c1cc[nH]c2c1ccs2	-2.81	-2.68	9.13	6.14	23.31	18.62	0.83	0.79
S932	O=c1nc[nH]c2c1scc2	-0.84	-0.85	11.61	10.78	27.24	23.96	0.32	0.45
S933	O=c1nc[nH]c2c1ccs2	-0.95	-0.85	11.15	9.39	26.03	23.38	0.48	0.63
S934	c1cnc2c(n1)scc2	-2.00	-1.62	2.24	3.02	6.98	9.39	0.34	0.46
S935	c1nnc2c(n1)ccs2	0.17	0.21	5.98	5.12	13.25	11.01	0.70	0.55
S936	c1nnc2c(n1)scc2	0.15	0.21	5.50	4.92	12.50	10.93	0.99	1.05
S937	O=c1[nH]cnc2c1scc2	-1.47	-0.85	6.32	5.45	15.10	12.50	0.68	0.58
S938	O=c1[nH]cnc2c1ccs2	-1.43	-0.85	6.72	5.62	14.55	12.48	0.69	0.54

S941	O=c1ocnc2c1scc2	0.21	0.75	4.67	5.33	12.76	11.01	0.45	0.56
S942	O=c1ocnc2c1ccs2	0.24	0.75	3.83	5.20	11.21	10.91	0.61	0.55
S945	O=c1scnc2c1scc2	-0.68	0.06	3.87	4.52	11.49	10.16	0.75	0.73
S946	O=c1scnc2c1ccs2	-0.63	0.06	3.37	4.41	10.13	10.06	0.68	0.62
S947	n1nnc2c(n1)scc2	2.42	2.04	9.30	8.04	17.50	14.80	0.42	0.53
S954	O=c1[nH]nnc2c1ccs2	0.48	0.98	4.98	6.52	10.95	11.80	0.74	0.62
S955	O=c1[nH]nnc2c1scc2	0.45	0.98	5.29	6.15	11.91	11.75	0.31	0.42
S964	O=c1ccoc2c1scc2	-1.47	-1.08	4.37	4.30	15.56	12.71	0.33	0.44
S965	O=c1ccoc2c1ccs2	-1.47	-1.08	4.56	3.92	14.86	12.43	0.61	0.70
S966	O=c1ncoc2c1scc2	0.39	0.75	5.95	6.86	17.60	16.30	0.63	0.51
S967	O=c1ncoc2c1ccs2	0.34	0.75	5.63	6.28	16.58	15.94	0.61	0.70
S968	O=c1ccsc2c1ccs2	-2.01	-1.77	3.93	3.25	14.02	12.16	0.29	0.41
S9686	n1cnc2c(c1)c[nH]c2	-3.16	-2.53	8.39	5.71	18.06	15.15	0.45	0.60
S9687	n1cnc2c(c1)coc2	-1.04	-0.93	4.69	3.90	10.64	10.73	0.36	0.47
S9688	n1cnc2c(c1)csc2	-1.55	-1.62	4.29	3.20	10.70	10.24	0.70	0.56
S9689	c1ncc2c(n1)c[nH]n2	-1.52	-0.70	8.07	6.02	14.59	13.39	0.38	0.37
S969	O=c1ccsc2c1scc2	-1.98	-1.77	3.69	3.68	14.71	12.46	0.65	0.51
S9690	c1ncc2c(n1)n[nH]c2	-1.28	-0.70	8.86	7.19	18.99	15.95	1.00	0.82
S9692	c1ncc2c(n1)noc2	1.19	0.90	8.87	6.33	16.81	12.86	0.71	0.58
S9694	c1ncc2c(n1)nsc2	0.30	0.21	7.78	5.57	15.92	12.21	0.43	0.59
S9695	n1cnc2c(c1)n[nH]n2	0.38	1.13	7.11	6.48	13.13	11.94	0.41	0.53
S9696	n1cnc2c(c1)non2	3.14	2.73	7.80	6.58	11.58	10.19	0.24	0.36
S9697	n1cnc2c(c1)nsn2	1.89	2.04	5.08	5.76	9.53	9.37	0.61	0.54
S97	O=c1ccoccl	-0.58	-0.65	4.94	4.06	15.76	13.46	0.52	0.40
S970	O=c1cn[nH]c2c1scc2	-0.92	-0.85	8.25	7.01	20.28	16.12	0.73	0.81
S9704	c1ncc2c(n1)ncnc2	1.76	1.51	7.55	6.21	13.33	11.62	0.71	0.53
S9705	n1cnc2c(c1)ncnc2	1.49	1.51	4.03	5.47	5.43	9.99	0.68	0.61
S9706	n1cnc2c(c1)cnnc2	3.99	3.34	11.33	9.69	18.44	16.37	0.47	0.62
S9707	n1cnc2c(c1)nnnc2	3.68	3.34	8.36	8.50	14.26	13.75	0.29	0.41
S9708	O=c1[nH]ncc2c1ncnc2	1.99	2.28	7.91	7.19	17.06	13.31	0.62	0.55
S9709	O=c1[nH]ncc2c1cncn2	2.04	2.28	5.53	6.83	10.49	11.41	0.76	0.69

S971	<chem>O=c1cn[nH]c2c1ccs2</chem>	-0.98	-0.85	7.33	6.01	18.37	15.70	0.62	0.60
S9712	<chem>O=c1ncc2c([nH]1)ncnc2</chem>	3.30	2.28	8.61	8.56	17.71	16.29	0.84	0.73
S9713	<chem>O=c1ncc2c([nH]1)cncn2</chem>	3.40	2.28	9.88	9.85	18.63	17.96	0.53	0.70
S9732	<chem>O=c1cnc2c([nH]1)cncn2</chem>	3.00	2.28	9.91	9.55	14.20	15.92	0.69	0.83
S9733	<chem>O=c1cnc2c([nH]1)ncnc2</chem>	2.66	2.28	6.91	7.52	11.44	12.63	0.53	0.71
S9734	<chem>O=c1nnc2c([nH]1)cncn2</chem>	4.84	4.11	13.28	13.80	19.66	22.59	0.70	0.52
S9735	<chem>O=c1nnc2c([nH]1)ncnc2</chem>	4.49	4.11	10.16	11.32	16.81	18.31	0.41	0.54
S9736	<chem>O=c1[nH]c2cncnc2c(=O)[nH]1</chem>	3.46	3.05	10.85	9.78	18.04	16.60	0.73	0.65
S9737	<chem>O=c1[nH]c2ncncc2c(=O)[nH]1</chem>	3.44	3.05	8.55	8.14	11.89	13.03	0.62	0.56
S9738	<chem>O=c1[nH]c2ncncc2[nH]c1=O</chem>	3.80	3.05	9.94	10.43	17.61	21.05	0.72	0.68
S9740	<chem>O=c1oc(=O)c2c([nH]1)ncnc2</chem>	4.93	4.65	11.22	10.57	15.91	15.45	0.28	0.40
S9743	<chem>O=c1sc(=O)c2c([nH]1)cncn2</chem>	3.90	3.96	11.88	11.88	17.89	18.52	0.50	0.63
S9744	<chem>O=c1sc(=O)c2c([nH]1)ncnc2</chem>	3.88	3.96	9.35	9.60	12.91	14.12	0.76	0.61
S9746	<chem>O=c1[nH]c2ncncc2sc1=O</chem>	3.94	3.96	9.47	10.43	15.37	19.04	0.59	0.82
S9747	<chem>O=c1cc[nH]c2c1cncn2</chem>	0.19	0.45	9.41	8.08	19.05	17.21	0.76	0.68
S9748	<chem>O=c1cc[nH]c2c1ncnc2</chem>	0.20	0.45	12.70	10.72	26.58	22.94	0.52	0.65
S9749	<chem>O=c1nc[nH]c2c1cncn2</chem>	2.07	2.28	11.40	10.85	21.89	20.64	0.86	0.71
S9750	<chem>O=c1nc[nH]c2c1ncnc2</chem>	2.11	2.28	14.87	13.94	28.50	27.36	0.37	0.50
S9751	<chem>c1ncc2c(n1)ncn2</chem>	0.99	1.51	6.18	6.03	12.12	11.23	0.70	0.56
S9752	<chem>c1ncc2c(n1)ncnn2</chem>	3.07	3.34	7.03	7.45	9.26	11.44	0.57	0.48
S9753	<chem>n1cnc2c(c1)ncnn2</chem>	3.09	3.34	7.42	7.90	12.44	12.42	0.70	0.60
S9754	<chem>O=c1[nH]cnc2c1cncn2</chem>	1.62	2.28	10.47	9.15	16.01	15.05	0.41	0.51
S9755	<chem>O=c1[nH]cnc2c1ncnc2</chem>	1.33	2.28	9.96	8.77	18.15	15.33	0.77	0.66
S9758	<chem>O=c1ocnc2c1cncn2</chem>	3.33	3.88	8.42	8.00	11.55	12.21	0.94	0.87
S9759	<chem>O=c1ocnc2c1ncnc2</chem>	3.03	3.88	8.17	8.30	14.79	13.43	0.61	0.80
S976	<chem>O=c1ncsc2c1scc2</chem>	-0.29	0.06	5.70	6.30	17.50	16.21	0.32	0.45
S977	<chem>O=c1ncsc2c1ccs2</chem>	-0.35	0.06	4.56	5.67	15.69	15.82	0.33	0.47
S9771	<chem>O=c1[nH]nnc2c1ncnc2</chem>	3.22	4.11	7.73	8.99	13.62	13.25	0.31	0.43
S978	<chem>O=c1nn[nH]c2c1scc2</chem>	0.95	0.98	10.79	11.48	23.97	23.21	0.57	0.43
S9781	<chem>O=c1ccoc2c1cncn2</chem>	1.64	2.05	6.61	6.61	12.69	12.61	0.86	0.68
S9782	<chem>O=c1ccoc2c1ncnc2</chem>	1.40	2.05	7.79	7.45	18.00	15.82	0.58	0.43

S9783	O=c1ncoc2c1cnnc2	3.49	3.88	8.96	8.49	15.78	14.79	0.62	0.89
S9784	O=c1ncoc2c1ncnc2	3.28	3.88	10.36	9.78	20.21	18.99	0.52	0.67
S9787	O=c1cn[nH]c2c1cnnc2	2.03	2.28	6.33	7.73	12.60	13.87	0.81	0.93
S979	O=c1nn[nH]c2c1ccs2	0.85	0.98	9.89	10.29	22.31	22.71	0.51	0.66
S9795	O=c1nn[nH]c2c1cnnc2	3.88	4.11	9.74	11.52	17.42	19.55	0.71	0.67
S98	O=c1ccocn1	1.24	1.18	7.88	6.57	19.00	17.03	0.65	0.55
S9802	O=c1oc2ncncc2c(=O)[nH]1	4.68	4.65	10.72	9.36	14.61	12.44	0.63	0.79
S9803	O=c1oc2cncnc2c(=O)[nH]1	4.47	4.65	10.75	9.21	15.27	13.49	0.43	0.62
S9805	O=c1sc2cncnc2c(=O)[nH]1	3.63	3.96	8.68	8.43	13.91	12.84	0.38	0.50
S9816	O=c1sc2c(s1)cnnc2	2.17	1.89	5.76	6.10	10.00	11.02	0.73	0.57
S9822	n1nnc2c(c1)c[nH]c2	-0.93	-0.70	11.81	9.97	25.88	21.22	0.78	0.71
S9823	n1nnc2c(c1)coc2	1.11	0.90	7.68	7.35	17.68	15.67	0.91	0.74
S9824	n1nnc2c(c1)csc2	0.63	0.21	7.40	6.71	18.22	15.31	0.70	0.55
S9826	n1nnc2c(c1)c[nH]n2	0.95	1.13	12.40	11.61	24.44	22.37	0.69	0.49
S9828	n1nnc2c(c1)con2	3.30	2.73	12.20	9.95	19.67	18.15	0.29	0.48
S9830	n1nnc2c(c1)csn2	2.49	2.04	11.16	9.24	20.79	17.63	0.74	0.74
S9831	n1nnc2c(c1)n[nH]n2	2.57	2.96	10.80	10.39	19.40	17.24	0.25	0.36
S985	O=c1oc2ccsc2c(=O)[nH]1	1.63	1.52	6.47	6.33	12.59	11.91	0.40	0.58
S986	O=c1oc2sccc2c(=O)[nH]1	1.65	1.52	5.37	6.38	11.01	11.81	0.52	0.75
S9867	O=c1cnc2c([nH]1)nnnc2	4.88	4.11	11.28	10.10	16.75	15.46	0.97	0.77
S9869	O=c1nnc2c([nH]1)nnnc2	6.63	5.94	14.12	13.33	17.41	19.90	0.76	0.70
S987	O=c1sc2ccsc2c(=O)[nH]1	0.83	0.83	6.16	5.54	12.08	11.17	0.59	0.79
S9871	O=c1[nH]c2nnncc2c(=O)[nH]1	5.71	4.88	12.86	11.31	16.97	16.55	0.38	0.56
S9878	O=c1sc(=O)c2c([nH]1)nnnc2	6.10	5.79	13.38	11.98	16.17	16.59	0.82	0.80
S988	O=c1sc2sccc2c(=O)[nH]1	0.85	0.83	5.10	5.54	10.56	11.04	0.77	0.80
S9885	c1cnc2c(n1)nnnc2	3.28	3.34	10.35	9.74	18.87	16.47	0.74	0.56
S989	O=c1oc2c(o1)ccs2	0.88	0.14	5.39	5.53	13.53	13.37	0.79	0.76
S99	O=c1ncocn1	3.05	3.01	10.76	8.49	21.30	19.31	0.30	0.51
S992	O=c1oc2sccc2oc1=O	2.74	3.12	7.68	9.62	14.35	20.63	0.88	0.62
S993	O=c1oc(=O)c2c(o1)ccs2	3.13	3.12	8.95	8.44	16.05	14.48	0.79	0.65
S994	O=c1oc(=O)c2c(o1)scc2	3.15	3.12	7.80	8.20	14.37	14.30	0.93	0.95

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Converting SMILES to Stacking Interaction Energies

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Abstract

Predicting the strength of stacking interactions involving heterocycles is vital for several fields, including structure-based drug design. While quantum chemical computations can provide accurate stacking interaction energies, these come at a steep computational cost. To address this challenge, we recently developed quantitative predictive models of stacking interactions between drug-like heterocycles and the aromatic amino acids Phe, Tyr, and Trp (DOI: 10.26434/chemrxiv.7628939.v4). These models depend on heterocycle descriptors derived from electrostatic potentials (ESPs) computed using density functional theory and provide accurate stacking interactions without the need for expensive computations on stacked dimers. Herein, we show that these ESP-based descriptors can be reliably evaluated directly from the atom connectivity of the heterocycle, providing a means of predicting both the descriptors and the potential for a given heterocycle to engage in stacking interactions without resorting to any quantum chemical computations. This enables the conversion of simple molecular representations (*e.g.* SMILES) directly into accurate stacking interaction energies using a freely-available online tool, thereby providing a way to rapidly rank the stacking abilities of large sets of heterocycles.

Introduction

Stacking interactions (*i.e.* roughly parallel face-to-face interactions between planar π -systems)¹⁻³ play vital roles in many chemical and biological systems, and the ability to predict and rationally tune the strength of these interactions is important in everything from asymmetric catalysis⁴⁻⁷ to structure based drug design.⁸⁻¹⁰ Various types of stacking interactions can contribute to the binding of ligands by proteins, and harnessing these interactions can provide a powerful means of tuning inhibitor binding.¹¹⁻²² Chief among these are stacking interactions of heterocycles with the aromatic amino acid side chains Phe, Tyr, and Trp (see Figure 1).^{8-10,23}

Figure 1. A) Pteridine fragment of methotrexate stacking with Tyr and Trp residues in the human folate receptor (PDB: 4KNO);²⁴ B) model stacked dimer of pyrimidine with Tyr; and C) model amino acid side chains Phe, Tyr, and Trp and selected heterocycles (**1 – 5**).

Tools exist for enumerating regioisomeric structures of heterocycles in order to build greater structural complexity during exploratory chemistry and lead optimization.²⁵⁻²⁶ However, there is currently no means of rapidly predicting how strongly such heterocyclic fragments will stack with binding site aromatic amino acid side chains. This limits our ability to choose heterocyclic fragments that maximize stacking interactions with binding site residues. While quantum mechanical methods can accurately predict accurate gas-phase stacking energies, this typically requires expensive *ab initio* methods paired with large basis sets or dispersion-corrected density functional theory (DFT) methods.²⁷⁻²⁹ Moreover, finding the maximum possible stacking interaction between a heterocycle and an aromatic amino acid side chain requires the systematic exploration of local stacked energy minima in order to identify the global minimum energy stacked structure.^{23,30-33} This is a time consuming and computationally costly process.

Recently, we introduced a series of heterocycle descriptors based on the electrostatic potential (ESP) and electric field in the plane 3.25 Å from the heterocycle.³² These descriptors, which are similar in spirit to the statistical interaction indices of Politzer *et al.*,³⁴⁻³⁵ have proved useful in the development of quantitative predictive models of the strength of stacking interactions between drug-like heterocycles and protein amide backbones,³³ Asp-Arg salt-bridges,³² and aromatic amino acid side chains.³⁰ For example, equation 1 (from Ref. 30) relies on two of these descriptors (ESP_{mean} and ESP_{max}) and was fit based on stacking interaction energies for a training set of 46 drug-like heterocycles with the aromatic amino acid side chains Phe, Tyr, and Trp:

$$\Delta E_{\text{pred}} = N_{\text{HA}}^{\text{AA}}(-0.022ESP_{\text{mean}} - 0.022ESP_{\text{max}} - 0.095N_{\text{HA}}^{\text{Het}}) - 1.67 \quad (1)$$

In equation 1, ESP_{mean} is the mean value of the ESP within the projection of the van der Waals (vdW) volume³⁶ of the heterocycle onto the plane 3.25 Å from the heterocycle, ESP_{max} is the maximum ESP value in this area,³² and $N_{\text{HA}}^{\text{Het}}$ and $N_{\text{HA}}^{\text{AA}}$ are the heavy atom counts⁶⁰ of the heterocycle and amino acid side chain, respectively. Similar predictive models of stacking interactions with Phe, Tyr, and Trp were developed that utilize the mean electric field (F_{mean}) and the range of ESP values (ESP_{range}) in place of ESP_{max} .³⁰

Figure 2A shows the correlation between stacking interaction energies for a representative set of 54 drug-like heterocycles predicted using equation 1 with highly-accurate DLPNO-CCSD(T)/cc-pVQZ interaction energies³⁷⁻⁴¹ from Ref.³⁰. This model not only provides accurate stacking interaction energies (RMSE 0.7 kcal mol⁻¹) but also reliable rankings of the relative stacking interactions of different heterocycles with Phe, Tyr, and Trp, as indicated by the Spearman's rank coefficient (ρ^2) of 0.91 and Kendall τ of 0.83. Equation 1, which utilizes ESP_{mean} and ESP_{max} values computed using DFT, indicates that stacking interactions with aromatic amino acid residues can be maximized by choosing heterocycles with large values of these two descriptors. More practically, equation 1 predicts the maximum possible stacking ability of a given heterocycle without the need to explore potential stacked dimer geometries. Instead, one needs to simply compute the ESP of the isolated heterocycle. The result is a reduction by a factor of 10⁴ in computational cost, compared to DFT optimizations of stacked dimers followed by the evaluation of high-accuracy *ab initio* interaction energies.

Despite the potential utility of equation 1, its dependence on DFT-computed ESPs renders its use in the prediction of stacking interactions for large sets of heterocycles impractical.

Herein, we show that ESP_{mean} and ESP_{max} , and the corresponding stacking interaction energies, can be accurately evaluated directly from the atom connectivity⁴² by exploiting systematic variations in ESPs arising from the introduction of different heteroatom types. This provides a means of converting simple molecular representations (*e.g.* SMILES) directly into reliable stacking interactions without any quantum chemical computations.

Figure 2. DLPNO-CCSD(T)/cc-pVQZ interaction energies versus values predicted based on equation 1 for 54 drug-like heterocycles stacked with model Phe, Tyr, and Trp side chains using A) DFT-computed ESP_{mean} and ESP_{max} values from Ref. 30 and B) ESP_{mean} and ESP_{max} values evaluated directly from SMILES using equations 2 and 3.

Results and Discussion

Below, we develop predictive models of the heterocycle descriptors ESP_{mean} and ESP_{max} based on atom connectivity. These physically-motivated models (*vide infra*) were parameterized based on a diverse set of 1854 heterocycles from the VEHICLE database of Pitt *et al.*⁴³ (see Computational Methods and Supporting Information for more details). The distribution of DFT-

computed ESP_{mean} and ESP_{max} values for these 1854 heterocycles are presented in Figure 3, grouped by whether or not the heterocycle had been synthesized as of publication of Ref. 43. Predicted stacking interaction energies with Phe, Tyr, and Trp, based on equation 1 using DFT-computed ESP_{mean} and ESP_{max} values, are plotted in Figure 4.

Figure 3. Distribution of DFT-computed values of A) ESP_{mean} and B) ESP_{max} , grouped by whether the heterocycles were known or unknown as of publication of Ref. 43.

The data in Figures 3 and 4 enable comparison of the electrostatic properties and stacking propensities of known versus unknown heterocycles. For instance, although the ESP_{max} values (see strip plot in Figure 3B) of the known heterocycles span a larger range than the unknown heterocycles, from $-1.4 \text{ kcal mol}^{-1}$ for benzene to $+19.5 \text{ kcal mol}^{-1}$ for **1** (see Figure 1C), the values for the unknown heterocycles are systematically slightly higher. Values of ESP_{mean} (Figure 3A) are also higher for the unknown compared to the previously synthesized heterocycles and there are several synthetically tractable, yet not previously synthesized, heterocycles that exhibit very large ESP_{mean} values. For instance, whereas ESP_{mean} values for known heterocycles range from $-7.6 \text{ kcal mol}^{-1}$ for **2** to $+5.7 \text{ kcal mol}^{-1}$ for **3**, ESP_{mean} for the unknown heterocycles are as large as $+8.0 \text{ kcal mol}^{-1}$. However, the heterocycles with very large ESP_{mean} values tend to include extreme degrees of functionalization with clustered carbonyl groups (*e.g.* **4**), so are likely not attractive synthetic targets. Moreover, while unknown heterocycles are among those predicted to exhibit very strong stacking interactions (see Figure

4), none are predicted to stack more strongly than known heterocycles. For example, the strongest predicted stacking interaction occurs for **1**, which has previously been synthesized and has a predicted stacking interaction with Trp of $-19.1 \text{ kcal mol}^{-1}$. This can be compared with the strongest stacking of the unknown heterocycles (**5**), for which the predicted interaction with Trp is $-18.8 \text{ kcal mol}^{-1}$. Of course, the range of gas-phase interaction energies displayed in Figure 4 is larger than what will be possible in the dielectric environment of a protein; however, previous solution-phase computations³⁰ suggest that the trends exhibited in Figure 4 will be similar in protein-like dielectric environments.

Figure 4. Predicted stacking interactions of 1854 known and unknown heterocycles⁴³ with Phe, Tyr, and Trp based on equation 1 using DFT-computed ESP_{mean} and ESP_{max} values, grouped by whether the heterocycles were known or unknown as of publication of Ref. 43.

A. Heteroatom Effects on ESP_{mean} and ESP_{max}

Previously, we showed³⁰ qualitatively that ESP_{mean} reflects the number of O, S, imino N ($-\text{N}=\text{}$), amino N ($-\text{NH}-$), and carbonyl groups within a heterocycle, while ESP_{max} depends on both the number and relative positions of these heteroatoms (throughout, carbonyl groups are considered a single ‘heteroatom’ located at the position of the carbonyl carbon). In order to develop a quantitative relationship between these descriptors and atom connectivity, we must first understand the impact of heteroatoms on these descriptors. These descriptors are statistical

measures of the distribution of ESP values in the vdW projection onto a plane 3.25 Å from the heterocycle. This is different from the more conventional depictions in which the ESP is mapped onto an electron density isosurface (*e.g.* Figure 5A). A top-down view of the ESP of benzene in the plane 3.25 Å away is depicted in Figure 5B, along with the projection of the van der Waals (vdW) volume of benzene onto this plane; the values of ESP_{mean} and ESP_{max} are determined by the ESP within this area. For benzene, the ESP in this area is negative, with ESP_{mean} and ESP_{max} values of -4.7 and -1.4 kcal mol $^{-1}$, respectively.

Figure 5. A) The ESP of benzene mapped onto an electron density isosurface ($\rho = 0.001$ e/bohr 3) and in the plane 3.25Å away from the ring. B) Top view of the ESP in the plane 3.25 Å from the plane of benzene, with the projection of the van der Waals volume onto this plane outlined in black. ESPs in kcal mol $^{-1}$, according to the scale shown.

The introduction of heteroatoms leads to significant perturbations of the ESP, and the ability to evaluate ESP_{mean} and ESP_{max} directly from atom connectivity stems from the systematic nature of these changes. Figure 6A shows the ESP of pyridine. To quantify the impact of replacing a CH group with an imino nitrogen, Figure 6A also shows the difference in electrostatic potential between pyridine and benzene. This ESP difference closely resembles that of a physical dipole located at the position of the nitrogen, reflecting the difference in the in-plane charge distribution between a C–H group and an imino nitrogen.⁴⁴ Consequently, the impact of introducing an imino nitrogen on the ESP can be approximated by a *local* dipole at the position of the heteroatom with the negative end of the dipole facing away from the ring

centroid. Because this local radial dipole is located at the periphery of the ring, the associated region of positive ESP is located within the vdW area while the negative portion of the ESP is primarily outside of this region. The net result is that the replacement of a CH group with an imino N provides a ~ 1.4 kcal mol⁻¹ increase in ESP_{mean}, regardless of the size of the heterocycle. The effects of other heteroatoms are similar, with the magnitude of the effect reflecting the size of the local dipole associated with each heteroatom (S < O < imino N < C=O). Amino NH groups have the opposite effect owing to the oppositely oriented local dipole.⁴⁵

Figure 6. A) ESP of pyridine (left) and the difference in ESP between pyridine and benzene (right); B-D) ESPs of pyridazine, pyrimidine, and pyrazine, respectively, with the orientation of local dipoles associated with each imino nitrogen depicted with a grey arrow; E) construction of approximate ESP of pyrimidine (far right) by adding the ESPs of two pyridines at 120° relative orientations and subtracting the ESP of benzene; F) construction of approximate ESP of 1,6-naphthyridin-5(6H)-one (2nd from right) by adding the ESPs of quinoline (left) and isoquinolin-1(2H)-one (2nd from left) and subtracting the ESP of naphthalene (middle). The true ESP of 1,6-naphthyridin-5(6H)-one is on the far right. All ESPs in kcal mol⁻¹ according to the scale shown.

Figures 6B-D show the ESPs of the diazines pyridazine, pyrimidine, and pyrazine, respectively, which reflect the effects of two imino nitrogens. These ESPs can be quantitatively reproduced by simply adding together the ESPs of two pyridines (with the appropriate relative orientations) and subtracting the effect of benzene, as shown previously for substituted arenes.⁴⁶ This is demonstrated for pyrimidine in Figure 6E; the additive ESP (far right) is nearly identical to the computed ESP for pyrimidine (Figure 6C). As a result of this additivity, ESP_{mean} can be accurately predicted by simply summing up the contributions of each CH group and each heteroatom (*vide infra*).

Each heteroatom type also has an inherent impact on ESP_{max} . For example, replacing a CH group with an imino N leads to a $\sim 1.6 \text{ kcal mol}^{-1}$ increase in ESP_{max} . However, to accurately predict ESP_{max} for systems with multiple heteroatoms, one must account for the constructive or destructive interaction of all pairs of heteroatom dipoles. Pairs of heteroatoms with parallel local dipoles add constructively, increasing ESP_{max} beyond what would be expected based on simple scalar additivity. Conversely, anti-parallel dipoles add destructively, diminishing their impact on ESP_{max} . The extent of this constructive/destructive additivity varies inversely with the distance between the atoms. This is reflected in the ESPs of the diazines depicted in Figures 6B-D. Based solely on the presence of two imino nitrogens, one would expect ESP_{max} values of $3.9 \text{ kcal mol}^{-1}$ for all three diazines. However, for pyridazine (Figure 6B), the two amino nitrogens are at a relative orientation of 60° and located at adjacent positions. This leads to a strong constructive additivity and an ESP_{max} of $5.5 \text{ kcal mol}^{-1}$. This can be contrasted with pyrazine (Figure 6D), for which the two imino nitrogen dipoles are oppositely oriented, leading to significant cancelation and an ESP_{max} of only $1.6 \text{ kcal mol}^{-1}$. The 120° relative orientation of the imino nitrogen dipoles in pyrimidine leads to an intermediate value of 4.1 for ESP_{max} . These effects can be modeled by assuming a $\cos(\alpha)/R$ dependence, where α is the angle between radial dipoles at the positions of the two heteroatoms and R is the distance between these points. Moreover, explicitly computed α or R values from heterocycle structures are not necessary; instead, one can simply use angles and distances derived from idealized hexagonal and pentagonal rings (*vide infra*).

While the above discussion focused on simple rings containing only imino nitrogens, these same trends apply to different heteroatom types and different ring sizes. For example, even for more complex heterocycles the overall ESP can be reproduced by considering the impact of each heteroatom separately. For example, the ESP of 1,6-naphthyridin-5(6*H*)-one can be reproduced by adding the ESP of quinoline with isoquinolin-1(2*H*)-one and subtracting the

impact of naphthalene (see Figure 6F). Furthermore, the values of ESP_{mean} and ESP_{max} of 1,6-naphthyridin-5(6*H*)-one and other complex heterocycles can be evaluated by simply accounting for the impact of each heteroatom and each unique pair of heteroatoms, as shown below.

B. Prediction of ESP_{mean} and ESP_{max} from Atom Connectivity

Guided by the above results, we defined seven atom types covering those present in drug-like heterocycles (see Table 1). We then fit a_0 as well as parameters for each of the seven atom types (a_i) to ω B97X-D/def2-TZVP computed ESP_{mean} values for the full set of 1854 heterocycles according to equation 2 (see Table 1 for fit parameters):

$$ESP_{\text{mean}}^{\text{pred}} = a_0 + \sum_i^{\text{atoms}} a_i \quad (2)$$

The application of equation 2 to predict ESP_{mean} for two representative heterocycles is demonstrated in Figure 7. ESP_{mean} values predicted from equation 2 are plotted versus the DFT computed values in Figure 8A. Errors in ESP_{mean} values predicted from equation 2, compared to the DFT-computed data, are as large as 3.7 kcal mol⁻¹. These errors grow with the size of ESP_{mean} (see SI Figure S1 and S2), which arises because the heterocycles with large positive ESP_{mean} values tend to have a large proportion of heteroatoms. Equation 2 assumes additivity of effects for each heteroatom, but as the relative number of heteroatoms grows this additivity assumption slowly begins to break down. However, overall this fit is highly accurate ($R^2 = 0.93$ and RMSE = 0.63 kcal mol⁻¹) and robust to cross validation. Moreover, it applies equally well to different classes of heterocycles, including all different sizes of ring systems levels of substitution (see SI Figure S3).

Table 1. Optimized parameters for each atom type for equations 2 and 3.

Atom types	a_i	b_i	c_i
C (aryl)	-0.24	-	-
C=O	2.98	3.04	1.57
N: (imino)	1.59	1.62	1.43
O	0.74	0.73	0.56
S	0.05	-0.02	0.42
NH (amino)	-0.86	1.73	-1.60
N (ring fusion)	-0.11	1.11	-0.66
$a_0 = -3.41$		$b_0 = 0.73$

Figure 7. Application of equations 2 and 3 to evaluate ESP_{mean} and ESP_{max} (in kcal mol^{-1}) for A) 1,2,4-triazine and B) 1,6-naphthyridin-5(6H)-one. DFT-computed values are also provided for comparison.

As noted above, ESP_{max} reflects both the number of each heteroatom type (aryl carbons contribute a relatively constant amount to ESP_{max} , regardless of their number) and the relative position of pairs of heteroatoms. Accordingly, we fit b_0 , coefficients for each of the six heteroatom types (b_i and c_i), to DFT-computed ESP_{max} values for the set of 1854 heterocycles according to equation 3 (see Table 1 for values of fit parameters)⁴⁷:

$$ESP_{\text{max}}^{\text{pred}} = b_0 + \sum_i^{\text{hetatm}} b_i + \sum_{i < j}^{\text{hetatm}} \frac{\cos(\alpha_{ij})}{R_{ij}} c_i c_j \quad (3)$$

The constants α_{ij} and R_{ij} in equation 3 are the relative angle and distance between radial vectors located at the positions of heteroatoms i and j derived from idealized hexagonal and pentagonal rings of edge length 1.0 and were not fit (see SI Table S1 for values of α_{ij} and R_{ij}). The use of equation 3 to evaluate ESP_{max} for two representative heterocycles is shown in Figure 7. Essentially, equation 3 accounts for the inherent impact of each heteroatom on ESP_{max} and then

corrects this value for the constructive or destructive additivity of each pair of the corresponding local dipoles. Values of ESP_{max} predicted from equation 3 are plotted against the DFT computed values in Figure 8B. While the mean errors in predicted ESP_{max} values, compared to the DFT-computed data, are slightly larger than observed for ESP_{mean} , this fit is still accurate ($R^2 = 0.81$ and $\text{RMSE} = 1.45 \text{ kcal mol}^{-1}$) and robust to cross-validation. It also applies equally well across different classes of heterocycles (see SI Figure S4). More importantly, as shown below, errors in predicted ESP_{max} values lead to relatively small errors in predicted stacking interaction energies due to the form of equation 1. The descriptors $\text{ESP}_{\text{range}}$ and F_{mean} , which appear in alternative models of stacking interactions,³⁰ follow similar trends as ESP_{max} and can be reliably predicted from atom connectivity based on analogs of equation 3 (see SI Figure S5-S6).

Figure 8. DFT computed values versus values from equations 2 and 3 for A) ESP_{mean} and B) ESP_{max} , grouped by whether the heterocycles were known or unknown as of publication of Ref. 43.

C. Converting SMILES to Stacking Interaction Energies

The heterocycle descriptors ESP_{mean} and ESP_{max} can be reliably predicted using equations 2 and 3 based on the number of heteroatom types and their relative positions, which can be readily derived from the connectivity information contained in SMILES representations. The resulting SMILES-based descriptors (along with the heavy atom count) can then be used to predict the ability of a given heterocycle to engage in stacking interactions with Phe, Tyr, and Trp based on equation 1. This provides a means of rapidly converting SMILES representations directly into stacking interaction energies without resolving three dimensional molecular structures or resorting to any quantum chemical computations. A free, online implementation of this procedure (SMILES2stacking) is available as part of FrOST (Free Online Stacking Tools).⁴⁸

To demonstrate this process, Figure 2B shows stacking interactions evaluated directly from heterocycle SMILES representations via equations 1-3 plotted against the high-level DLPNO-CCSD(T)/cc-pVQZ data from Ref. 30. Both quantitative stacking interaction energies and relative rankings are captured with negligible loss in accuracy compared to those predicted using DFT-based descriptors. Moreover, while the use of DFT-based descriptors provided a 10^4 -fold reduction in computational cost, compared to explicit optimizations of stacked dimers, the evaluation of stacking interactions directly from SMILES provides an additional 10^5 -fold speedup. The net result is that stacking interaction energies with Phe, Tyr, and Trp can be evaluated directly from SMILES using equations 1-3 at a rate of ~ 7500 heterocycles per second on a single CPU, with mean errors below 1 kcal mol^{-1} . This can be used to rapidly evaluate stacking interactions for large libraries of heterocycles. For example, Figure 9 shows interaction energies for the set of 1854 heterocycles stacked with Trp computed via equation 1 using DFT computed heterocycle descriptors versus those evaluated directly from SMILES. Overall, there is excellent agreement both in terms of quantitative predictions and ranking, with the SMILES derived stacking interactions exhibiting a RMSE of only $0.3 \text{ kcal mol}^{-1}$ compared to those based on DFT-computed descriptors. That is, the errors arising from the use of SMILES-derived descriptors, rather than those from DFT-computed ESPs, are smaller than the errors inherent in equation 1.

Figure 9. Stacking interactions of 1854 known and unknown⁴³ heterocycles with Trp predicted with equation 1 using DFT-based ESP descriptors compared to those evaluated directly from SMILES representations, grouped by whether the heterocycles were known or unknown as of publication of Ref. 43.

Summary and Concluding Remarks

Predicting the potential strength of stacking interactions between heterocyclic systems is vital for several fields, including drug design. We previously showed that the heterocycle descriptors ESP_{mean} and ESP_{max} can be used to predict the strength of stacking interactions of drug-like heterocycles with the aromatic amino acid side chains Phe, Tyr, and Trp.³⁰ This provided access to accurate stacking interaction energies based solely on computed electrostatic potentials of the isolated heterocycles, obviating the need for DFT-based geometry optimizations of stacked dimers and the computation of high-level *ab initio* interaction energies. However, the reliance on DFT computed ESPs prohibited the prediction of stacking interactions for large sets of heterocycles. Here, we developed a physical model of the impact of multiple heteroatoms on the ESP near mono- and bicyclic heterocycles that enables the evaluation of ESP_{mean} and ESP_{max} based solely on atom connectivity. Consequently, one can convert simple molecular representations (*e.g.* SMILES) directly into high-level *ab initio* quality stacking interactions with minimal loss in accuracy using a freely available online tool.⁴⁸ This opens the door for the scoring of large sets of heterocycles with regard to their ability to engage in stacking interactions with aromatic amino acid side chains. While such predictions correspond to idealized stacked dimers in the gas-phase, they should help guide the choice of heterocyclic fragments of potential inhibitors that will enhance stacking interactions with binding site aromatic residues.

Computational Methods

We selected 1854 heterocycles (51 monocycles and 1803 bicycles) from the VEHICLE database of Pitt *et al.*⁴³ with high synthetic tractability scores [$p(\text{good}) > 0.95$], a fully aromatic canonical SMILES string, at least two (for monocycles) or three (for bicycles) unsubstituted positions, fewer than four carbonyl groups, and fewer than six imino nitrogen atoms. This provides a diverse set of heterocycles comprising 1174 previously synthesized (known) heterocycles and 680 heterocycles that had not been synthesized as of 2009 but should be synthetically viable.⁴³ Initial three dimensional structures of these heterocycles were generated from the SMILES representations in the VEHICLE database⁴³ using OpenBabel.⁴⁹ These structures were then optimized at the ω B97X-D/def2-TZVP level of theory⁵⁰⁻⁵¹ using Gaussian09.⁵² All heterocycles were considered to be planar (*e.g.* no pyramidalization of amino nitrogens, *etc.*). Values for ESP_{mean} and ESP_{max} were evaluated for each heterocycle by first computing the ESP on a grid of points (0.1 Å spacing) located 3.25 Å from the heterocycle at the ω B97X-D/def2-TZVP level of theory, and then computing the mean and maximum values within the projection of the van der Waals volume³⁶ of the heterocycle onto this plane, as done previously.³²

In order to identify all heteroatom types and heteroatom pairs, SMILES strings from the VEHICLE database were first canonicalized and then converted to connectivity tables using OpenBabel.⁴⁹ Atom types and pairs were then identified using a Perl script based on these connectivities. The angles (α_{ij}) and distances (R_{ij}) in equation 3 were derived from idealized pentagonal and hexagonal rings and are listed in SI Table S1. The fits of equations 2 and 3 were subjected to 5-fold cross-validation. To confirm that equations 2 and 3 were not over-fit, we performed two sets of fits to randomized data. First, we generated random sets of heteroatom and pair counts according to a gamma distribution with $k = 0.7$ and $\theta = 1$ for the heteroatom counts and $k = 0.15$, $\theta = 1$ for the pair counts. This resulted in a distribution of digits that match the distribution found in the initial data set. We refit equations 2 and 3 to three such random data sets. Second, we utilized the actual heteroatom and pair counts but fit to randomized ESP_{mean} and ESP_{max} values taken from Gaussian distributions with the same mean and standard deviation as the DFT-computed data. In both cases, there was no correlation; the average RMSE for equations 2 and 3 were 2.3 kcal mol⁻¹ and 3.3 kcal mol⁻¹, respectively.

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Supporting Information Available: Additional computational data and figures.

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TOC Graphic

c1cc2c(o1)occ2
c1cn2c(c1)snn2
c1cc2c(o1)scn2
c1nn2c(c1)snc2
c1cn2c(c1)onn2
s1cc2c(c1)nco2
c1oc2c(c1)ocn2
o1cc2c(c1)cn[nH]2
c1cnc2c(c1)coc2
c1cc2n(c1)occ2
[nH]1nc2c(n1)cco2

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