Supplementary material to: SCAN-based hybrid and double-hybrid density functionals from models without fitted parameters

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[1] Y. Zhao, N. González-García, and D. G. Truhlar, J. Phys. Chem. A **109**, 2012 (2005); **110**, 4942(E) (2006).

[2] Y. Zhao, B. J. Lynch, and D. G. Truhlar, J. Phys. Chem. A **108**, 2715 (2004).

[3] P. Jurečka, J. Šponer, J. Černý, and P. Hobza, Phys. Chem. Chem. Phys. **8**, 1985 (2006).

[4] T. Takatani, E. G. Hohenstein, M. Malagoli, M. S. Marshall, and C. D. Sherrill, J. Chem. Phys. **132**, 144104 (2010).

[5] J. Rezac, K. E. Riley, and P. Hobza, J. Chem. Theory Comput. **7**, 2427 (2011).

TABLES

TABLE I: Nonhydrogen transfer barrier heights (in kcal/mol) of the NHTBH38/04 set [1].

Reaction	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
Heavy-atom transfer reactions											
$H + N_2O \longrightarrow OH + N_2$											
	V^f	18.14	9.97	9.57	13.91	12.08	17.41	15.34	20.83	19.30	23.58	22.66
	V^r	83.22	52.46	64.71	68.79	76.54	76.63	81.26	79.93	82.69	81.25	83.28
$H + FH \longrightarrow HF + H$											
	V^f	42.18	27.07	28.83	33.74	33.42	38.71	37.24	41.88	40.16	43.35	41.87
	V^r	42.18	27.07	28.83	33.74	33.42	38.71	37.24	41.88	40.16	43.35	41.87
$H + ClH \longrightarrow HCl + H$											
	V^f	18.00	9.64	9.51	13.38	11.59	16.03	13.85	18.06	16.14	19.26	17.78
	V^r	18.00	9.64	9.51	13.38	11.59	16.03	13.85	18.06	16.14	19.26	17.78
$H + FCH_3 \longrightarrow HF + CH_3$											
	V^f	30.38	18.51	20.38	25.71	25.25	30.23	28.79	32.79	31.06	33.87	32.35
	V^r	57.02	40.99	46.44	49.75	53.03	54.86	56.60	57.43	58.24	58.38	58.85
$H + F_2 \longrightarrow HF + F$											
	V^f	2.27	-9.86	-11.36	-4.60	-8.46	-0.44	-4.25	5.79	2.74	11.20	8.89
	V^r	106.18	80.86	89.93	99.03	103.53	109.15	111.27	116.64	117.43	121.25	121.59

Table I: NHTBH38/04 (continued).

Reaction	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
$CH_3 + FCl \longrightarrow CH_3F + Cl$											
V^f	7.43	-6.47	-4.62	0.79	1.39	4.97	5.08	7.86	7.84	10.02	10.03
V^r	60.17	41.63	45.99	53.46	55.24	60.14	60.54	64.14	63.88	66.55	66.21
Nucleophilic substitution reactions											
$F^- + CH_3F \longrightarrow FCH_3 + F^-$											
V^f	-0.34	-8.31	-8.37	-2.67	-3.20	-0.70	-1.16	-0.07	-0.40	-0.00	-0.17
V^r	-0.34	-8.31	-8.37	-2.67	-3.20	-0.70	-1.16	-0.07	-0.40	-0.00	-0.17
$F^-\cdots CH_3F \longrightarrow FCH_3\cdots F^-$											
V^f	13.38	7.06	8.03	11.69	12.24	13.57	13.94	14.25	14.48	14.40	14.58
V^r	13.38	7.06	8.03	11.69	12.24	13.57	13.94	14.25	14.48	14.40	14.58
$Cl^- + CH_3Cl \longrightarrow ClCH_3 + Cl^-$											
V^f	3.10	-3.80	-5.10	0.87	-0.53	2.92	1.92	3.89	3.27	4.32	3.91
V^r	3.10	-3.80	-5.10	0.87	-0.53	2.92	1.92	3.89	3.27	4.32	3.91
$Cl^-\cdots CH_3Cl \longrightarrow ClCH_3\cdots Cl^-$											
V^f	13.61	7.15	6.95	11.29	10.88	13.41	13.13	14.58	14.42	15.14	15.04
V^r	13.61	7.15	6.95	11.29	10.88	13.41	13.13	14.58	14.42	15.14	15.04
$F^- + CH_3Cl \longrightarrow FCH_3 + Cl^-$											
V^f	-12.54	-19.52	-21.98	-15.45	-17.67	-13.75	-15.21	-12.68	-13.56	-12.13	-12.64

Table I: NHTBH38/04 (continued).

Reaction	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
V^r	20.11	12.31	15.14	19.44	20.56	21.77	22.08	22.10	22.05	21.83	21.69
$F^-\cdots CH_3Cl \longrightarrow FCH_3\cdots Cl^-$											
V^f	2.89	-0.67	-1.65	1.66	0.94	2.95	2.56	3.82	3.63	4.29	4.20
V^r	29.62	21.45	25.09	28.35	30.19	30.86	31.73	31.47	31.80	31.38	31.51
$OH^- + CH_3F \longrightarrow HOCH_3 + F^-$											
V^f	-2.78	-10.59	-10.24	-4.97	-5.24	-2.97	-3.27	-2.34	-2.56	-2.20	-2.34
V^r	17.33	9.14	9.15	15.94	15.34	18.22	17.64	18.70	18.23	18.50	18.22
$OH^-\cdots CH_3F \longrightarrow HOCH_3\cdots F^-$											
V^f	10.96	3.89	5.16	8.82	9.54	10.87	11.35	11.68	11.99	11.94	12.16
V^r	47.2	43.21	44.02	49.06	49.29	51.09	51.18	51.44	51.47	51.22	51.22
Unimolecular and association reactions											
$H + N_2 \longrightarrow HN_2$											
V^f	14.69	5.19	4.35	8.50	6.40	11.54	9.42	14.77	13.19	17.32	16.25
V^r	10.72	9.08	9.70	11.64	11.75	12.55	12.48	12.41	12.32	11.91	11.71
$H + CO \longrightarrow HCO$											
V^f	3.17	-1.69	-3.48	0.31	-2.18	1.83	-0.41	3.08	1.37	3.85	2.59
V^r	22.68	24.66	24.12	25.47	24.68	25.51	24.71	25.03	24.42	24.52	24.10
$H + C_2H_4 \longrightarrow CH_3CH_2$											

Table I: NHTBH38/04 (continued).

Reaction	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
V^f	1.72	-0.14	-4.01	0.67	-3.68	1.50	-1.73	2.89	0.76	4.24	2.80
V^r	41.75	40.20	43.00	44.12	45.16	45.72	46.03	46.14	46.31	46.18	46.38
$CH_3 + C_2H_4 \longrightarrow CH_3CH_2CH_2$											
V^f	6.85	1.50	0.93	4.02	2.47	5.24	4.28	6.64	6.15	7.93	7.67
V^r	32.97	29.76	30.62	34.47	33.72	36.89	35.78	38.33	37.45	39.12	38.50
$HCN \longrightarrow HCN$											
V^f	48.16	45.60	46.27	46.37	46.47	47.30	47.11	48.45	48.18	49.35	49.09
V^r	33.11	30.50	32.14	32.51	33.42	33.31	33.69	33.71	33.79	33.92	33.90
	MSE	-8.52	-7.48	-3.13	-3.28	-0.32	-0.83	1.39	0.87	2.34	1.94
	MAE	8.62	7.62	3.63	3.84	1.57	2.24	1.62	1.63	2.44	2.03
	rms	10.61	8.72	4.63	4.63	2.19	2.82	2.58	2.55	3.71	3.43
	Max(−)	-30.76	-18.51	-14.43	-10.73	-6.59	-6.52	-3.29	-2.02	-1.97	-0.58
	Max(+)	1.98	1.44	2.79	3.41	3.97	5.09	10.46	11.25	15.07	15.41

TABLE II: Hydrogen transfer barrier heights (in kcal/mol) of the HTBH38/04 set [1, 2].

Reaction	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
$H + HCl \longrightarrow H_2 + Cl$											
V^f	5.70	0.56	-1.05	2.94	0.31	4.88	2.18	6.56	4.26	7.64	5.83

Table II: HTBH38/04 (continued).

Reaction	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
V^r	8.70	-1.95	0.09	1.66	2.39	3.90	4.23	5.26	5.20	5.90	5.79
$OH + H_2 \longrightarrow H + H_2O$											
V^f	5.10	-6.36	-2.01	-0.02	1.98	3.16	4.11	4.79	4.95	5.51	5.45
V^r	21.20	13.69	11.36	17.31	14.02	20.24	17.06	23.24	20.58	25.39	23.30
$CH_3 + H_2 \longrightarrow H + CH_4$											
V^f	12.10	3.82	7.47	6.89	8.99	8.83	10.21	10.13	10.81	10.84	11.26
V^r	15.30	9.32	7.36	11.90	9.18	13.92	11.47	15.64	13.55	16.72	15.05
$OH + CH_4 \longrightarrow CH_3 + H_2O$											
V^f	6.70	-5.65	-1.58	1.62	3.48	4.91	5.87	6.17	6.44	6.50	6.53
V^r	19.60	8.91	11.90	13.94	15.33	16.90	17.56	19.10	19.34	20.50	20.59
$H + H_2 \longrightarrow H_2 + H$											
V^f	9.60	3.64	2.53	5.63	3.58	7.46	5.59	9.15	7.56	10.24	9.03
V^r	9.60	3.64	2.53	5.63	3.58	7.46	5.59	9.15	7.56	10.24	9.03
$OH + NH_3 \longrightarrow H_2O + NH_2$											

Table II: HTBH38/04 (continued).

Reaction	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
V^f	3.20	-11.94	-7.40	-2.28	-0.07	2.16	3.31	3.97	4.43	4.60	4.78
V^r	12.70	-0.71	3.31	7.41	9.37	11.49	12.47	13.73	14.13	14.91	15.07
$HCl + CH_3 \longrightarrow Cl + CH_4$											
V^f	1.70	-5.94	-3.08	-2.49	-0.90	-0.67	0.21	0.30	0.67	0.74	0.91
V^r	7.90	-2.95	-2.04	1.25	1.38	3.45	3.51	4.51	4.34	4.88	4.66
$OH + C_2H_6 \longrightarrow H_2O + C_2H_5$											
V^f	3.40	-9.03	-4.49	-1.23	0.77	2.22	3.37	3.58	3.96	4.00	4.08
V^r	19.90	10.75	13.13	15.65	16.62	18.30	18.71	20.25	20.34	21.52	21.51
$F + H_2 \longrightarrow HF + H$											
V^f	1.80	-12.97	-7.77	-4.90	-2.56	-0.73	0.29	1.48	1.67	2.44	2.44
V^r	33.40	25.12	22.61	28.40	24.89	31.46	28.03	35.11	32.33	37.88	35.75
$O + CH_4 \longrightarrow OH + CH_3$											
V^f	13.70	-0.79	1.76	7.16	7.98	11.53	11.82	13.66	13.56	14.42	14.23
V^r	8.10	-0.57	3.31	3.94	6.33	6.48	7.86	8.07	8.83	8.93	9.43

Table II: HTBH38/04 (continued).

Reaction	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
$H + PH_3 \longrightarrow PH_2 + H_2$											
V^f	3.10	-1.78	-2.65	0.35	-1.67	1.86	-0.08	3.02	1.28	3.70	2.29
V^r	23.20	17.91	19.24	20.12	20.47	21.43	21.69	22.31	22.36	22.79	22.82
$H + HO \longrightarrow H_2 + O$											
V^f	10.70	3.74	3.39	7.13	5.69	9.66	7.81	11.87	10.16	13.34	11.94
V^r	13.10	-1.98	1.94	5.33	7.14	9.62	10.52	11.95	12.15	12.94	12.95
$H + H_2S \longrightarrow H_2 + HS$											
V^f	3.50	-1.22	-2.43	1.05	-1.10	2.69	0.56	3.95	2.10	4.69	3.21
V^r	17.30	9.10	11.25	12.06	13.02	13.75	14.34	14.70	14.88	15.12	15.20
$O + HCl \longrightarrow OH + Cl$											
V^f	9.80	-10.54	-3.88	2.22	4.86	8.05	9.21	11.10	11.44	12.38	12.46
V^r	10.40	-7.33	-1.30	2.74	5.48	7.12	8.55	9.71	10.39	11.04	11.42
$NH_2 + CH_3 \longrightarrow CH_4 + NH$											
V^f	8.00	0.71	4.52	5.05	7.38	7.26	8.59	8.44	9.15	9.00	9.44
V^r	22.40	10.56	12.29	16.42	16.77	19.62	19.63	21.32	21.03	22.03	21.69

Table II: HTBH38/04 (continued).

Reaction	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
$NH_2 + C_2H_5 \longrightarrow C_2H_6 + NH$											
	V^f	7.50	2.89	5.99	6.88	8.82	8.71	9.85	9.53	10.16	9.86	10.27
	V^r	18.30	7.50	9.61	13.69	14.21	16.98	17.24	18.67	18.55	19.38	19.15
$C_2H_6 + NH_2 \longrightarrow NH_3 + C_2H_5$											
	V^f	10.40	1.43	5.26	7.25	9.01	9.81	10.88	10.69	11.07	10.87	10.97
	V^r	17.40	9.98	12.17	14.45	15.41	16.57	17.06	17.60	17.76	18.08	18.12
$NH_2 + CH_4 \longrightarrow CH_3 + NH_3$											
	V^f	14.50	4.39	7.85	9.87	11.51	12.37	13.25	13.29	13.55	13.49	13.53
	V^r	17.80	7.71	10.62	12.50	13.92	15.03	15.78	16.47	16.75	17.18	17.30
s-trans cis-$C_5H_8 \longrightarrow$ *s-trans cis*-C_5H_8											
	V^f	38.40	31.20	33.63	35.58	37.16	37.35	38.19	37.23	37.54	36.46	36.57
	V^r	38.40	31.20	33.63	35.58	37.16	37.35	38.19	37.23	37.54	36.46	36.57

Table II: HTBH38/04 (continued).

Reaction	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
	MSE	-9.67	-7.49	-4.60	-3.99	-1.87	-1.81	-0.28	-0.56	0.50	0.19
	MSE	9.67	7.49	4.60	4.06	1.93	2.00	0.99	1.14	1.39	1.18
	rms	10.37	7.94	4.88	4.46	2.19	2.48	1.30	1.43	1.74	1.45
	Max(−)	-20.34	-13.68	-7.77	-8.51	-4.80	-5.37	-3.44	-3.56	-3.02	-3.24
	Max(+)	-4.61	-1.51	-0.62	1.32	1.21	2.35	2.04	2.66	4.48	2.77

TABLE III: Interaction energies (in kcal/mol) of the S22 set [3, 4].

Complex	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
Hydrogen bonded complexes											
NH_3 dimer (C2h)	-3.17	-2.83	-3.14	-2.77	-3.11	-2.83	-3.15	-2.90	-3.15	-2.93	-3.12
H_2O dimer (Cs)	-5.02	-4.91	-5.39	-4.92	-5.38	-4.96	-5.34	-4.94	-5.22	-4.89	-5.09
Formic acid dimer (C2h)	-18.80	-18.08	-20.63	-18.86	-20.75	-19.21	-20.49	-19.08	-19.87	-18.75	-19.28
Formamide dimer (C2h)	-16.12	-14.69	-16.38	-15.27	-16.59	-15.64	-16.60	-15.69	-16.34	-15.55	-16.01
Uracil dimer (C2h)	-20.69	-18.45	-20.32	-19.16	-20.65	-19.72	-20.81	-19.95	-20.68	-19.91	-20.43
2-pyridone ... 2-aminopyridine (C1)	-17.00	-15.27	-16.69	-15.35	-16.53	-15.84	-16.73	-16.26	-16.88	-16.42	-16.86
Adenine ... thymine WC (C1)	-16.74	-14.29	-15.88	-14.50	-15.83	-15.09	-16.10	-15.54	-16.25	-15.69	-16.17
Dispersion complexes											

Table III: S22 interaction energies (continued).

Complex	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
CH_4 dimer (D3d)	-0.53	-0.08	-0.37	-0.04	-0.31	-0.09	-0.32	-0.18	-0.36	-0.25	-0.38
C_2H_4 dimer (D2d)	-1.50	-0.31	-1.07	-0.35	-1.04	-0.58	-1.15	-0.84	-1.26	-1.00	-1.31
Benzene ... CH_4	-1.45	-0.01	-0.89	-0.08	-0.82	-0.41	-0.97	-0.79	-1.19	-1.04	-1.33
Benzene dimer (C2h)	-2.62	1.90	-1.13	1.80	-0.57	0.60	-1.03	-0.91	-1.95	-1.94	-2.66
Pyrazine dimer (Cs)	-4.20	0.73	-2.71	0.53	-2.14	-0.82	-2.64	-2.45	-3.61	-3.57	-4.35
Uracil dimer (C2)	-9.74	-2.69	-8.00	-3.30	-7.32	-4.99	-7.76	-6.81	-8.57	-7.91	-9.14
Indole Benzene (C1)	-4.59	2.24	-2.19	2.02	-1.39	0.17	-2.17	-2.12	-3.59	-3.67	-4.68
Adenine ... thymine (C1)	-11.66	-1.32	-8.69	-2.14	-7.73	-4.86	-8.65	-7.83	-10.21	-9.69	-11.32
Mixed complexes											
Ethene ... Ethine (C2v)	-1.51	-1.16	-1.35	-1.18	-1.38	-1.26	-1.46	-1.36	-1.51	-1.41	-1.53
Benzene ... H_2O (Cs)	-3.29	-2.04	-3.30	-2.21	-3.19	-2.54	-3.23	-2.83	-3.28	-2.98	-3.30
Benzene ... NH_3 (Cs)	-2.32	-0.92	-2.00	-1.03	-1.89	-1.36	-1.99	-1.72	-2.14	-1.94	-2.24
Benzene ... HCN (Cs)	-4.55	-2.81	-4.08	-3.28	-4.29	-3.83	-4.55	-4.25	-4.73	-4.46	-4.79
Benzene dimer (C2v)	-2.71	-0.10	-1.50	-0.28	-1.43	-0.95	-1.79	-1.70	-2.28	-2.19	-2.60
Indole ... Benzene (Cs)	-5.62	-2.03	-4.07	-2.36	-3.97	-3.32	-4.48	-4.37	-5.14	-5.03	-5.57
Phenol dimer (C1)	-7.09	-3.87	-5.92	-4.18	-5.83	-4.96	-6.18	-5.76	-6.58	-6.23	-6.82

Table III: S22 interaction energies (continued).

Complex	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
	MSE	2.72	0.69	2.45	0.85	1.75	0.60	1.03	0.28	0.61	0.09
	MAE	2.72	0.92	2.46	1.11	1.78	0.84	1.05	0.43	0.61	0.19
	rms	3.73	1.22	3.45	1.54	2.49	1.19	1.42	0.59	0.78	0.25
	Max(−)	0.11	-1.83	-0.06	-1.95	-0.41	-1.69	-0.28	-1.07	0.05	-0.48
	Max(+)	10.34	2.97	9.52	3.93	6.80	3.01	3.83	1.45	1.97	0.60

TABLE IV: Interaction energies (in kcal/mol) of the S66 set [5].

Complex	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
Hydrogen bonded complexes											
Water ... Water	-4.918	-4.87	-5.32	-4.90	-5.33	-4.94	-5.30	-4.93	-5.20	-4.88	-5.08
Water ... MeOH	-5.592	-5.16	-5.95	-5.20	-5.88	-5.33	-5.86	-5.42	-5.79	-5.43	-5.70
Water ... MeNH2	-6.908	-7.15	-7.46	-7.01	-7.36	-7.01	-7.33	-6.99	-7.24	-6.94	-7.13
Water ... Peptide	-8.103	-7.28	-8.68	-7.49	-8.63	-7.72	-8.56	-7.83	-8.39	-7.82	-8.21
MeOH ... MeOH	-5.757	-5.08	-5.89	-5.10	-5.80	-5.26	-5.82	-5.40	-5.80	-5.46	-5.75
MeOH ... MeNH2	-7.554	-7.19	-7.83	-7.05	-7.67	-7.16	-7.69	-7.28	-7.68	-7.32	-7.62
MeOH ... Peptide	-8.230	-7.18	-8.53	-7.30	-8.43	-7.56	-8.42	-7.74	-8.33	-7.78	-8.20
MeOH ... Water	-5.009	-4.78	-5.27	-4.79	-5.26	-4.85	-5.26	-4.88	-5.18	-4.87	-5.09
MeNH2 ... MeOH	-3.059	-2.22	-2.76	-2.17	-2.68	-2.31	-2.76	-2.50	-2.84	-2.61	-2.86

Table IV: S66 interaction energies (continued).

Complex	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
MeNH2 ... MeNH2	-4.160	-3.08	-3.87	-3.01	-3.75	-3.24	-3.86	-3.51	-3.97	-3.67	-4.01
MeNH2 ... Peptide	-5.419	-3.39	-4.96	-3.53	-4.84	-3.98	-4.98	-4.43	-5.12	-4.67	-5.17
MeNH2 ... Water	-7.266	-7.14	-7.87	-7.06	-7.72	-7.15	-7.68	-7.22	-7.59	-7.22	-7.49
Peptide ... MeOH	-6.187	-4.53	-5.69	-4.72	-5.69	-5.09	-5.85	-5.44	-5.98	-5.63	-6.02
Peptide ... MeNH2	-7.454	-6.12	-7.06	-6.12	-6.96	-6.44	-7.12	-6.78	-7.27	-6.96	-7.32
Peptide ... Peptide	-8.630	-6.36	-8.00	-6.64	-7.98	-7.16	-8.16	-7.62	-8.31	-7.84	-8.34
Peptide ... Water	-5.124	-4.32	-4.88	-4.46	-4.98	-4.64	-5.08	-4.78	-5.11	-4.83	-5.08
Uracil ... Uracil (BP)	-17.182	-15.49	-17.25	-15.98	-17.41	-16.47	-17.53	-16.70	-17.42	-16.69	-17.20
Water ... Pyridine	-6.857	-6.82	-7.13	-6.64	-7.01	-6.69	-7.02	-6.75	-7.01	-6.76	-6.96
MeOH ... Pyridine	-7.410	-6.92	-7.42	-6.73	-7.24	-6.86	-7.31	-7.04	-7.38	-7.14	-7.39
AcOH ... AcOH	-19.093	-18.59	-21.09	-19.24	-21.12	-19.58	-20.87	-19.49	-20.29	-19.20	-19.73
AcNH2 ... AcNH2	-16.265	-15.02	-16.64	-15.48	-16.78	-15.85	-16.81	-15.94	-16.59	-15.85	-16.30
AcOH ... Uracil	-19.491	-18.31	-20.45	-18.96	-20.62	-19.39	-20.56	-19.45	-20.21	-19.28	-19.81
AcNH2 ... Uracil	-19.189	-17.67	-19.53	-18.31	-19.78	-18.79	-19.85	-18.93	-19.64	-18.83	-19.33
Dispersion complexes											
Benzene ... Benzene (pi-pi)	-2.822	1.22	-1.34	1.18	-0.83	0.18	-1.24	-1.13	-2.05	-2.04	-2.68
Pyridine ... Pyridine (pi-pi)	-3.895	0.48	-2.39	0.34	-1.90	-0.79	-2.34	-2.20	-3.20	-3.17	-3.86
Uracil ... Uracil (pi-pi)	-9.829	-2.51	-8.00	-3.15	-7.30	-4.91	-7.75	-6.77	-8.58	-7.90	-9.15

Table IV: S66 interaction energies (continued).

Complex	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
Benzene ... Pyridine (pi-pi)	-3.439	0.81	-1.94	0.71	-1.44	-0.37	-1.87	-1.74	-2.71	-2.68	-3.35
Benzene ... Uracil (pi-pi)	-5.713	0.36	-3.81	0.01	-3.18	-1.49	-3.69	-3.22	-4.62	-4.34	-5.30
Pyridine ... Uracil (pi-pi)	-6.819	-0.74	-4.97	-1.12	-4.37	-2.62	-4.86	-4.34	-5.76	-5.44	-6.42
Benzene ... Ethene	-1.432	0.76	-0.81	0.82	-0.45	0.32	-0.60	-0.36	-0.97	-0.84	-1.27
Uracil ... Ethene	-3.380	-0.34	-2.56	-0.52	-2.27	-1.22	-2.47	-2.01	-2.83	-2.51	-3.08
Uracil ... Ethyne	-3.738	-1.03	-3.16	-1.24	-2.92	-1.88	-3.06	-2.57	-3.34	-3.00	-3.54
Pyridine ... Ethene	-1.872	0.45	-1.24	0.48	-0.88	-0.06	-1.04	-0.77	-1.43	-1.27	-1.73
Pentane ... Pentane	-3.776	0.42	-1.90	0.38	-1.61	-0.45	-2.02	-1.46	-2.59	-2.12	-2.95
Neopentane ... Pentane	-2.613	0.18	-0.98	0.23	-0.82	-0.26	-1.14	-0.89	-1.55	-1.31	-1.80
Neopentane ... Neopentane	-1.777	0.14	-1.16	0.18	-0.99	-0.35	-1.31	-1.01	-1.72	-1.45	-1.98
Cyclopentane ... Neopentane	-2.404	0.11	-1.25	0.18	-1.07	-0.41	-1.45	-1.18	-1.96	-1.69	-2.27
Cyclopentane ... Cyclopentane	-2.997	0.05	-0.59	0.16	-0.48	-0.16	-0.73	-0.59	-1.04	-0.89	-1.24
Benzene ... Cyclopentane	-3.575	0.30	-1.96	0.18	-1.66	-0.72	-2.07	-1.80	-2.72	-2.52	-3.17
Benzene ... Neopentane	-2.895	0.09	-1.57	0.00	-1.36	-0.67	-1.70	-1.49	-2.20	-2.04	-2.54
Uracil ... Pentane	-4.848	0.52	-2.89	0.27	-2.43	-0.91	-2.88	-2.25	-3.58	-3.09	-4.04
Uracil ... Cyclopentane	-4.138	0.58	-2.25	0.44	-1.83	-0.58	-2.24	-1.77	-2.90	-2.54	-3.35
Uracil ... Neopentane	-3.712	0.08	-2.26	-0.07	-1.93	-0.87	-2.24	-1.80	-2.73	-2.39	-3.06
Ethene ... Pentane	-2.005	0.01	-1.12	0.03	-0.98	-0.36	-1.18	-0.85	-1.45	-1.17	-1.62
Ethyne ... Pentane	-1.748	-0.09	-1.14	-0.06	-0.96	-0.39	-1.10	-0.82	-1.33	-1.12	-1.49

Table IV: S66 interaction energies (continued).

Complex	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
Peptide ... Pentane	-4.264	0.07	-2.69	-0.07	-2.34	-0.97	-2.68	-2.00	-3.19	-2.65	-3.51
Mixed complexes											
Benzene ... Benzene (TS)	-2.876	-0.19	-1.66	-0.36	-1.56	-1.03	-1.92	-1.79	-2.40	-2.29	-2.72
Pyridine ... Pyridine (TS)	-3.535	-0.75	-2.31	-0.97	-2.26	-1.68	-2.64	-2.46	-3.11	-2.95	-3.42
Benzene ... Pyridine (TS)	-3.331	-0.61	-2.13	-0.84	-2.08	-1.53	-2.45	-2.30	-2.91	-2.78	-3.22
Benzene ... Ethyne (CH-pi)	-2.867	-1.23	-2.31	-1.48	-2.36	-1.94	-2.59	-2.38	-2.82	-2.64	-2.95
Ethyne ... Ethyne (TS)	-1.524	-1.20	-1.38	-1.21	-1.41	-1.28	-1.47	-1.35	-1.51	-1.39	-1.51
Benzene ... AcOH (OH-pi)	-4.707	-2.32	-4.31	-2.65	-4.16	-3.28	-4.31	-3.86	-4.52	-4.18	-4.63
Benzene ... AcNH2 (NH-pi)	-4.361	-2.34	-3.82	-2.59	-3.78	-3.10	-3.98	-3.59	-4.18	-3.86	-4.28
Benzene ... Water (OH-pi)	-3.277	-1.98	-3.33	-2.17	-3.21	-2.52	-3.25	-2.82	-3.30	-2.98	-3.31
Benzene ... MeOH (OH-pi)	-4.188	-1.86	-3.75	-2.03	-3.52	-2.61	-3.66	-3.21	-3.91	-3.58	-4.06
Benzene ... MeNH2 (NH-pi)	-3.231	-0.77	-2.52	-0.90	-2.30	-1.48	-2.50	-2.13	-2.81	-2.55	-3.03
Benzene ... Peptide (NH-pi)	-5.282	-1.68	-4.05	-2.01	-3.87	-2.90	-4.23	-3.86	-4.73	-4.45	-5.06
Pyridine ... Pyridine (CH-N)	-4.146	-2.49	-3.01	-2.60	-3.15	-3.02	-3.51	-3.43	-3.81	-3.66	-3.95
Ethyne ... Water (CH-O)	-2.850	-2.63	-2.82	-2.74	-2.96	-2.81	-3.03	-2.83	-3.01	-2.81	-2.95
Ethyne ... AcOH (OH-pi)	-4.868	-4.10	-5.23	-4.30	-5.21	-4.50	-5.18	-4.61	-5.07	-4.62	-4.94
Pentane ... AcOH	-2.912	0.07	-1.82	0.02	-1.54	-0.57	-1.76	-1.26	-2.10	-1.71	-2.31
Pentane ... AcNH2	-3.534	-0.26	-2.35	-0.32	-2.05	-0.98	-2.31	-1.75	-2.68	-2.23	-2.91

Table IV: S66 interaction energies (continued).

Complex	Reference	PBE	SCAN	PBE0	SCAN0	PBE0-DH	SCAN0-DH	PBE-QIDH	SCAN-QIDH	PBE0-2	SCAN0-2
Benzene ... AcOH	-3.801	-0.53	-2.83	-0.81	-2.61	-1.60	-2.88	-2.46	-3.29	-2.99	-3.57
Peptide ... Ethene	-2.999	-0.95	-2.34	-1.06	-2.22	-1.49	-2.38	-1.96	-2.58	-2.25	-2.70
Pyridine ... Ethyne	-3.991	-3.64	-3.73	-3.65	-3.82	-3.78	-3.97	-3.89	-4.06	-3.94	-4.07
MeNH2 ... Pyridine	-3.968	-1.73	-3.30	-1.73	-3.05	-2.25	-3.24	-2.88	-3.56	-3.28	-3.77
	MSE	2.22	0.61	2.09	0.77	1.56	0.58	1.00	0.33	0.66	0.19
	MAE	2.23	0.85	2.10	1.01	1.58	0.81	1.01	0.49	0.67	0.27
	rms	2.75	1.04	2.61	1.25	1.98	1.01	1.27	0.63	0.83	0.40
	Max(−)	-0.24	-2.00	-0.15	-2.03	-0.49	-1.77	-0.40	-1.20	-0.10	-0.64
	Max(+)	7.32	2.41	6.68	2.53	4.92	2.27	3.06	1.95	2.11	1.76