Supplementary Information: Accurate and Efficient Polymorph Energy Ranking with XDM-corrected hybrid DFT

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For the crystal structures belonging to the first to fifth blind tests (molecules I to XXI), duplicates were removed before the FHIaims calculations were performed. Two structures were considered replicas if their powder diffraction pattern difference measure (POWDIFF) as computed using the critic2 program with no volume correction applied was lower than 0.001.

An in-house script was subseqently used to identify and remove duplicates from the list of candidate structures after optimization for each target for compounds from all six blind tests. The structures within a 2 kJ/mol range of the structure being checked were compared by their POWDIFF values, again with no volume correction. If a value ≤ 0.07 was obtained, then the structure pair were compared with COMPACK (Mercury implementation via the CSD Python API) with a cluster size of 20 molecules and tolerances of $\pm$ 30% on the distances and $\pm$ 30° on the angles. If the structure pair yielded a match of 20/20 molecules by COMPACK, then they were considered duplicates and the higher energy structure was removed from the list. The number of replicates of a structure was also recorded.

TABLE I: Summary of the previous blind test results and numbers of structures considered. Reported are the number of matching structures identified in the previous blind test publications, the total number of candidate structures considered (after initial pruning of duplicates for BT1-5), and the number of unique candidate structures obtained after DFT optimization by removing duplicates.

Compound	BT	Year	Matches	Candidates	Unique
I	1	1999	4[a]	33	26
II	1	1999	1	24	22
III	1	1999	2	29	25
IV	2	2001	2	43	22
V	2	2001	4	39	23
VI	2	2001	0	33	31
VII	1	1999	1	18	11
VIII	3	2004	4	19	12
IX	3	2004	1	27	18
X	3	2004	0	24	22
XI	3	2004	0	30	23
XII	4	2007	4	37	27
XIII	4	2007	4	38	23
XIV	4	2007	3	35	22
XV	4	2007	2	32	27
XVI	5	2010	2	39	28
XVII	5	2010	2	36	21
XVIII	5	2010	1	37	30
XIX	5	2010	2	28	23
XX	5	2010	2	29	23
XXI	5	2010	0	19	19
XXII	6	2014	18	216	124
XXIII	6	2014	29[b]	201	131
XXIV	6	2014	1	163	129
XXV	6	2014	8	184	118
XXVI	6	2014	6	170	121

[a] All matches were for Form II. [b] Matches were 5 for Form A, 14 for Form B, 1 for Form C, 9 for Form D, and 0 for Form E.

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TABLE II: Computed energy ranking for unique candidate structures of compound I, 3-oxabicyclo[3.2.0]hepta-1,4-diene. Energies are expressed relative to the experimental form 1, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	i-expt-1	2	0.0	i-expt-2	0	-0.2	i-expt-2	0	-0.8
2	i-vaneijck-3	0	0.1	i-vaneijck-3	0	-0.0	i-vaneijck-3	0	-0.2
3	i-expt-2	0	0.2	i-expt-1	2	0.0	i-expt-1	2	0.0
4	i-williams-2	0	0.9	i-williams-2	0	0.8	i-williams-2	0	0.7
5	i-ammon-2	0	1.3	i-ammon-2	0	1.3	i-ammon-2	0	1.2
6	i-mooij-1	2	1.8	i-gavezzotti-3	0	1.9	i-gavezzotti-3	0	1.7
7	i-schmidt-1	0	1.8	i-schmidt-1	0	1.9	i-schmidt-1	0	2.0
8	i-gavezzotti-3	0	2.0	i-mooij-1	2	2.1	i-schmidt-3	2	2.4
9	i-mooij-2	0	2.3	i-mooij-2	0	2.6	i-mooij-2	0	2.9
10	i-verwer-2	0	2.4	i-verwer-2	0	2.8	i-verwer-2	0	3.1
11	i-mooij-3	0	2.8	i-hofmann-1	0	3.1	i-gavezzotti-2	1	3.2
12	i-hofmann-1	0	2.8	i-mooij-3	0	3.3	i-hofmann-1	0	3.5
13	i-motherwell-1	1	3.2	i-gavezzotti-2	1	3.3	i-price-3	0	3.6
14	i-price-3	0	3.2	i-price-3	0	3.4	i-lommerse-3	0	3.7
15	i-ammon-1	0	3.8	i-lommerse-3	0	3.9	i-mooij-3	0	3.7
16	i-lommerse-3	0	3.8	i-ammon-1	0	3.9	i-ammon-1	0	3.9
17	i-price-2	0	4.0	i-price-2	0	4.3	i-price-2	0	4.6
18	i-vaneijck-2	0	6.4	i-verwer-3	0	6.5	i-verwer-3	0	6.5
19	i-verwer-3	0	6.4	i-vaneijck-2	0	6.8	i-lommerse-1	0	7.2
20	i-hofmann-3	1	6.5	i-lommerse-1	0	7.0	i-vaneijck-2	0	7.3
21	i-motherwell-2	0	6.6	i-motherwell-2	0	7.2	i-schmidt-2	0	7.5
22	i-lommerse-1	0	6.6	i-schmidt-2	0	7.2	i-motherwell-2	0	7.7
23	i-schmidt-2	0	6.7	i-hofmann-3	1	7.4	i-vaneijck-1	0	7.8
24	i-lommerse-2	1	7.1	i-vaneijck-1	0	7.5	i-hofmann-3	1	8.1
25	i-vaneijck-1	0	7.2	i-ammon-3	1	7.9	i-ammon-3	1	8.7
26	i-motherwell-3	0	11.0	i-motherwell-3	0	11.4	i-motherwell-3	0	11.8

TABLE III: Computed energy ranking for unique candidate structures of compound II, 4-hydroxy-2-thiophenecarbonitrile. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	ii-verwer-3	0	-1.1	ii-verwer-3	0	-0.7	ii-verwer-3	0	-0.5
2	ii-price-1	0	-0.1	ii-expt	0	0.0	ii-expt	0	0.0
3	ii-verwer-1	0	-0.0	ii-price-1	0	0.3	ii-price-1	0	0.7
4	ii-expt	0	0.0	ii-motherwell-1	0	0.9	ii-motherwell-1	0	1.6
5	ii-williams-2	1	0.1	ii-verwer-1	0	1.1	ii-williams-1	0	1.8
6	ii-motherwell-1	0	0.2	ii-williams-2	1	1.2	ii-price-2	0	2.1
7	ii-verwer-2	0	0.3	ii-verwer-2	0	1.3	ii-williams-2	1	2.3
8	ii-price-2	0	0.9	ii-williams-1	0	1.5	ii-verwer-1	0	2.3
9	ii-williams-1	0	1.0	ii-price-2	0	1.5	ii-verwer-2	0	2.4
10	ii-motherwell-2	0	2.7	ii-motherwell-2	0	3.3	ii-motherwell-2	0	3.9
11	ii-price-3	0	4.7	ii-price-3	0	5.3	ii-price-3	0	5.8
12	ii-lommerse-3	0	6.4	ii-hofmann-1	0	7.6	ii-hofmann-1	0	8.1
13	ii-hofmann-1	0	6.8	ii-lommerse-3	0	7.6	ii-lommerse-3	0	8.8
14	ii-lommerse-2	0	10.7	ii-schmidt-3	0	12.1	ii-schmidt-3	0	12.6
15	ii-lommerse-1	1	11.3	ii-lommerse-2	0	12.2	ii-schmidt-2	0	12.9
16	ii-schmidt-3	0	11.7	ii-schmidt-2	0	12.4	ii-lommerse-2	0	13.7
17	ii-schmidt-2	0	12.0	ii-motherwell-3	1	12.8	ii-motherwell-3	1	14.2
18	ii-ammon-1	0	18.6	ii-ammon-1	0	18.5	ii-ammon-1	0	18.9
19	ii-hofmann-2	0	20.8	ii-ammon-2	0	21.0	ii-ammon-2	0	20.8
20	ii-ammon-2	0	21.6	ii-hofmann-2	0	21.7	ii-hofmann-2	0	22.9
21	ii-ammon-3	0	25.8	ii-ammon-3	0	24.4	ii-ammon-3	0	23.5
22	ii-hofmann-3	0	26.8	ii-hofmann-3	0	25.9	ii-hofmann-3	0	25.4

TABLE IV: Computed energy ranking for unique candidate structures of compound III, 2-(2-phenylethenyl)-1,3,2-benzodioxaborole. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	iii-expt	0	0.0	iii-expt	0	0.0	iii-expt	0	0.0
2	iii-williams-2	0	0.5	iii-williams-2	0	0.6	iii-williams-2	0	0.5
3	iii-price-1	1	0.8	iii-price-3	1	1.1	iii-price-3	1	1.2
4	iii-mooij-2	0	2.5	iii-mooij-2	0	2.7	iii-mooij-2	0	2.7
5	iii-lommerse-1	0	4.6	iii-vaneijck-3	0	4.4	iii-vaneijck-3	0	3.8
6	iii-vaneijck-3	0	4.7	iii-lommerse-1	0	4.7	iii-lommerse-1	0	4.4
7	iii-verwer-2	0	5.2	iii-verwer-2	0	5.3	iii-verwer-2	0	5.2
8	iii-vaneijck-2	2	5.4	iii-ammon-2	2	6.0	iii-mooij-3	0	6.4
9	iii-mooij-3	0	6.1	iii-mooij-3	0	6.3	iii-price-2	2	6.5
10	iii-lommerse-3	0	6.4	iii-lommerse-3	0	6.7	iii-lommerse-3	0	6.7
11	iii-verwer-1	0	6.6	iii-verwer-1	0	7.1	iii-verwer-1	0	7.8
12	iii-schmidt-3	0	6.7	iii-schmidt-3	0	7.3	iii-motherwell-3	0	7.8
13	iii-motherwell-3	0	7.0	iii-motherwell-3	0	7.7	iii-schmidt-3	0	8.0
14	iii-motherwell-2	0	8.3	iii-motherwell-2	0	8.7	iii-motherwell-2	0	9.0
15	iii-ammon-3	1	8.5	iii-hofmann-1	1	9.1	iii-hofmann-1	1	9.6
16	iii-gavezzotti-1	0	9.0	iii-gavezzotti-1	0	9.7	iii-gavezzotti-1	0	10.4
17	iii-verwer-3	0	9.1	iii-verwer-3	0	9.9	iii-verwer-3	0	10.8
18	iii-schmidt-2	0	9.7	iii-schmidt-2	0	10.5	iii-schmidt-2	0	11.2
19	iii-ammon-1	0	10.0	iii-schmidt-1	0	11.0	iii-schmidt-1	0	11.9
20	iii-schmidt-1	0	10.2	iii-ammon-1	0	11.1	iii-gavezzotti-2	0	12.2
21	iii-gavezzotti-2	0	10.2	iii-gavezzotti-2	0	11.2	iii-ammon-1	0	12.2
22	iii-lommerse-2	0	15.1	iii-lommerse-2	0	16.5	iii-lommerse-2	0	17.7
23	iii-motherwell-1	0	17.0	iii-motherwell-1	0	18.6	iii-motherwell-1	0	19.8
24	iii-hofmann-2	0	23.0	iii-hofmann-2	0	25.5	iii-hofmann-2	0	27.3
25	iii-hofmann-3	0	25.2	iii-hofmann-3	0	27.1	iii-hofmann-3	0	28.1

TABLE V: Computed energy ranking for unique candidate structures of compound IV, 3-azabicyclo[3.3.1]nonane-2,4-dione. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	iv-expt	1	0.0	iv-expt	1	0.0	iv-expt	1	0.0
2	iv-ammon-1	7	2.6	iv-ammon-1	7	2.1	iv-schmidt-1	7	1.7
3	iv-ammon-2	0	3.3	iv-ammon-2	0	3.3	iv-ammon-2	0	3.2
4	iv-scheraga-3	2	4.8	iv-ammon-3	2	4.6	iv-ammon-3	2	4.3
5	iv-motherwell-3	6	5.3	iv-price-3	6	5.5	iv-lommerse-3	1	5.5
6	iv-motherwell-2	0	5.4	iv-motherwell-2	0	5.6	iv-motherwell-2	0	5.7
7	iv-williams-2	0	5.8	iv-lommerse-3	1	5.8	iv-price-3	6	5.7
8	iv-lommerse-1	0	5.9	iv-lommerse-1	0	6.2	iv-lommerse-1	0	6.3
9	iv-lommerse-3	1	6.0	iv-williams-2	0	6.2	iv-williams-2	0	6.6
10	iv-erk-1	2	6.5	iv-erk-1	2	6.7	iv-erk-1	2	6.9
11	iv-schweizer-2	0	6.8	iv-price-2	0	7.2	iv-price-2	0	7.5
12	iv-price-2	0	6.9	iv-schweizer-2	0	7.2	iv-schweizer-2	0	7.8
13	iv-motherwell-1	0	7.4	iv-motherwell-1	0	7.6	iv-motherwell-1	0	7.9
14	iv-price-1	0	8.5	iv-price-1	0	8.9	iv-leusen-2	1	9.1
15	iv-schmidt-3	1	8.9	iv-leusen-2	1	9.0	iv-schmidt-3	1	9.3
16	iv-vaneijck-2	1	9.0	iv-schmidt-3	1	9.1	iv-price-1	0	9.4
17	iv-hofmann-3	0	9.3	iv-hofmann-3	0	9.6	iv-hofmann-3	0	9.8
18	iv-dzyabchenko-3	0	9.9	iv-dzyabchenko-3	0	10.1	iv-dzyabchenko-3	0	9.9
19	iv-schweizer-3	0	10.2	iv-schweizer-3	0	10.4	iv-williams-3	0	10.1
20	iv-schweizer-1	0	10.4	iv-williams-3	0	10.5	iv-schweizer-3	0	10.6
21	iv-williams-3	0	10.9	iv-schweizer-1	0	10.7	iv-schweizer-1	0	11.0
22	iv-hofmann-2	0	11.1	iv-hofmann-2	0	11.2	iv-hofmann-2	0	11.4

TABLE VI: Computed energy ranking for unique candidate structures of compound V, 7-endo-(bromocamphorylsulfonyl)imine. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	v-leusen-1	0	-1.9	v-williams-1	0	-1.9	v-williams-1	0	-1.5
2	v-williams-1	0	-1.9	v-leusen-1	0	-1.6	v-leusen-1	0	-1.1
3	v-scheraga-1	2	-1.4	v-mooy-2	2	-1.1	v-mooy-2	2	-0.7
4	v-expt	4	0.0	v-expt	4	0.0	v-expt	4	0.0
5	v-price-3	2	1.2	v-price-3	2	0.6	v-price-3	2	0.3
6	v-dzyabchenko-2	1	1.5	v-dzyabchenko-2	1	1.3	v-vaneijck-3	0	1.3
7	v-vaneijck-3	0	1.7	v-vaneijck-3	0	1.5	v-dzyabchenko-2	1	1.3
8	v-scheraga-2	1	2.2	v-scheraga-2	1	1.6	v-ammon-3	1	1.3
9	v-motherwell-2	0	3.5	v-motherwell-2	0	3.5	v-motherwell-2	0	3.8
10	v-erk-3	0	3.5	v-erk-1	3	4.1	v-erk-1	3	4.6
11	v-erk-1	3	3.9	v-erk-3	0	4.3	v-erk-3	0	5.3
12	v-lommerse-2	0	5.9	v-lommerse-2	0	5.9	v-lommerse-2	0	6.1
13	v-hofmann-1	0	6.8	v-hofmann-1	0	7.2	v-hofmann-1	0	8.0
14	v-schmidt-1	0	8.5	v-schmidt-1	0	8.8	v-schmidt-3	0	9.4
15	v-schmidt-3	0	9.0	v-schmidt-3	0	9.0	v-schmidt-1	0	9.6
16	v-gavezzotti-1	3	9.4	v-erk-2	3	10.2	v-dzyabchenko-3	0	10.2
17	v-hofmann-3	0	10.0	v-hofmann-3	0	10.4	v-hofmann-3	0	10.7
18	v-dzyabchenko-3	0	11.4	v-dzyabchenko-3	0	10.6	v-erk-2	3	11.3
19	v-schmidt-2	0	11.8	v-schmidt-2	0	13.0	v-schmidt-2	0	14.6
20	v-gavezzotti-2	0	12.6	v-gavezzotti-2	0	14.0	v-gavezzotti-2	0	15.6
21	v-hofmann-2	0	16.5	v-hofmann-2	0	17.6	v-hofmann-2	0	18.9
22	v-lommerse-1	0	20.4	v-lommerse-1	0	20.8	v-lommerse-1	0	21.6
23	v-vaneick-2	0	22.1	v-vaneick-2	0	22.1	v-vaneick-2	0	22.7

TABLE VII: Computed energy ranking for unique candidate structures of compound VI, 6-amino-2-phenylsulfonylimino-1,2-dihydropyridine. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	vi-expt	0	0.0	vi-expt	0	0.0	vi-expt	0	0.0
2	vi-erk-1	0	7.5	vi-mooy-3	0	8.1	vi-mooy-3	0	8.0
3	vi-mooy-3	0	8.6	vi-erk-1	0	8.2	vi-erk-1	0	8.7
4	vi-vaneijck-3	0	11.9	vi-vaneijck-3	0	12.4	vi-vaneijck-3	0	12.6
5	vi-mooy-1	1	13.6	vi-vaneick-2	1	14.2	vi-vaneick-2	1	14.6
6	vi-vaneijck-1	0	14.7	vi-vaneijck-1	0	15.8	vi-schmidt-1	0	15.7
7	vi-dzyabchenko-2	0	15.1	vi-dzyabchenko-2	0	16.1	vi-vaneijck-1	0	16.5
8	vi-schmidt-1	0	16.7	vi-schmidt-1	0	16.1	vi-dzyabchenko-2	0	16.6
9	vi-leusen-2	0	18.6	vi-dzyabchenko-3	0	18.4	vi-dzyabchenko-3	0	17.8
10	vi-dzyabchenko-3	0	18.9	vi-leusen-2	0	19.6	vi-leusen-2	0	20.6
11	vi-scheraga-2	0	19.2	vi-schmidt-3	0	20.4	vi-schmidt-3	0	21.0
12	vi-schmidt-3	0	19.7	vi-scheraga-2	0	20.7	vi-scheraga-2	0	21.9
13	vi-dzyabchenko-1	0	20.7	vi-dzyabchenko-1	0	21.8	vi-dzyabchenko-1	0	22.6
14	vi-williams-1	0	20.7	vi-williams-1	0	22.6	vi-williams-1	0	24.3
15	vi-mooy-2	0	24.4	vi-verwer-1	0	24.8	vi-verwer-1	0	25.3
16	vi-verwer-1	0	24.4	vi-verwer-3	0	25.6	vi-verwer-3	0	26.0
17	vi-verwer-3	0	25.1	vi-ammon-2	0	25.9	vi-ammon-2	0	26.0
18	vi-verwer-2	0	25.4	vi-verwer-2	0	26.2	vi-verwer-2	0	26.7
19	vi-ammon-2	0	26.0	vi-mooy-2	0	26.9	vi-mooy-2	0	29.2
20	vi-scheraga-1	0	27.8	vi-ammon-1	0	28.7	vi-ammon-1	0	29.6
21	vi-erk-2	0	28.0	vi-scheraga-1	0	29.7	vi-scheraga-1	0	31.1
22	vi-williams-2	0	28.1	vi-williams-2	0	30.2	vi-williams-2	0	32.1
23	vi-ammon-1	0	28.2	vi-erk-2	0	30.7	vi-erk-2	0	33.0
24	vi-hofmann-3	1	29.0	vi-hofmann-3	1	31.6	vi-hofmann-3	1	33.7
25	vi-ammon-3	0	32.0	vi-ammon-3	0	33.7	vi-ammon-3	0	35.7
26	vi-hofmann-1	0	38.5	vi-hofmann-1	0	41.2	vi-hofmann-1	0	43.8
27	vi-schmidt-2	0	40.7	vi-schmidt-2	0	43.9	vi-schmidt-2	0	47.1
28	vi-leusen-1	0	42.2	vi-leusen-1	0	45.7	vi-leusen-1	0	48.7
29	vi-scheraga-3	0	43.7	vi-scheraga-3	0	46.5	vi-scheraga-3	0	49.5
30	vi-leusen-3	0	46.1	vi-leusen-3	0	49.2	vi-leusen-3	0	52.5
31	vi-hofmann-2	0	54.0	vi-hofmann-2	0	56.3	vi-hofmann-2	0	58.5

TABLE VIII: Computed energy ranking for unique candidate structures of compound VII, propane. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	vii-expt	2	0.0	vii-expt	2	0.0	vii-expt	2	0.0
2	vii-williams-1	1	0.3	vii-mooij-2	2	0.3	vii-mooij-2	2	0.3
3	vii-mooij-2	2	0.3	vii-williams-1	1	0.4	vii-williams-1	1	0.4
4	vii-verwer-1	2	0.8	vii-verwer-1	2	1.0	vii-verwer-1	2	1.2
5	vii-verwer-2	0	1.2	vii-verwer-2	0	1.4	vii-verwer-2	0	1.7
6	vii-verwer-3	0	1.3	vii-lommerse-2	0	1.6	vii-lommerse-2	0	1.7
7	vii-lommerse-1	0	1.4	vii-lommerse-1	0	1.6	vii-lommerse-1	0	1.8
8	vii-lommerse-2	0	1.4	vii-verwer-3	0	1.7	vii-verwer-3	0	2.0
9	vii-motherwell-2	0	1.8	vii-motherwell-2	0	2.1	vii-motherwell-2	0	2.4
10	vii-motherwell-1	0	2.0	vii-motherwell-1	0	2.3	vii-motherwell-1	0	2.7
11	vii-lommerse-3	0	3.8	vii-lommerse-3	0	4.2	vii-lommerse-3	0	4.4

TABLE IX: Computed energy ranking for unique candidate structures of compound VIII, hydantoin. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
sh maketable 1	viii-expt	1	0.0	viii-expt	1	0.0	viii-expt	1	0.0
2	viii-day-2	0	0.6	viii-day-2	0	0.9	viii-day-2	0	1.1
3	viii-day-3	1	0.7	viii-day-3	1	1.3	viii-day-3	1	1.9
4	viii-vaneijck-3	0	2.0	viii-vaneijck-3	0	2.6	viii-vaneijck-3	0	3.2
5	viii-boerrigter-2	0	4.0	viii-boerrigter-2	0	5.1	viii-boerrigter-1	0	5.0
6	viii-hofmann-2	1	6.4	viii-boerrigter-1	0	6.0	viii-liang-3	0	5.9
7	viii-erk-1	0	6.7	viii-erk-1	0	6.3	viii-erk-1	0	5.9
8	viii-boerrigter-1	0	7.2	viii-liang-3	0	6.6	viii-boerrigter-2	0	6.0
9	viii-liang-3	0	7.6	viii-hofmann-2	1	8.0	viii-liang-2	1	8.4
10	viii-liang-2	1	9.3	viii-liang-2	1	8.8	viii-valle-1	3	8.9
11	viii-valle-2	3	9.6	viii-valle-1	3	9.2	viii-hofmann-2	1	9.6
12	viii-valle-3	0	13.0	viii-valle-3	0	14.5	viii-valle-3	0	16.0

TABLE X: Computed energy ranking for unique candidate structures of compound IX, 2,9-diiodoanthanthrone. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	ix-expt	1	0.0	ix-expt	1	0.0	ix-expt	1	0.0
2	ix-day-3	1	5.7	ix-vaneijck-3	1	5.9	ix-vaneijck-3	1	5.6
3	ix-vaneijck-3	1	6.4	ix-day-3	1	6.2	ix-day-3	1	6.4
4	ix-valle-1	1	9.4	ix-liang-1	1	8.7	ix-liang-1	1	8.2
5	ix-day-2	0	12.5	ix-day-2	0	12.4	ix-liang-2	0	11.9
6	ix-liang-2	0	13.4	ix-liang-2	0	12.6	ix-day-2	0	12.2
7	ix-boerrigter-3	0	13.4	ix-boerrigter-3	0	13.2	ix-boerrigter-3	0	13.0
8	ix-liang-3	0	17.0	ix-boerrigter-1	1	15.9	ix-boerrigter-1	1	14.2
9	ix-boerrigter-1	1	18.2	ix-liang-3	0	16.4	ix-liang-3	0	15.8
10	ix-valle-2	0	19.4	ix-valle-2	0	18.9	ix-valle-2	0	18.7
11	ix-hofmann-2	0	23.6	ix-hofmann-1	1	21.9	ix-hofmann-1	1	20.3
12	ix-hofmann-3	1	23.9	ix-hofmann-2	0	23.0	ix-hofmann-2	0	22.6
13	ix-motherwell-3	2	27.5	ix-motherwell-1	2	26.5	ix-vaneijck-2	1	25.4
14	ix-vaneijck-2	1	28.4	ix-vaneijck-2	1	26.7	ix-motherwell-1	2	25.8
15	ix-erk-3	0	28.6	ix-erk-3	0	27.7	ix-erk-3	0	27.3
16	ix-dzyabchenko-1	0	30.4	ix-dzyabchenko-1	0	29.7	ix-dzyabchenko-1	0	28.3
17	ix-erk-2	0	32.9	ix-erk-2	0	32.1	ix-erk-2	0	31.7
18	ix-dzyabchenko-2	0	35.4	ix-dzyabchenko-2	0	34.8	ix-dzyabchenko-2	0	33.4

TABLE XI: Computed energy ranking for unique candidate structures of compound X, 2-acetamido-4,5,-dinitrotoluene. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	x-vaneijck-3	0	-0.9	x-vaneijck-3	0	-0.4	x-expt	0	0.0
2	x-expt	0	0.0	x-expt	0	0.0	x-vaneijck-3	0	0.6
3	x-dzyabchenko-3	1	2.1	x-dzyabchenko-3	1	2.4	x-dzyabchenko-3	1	2.6
4	x-day-1	0	2.7	x-ammon-2	0	3.3	x-ammon-2	0	2.8
5	x-day-2	0	2.8	x-day-1	0	3.4	x-dzyabchenko-2	0	3.1
6	x-ammon-2	0	4.4	x-day-2	0	3.5	x-day-1	0	4.1
7	x-dzyabchenko-2	0	4.4	x-dzyabchenko-2	0	3.6	x-day-2	0	4.5
8	x-vaneijck-1	1	4.9	x-vaneijck-1	1	5.7	x-erk-2	0	6.6
9	x-day-3	0	5.1	x-erk-2	0	6.0	x-ammon-3	1	6.7
10	x-erk-2	0	5.2	x-day-3	0	6.1	x-day-3	0	7.2
11	x-dzyabchenko-1	0	5.7	x-dzyabchenko-1	0	7.0	x-ammon-1	0	8.1
12	x-ammon-1	0	9.4	x-ammon-1	0	8.5	x-dzyabchenko-1	0	8.1
13	x-erk-1	0	9.5	x-erk-1	0	9.3	x-erk-1	0	9.7
14	x-hofmann-2	0	12.5	x-hofmann-3	0	13.7	x-liang-1	0	14.2
15	x-hofmann-3	0	12.7	x-hofmann-2	0	13.7	x-hofmann-3	0	14.4
16	x-liang-1	0	13.9	x-liang-1	0	13.9	x-liang-2	0	14.7
17	x-liang-2	0	14.3	x-liang-2	0	14.3	x-hofmann-2	0	14.9
18	x-hofmann-1	0	15.6	x-hofmann-1	0	17.2	x-liang-3	0	18.5
19	x-liang-3	0	17.5	x-liang-3	0	18.1	x-hofmann-1	0	18.6
20	x-boerrigter-1	0	18.6	x-boerrigter-1	0	22.2	x-boerrigter-2	0	24.9
21	x-boerrigter-2	0	19.3	x-boerrigter-2	0	22.3	x-boerrigter-1	0	26.3
22	x-boerrigter-3	0	28.9	x-boerrigter-3	0	31.3	x-boerrigter-3	0	33.2

TABLE XII: Computed energy ranking for unique candidate structures of compound XI, azetidine. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	xi-expt	0	0.0	xi-expt	0	0.0	xi-expt	0	0.0
2	xi-liang-2	1	0.7	xi-liang-2	1	0.5	xi-liang-2	1	0.4
3	xi-liang-1	0	0.7	xi-liang-1	0	0.6	xi-liang-1	0	0.5
4	xi-boerrigter-3	0	0.7	xi-liang-3	1	0.8	xi-liang-3	1	0.8
5	xi-vaneijck-3	0	0.8	xi-boerrigter-3	0	0.8	xi-valle-3	1	0.8
6	xi-motherwell-2	1	0.9	xi-vaneijck-3	0	0.9	xi-boerrigter-2	0	0.9
7	xi-boerrigter-2	0	1.2	xi-boerrigter-2	0	1.0	xi-vaneijck-3	0	0.9
8	xi-ammon-1	2	1.5	xi-valle-3	1	1.2	xi-boerrigter-3	0	0.9
9	xi-ammon-2	2	1.5	xi-erk-3	0	1.5	xi-erk-3	0	1.4
10	xi-erk-2	0	1.5	xi-day-2	2	1.6	xi-dzyabchenko-3	0	1.5
11	xi-valle-3	1	1.6	xi-ammon-3	0	1.7	xi-ammon-3	0	1.6
12	xi-erk-3	0	1.6	xi-ammon-1	2	1.7	xi-day-2	2	1.7
13	xi-vaneijck-2	0	1.7	xi-vaneijck-2	0	1.7	xi-erk-1	1	1.8
14	xi-ammon-3	0	1.8	xi-erk-2	0	1.8	xi-vaneijck-2	0	1.8
15	xi-motherwell-3	0	1.9	xi-motherwell-3	0	1.9	xi-ammon-1	2	1.9
16	xi-erk-1	1	2.1	xi-erk-1	1	2.0	xi-motherwell-3	0	1.9
17	xi-dzyabchenko-3	0	2.6	xi-dzyabchenko-3	0	2.1	xi-erk-2	0	1.9
18	xi-valle-1	0	6.3	xi-valle-1	0	5.2	xi-valle-1	0	4.3
19	xi-hofmann-3	0	10.1	xi-hofmann-3	0	8.8	xi-hofmann-3	0	7.8
20	xi-hofmann-1	0	10.2	xi-hofmann-1	0	9.4	xi-hofmann-2	0	8.8
21	xi-hofmann-2	0	10.9	xi-hofmann-2	0	9.6	xi-hofmann-1	0	8.9
22	xi-day-3	0	33.6	xi-day-3	0	37.5	xi-day-3	0	41.8

TABLE XIII: Computed energy ranking for unique candidate structures of compound XII, 2-propenal. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	xii-expt	3	0.0	xii-expt	3	0.0	xii-expt	3	0.0
2	xii-neumann-2	1	1.3	xii-neumann-2	1	1.2	xii-ammon-3	0	1.2
3	xii-day-1	0	1.7	xii-ammon-3	0	1.7	xii-price-3	1	1.3
4	xii-neumann-3	0	1.8	xii-scheraga-3	1	1.7	xii-scheraga-3	1	1.4
5	xii-boerrigter-2	0	2.2	xii-day-1	0	1.7	xii-day-1	0	1.7
6	xii-day-2	0	2.2	xii-neumann-3	0	1.7	xii-neumann-3	0	1.9
7	xii-price-2	0	2.2	xii-price-2	0	1.9	xii-price-2	0	1.9
8	xii-ammon-3	0	2.3	xii-boerrigter-2	0	1.9	xii-boerrigter-2	0	1.9
9	xii-scheraga-3	1	2.3	xii-day-2	0	2.3	xii-day-2	0	2.6
10	xii-price-1	2	2.3	xii-price-1	2	2.6	xii-jose-3	0	2.9
11	xii-schmidt-3	0	2.6	xii-schmidt-3	0	2.9	xii-price-1	2	3.0
12	xii-jose-3	0	3.3	xii-jose-3	0	3.0	xii-schmidt-3	0	3.0
13	xii-valle-2	0	3.4	xii-valle-2	0	3.2	xii-valle-2	0	3.1
14	xii-vaneijck-2	1	3.7	xii-boerrigter-3	1	3.6	xii-boerrigter-3	1	3.7
15	xii-day-3	0	3.8	xii-day-3	0	4.0	xii-vaneijck-1	2	3.8
16	xii-schmidt-2	0	4.4	xii-vaneijck-1	2	4.1	xii-schmidt-2	0	4.0
17	xii-vaneijck-1	2	4.4	xii-schmidt-2	0	4.2	xii-day-3	0	4.5
18	xii-schweizer-3	0	4.7	xii-schmidt-1	0	4.8	xii-schmidt-1	0	4.7
19	xii-jose-2	0	4.7	xii-schweizer-3	0	5.2	xii-jose-2	0	5.8
20	xii-schmidt-1	0	5.0	xii-jose-2	0	5.2	xii-schweizer-3	0	5.8
21	xii-valle-3	0	7.3	xii-valle-3	0	7.1	xii-valle-3	0	7.4
22	xii-jose-1	0	7.9	xii-jose-1	0	8.1	xii-jose-1	0	8.4
23	xii-hofmann-1	0	8.2	xii-hofmann-1	0	8.4	xii-hofmann-1	0	8.6
24	xii-hofmann-2	0	9.1	xii-hofmann-2	0	9.7	xii-hofmann-2	0	9.7
25	xii-hofmann-3	0	10.6	xii-hofmann-3	0	10.3	xii-hofmann-3	0	10.4
26	xii-facelli-3	0	12.2	xii-facelli-3	0	12.0	xii-facelli-3	0	12.1
27	xii-facelli-1	0	12.3	xii-facelli-1	0	12.2	xii-facelli-1	0	12.4

TABLE XIV: Computed energy ranking for unique candidate structures of compound XIII, 1,3-dibromo-2-chloro-5-fluorobenzene. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
sh maketable 1	xiii-expt	1	0.0	xiii-expt	1	0.0	xiii-expt	1	0.0
2	xiii-neumann-3	1	1.2	xiii-neumann-2	0	1.2	xiii-neumann-2	0	1.2
3	xiii-neumann-2	0	1.3	xiii-neumann-3	1	2.3	xiii-neumann-3	1	3.0
4	xiii-price-2	0	3.9	xiii-price-2	0	3.3	xiii-price-2	0	3.1
5	xiii-day-2	0	4.8	xiii-ammon-3	0	5.1	xiii-ammon-3	0	5.4
6	xiii-ammon-3	0	5.1	xiii-day-2	0	5.6	xiii-schweizer-3	0	6.0
7	xiii-scheraga-2	3	5.6	xiii-scheraga-2	3	5.9	xiii-scheraga-2	3	6.4
8	xiii-boerrigter-3	0	6.3	xiii-schweizer-3	0	6.3	xiii-facelli-1	0	6.4
9	xiii-boerrigter-2	1	6.8	xiii-boerrigter-3	0	6.5	xiii-boerrigter-2	1	6.4
10	xiii-schweizer-3	0	6.9	xiii-boerrigter-2	1	6.6	xiii-boerrigter-3	0	6.6
11	xiii-facelli-1	0	7.2	xiii-facelli-1	0	6.7	xiii-day-2	0	6.6
12	xiii-schweizer-2	0	7.3	xiii-schweizer-2	0	7.1	xiii-schweizer-2	0	7.3
13	xiii-day-3	0	7.4	xiii-desiraju-1	5	7.5	xiii-desiraju-1	5	7.8
14	xiii-facelli-2	5	7.4	xiii-day-3	0	7.7	xiii-day-3	0	8.3
15	xiii-hofmann-1	1	8.5	xiii-hofmann-1	1	8.4	xiii-hofmann-1	1	8.6
16	xiii-desiraju-3	0	8.7	xiii-desiraju-3	0	9.1	xiii-desiraju-3	0	9.6
17	xiii-jose-1	1	9.2	xiii-jose-1	1	9.6	xiii-jose-1	1	10.3
18	xiii-facelli-3	0	10.1	xiii-facelli-3	0	10.4	xiii-facelli-3	0	10.8
19	xiii-valle-2	1	12.4	xiii-valle-2	1	12.2	xiii-valle-2	1	12.5
20	xiii-hofmann-2	0	13.2	xiii-hofmann-2	0	14.0	xiii-hofmann-2	0	15.1
21	xiii-vaneijck-3	0	13.6	xiii-vaneijck-1	1	14.6	xiii-vaneijck-1	1	15.6
22	xiii-vaneijck-1	1	13.7	xiii-vaneijck-3	0	14.7	xiii-vaneijck-3	0	15.9
23	xiii-jose-2	0	16.1	xiii-jose-2	0	17.4	xiii-jose-2	0	18.8

TABLE XV: Computed energy ranking for unique candidate structures of compound XIV, N-(dimethylthiocarbamoyl)benzothiazole-2-thione. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	xiv-expt	1	0.0	xiv-expt	1	0.0	xiv-expt	1	0.0
2	xiv-kendrick-2	0	3.2	xiv-kendrick-3	0	4.3	xiv-kendrick-3	0	4.4
3	xiv-price-3	1	3.8	xiv-kendrick-2	0	4.5	xiv-kendrick-2	0	5.2
4	xiv-kendrick-3	0	4.1	xiv-price-3	1	4.5	xiv-price-3	1	5.2
5	xiv-vaneijck-2	4	6.6	xiv-schmidt-2	4	6.4	xiv-schmidt-2	4	5.8
6	xiv-ammon-3	0	6.8	xiv-scheraga-1	1	6.7	xiv-scheraga-1	1	6.2
7	xiv-scheraga-1	1	6.8	xiv-ammon-3	0	7.5	xiv-ammon-3	0	7.7
8	xiv-facelli-3	0	7.2	xiv-facelli-3	0	7.9	xiv-facelli-3	0	8.4
9	xiv-schmidt-1	1	9.8	xiv-facelli-1	1	10.1	xiv-facelli-1	1	9.8
10	xiv-facelli-1	1	10.2	xiv-facelli-2	2	10.1	xiv-facelli-2	2	9.8
11	xiv-facelli-2	2	10.2	xiv-scheraga-2	1	10.9	xiv-scheraga-2	1	11.0
12	xiv-scheraga-2	1	10.5	xiv-schmidt-1	1	11.1	xiv-schmidt-1	1	11.7
13	xiv-price-2	0	11.5	xiv-boerrigter-3	0	13.0	xiv-boerrigter-3	0	12.2
14	xiv-boerrigter-3	0	13.3	xiv-price-2	0	13.1	xiv-hofmann-1	1	13.6
15	xiv-schmidt-3	1	14.5	xiv-hofmann-1	1	14.2	xiv-price-2	0	14.2
16	xiv-desiraju-2	0	17.7	xiv-desiraju-2	0	18.5	xiv-desiraju-2	0	18.7
17	xiv-jose-2	0	17.9	xiv-jose-2	0	19.6	xiv-jose-2	0	20.5
18	xiv-jose-3	0	22.6	xiv-jose-3	0	24.4	xiv-jose-3	0	25.1
19	xiv-desiraju-3	0	25.5	xiv-desiraju-3	0	27.8	xiv-desiraju-3	0	29.4
20	xiv-desiraju-1	0	25.6	xiv-hofmann-2	0	28.4	xiv-hofmann-2	0	30.1
21	xiv-hofmann-2	0	26.1	xiv-desiraju-1	0	29.0	xiv-desiraju-1	0	31.5
22	xiv-jose-1	0	33.3	xiv-jose-1	0	36.6	xiv-jose-1	0	39.0

TABLE XVI: Computed energy ranking for unique candidate structures of compound XV, 2-amino-4-methylpyrimidine:2-methylbenzoic acid. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	xv-ammon-1	2	-0.3	xv-ammon-1	2	-0.8	xv-desiraju-3	2	-1.2
2	xv-expt	1	0.0	xv-expt	1	0.0	xv-expt	1	0.0
3	xv-neumann-2	0	1.9	xv-neumann-2	0	2.9	xv-schmidt-1	1	3.6
4	xv-neumann-3	0	2.5	xv-neumann-3	0	3.6	xv-neumann-2	0	4.0
5	xv-desiraju-2	0	4.1	xv-schmidt-1	1	3.6	xv-neumann-3	0	4.7
6	xv-ammon-2	1	4.1	xv-desiraju-2	0	4.3	xv-desiraju-2	0	4.8
7	xv-price-2	1	5.0	xv-day-2	0	5.2	xv-day-2	0	5.7
8	xv-day-2	0	5.1	xv-price-2	1	5.6	xv-price-2	1	6.6
9	xv-day-3	0	6.7	xv-day-3	0	6.8	xv-boerrigter-1	0	7.2
10	xv-boerrigter-1	0	7.4	xv-boerrigter-1	0	7.1	xv-day-3	0	7.4
11	xv-schmidt-3	0	8.1	xv-facelli-3	0	7.6	xv-facelli-3	0	7.5
12	xv-price-3	0	8.2	xv-schmidt-3	0	8.3	xv-schmidt-3	0	9.1
13	xv-facelli-3	0	8.3	xv-price-3	0	8.8	xv-valle-2	0	9.3
14	xv-ammon-3	0	9.6	xv-valle-2	0	9.6	xv-price-3	0	9.8
15	xv-price-1	0	9.7	xv-facelli-2	0	10.2	xv-facelli-2	0	10.0
16	xv-boerrigter-3	0	9.7	xv-boerrigter-3	0	10.3	xv-schweizer-3	0	10.8
17	xv-boerrigter-2	0	10.0	xv-ammon-3	0	10.3	xv-boerrigter-3	0	10.8
18	xv-facelli-2	0	10.7	xv-price-1	0	10.3	xv-ammon-3	0	10.8
19	xv-valle-2	0	10.8	xv-valle-1	0	11.2	xv-price-1	0	11.0
20	xv-desiraju-1	0	11.3	xv-boerrigter-2	0	11.3	xv-valle-1	0	11.4
21	xv-valle-1	0	11.8	xv-schweizer-3	0	11.3	xv-schweizer-1	0	11.4
22	xv-schweizer-3	0	12.6	xv-desiraju-1	0	11.4	xv-desiraju-1	0	12.0
23	xv-schweizer-1	0	12.7	xv-schweizer-1	0	11.8	xv-boerrigter-2	0	12.3
24	xv-facelli-1	0	14.1	xv-facelli-1	0	13.5	xv-facelli-1	0	13.2
25	xv-valle-3	0	15.2	xv-schweizer-2	0	15.2	xv-valle-3	0	15.4
26	xv-schweizer-2	0	15.5	xv-valle-3	0	15.3	xv-schweizer-2	0	15.5
27	xv-jose-3	0	68.2	xv-jose-3	0	69.4	xv-jose-3	0	71.2

TABLE XVII: Computed energy ranking for unique candidate structures of compound XVI, 2-diazo-3,5-cyclohexadiene-2-one. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	xvi-expt	2	0.0	xvi-expt	2	0.0	xvi-expt	2	0.0
2	xvi-neumann-2	1	0.8	xvi-scheraga-2	1	0.8	xvi-scheraga-2	1	0.9
3	xvi-misquitta-1	1	0.9	xvi-day-3	0	2.6	xvi-day-3	0	2.8
4	xvi-desiraju-2	1	1.6	xvi-price-3	1	3.1	xvi-vaneijck-3	2	4.1
5	xvi-day-3	0	2.9	xvi-day-2	0	3.7	xvi-day-2	0	4.4
6	xvi-day-2	0	3.3	xvi-neumann-3	1	3.8	xvi-facelli-2	1	4.7
7	xvi-boerrigter-3	0	3.5	xvi-vaneijck-3	2	4.3	xvi-price-3	1	4.8
8	xvi-facelli-1	0	4.3	xvi-facelli-2	1	4.5	xvi-price-1	1	5.5
9	xvi-ammon-3	1	4.6	xvi-boerrigter-3	0	5.0	xvi-neumann-3	1	5.6
10	xvi-vaneijck-3	2	4.8	xvi-price-1	1	5.0	xvi-desiraju-1	0	5.8
11	xvi-desiraju-1	0	4.9	xvi-desiraju-1	0	5.1	xvi-misquitta-3	0	6.5
12	xvi-misquitta-3	0	4.9	xvi-misquitta-3	0	5.4	xvi-boerrigter-3	0	6.8
13	xvi-vaneijck-1	1	4.9	xvi-facelli-1	0	5.8	xvi-boerrigter-2	1	6.8
14	xvi-boerrigter-2	1	5.4	xvi-boerrigter-2	1	5.9	xvi-desiraju-3	0	6.9
15	xvi-desiraju-3	0	5.7	xvi-desiraju-3	0	6.0	xvi-facelli-1	0	7.2
16	xvi-boerrigter-1	0	6.5	xvi-facelli-3	0	7.7	xvi-facelli-3	0	8.5
17	xvi-facelli-3	0	7.1	xvi-boerrigter-1	0	7.8	xvi-boerrigter-1	0	9.1
18	xvi-maleev-1	0	7.7	xvi-maleev-1	0	8.9	xvi-maleev-1	0	10.3
19	xvi-valle-3	0	8.8	xvi-hofmann-2	1	10.3	xvi-hofmann-2	1	11.1
20	xvi-hofmann-2	1	10.1	xvi-hofmann-3	0	11.6	xvi-hofmann-3	0	12.7
21	xvi-hofmann-3	0	11.2	xvi-valle-3	0	12.2	xvi-valle-3	0	14.8
22	xvi-nikylov-1	0	11.3	xvi-nikylov-3	0	13.3	xvi-nikylov-3	0	15.3
23	xvi-nikylov-3	0	11.4	xvi-nikylov-2	0	14.2	xvi-nikylov-2	0	16.8
24	xvi-nikylov-2	0	11.7	xvi-nikylov-1	0	14.5	xvi-nikylov-1	0	17.2
25	xvi-valle-1	0	17.8	xvi-valle-1	0	21.7	xvi-valle-2	0	24.6
26	xvi-maleev-2	0	20.6	xvi-maleev-2	0	23.0	xvi-valle-1	0	25.2
27	xvi-hofmann-1	0	22.1	xvi-valle-2	0	23.9	xvi-maleev-2	0	25.4
28	xvi-valle-2	0	23.6	xvi-hofmann-1	0	24.7	xvi-hofmann-1	0	27.4

TABLE XVIII: Computed energy ranking for unique candidate structures of compound XVII, 1,2-dichloro4,5-dinitrobenzene. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	xvii-expt	2	0.0	xvii-expt	2	0.0	xvii-expt	2	0.0
2	xvii-neumann-2	0	1.5	xvii-neumann-2	0	1.9	xvii-neumann-3	1	2.2
3	xvii-day-2	1	1.8	xvii-neumann-3	1	2.0	xvii-neumann-2	0	2.3
4	xvii-price-3	0	2.6	xvii-price-3	0	2.5	xvii-price-3	0	2.7
5	xvii-vaneijck-3	2	2.9	xvii-desiraju-2	2	2.6	xvii-desiraju-2	2	2.8
6	xvii-price-1	5	3.1	xvii-day-1	5	2.7	xvii-day-1	5	2.9
7	xvii-day-3	2	3.5	xvii-vaneijck-2	2	3.5	xvii-vaneijck-2	2	3.8
8	xvii-facelli-1	2	4.6	xvii-facelli-1	2	4.5	xvii-facelli-1	2	4.6
9	xvii-ammon-1	0	4.6	xvii-ammon-1	0	5.0	xvii-boerrigter-2	0	5.5
10	xvii-boerrigter-2	0	5.1	xvii-boerrigter-2	0	5.1	xvii-ammon-1	0	5.6
11	xvii-scheraga-3	0	6.4	xvii-scheraga-3	0	7.2	xvii-facelli-2	0	7.5
12	xvii-valle-1	0	6.6	xvii-facelli-2	0	7.3	xvii-scheraga-3	0	8.2
13	xvii-facelli-2	0	6.8	xvii-valle-1	0	7.4	xvii-ammon-2	0	8.3
14	xvii-ammon-2	0	7.1	xvii-ammon-2	0	7.8	xvii-valle-1	0	8.4
15	xvii-hofmann-3	0	9.9	xvii-hofmann-3	0	10.1	xvii-hofmann-3	0	10.3
16	xvii-valle-2	0	9.9	xvii-valle-2	0	10.8	xvii-boerrigter-3	0	11.5
17	xvii-boerrigter-3	0	10.5	xvii-boerrigter-3	0	10.9	xvii-valle-2	0	11.7
18	xvii-maleev-1	0	13.3	xvii-maleev-1	0	14.8	xvii-valle-3	0	16.5
19	xvii-valle-3	0	13.3	xvii-valle-3	0	15.1	xvii-maleev-1	0	16.6
20	xvii-maleev-3	0	20.2	xvii-maleev-3	0	22.0	xvii-maleev-3	0	24.0
21	xvii-hofmann-2	1	28.6	xvii-hofmann-2	1	30.5	xvii-hofmann-2	1	32.1

TABLE XIX: Computed energy ranking for unique candidate structures of compound XVIII, (1-((4-chlorophenyl)sulfonyl)-2-oxopropylidene)diazenium. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	xviii-expt	1	0.0	xviii-expt	1	0.0	xviii-expt	1	0.0
2	xviii-kendrick-3	0	1.2	xviii-kendrick-2	0	0.9	xviii-kendrick-2	0	0.7
3	xviii-kendrick-2	0	1.2	xviii-ammon-1	5	2.7	xviii-ammon-1	5	3.4
4	xviii-ammon-1	5	1.9	xviii-kendrick-3	0	3.0	xviii-vaneijck-1	0	4.1
5	xviii-day-3	0	2.7	xviii-day-3	0	3.8	xviii-day-3	0	5.0
6	xviii-price-3	0	3.9	xviii-price-3	0	5.0	xviii-kendrick-3	0	5.1
7	xviii-scheraga-3	0	6.4	xviii-vaneijck-1	0	6.0	xviii-price-1	0	5.6
8	xviii-orendt-2	0	6.4	xviii-price-1	0	6.6	xviii-vaneijck-3	0	6.1
9	xviii-desiraju-2	1	6.5	xviii-orendt-2	0	7.2	xviii-price-3	0	6.2
10	xviii-boerrigter-2	0	7.1	xviii-desiraju-2	1	7.3	xviii-orendt-2	0	8.0
11	xviii-scheraga-2	0	7.2	xviii-vaneijck-3	0	7.6	xviii-desiraju-2	1	8.1
12	xviii-ammon-2	0	7.8	xviii-scheraga-3	0	7.6	xviii-venuti-3	0	8.8
13	xviii-day-2	0	7.8	xviii-venuti-3	0	8.5	xviii-scheraga-3	0	9.0
14	xviii-boerrigter-1	0	7.9	xviii-day-2	0	8.5	xviii-price-2	0	9.2
15	xviii-orendt-3	0	9.2	xviii-boerrigter-2	0	8.6	xviii-vaneijck-2	0	9.2
16	xviii-vaneijck-1	0	9.3	xviii-boerrigter-1	0	9.1	xviii-day-2	0	9.3
17	xviii-price-1	0	9.3	xviii-price-2	0	9.2	xviii-venuti-1	0	9.4
18	xviii-venuti-3	0	9.7	xviii-ammon-2	0	9.3	xviii-boerrigter-2	0	10.0
19	xviii-maleev-2	0	10.1	xviii-scheraga-2	0	9.4	xviii-boerrigter-1	0	10.4
20	xviii-vaneijck-3	0	10.8	xviii-venuti-1	0	9.7	xviii-ammon-2	0	10.6
21	xviii-price-2	0	11.0	xviii-vaneijck-2	0	10.8	xviii-scheraga-2	0	11.4
22	xviii-desiraju-3	0	11.1	xviii-maleev-2	0	11.5	xviii-maleev-2	0	13.2
23	xviii-venuti-1	0	11.4	xviii-orendt-3	0	11.6	xviii-orendt-3	0	14.1
24	xviii-maleev-1	0	12.5	xviii-desiraju-3	0	12.9	xviii-maleev-1	0	14.2
25	xviii-vaneijck-2	0	13.9	xviii-maleev-1	0	13.4	xviii-desiraju-3	0	14.5
26	xviii-maleev-3	0	15.2	xviii-maleev-3	0	17.6	xviii-hofmann-2	0	17.1
27	xviii-hofmann-2	0	21.4	xviii-hofmann-2	0	18.5	xviii-maleev-3	0	19.5
28	xviii-venuti-2	0	27.8	xviii-venuti-2	0	27.5	xviii-venuti-2	0	28.3
29	xviii-hofmann-3	0	33.7	xviii-hofmann-3	0	32.5	xviii-hofmann-3	0	32.9
30	xviii-hofmann-1	0	40.1	xviii-hofmann-1	0	38.8	xviii-hofmann-1	0	39.3

TABLE XX: Computed energy ranking for unique candidate structures of compound XIX, 1,8-naphthyridinium fumarate. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	Δ*E*	Structure	# Duplicates	Δ*E*	Structure	# Duplicates	Δ*E*
1	xix-neumann-1	0	-4.3	xix-neumann-1	0	-2.2	xix-neumann-1	0	-0.1
2	xix-neumann-2	0	-4.0	xix-neumann-2	0	-1.7	xix-expt	2	0.0
3	xix-price-1	1	-2.6	xix-day-1	1	-0.3	xix-neumann-2	0	0.5
4	xix-day-2	0	-1.1	xix-expt	2	0.0	xix-vaneijck-1	0	1.8
5	xix-facelli-3	0	-0.2	xix-vaneijck-1	0	1.0	xix-boerrigter-1	0	1.9
6	xix-expt	2	0.0	xix-day-2	0	1.3	xix-day-1	1	2.1
7	xix-vaneijck-1	0	0.4	xix-facelli-3	0	2.0	xix-day-2	0	3.7
8	xix-boerrigter-3	0	0.7	xix-boerrigter-1	0	2.0	xix-facelli-3	0	4.2
9	xix-day-3	0	1.3	xix-boerrigter-3	0	3.1	xix-boerrigter-3	0	5.4
10	xix-boerrigter-1	0	2.1	xix-day-3	0	3.4	xix-day-3	0	5.5
11	xix-price-2	0	3.2	xix-price-2	0	6.2	xix-price-2	0	8.8
12	xix-scheraga-3	0	4.9	xix-scheraga-3	0	7.3	xix-scheraga-3	0	9.9
13	xix-desiraju-2	1	5.4	xix-desiraju-1	1	8.1	xix-desiraju-1	1	10.2
14	xix-facelli-2	0	6.0	xix-facelli-2	0	8.3	xix-facelli-2	0	10.5
15	xix-boerrigter-2	0	12.3	xix-boerrigter-2	0	12.2	xix-boerrigter-2	0	12.0
16	xix-price-3	0	12.5	xix-price-3	0	14.8	xix-price-3	0	16.9
17	xix-scheraga-2	1	13.8	xix-facelli-1	0	16.5	xix-facelli-1	0	18.3
18	xix-facelli-1	0	14.8	xix-scheraga-1	1	17.3	xix-scheraga-1	1	20.9
19	xix-valle-2	0	29.0	xix-valle-2	0	34.1	xix-valle-2	0	37.4
20	xix-desiraju-3	0	33.5	xix-desiraju-3	0	35.9	xix-desiraju-3	0	38.2
21	xix-valle-3	0	45.2	xix-valle-3	0	52.3	xix-maleev-3	0	56.4
22	xix-maleev-3	0	47.8	xix-maleev-3	0	52.4	xix-valle-3	0	56.7
23	xix-valle-1	0	63.3	xix-valle-1	0	64.3	xix-valle-1	0	64.6

TABLE XXI: Computed energy ranking for unique candidate structures of compound XX, benzyl-(4-(4-methyl-5-(p-tolyl-sulfonyl)-1,3-thiazol-2-yl)phenyl)carbamate. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	Δ*E*	Structure	# Duplicates	Δ*E*	Structure	# Duplicates	Δ*E*
1	xx-price-2	0	-6.7	xx-price-2	0	-6.5	xx-price-2	0	-6.7
2	xx-kendrick-3	2	-4.8	xx-kendrick-3	2	-4.8	xx-kendrick-2	0	-5.5
3	xx-kendrick-2	0	-4.4	xx-kendrick-2	0	-4.7	xx-vaneijck-2	2	-5.3
4	xx-expt	2	0.0	xx-expt	2	0.0	xx-day-2	0	-1.3
5	xx-kendrick-1	0	2.1	xx-day-2	0	0.4	xx-kendrick-1	0	-0.9
6	xx-day-2	0	2.4	xx-kendrick-1	0	0.8	xx-expt	2	0.0
7	xx-vaneijck-1	0	3.8	xx-vaneijck-1	0	4.7	xx-vaneijck-1	0	5.3
8	xx-price-3	0	5.6	xx-price-3	0	7.4	xx-price-3	0	8.3
9	xx-boerrigter-3	0	12.4	xx-orendt-1	1	11.0	xx-orendt-1	1	9.1
10	xx-orendt-1	1	12.5	xx-ammon-2	0	12.7	xx-ammon-2	0	11.3
11	xx-maleev-1	0	12.6	xx-boerrigter-3	0	13.0	xx-boerrigter-3	0	12.8
12	xx-ammon-2	0	14.6	xx-maleev-1	0	13.7	xx-maleev-1	0	14.3
13	xx-day-3	0	17.4	xx-day-3	0	17.1	xx-ammon-3	0	16.0
14	xx-orendt-2	0	18.4	xx-ammon-3	0	17.5	xx-day-3	0	16.2
15	xx-ammon-3	0	19.5	xx-orendt-2	0	18.2	xx-orendt-2	0	17.3
16	xx-orendt-3	0	19.8	xx-orendt-3	0	19.7	xx-orendt-3	0	19.1
17	xx-hofmann-2	0	25.2	xx-maleev-2	0	25.7	xx-maleev-2	0	25.2
18	xx-maleev-2	0	25.6	xx-hofmann-2	0	27.3	xx-hofmann-2	0	28.8
19	xx-maleev-3	0	32.3	xx-venuti-2	1	31.4	xx-venuti-2	1	30.1
20	xx-venuti-3	1	32.5	xx-hofmann-3	0	32.6	xx-hofmann-3	0	31.3
21	xx-hofmann-3	0	33.0	xx-venuti-1	0	33.6	xx-venuti-1	0	33.8
22	xx-venuti-1	0	33.4	xx-maleev-3	0	35.0	xx-maleev-3	0	38.0
23	xx-hofmann-1	0	40.1	xx-hofmann-1	0	41.9	xx-hofmann-1	0	43.0

TABLE XXII: Computed energy ranking for unique candidate structures of compound XXI, gallic acid monohydrate. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	xxi-expt	0	0.0	xxi-expt	0	0.0	xxi-expt	0	0.0
2	xxi-price-1	0	0.9	xxi-price-1	0	1.9	xxi-day-2	0	2.6
3	xxi-day-2	0	1.7	xxi-day-2	0	2.2	xxi-vaneijck-1	0	2.8
4	xxi-vaneijck-1	0	2.4	xxi-vaneijck-1	0	2.6	xxi-price-1	0	2.9
5	xxi-facelli-3	0	4.1	xxi-facelli-1	0	3.7	xxi-facelli-1	0	3.3
6	xxi-facelli-1	0	4.5	xxi-facelli-3	0	4.0	xxi-facelli-3	0	4.4
7	xxi-desiraju-1	0	4.6	xxi-facelli-2	0	7.0	xxi-facelli-4	0	7.0
8	xxi-facelli-2	0	6.1	xxi-desiraju-1	0	7.2	xxi-boerrigter-1	0	7.3
9	xxi-facelli-4	0	8.2	xxi-facelli-4	0	7.5	xxi-facelli-2	0	7.4
10	xxi-boerrigter-1	0	9.6	xxi-boerrigter-1	0	8.3	xxi-desiraju-1	0	9.2
11	xxi-day-3	0	14.3	xxi-day-3	0	13.5	xxi-day-3	0	13.0
12	xxi-boerrigter-2	0	16.5	xxi-desiraju-2	0	18.4	xxi-desiraju-2	0	19.3
13	xxi-desiraju-2	0	17.1	xxi-boerrigter-2	0	19.7	xxi-boerrigter-2	0	22.3
14	xxi-desiraju-3	0	26.2	xxi-desiraju-3	0	25.5	xxi-desiraju-3	0	25.4
15	xxi-valle-2	0	28.4	xxi-valle-2	0	28.8	xxi-valle-2	0	28.8
16	xxi-hofmann-2	0	35.6	xxi-hofmann-2	0	35.4	xxi-hofmann-2	0	35.2
17	xxi-hofmann-1	0	36.8	xxi-hofmann-1	0	39.3	xxi-hofmann-1	0	41.2
18	xxi-hofmann-3	0	49.6	xxi-hofmann-3	0	51.0	xxi-hofmann-3	0	52.2
19	xxi-valle-3	0	51.3	xxi-valle-3	0	51.9	xxi-valle-3	0	52.5

TABLE XXIII: Computed energy ranking for unique candidate structures of compound XXII, tricyano1,4-dithiino[c]-isothiazole. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	xxii-szalewicz-price1-1	10	-2.7	xxii-004	2	-0.4	xxii-004	2	-0.1
2	xxii-goto-obata1-1	2	-1.2	xxii-001	10	-0.2	xxii-expt	10	0.0
3	xxii-elking-fustimolnar1-3	16	-0.9	xxii-expt	10	0.0	xxii-marom1-2	16	0.9
4	xxii-006	2	-0.7	xxii-zhu1-1	16	0.1	xxii-001	10	1.7
5	xxii-marom2-3	2	-0.4	xxii-006	2	1.4	xxii-poly59-22-4	2	2.9
6	xxii-005	0	-0.4	xxii-005	0	2.1	xxii-019	2	3.0
7	xxii-103	6	-0.3	xxii-008	6	2.2	xxii-025	0	3.9
8	xxii-024	0	-0.1	xxii-025	0	2.2	xxii-price2-3	0	3.9
9	xxii-expt	10	0.0	xxii-007	2	2.4	xxii-008	6	4.0
10	xxii-025	0	0.2	xxii-024	0	2.6	xxii-005	0	4.0
11	xxii-011	0	0.5	xxii-019	2	2.7	xxii-027	0	4.2
12	xxii-030	0	0.7	xxii-price2-3	0	2.7	xxii-007	2	4.4
13	xxii-010	0	0.8	xxii-011	0	3.1	xxii-mohamed1-2	3	4.5
14	xxii-lv-wang-ma1-3	4	1.1	xxii-030	0	3.5	xxii-024	0	4.8
15	xxii-price2-3	0	1.1	xxii-lv-wang-ma1-2	4	3.6	xxii-011	0	4.9
16	xxii-009	0	1.3	xxii-009	0	3.7	xxii-038	1	5.0
17	xxii-105	1	1.5	xxii-mohamed1-2	3	3.8	xxii-009	0	5.4
18	xxii-boese-hofmann1-3	0	1.7	xxii-063	2	3.9	xxii-brandenburg-grimme1-3	0	5.5
19	xxii-079	0	1.7	xxii-027	0	3.9	xxii-036	0	5.6
20	xxii-boese-hofmann1-2	2	1.9	xxii-035	1	4.0	xxii-063	2	5.6
21	xxii-071	0	1.9	xxii-087	2	4.2	xxii-088	4	5.6
22	xxii-012	0	2.0	xxii-brandenburg-grimme1-3	0	4.3	xxii-030	0	5.6
23	xxii-074	0	2.0	xxii-072	0	4.4	xxii-052	1	5.8
24	xxii-040	0	2.1	xxii-041	0	4.5	xxii-lv-wang-ma2-2	3	5.8
25	xxii-072	0	2.2	xxii-036	0	4.5	xxii-046	0	5.9
26	xxii-108	2	2.3	xxii-boese-hofmann1-3	0	4.5	xxii-041	0	5.9
27	xxii-pickard-et-al1-1	3	2.3	xxii-010	0	4.5	xxii-020	0	6.0
28	xxii-022	0	2.3	xxii-040	0	4.6	xxii-087	2	6.1
29	xxii-109	2	2.3	xxii-078	3	4.6	xxii-053	2	6.1
30	xxii-102	8	2.4	xxii-079	0	4.6	xxii-037	0	6.2
31	xxii-mohamed1-2	3	2.7	xxii-022	0	4.7	xxii-034	0	6.2
32	xxii-brandenburg-grimme1-3	0	2.7	xxii-052	1	4.7	xxii-013	2	6.3
33	xxii-035	1	2.7	xxii-071	0	4.7	xxii-022	0	6.4
34	xxii-041	0	2.8	xxii-adjiman-pantelides1-1	8	4.9	xxii-072	0	6.5
35	xxii-zhu2-1	2	3.1	xxii-lv-wang-ma2-2	3	5.0	xxii-073	0	6.5
36	xxii-036	0	3.2	xxii-012	0	5.0	xxii-078	3	6.6
37	xxii-026	0	3.2	xxii-074	0	5.0	xxii-040	0	6.6
38	xxii-029	0	3.3	xxii-013	2	5.0	xxii-boese-hofmann1-3	0	6.7
39	xxii-vandenende-cuppen2-3	1	3.3	xxii-046	0	5.0	xxii-047	0	6.7
40	xxii-045	0	3.4	xxii-034	0	5.1	xxii-042	0	6.8
41	xxii-039	1	3.5	xxii-020	0	5.1	xxii-092	0	6.8
42	xxii-zhu2-3	1	3.5	xxii-053	2	5.2	xxii-021	1	6.9
43	xxii-027	0	3.6	xxii-029	0	5.3	xxii-price1-3	8	6.9
44	xxii-069	0	3.6	xxii-042	0	5.3	xxii-facelli2-3	0	7.0
45	xxii-034	0	3.6	xxii-poly59-22-5	1	5.3	xxii-029	0	7.0
46	xxii-042	0	3.6	xxii-073	0	5.3	xxii-079	0	7.1
47	xxii-028	0	3.7	xxii-037	0	5.4	xxii-069	0	7.1
48	xxii-061	0	3.7	xxii-047	0	5.4	xxii-071	0	7.2
49	xxii-048	0	3.7	xxii-zhu2-3	1	5.4	xxii-064	0	7.3
50	xxii-064	0	3.8	xxii-069	0	5.5	xxii-044	0	7.3
51	xxii-107	3	3.8	xxii-039	1	5.7	xxii-074	0	7.3
52	xxii-boese-hofmann1-1	0	3.8	xxii-064	0	5.7	xxii-039	1	7.4
53	xxii-055	0	3.8	xxii-045	0	5.8	xxii-012	0	7.4
54	xxii-080	0	3.9	xxii-026	0	5.8	xxii-tuckerman-szalewicz1-1	1	7.5
55	xxii-073	0	3.9	xxii-044	0	5.9	xxii-067	0	7.5
56	xxii-054	0	3.9	xxii-092	0	5.9	xxii-010	0	7.5
57	xxii-047	0	3.9	xxii-facelli2-3	0	6.0	xxii-045	0	7.6
58	xxii-020	0	3.9	xxii-058	0	6.1	xxii-085	0	7.7
59	xxii-068	0	3.9	xxii-061	0	6.2	xxii-026	0	7.8
60	xxii-044	0	3.9	xxii-086	0	6.3	xxii-061	0	7.9
61	xxii-046	0	4.0	xxii-boese-hofmann1-1	0	6.4	xxii-058	0	8.0
62	xxii-015	0	4.0	xxii-043	0	6.4	xxii-086	0	8.2

Continued

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
63	xxii-016	0	4.0	xxii-067	0	6.5	xxii-083	0	8.3
64	xxii-110	2	4.0	xxii-085	0	6.5	xxii-043	0	8.3
65	xxii-031	0	4.0	xxii-016	0	6.6	xxii-070	0	8.4
66	xxii-058	0	4.1	xxii-031	0	6.7	xxii-poly59-22-5	1	8.5
67	xxii-086	0	4.2	xxii-070	0	6.7	xxii-016	0	8.5
68	xxii-043	0	4.2	xxii-083	0	6.8	xxii-031	0	8.5
69	xxii-018	0	4.3	xxii-tuckerman-szalewicz1-1	1	6.8	xxii-boese-hofmann1-1	0	8.6
70	xxii-goto-obata2-2	0	4.3	xxii-048	0	6.9	xxii-059	0	8.7
71	xxii-051	0	4.4	xxii-goto-obata2-2	0	6.9	xxii-goto-obata2-3	0	8.7
72	xxii-097	0	4.5	xxii-055	0	6.9	xxii-goto-obata2-2	0	8.9
73	xxii-037	0	4.5	xxii-018	0	6.9	xxii-050	0	9.0
74	xxii-050	0	4.5	xxii-050	0	6.9	xxii-018	0	9.0
75	xxii-092	0	4.7	xxii-059	0	7.0	xxii-dzyabchenko-3	0	9.0
76	xxii-075	0	4.7	xxii-015	0	7.2	xxii-048	0	9.1
77	xxii-brandenburg-grimme1-2	0	4.7	xxii-097	0	7.2	xxii-097	0	9.3
78	xxii-cole-1	1	4.7	xxii-054	0	7.2	xxii-055	0	9.4
79	xxii-023	1	4.8	xxii-080	0	7.3	xxii-062	0	9.4
80	xxii-090	0	4.8	xxii-100	0	7.4	xxii-100	0	9.5
81	xxii-077	0	4.8	xxii-brandenburg-grimme1-2	0	7.4	xxii-brandenburg-grimme1-2	0	9.6
82	xxii-070	0	4.9	xxii-068	0	7.6	xxii-015	0	9.7
83	xxii-100	0	4.9	xxii-077	0	7.7	xxii-077	0	10.0
84	xxii-083	0	4.9	xxii-028	0	7.7	xxii-076	0	10.0
85	xxii-065	0	4.9	xxii-goto-obata2-3	0	7.7	xxii-084	0	10.0
86	xxii-076	0	5.0	xxii-062	0	7.7	xxii-054	0	10.1
87	xxii-067	0	5.1	xxii-076	0	7.9	xxii-080	0	10.1
88	xxii-059	0	5.1	xxii-051	0	7.9	xxii-065	0	10.3
89	xxii-094	0	5.1	xxii-cole-1	1	7.9	xxii-090	0	10.5
90	xxii-facelli2-3	0	5.2	xxii-065	0	7.9	xxii-093	0	10.5
91	xxii-095	0	5.2	xxii-090	0	7.9	xxii-adjiman-pantelides1-3	0	10.5
92	xxii-089	0	5.3	xxii-023	1	8.0	xxii-049	1	10.6
93	xxii-085	0	5.3	xxii-075	0	8.1	xxii-091	1	10.6
94	xxii-082	0	5.4	xxii-084	0	8.4	xxii-051	0	10.8
95	xxii-062	0	5.4	xxii-095	0	8.4	xxii-068	0	10.8
96	xxii-066	0	5.5	xxii-082	0	8.4	xxii-082	0	10.9
97	xxii-podeszwa1-3	1	5.8	xxii-dzyabchenko-3	0	8.5	xxii-028	0	10.9
98	xxii-081	0	5.8	xxii-066	0	8.6	xxii-lv-wang-ma2-3	1	10.9
99	xxii-060	1	5.8	xxii-093	0	8.7	xxii-066	0	11.0
100	xxii-098	0	6.0	xxii-094	0	8.9	xxii-facelli2-1	0	11.0
101	xxii-084	0	6.3	xxii-089	0	9.1	xxii-075	0	11.1
102	xxii-093	0	6.4	xxii-081	0	9.1	xxii-095	0	11.1
103	xxii-goto-obata2-3	0	6.4	xxii-szalewicz-price1-2	0	9.2	xxii-szalewicz-price1-2	0	11.2
104	xxii-szalewicz-price1-2	0	6.8	xxii-060	1	9.2	xxii-094	0	11.7
105	xxii-dzyabchenko-3	0	7.3	xxii-adjiman-pantelides1-3	0	9.3	xxii-081	0	11.8
106	xxii-096	0	7.5	xxii-facelli2-1	0	9.4	xxii-060	1	12.0
107	xxii-facelli2-1	0	7.6	xxii-lv-wang-ma2-3	1	9.4	xxii-089	0	12.3
108	xxii-lv-wang-ma2-3	1	7.9	xxii-098	0	10.3	xxii-vandenende-cuppen2-1	0	12.6
109	xxii-099	0	7.9	xxii-facelli1-3	0	11.0	xxii-goto-obata2-1	0	13.5
110	xxii-facelli1-3	0	7.9	xxii-099	0	11.1	xxii-facelli1-3	0	13.7
111	xxii-adjiman-pantelides1-3	0	8.0	xxii-vandenende-cuppen2-1	0	11.7	xxii-099	0	13.9
112	xxii-goto-obata2-1	0	9.0	xxii-goto-obata2-1	0	11.7	xxii-098	0	13.9
113	xxii-lv-wang-ma2-1	0	9.1	xxii-096	0	12.2	xxii-podeszwa1-1	3	15.3
114	xxii-hofmann1-3	0	9.9	xxii-lv-wang-ma2-1	0	13.1	xxii-096	0	15.9
115	xxii-vandenende-cuppen2-1	0	10.8	xxii-hofmann1-3	0	14.0	xxii-lv-wang-ma2-1	0	16.1
116	xxii-vaneijck1-1	3	12.9	xxii-podeszwa1-1	3	14.1	xxii-brandenburg-grimme1-1	0	16.7
117	xxii-cole-3	0	15.2	xxii-brandenburg-grimme1-1	0	16.0	xxii-hofmann1-3	0	17.3
118	xxii-brandenburg-grimme1-1	0	15.2	xxii-chadha-singh-2	0	16.9	xxii-chadha-singh-2	0	18.0
119	xxii-chadha-singh-2	0	15.3	xxii-vaneijck1-3	0	16.9	xxii-vaneijck1-3	0	18.3
120	xxii-vaneijck1-3	0	15.4	xxii-cole-3	0	17.5	xxii-cole-3	0	19.4
121	xxii-cole-2	0	18.1	xxii-cole-2	0	19.7	xxii-cole-2	0	21.2
122	xxii-chadha-singh-3	0	20.7	xxii-chadha-singh-3	0	22.4	xxii-chadha-singh-3	0	23.9
123	xxii-chadha-singh-1	0	21.2	xxii-chadha-singh-1	0	23.9	xxii-chadha-singh-1	0	26.4
124	xxii-hofmann1-2	0	27.2	xxii-hofmann1-2	0	33.7	xxii-hofmann1-2	0	38.8

TABLE XXIV: Computed energy ranking for unique candidate structures of compound XXIII, 2-((4-(3,4-dicholorophenethyl)phenyl)amino)benzoic acid. Energies are expressed relative to the experimental form c, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	xxiii-neumann2-2	1	-0.8	xxiii-005	0	0.0	xxiii-005	0	0.0
2	xxiii-005	0	-0.0	xxiii-expt-c	2	0.0	xxiii-expt-c	2	0.0
3	xxiii-expt-c	2	0.0	xxiii-expt-b	8	0.8	xxiii-expt-b	8	1.3
4	xxiii-expt-b	8	0.3	xxiii-018	1	1.5	xxiii-018	1	1.8
5	xxiii-070	0	0.6	xxiii-011	6	1.6	xxiii-011	6	2.3
6	xxiii-neumann1-3	6	0.7	xxiii-070	0	1.8	xxiii-070	0	3.0
7	xxiii-neumann2-1	1	0.7	xxiii-neumann2-2	1	1.9	xxiii-expt-e	1	3.0
8	xxiii-003	1	0.8	xxiii-expt-e	1	2.1	xxiii-026	0	3.3
9	xxiii-015	1	0.9	xxiii-expt-a	2	2.2	xxiii-expt-a	2	3.4
10	xxiii-expt-a	2	1.0	xxiii-026	0	2.5	xxiii-025	0	3.9
11	xxiii-expt-e	1	1.0	xxiii-neumann2-1	1	2.7	xxiii-poly59-23-2	3	4.0
12	xxiii-expt-d	3	1.0	xxiii-expt-d	3	3.0	xxiii-030	0	4.2
13	xxiii-024	0	1.4	xxiii-022	0	3.2	xxiii-neumann2-1	1	4.2
14	xxiii-022	0	1.6	xxiii-025	0	3.2	xxiii-neumann2-2	1	4.5
15	xxiii-007	0	1.7	xxiii-007	0	3.3	xxiii-expt-d	3	4.7
16	xxiii-008	0	1.7	xxiii-042	7	3.4	xxiii-042	7	4.7
17	xxiii-026	0	1.8	xxiii-030	0	3.5	xxiii-007	0	4.8
18	xxiii-020	0	1.8	xxiii-poly59-23-2	3	3.7	xxiii-022	0	5.0
19	xxiii-023	0	1.9	xxiii-neumann1-1	1	3.8	xxiii-100	0	5.0
20	xxiii-010	0	2.0	xxiii-tkatchenko2-1	4	4.1	xxiii-080	1	5.1
21	xxiii-038	0	2.1	xxiii-013	1	4.2	xxiii-063	0	5.1
22	xxiii-013	1	2.2	xxiii-021	0	4.2	xxiii-067	0	5.3
23	xxiii-vaneijck1-1	2	2.3	xxiii-068	3	4.2	xxiii-057	0	5.5
24	xxiii-042	7	2.3	xxiii-080	1	4.2	xxiii-tkatchenko2-1	4	5.5
25	xxiii-025	0	2.4	xxiii-033	0	4.2	xxiii-021	0	5.5
26	xxiii-021	0	2.4	xxiii-008	0	4.3	xxiii-033	0	5.5
27	xxiii-053	0	2.5	xxiii-100	0	4.3	xxiii-013	1	5.6
28	xxiii-030	0	2.6	xxiii-053	0	4.3	xxiii-097	0	5.6
29	xxiii-mohamed1-2	4	2.7	xxiii-024	0	4.3	xxiii-tkatchenko1-3	3	5.6
30	xxiii-062	0	2.7	xxiii-063	0	4.4	xxiii-047	0	5.6
31	xxiii-056	1	2.8	xxiii-010	0	4.4	xxiii-059	0	5.7
32	xxiii-brandenburg-grimme1-2	3	2.8	xxiii-067	0	4.4	xxiii-052	0	5.7
33	xxiii-048	0	3.0	xxiii-poly59-23-1	3	4.4	xxiii-060	0	5.7
34	xxiii-036	0	3.0	xxiii-boese-hofmann1-1	1	4.5	xxiii-poly59-23-1	3	5.7
35	xxiii-027	0	3.0	xxiii-036	0	4.5	xxiii-036	0	5.9
36	xxiii-adjiman-pantelides1-2	3	3.0	xxiii-057	0	4.7	xxiii-095	0	6.0
37	xxiii-033	0	3.0	xxiii-097	0	4.7	xxiii-035	0	6.1
38	xxiii-080	1	3.2	xxiii-059	0	4.7	xxiii-065	0	6.1
39	xxiii-034	0	3.3	xxiii-vaneijck1-1	2	4.7	xxiii-053	0	6.1
40	xxiii-102	3	3.3	xxiii-047	0	4.7	xxiii-010	0	6.4
41	xxiii-046	0	3.3	xxiii-060	0	4.7	xxiii-boese-hofmann1-1	1	6.5
42	xxiii-044	0	3.3	xxiii-052	0	4.7	xxiii-008	0	6.5
43	xxiii-041	0	3.4	xxiii-035	0	4.8	xxiii-043	0	6.7
44	xxiii-029	0	3.4	xxiii-020	0	4.9	xxiii-083	0	6.7
45	xxiii-043	0	3.4	xxiii-095	0	4.9	xxiii-neumann1-1	1	7.0
46	xxiii-067	0	3.5	xxiii-065	0	4.9	xxiii-024	0	7.2
47	xxiii-076	0	3.5	xxiii-023	0	4.9	xxiii-091	0	7.2
48	xxiii-100	0	3.5	xxiii-043	0	5.1	xxiii-049	3	7.2
49	xxiii-063	0	3.6	xxiii-083	0	5.3	xxiii-054	0	7.2
50	xxiii-097	0	3.7	xxiii-038	0	5.3	xxiii-vaneijck1-1	2	7.5
51	xxiii-071	0	3.7	xxiii-046	0	5.4	xxiii-029	0	7.5
52	xxiii-095	0	3.8	xxiii-091	0	5.6	xxiii-046	0	7.6
53	xxiii-065	0	3.8	xxiii-054	0	5.6	xxiii-040	0	7.7
54	xxiii-goto-obata1-3	1	3.8	xxiii-049	3	5.6	xxiii-073	0	7.7
55	xxiii-045	1	3.8	xxiii-029	0	5.6	xxiii-038	0	7.9
56	xxiii-060	0	3.8	xxiii-048	0	5.8	xxiii-032	0	7.9
57	xxiii-059	0	3.8	xxiii-040	0	5.9	xxiii-087	0	7.9
58	xxiii-047	0	3.8	xxiii-044	0	5.9	xxiii-090	0	8.1
59	xxiii-052	0	3.9	xxiii-073	0	6.0	xxiii-044	0	8.1
60	xxiii-057	0	3.9	xxiii-090	0	6.1	xxiii-020	0	8.2
61	xxiii-035	0	3.9	xxiii-041	0	6.1	xxiii-023	0	8.3
62	xxiii-064	0	3.9	xxiii-032	0	6.1	xxiii-goto-obata2-1	2	8.3
63	xxiii-055	0	3.9	xxiii-062	0	6.1	xxiii-boese-hofmann1-2	0	8.5
64	xxiii-boese-hofmann1-3	3	3.9	xxiii-027	0	6.2	xxiii-048	0	8.6
65	xxiii-091	0	4.0	xxiii-goto-obata2-1	2	6.2	xxiii-041	0	8.9

Continued

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
66	xxiii-adjiman-pantelides1-1	2	4.0	xxiii-071	0	6.2	xxiii-071	0	8.9
67	xxiii-040	0	4.0	xxiii-076	0	6.3	xxiii-051	0	9.1
68	xxiii-054	0	4.2	xxiii-034	0	6.4	xxiii-089	0	9.1
69	xxiii-032	0	4.2	xxiii-boese-hofmann1-2	0	6.5	xxiii-poly59-23-6	1	9.2
70	xxiii-058	0	4.2	xxiii-087	0	6.5	xxiii-058	0	9.2
71	xxiii-083	0	4.2	xxiii-064	0	6.6	xxiii-062	0	9.3
72	xxiii-090	0	4.2	xxiii-045	1	6.8	xxiii-079	0	9.4
73	xxiii-109	1	4.4	xxiii-058	0	6.8	xxiii-076	0	9.4
74	xxiii-073	0	4.4	xxiii-082	1	7.0	xxiii-096	0	9.5
75	xxiii-072	0	4.5	xxiii-089	0	7.1	xxiii-086	1	9.6
76	xxiii-boese-hofmann1-2	0	4.5	xxiii-069	1	7.1	xxiii-027	0	9.6
77	xxiii-092	1	4.5	xxiii-poly59-23-9	1	7.2	xxiii-064	0	9.7
78	xxiii-075	0	4.6	xxiii-051	0	7.3	xxiii-034	0	9.7
79	xxiii-082	1	4.6	xxiii-072	0	7.3	xxiii-069	1	9.8
80	xxiii-069	1	4.6	xxiii-096	0	7.3	xxiii-poly59-23-9	1	9.9
81	xxiii-061	0	4.7	xxiii-055	0	7.3	xxiii-045	1	9.9
82	xxiii-077	0	4.8	xxiii-075	0	7.3	xxiii-075	0	10.0
83	xxiii-088	0	5.0	xxiii-077	0	7.4	xxiii-072	0	10.0
84	xxiii-084	0	5.0	xxiii-079	0	7.5	xxiii-077	0	10.2
85	xxiii-day1-1	1	5.1	xxiii-037	1	7.5	xxiii-078	1	10.2
86	xxiii-089	0	5.1	xxiii-093	0	7.6	xxiii-093	0	10.3
87	xxiii-079	0	5.2	xxiii-088	0	7.8	xxiii-poly59-23-8	1	10.8
88	xxiii-093	0	5.2	xxiii-poly59-23-6	1	7.8	xxiii-055	0	10.8
89	xxiii-096	0	5.2	xxiii-day2-1	1	7.9	xxiii-day2-1	1	10.9
90	xxiii-051	0	5.3	xxiii-078	1	8.2	xxiii-088	0	11.0
91	xxiii-087	0	5.3	xxiii-061	0	8.4	xxiii-zhu1-1	0	11.1
92	xxiii-081	0	5.8	xxiii-zhu1-1	0	8.5	xxiii-037	1	11.5
93	xxiii-goto-obata1-1	0	5.9	xxiii-092	1	8.8	xxiii-094	0	11.8
94	xxiii-078	1	6.2	xxiii-084	0	8.9	xxiii-061	0	12.0
95	xxiii-zhu1-1	0	6.2	xxiii-poly59-23-8	1	9.0	xxiii-zhu1-2	0	12.2
96	xxiii-094	0	6.3	xxiii-094	0	9.1	xxiii-110	1	12.5
97	xxiii-day2-2	0	6.9	xxiii-081	0	9.3	xxiii-elking-fustimolnar1-1	0	12.5
98	xxiii-poly59-23-6	1	6.9	xxiii-zhu1-2	0	9.5	xxiii-081	0	12.8
99	xxiii-zhu1-2	0	7.2	xxiii-goto-obata1-1	0	10.1	xxiii-084	0	13.0
100	xxiii-108	1	7.4	xxiii-day2-2	0	10.2	xxiii-day2-2	0	13.2
101	xxiii-zhu1-3	0	8.0	xxiii-zhu1-3	0	10.3	xxiii-zhu1-3	0	13.2
102	xxiii-vaneijck1-2	1	8.4	xxiii-110	1	10.6	xxiii-066	1	13.3
103	xxiii-elking-fustimolnar2-1	0	8.6	xxiii-vaneijck1-2	1	10.7	xxiii-elking-fustimolnar2-1	0	13.6
104	xxiii-vaneijck1-3	0	8.8	xxiii-elking-fustimolnar1-1	0	10.8	xxiii-vaneijck1-2	1	13.6
105	xxiii-110	1	8.9	xxiii-elking-fustimolnar2-1	0	11.0	xxiii-vaneijck1-3	0	13.8
106	xxiii-elking-fustimolnar1-1	0	9.0	xxiii-vaneijck1-3	0	11.0	xxiii-day2-3	1	14.5
107	xxiii-day1-2	1	9.9	xxiii-day2-3	1	12.3	xxiii-goto-obata1-1	0	14.6
108	xxiii-elking-fustimolnar1-3	0	10.9	xxiii-elking-fustimolnar1-3	0	14.5	xxiii-day1-3	0	17.9
109	xxiii-brandenburg-grimme1-1	0	12.2	xxiii-brandenburg-grimme1-1	0	15.0	xxiii-elking-fustimolnar1-3	0	18.3
110	xxiii-day1-3	0	12.7	xxiii-day1-3	0	15.3	xxiii-brandenburg-grimme1-1	0	18.3
111	xxiii-vandenende-cuppen2-1	0	13.1	xxiii-vandenende-cuppen2-1	0	16.6	xxiii-goto-obata2-2	0	19.2
112	xxiii-elking-fustimolnar1-2	0	14.7	xxiii-goto-obata2-2	0	17.3	xxiii-vandenende-cuppen2-1	0	20.5
113	xxiii-goto-obata2-2	0	15.4	xxiii-elking-fustimolnar1-2	0	19.7	xxiii-elking-fustimolnar2-3	0	23.9
114	xxiii-elking-fustimolnar2-3	0	15.5	xxiii-elking-fustimolnar2-3	0	19.7	xxiii-goto-obata2-3	0	24.1
115	xxiii-goto-obata2-3	0	16.0	xxiii-goto-obata2-3	0	20.3	xxiii-elking-fustimolnar1-2	0	24.8
116	xxiii-vandenende-cuppen1-2	0	18.4	xxiii-vandenende-cuppen1-2	0	21.6	xxiii-vandenende-cuppen1-2	0	25.0
117	xxiii-elking-fustimolnar2-2	0	18.5	xxiii-elking-fustimolnar2-2	0	22.3	xxiii-elking-fustimolnar2-2	0	25.8
118	xxiii-facelli1-1	0	21.8	xxiii-facelli1-1	0	25.1	xxiii-vandenende-cuppen2-2	0	25.8
119	xxiii-facelli1-3	0	22.2	xxiii-vandenende-cuppen2-2	0	25.4	xxiii-facelli1-1	0	28.0
120	xxiii-hofmann1-1	0	22.6	xxiii-facelli1-3	0	26.0	xxiii-facelli1-3	0	29.6
121	xxiii-facelli1-2	0	24.0	xxiii-hofmann1-1	0	26.2	xxiii-hofmann1-1	0	29.8
122	xxiii-vandenende-cuppen2-2	0	25.8	xxiii-facelli1-2	0	27.5	xxiii-facelli1-2	0	30.6
123	xxiii-vandenende-cuppen2-3	0	31.2	xxiii-vandenende-cuppen2-3	0	31.7	xxiii-vandenende-cuppen2-3	0	33.3
124	xxiii-hofmann1-3	0	33.8	xxiii-vandenende-cuppen1-3	0	34.9	xxiii-vandenende-cuppen1-3	0	36.5
125	xxiii-vandenende-cuppen1-3	0	33.9	xxiii-chadha-singh-1	1	36.5	xxiii-chadha-singh-1	1	37.5
126	xxiii-chadha-singh-1	1	35.3	xxiii-hofmann1-3	0	36.6	xxiii-hofmann1-3	0	39.8
127	xxiii-cole-1	0	39.1	xxiii-cole-1	0	41.5	xxiii-cole-1	0	44.3
128	xxiii-cole-2	0	45.6	xxiii-cole-2	0	47.9	xxiii-cole-2	0	50.4
129	xxiii-vandenende-cuppen1-1	0	45.8	xxiii-vandenende-cuppen1-1	0	48.1	xxiii-chadha-singh-3	0	50.8
130	xxiii-chadha-singh-3	0	46.4	xxiii-chadha-singh-3	0	48.2	xxiii-vandenende-cuppen1-1	0	51.2
131	xxiii-hofmann1-2	0	57.6	xxiii-hofmann1-2	0	60.9	xxiii-hofmann1-2	0	64.3

TABLE XXV: Computed energy ranking for unique candidate structures of compound XXIV, chloride salt hydrate of (Z)-3-((diaminomethyl)thio)acrylic acid. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	xxiv-zhu1-3	2	-2.0	xxiv-boese-hofmann1-1	1	-0.7	xxiv-boese-hofmann1-1	1	-0.4
2	xxiv-003	1	-1.3	xxiv-003	1	0.0	xxiv-expt	3	0.0
3	xxiv-boese-hofmann1-1	1	-1.1	xxiv-expt	3	0.0	xxiv-003	1	1.0
4	xxiv-010	0	-0.8	xxiv-010	0	0.6	xxiv-010	0	1.5
5	xxiv-016	0	-0.4	xxiv-012	1	1.6	xxiv-027	0	3.0
6	xxiv-012	1	-0.2	xxiv-001	2	1.7	xxiv-012	1	3.1
7	xxiv-005	0	-0.0	xxiv-018	1	2.3	xxiv-008	0	3.3
8	xxiv-expt	3	0.0	xxiv-016	0	2.3	xxiv-009	0	3.8
9	xxiv-015	1	0.0	xxiv-008	0	2.8	xxiv-019	0	3.9
10	xxiv-011	0	0.7	xxiv-027	0	3.1	xxiv-018	1	4.1
11	xxiv-022	0	1.1	xxiv-022	0	3.2	xxiv-001	2	4.5
12	xxiv-013	0	1.4	xxiv-021	0	3.3	xxiv-016	0	4.6
13	xxiv-037	0	1.5	xxiv-019	0	3.5	xxiv-021	0	4.9
14	xxiv-021	0	1.5	xxiv-009	0	3.6	xxiv-022	0	5.0
15	xxiv-007	0	1.6	xxiv-007	0	3.6	xxiv-055	0	5.2
16	xxiv-014	0	1.7	xxiv-005	0	3.6	xxiv-007	0	5.3
17	xxiv-028	1	1.7	xxiv-023	1	3.9	xxiv-042	0	5.5
18	xxiv-boese-hofmann1-2	1	1.8	xxiv-031	0	4.0	xxiv-045	0	5.6
19	xxiv-032	0	2.0	xxiv-028	1	4.2	xxiv-023	1	5.6
20	xxiv-031	0	2.0	xxiv-011	0	4.2	xxiv-031	0	5.6
21	xxiv-008	0	2.1	xxiv-zhu1-2	1	4.3	xxiv-028	1	5.7
22	xxiv-zhu1-1	1	2.4	xxiv-032	0	4.5	xxiv-043	0	5.8
23	xxiv-039	0	2.5	xxiv-040	0	4.7	xxiv-zhu1-2	1	5.8
24	xxiv-080	0	2.5	xxiv-042	0	4.8	xxiv-029	0	5.9
25	xxiv-019	0	2.6	xxiv-049	0	4.8	xxiv-tkatchenko1-1	4	6.1
26	xxiv-020	1	2.7	xxiv-055	0	5.3	xxiv-049	0	6.1
27	xxiv-040	0	2.9	xxiv-037	0	5.3	xxiv-032	0	6.1
28	xxiv-027	0	2.9	xxiv-043	0	5.4	xxiv-005	0	6.1
29	xxiv-049	0	3.0	xxiv-045	0	5.4	xxiv-040	0	6.2
30	xxiv-042	0	3.1	xxiv-058	0	5.6	xxiv-011	0	6.3
31	xxiv-035	0	3.1	xxiv-014	0	5.7	xxiv-053	0	7.1
32	xxiv-009	0	3.1	xxiv-029	0	5.8	xxiv-058	0	7.4
33	xxiv-054	0	3.4	xxiv-054	0	5.8	xxiv-024	0	7.5
34	xxiv-034	0	3.5	xxiv-013	0	5.9	xxiv-050	0	7.5
35	xxiv-058	0	3.8	xxiv-050	0	5.9	xxiv-052	0	7.6
36	xxiv-059	1	4.0	xxiv-039	0	6.0	xxiv-062	0	7.9
37	xxiv-067	0	4.1	xxiv-024	0	6.3	xxiv-054	0	7.9
38	xxiv-074	0	4.1	xxiv-063	4	6.4	xxiv-044	0	8.0
39	xxiv-050	0	4.2	xxiv-062	0	6.6	xxiv-033	0	8.0
40	xxiv-024	0	4.4	xxiv-034	0	6.9	xxiv-065	0	8.2
41	xxiv-062	0	4.4	xxiv-052	0	6.9	xxiv-039	0	8.3
42	xxiv-087	0	4.4	xxiv-035	0	6.9	xxiv-037	0	8.4
43	xxiv-038	0	4.4	xxiv-033	0	7.0	xxiv-030	0	8.6
44	xxiv-025	1	4.8	xxiv-030	0	7.1	xxiv-014	0	8.6
45	xxiv-045	0	4.8	xxiv-020	1	7.1	xxiv-108	1	8.7
46	xxiv-043	0	4.9	xxiv-073	0	7.5	xxiv-073	0	8.9
47	xxiv-030	0	4.9	xxiv-087	0	7.6	xxiv-089	0	9.1
48	xxiv-047	0	4.9	xxiv-044	0	7.7	xxiv-078	0	9.2
49	xxiv-017	0	5.0	xxiv-017	0	7.8	xxiv-013	0	9.3
50	xxiv-055	0	5.0	xxiv-074	0	7.8	xxiv-034	0	9.6
51	xxiv-029	0	5.1	xxiv-080	0	7.8	xxiv-081	0	9.6
52	xxiv-091	0	5.1	xxiv-089	0	7.9	xxiv-070	0	9.7
53	xxiv-079	0	5.2	xxiv-053	0	7.9	xxiv-017	0	10.0
54	xxiv-096	0	5.3	xxiv-078	0	8.1	xxiv-035	0	10.0
55	xxiv-077	0	5.4	xxiv-067	0	8.1	xxiv-087	0	10.0
56	xxiv-046	0	5.4	xxiv-081	0	8.2	xxiv-020	1	10.3
57	xxiv-048	0	5.4	xxiv-065	0	8.2	xxiv-100	0	10.4
58	xxiv-033	0	5.5	xxiv-070	0	8.3	xxiv-day1-2	0	10.4
59	xxiv-089	0	5.6	xxiv-047	0	8.4	xxiv-085	0	10.4
60	xxiv-061	0	5.7	xxiv-099	0	8.4	xxiv-074	0	10.5
61	xxiv-073	0	5.8	xxiv-day1-2	0	8.4	xxiv-099	0	10.8
62	xxiv-099	0	5.8	xxiv-077	0	8.5	xxiv-093	0	10.9
63	xxiv-tkatchenko1-2	0	5.8	xxiv-tkatchenko1-2	0	8.6	xxiv-tkatchenko1-2	0	10.9
64	xxiv-071	0	5.8	xxiv-091	0	8.7	xxiv-047	0	10.9

Continued

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
65	xxiv-052	0	5.9	xxiv-025	1	8.7	xxiv-brandenburg-grimme2-2	1	10.9
66	xxiv-068	0	5.9	xxiv-066	0	8.7	xxiv-067	0	11.0
67	xxiv-060	0	5.9	xxiv-096	0	8.8	xxiv-060	0	11.0
68	xxiv-069	1	6.0	xxiv-060	0	8.9	xxiv-077	0	11.0
69	xxiv-day1-2	0	6.0	xxiv-108	1	9.0	xxiv-day1-1	0	11.0
70	xxiv-066	0	6.0	xxiv-094	0	9.1	xxiv-064	0	11.1
71	xxiv-081	0	6.1	xxiv-085	0	9.2	xxiv-066	0	11.2
72	xxiv-094	0	6.2	xxiv-brandenburg-grimme2-2	1	9.2	xxiv-091	0	11.2
73	xxiv-070	0	6.2	xxiv-059	1	9.3	xxiv-096	0	11.3
74	xxiv-063	4	6.4	xxiv-048	0	9.4	xxiv-094	0	11.4
75	xxiv-076	0	6.6	xxiv-095	0	9.8	xxiv-brandenburg-grimme2-3	1	11.4
76	xxiv-083	0	6.8	xxiv-064	0	9.9	xxiv-025	1	11.6
77	xxiv-095	0	6.8	xxiv-068	0	10.1	xxiv-088	0	11.8
78	xxiv-brandenburg-grimme2-2	1	6.9	xxiv-051	1	10.1	xxiv-095	0	11.9
79	xxiv-078	0	6.9	xxiv-061	0	10.2	xxiv-110	1	12.1
80	xxiv-082	0	7.0	xxiv-brandenburg-grimme2-3	1	10.3	xxiv-051	1	12.1
81	xxiv-044	0	7.1	xxiv-069	1	10.4	xxiv-poly59-24-5	1	12.1
82	xxiv-092	1	7.1	xxiv-day1-1	0	10.5	xxiv-080	0	12.2
83	xxiv-051	1	7.2	xxiv-079	0	10.6	xxiv-048	0	12.2
84	xxiv-065	0	7.6	xxiv-093	0	10.7	xxiv-097	0	12.2
85	xxiv-064	0	7.8	xxiv-088	0	10.7	xxiv-084	0	12.4
86	xxiv-085	0	7.9	xxiv-086	1	10.8	xxiv-poly59-24-6	1	12.6
87	xxiv-090	0	8.3	xxiv-100	0	10.8	xxiv-tkatchenko1-3	0	12.9
88	xxiv-084	0	8.3	xxiv-tkatchenko1-3	0	10.8	xxiv-068	0	13.1
89	xxiv-053	0	8.3	xxiv-082	0	10.8	xxiv-059	1	13.2
90	xxiv-tkatchenko1-3	0	8.4	xxiv-084	0	10.8	xxiv-086	1	13.4
91	xxiv-075	0	8.9	xxiv-083	0	10.8	xxiv-083	0	13.6
92	xxiv-brandenburg-grimme2-3	1	8.9	xxiv-076	0	11.0	xxiv-082	0	13.7
93	xxiv-088	0	9.2	xxiv-097	0	11.0	xxiv-069	1	13.7
94	xxiv-097	0	9.3	xxiv-071	0	11.0	xxiv-061	0	13.7
95	xxiv-108	1	9.4	xxiv-038	0	11.5	xxiv-brandenburg-grimme1-3	2	14.1
96	xxiv-093	0	9.6	xxiv-poly59-24-5	1	11.6	xxiv-076	0	14.1
97	xxiv-day1-1	0	10.2	xxiv-090	0	11.7	xxiv-090	0	14.4
98	xxiv-100	0	10.4	xxiv-110	1	11.8	xxiv-boese-hofmann1-3	0	14.5
99	xxiv-poly59-24-5	1	10.6	xxiv-046	0	12.1	xxiv-brandenburg-grimme1-2	0	14.6
100	xxiv-brandenburg-grimme1-3	2	10.6	xxiv-106	1	12.3	xxiv-075	0	14.9
101	xxiv-poly59-24-9	2	10.9	xxiv-075	0	12.4	xxiv-079	0	14.9
102	xxiv-boese-hofmann1-3	0	11.0	xxiv-brandenburg-grimme1-3	2	12.6	xxiv-071	0	15.0
103	xxiv-107	1	11.0	xxiv-boese-hofmann1-3	0	13.0	xxiv-poly59-24-7	1	15.3
104	xxiv-110	1	11.3	xxiv-brandenburg-grimme1-2	0	13.3	xxiv-day1-3	2	15.5
105	xxiv-106	1	11.5	xxiv-poly59-24-7	1	13.5	xxiv-brandenburg-grimme1-1	0	16.3
106	xxiv-brandenburg-grimme1-2	0	11.8	xxiv-poly59-24-9	2	13.5	xxiv-vaneijck1-2	0	16.7
107	xxiv-brandenburg-grimme1-1	0	12.1	xxiv-brandenburg-grimme1-1	0	14.5	xxiv-vaneijck1-3	0	16.7
108	xxiv-vaneijck1-3	0	14.6	xxiv-vaneijck1-3	0	15.7	xxiv-038	0	16.9
109	xxiv-vaneijck1-2	0	14.7	xxiv-vaneijck1-2	0	15.8	xxiv-046	0	17.3
110	xxiv-price2-1	0	14.9	xxiv-price2-1	0	17.0	xxiv-price1-1	1	17.6
111	xxiv-price2-2	0	15.1	xxiv-price1-1	1	17.2	xxiv-price1-3	0	18.7
112	xxiv-vaneijck1-1	1	17.0	xxiv-price2-2	0	17.3	xxiv-price2-1	0	19.0
113	xxiv-facelli1-1	0	17.4	xxiv-price1-3	0	18.1	xxiv-price2-2	0	19.4
114	xxiv-price1-3	0	17.7	xxiv-facelli1-1	0	20.0	xxiv-facelli1-1	0	22.0
115	xxiv-hofmann1-1	0	19.4	xxiv-hofmann1-1	0	21.4	xxiv-hofmann1-1	0	22.9
116	xxiv-price2-3	0	19.8	xxiv-price2-3	0	21.5	xxiv-price2-3	0	23.3
117	xxiv-szalewicz1-3	0	21.6	xxiv-hofmann1-3	0	23.1	xxiv-hofmann1-3	0	24.0
118	xxiv-szalewicz1-1	0	21.9	xxiv-szalewicz1-3	0	24.3	xxiv-price1-2	0	25.6
119	xxiv-hofmann1-3	0	22.0	xxiv-price1-2	0	24.3	xxiv-szalewicz1-3	0	26.5
120	xxiv-szalewicz1-2	0	22.9	xxiv-szalewicz1-1	0	24.7	xxiv-facelli1-2	0	26.5
121	xxiv-price1-2	0	23.2	xxiv-szalewicz1-2	0	25.7	xxiv-szalewicz1-1	0	26.6
122	xxiv-hofmann1-2	0	24.3	xxiv-facelli1-2	0	26.7	xxiv-szalewicz1-2	0	28.1
123	xxiv-facelli1-2	0	26.8	xxiv-hofmann1-2	0	27.9	xxiv-elking-fustimolnar1-3	0	30.4
124	xxiv-elking-fustimolnar1-3	0	30.9	xxiv-elking-fustimolnar1-3	0	30.5	xxiv-hofmann1-2	0	31.0
125	xxiv-elking-fustimolnar2-2	0	35.6	xxiv-elking-fustimolnar2-2	0	35.4	xxiv-elking-fustimolnar2-2	0	35.0
126	xxiv-elking-fustimolnar2-1	0	36.3	xxiv-elking-fustimolnar1-1	0	37.1	xxiv-elking-fustimolnar1-1	0	37.7
127	xxiv-elking-fustimolnar1-1	0	36.6	xxiv-elking-fustimolnar2-1	0	37.3	xxiv-elking-fustimolnar2-1	0	37.8
128	xxiv-elking-fustimolnar2-3	0	39.3	xxiv-elking-fustimolnar1-2	0	41.1	xxiv-elking-fustimolnar1-2	0	39.3
129	xxiv-elking-fustimolnar1-2	0	43.6	xxiv-elking-fustimolnar2-3	0	41.7	xxiv-elking-fustimolnar2-3	0	43.7

TABLE XXVI: Computed energy ranking for unique candidate structures of compound XXV, 2,8-dimethyl-6H,12H-5,11-methanodibenzo[b,f][1,5]diazocine:3,5-dinitrobenzoic acid. Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	xxv-expt	10	0.0	xxv-expt	10	0.0	xxv-expt	10	0.0
2	xxv-poly59-25-1	5	0.8	xxv-mohamed1-2	5	2.9	xxv-021	5	4.7
3	xxv-poly59-25-4	2	3.4	xxv-goto-obata1-1	6	5.2	xxv-day2-1	6	5.0
4	xxv-facelli1-1	2	4.7	xxv-poly59-25-4	2	5.5	xxv-024	0	5.5
5	xxv-106	4	4.9	xxv-facelli1-2	4	5.6	xxv-011	0	5.9
6	xxv-brandenburg-grimme1-3	4	5.2	xxv-011	0	6.0	xxv-facelli1-2	4	6.1
7	xxv-104	0	5.2	xxv-012	0	6.5	xxv-poly59-25-4	2	6.3
8	xxv-goto-obata1-1	6	5.4	xxv-018	1	6.8	xxv-012	0	6.6
9	xxv-003	5	5.5	xxv-facelli1-1	2	6.9	xxv-018	1	6.9
10	xxv-013	0	5.7	xxv-015	0	7.0	xxv-015	0	7.1
11	xxv-025	0	5.8	xxv-024	0	7.1	xxv-110	2	7.3
12	xxv-011	0	6.0	xxv-poly59-25-2	5	7.1	xxv-poly59-25-2	5	8.0
13	xxv-012	0	6.1	xxv-110	2	7.3	xxv-facelli1-1	2	8.3
14	xxv-018	1	6.3	xxv-016	4	7.6	xxv-adjiman-pantelides1-2	8	8.4
15	xxv-neumann1-2	2	6.4	xxv-104	0	7.6	xxv-027	0	8.7
16	xxv-015	0	6.6	xxv-025	0	8.4	xxv-104	0	8.9
17	xxv-poly59-25-10	2	6.8	xxv-027	0	8.4	xxv-036	1	9.2
18	xxv-017	0	6.9	xxv-adjiman-pantelides1-2	8	8.4	xxv-029	0	9.2
19	xxv-007	1	7.1	xxv-033	0	9.0	xxv-041	2	9.3
20	xxv-poly59-25-5	1	7.4	xxv-029	0	9.2	xxv-033	0	9.5
21	xxv-048	0	7.6	xxv-poly59-25-5	1	9.2	xxv-016	4	9.9
22	xxv-026	0	7.6	xxv-013	0	9.2	xxv-066	2	10.2
23	xxv-027	0	7.7	xxv-035	1	9.3	xxv-048	0	10.2
24	xxv-024	0	8.0	xxv-026	0	9.4	xxv-020	1	10.4
25	xxv-039	0	8.3	xxv-neumann1-2	2	9.5	xxv-025	0	10.5
26	xxv-adjiman-pantelides1-2	8	8.4	xxv-007	1	9.6	xxv-056	0	10.6
27	xxv-009	0	8.5	xxv-048	0	9.7	xxv-026	0	10.7
28	xxv-033	0	8.5	xxv-041	2	9.8	xxv-poly59-25-5	1	10.9
29	xxv-099	0	8.9	xxv-066	2	10.0	xxv-008	1	11.1
30	xxv-036	1	9.0	xxv-020	1	10.3	xxv-042	1	11.3
31	xxv-029	0	9.2	xxv-017	0	10.4	xxv-043	0	11.5
32	xxv-poly59-25-9	2	9.3	xxv-099	0	10.6	xxv-neumann1-2	2	11.5
33	xxv-023	0	9.4	xxv-042	1	10.9	xxv-099	0	11.8
34	xxv-066	2	9.4	xxv-039	0	11.2	xxv-013	0	11.9
35	xxv-034	0	9.4	xxv-poly59-25-7	3	11.4	xxv-017	0	12.3
36	xxv-goto-obata1-2	1	9.5	xxv-034	0	11.5	xxv-038	0	12.6
37	xxv-047	0	9.9	xxv-047	0	11.6	xxv-080	0	12.6
38	xxv-poly59-25-7	3	10.2	xxv-056	0	11.8	xxv-poly59-25-7	3	12.6
39	xxv-adjiman-pantelides1-3	1	10.3	xxv-009	0	11.9	xxv-047	0	12.8
40	xxv-044	0	10.6	xxv-038	0	11.9	xxv-039	0	12.9
41	xxv-032	0	10.7	xxv-060	0	12.2	xxv-044	0	13.0
42	xxv-038	0	10.8	xxv-044	0	12.3	xxv-060	0	13.0
43	xxv-037	0	11.1	xxv-023	0	12.5	xxv-062	0	13.3
44	xxv-060	0	11.2	xxv-043	0	12.6	xxv-034	0	13.3
45	xxv-030	0	11.3	xxv-037	0	12.9	xxv-070	0	13.5
46	xxv-045	0	11.6	xxv-080	0	13.1	xxv-040	0	13.5
47	xxv-055	0	11.6	xxv-070	0	13.1	xxv-100	0	13.5
48	xxv-062	0	12.1	xxv-062	0	13.1	xxv-074	0	13.5
49	xxv-070	0	12.1	xxv-100	0	13.5	xxv-085	0	13.7
50	xxv-100	0	12.2	xxv-055	0	13.5	xxv-091	0	13.7
51	xxv-053	0	12.2	xxv-053	0	13.7	xxv-037	0	13.8
52	xxv-056	0	12.3	xxv-085	0	13.7	xxv-053	0	14.2
53	xxv-vandenende-cuppen1-2	0	12.3	xxv-074	0	13.9	xxv-055	0	14.4
54	xxv-061	0	12.6	xxv-030	0	14.0	xxv-009	0	14.5
55	xxv-054	0	12.9	xxv-032	0	14.1	xxv-052	0	14.5
56	xxv-068	0	13.0	xxv-040	0	14.1	xxv-023	0	15.3
57	xxv-052	0	13.1	xxv-052	0	14.1	xxv-096	0	15.3
58	xxv-080	0	13.2	xxv-091	0	14.3	xxv-030	0	15.4
59	xxv-085	0	13.2	xxv-045	0	14.6	xxv-067	1	15.5

Continued

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
60	xxv-083	0	13.3	xxv-vandenende-cuppen1-2	0	14.7	xxv-075	0	15.6
61	xxv-074	0	13.3	xxv-054	0	14.8	xxv-054	0	15.7
62	xxv-046	0	13.5	xxv-096	0	15.0	xxv-057	0	16.0
63	xxv-057	0	13.5	xxv-046	0	15.2	xxv-vandenende-cuppen1-2	0	16.2
64	xxv-043	0	13.5	xxv-075	0	15.2	xxv-079	1	16.2
65	xxv-050	0	13.5	xxv-089	0	15.3	xxv-089	0	16.2
66	xxv-067	1	13.7	xxv-057	0	15.3	xxv-032	0	16.5
67	xxv-059	0	13.7	xxv-067	1	15.4	xxv-046	0	16.5
68	xxv-040	0	13.8	xxv-079	1	15.5	xxv-072	0	16.6
69	xxv-075	0	13.9	xxv-068	0	15.6	xxv-045	0	16.8
70	xxv-065	0	13.9	xxv-061	0	15.8	xxv-073	0	17.2
71	xxv-096	0	14.0	xxv-050	0	15.8	xxv-068	0	17.2
72	xxv-081	0	14.1	xxv-072	0	16.0	xxv-elking-fustimolnar1-1	1	17.4
73	xxv-089	0	14.2	xxv-081	0	16.1	xxv-077	0	17.4
74	xxv-077	0	14.2	xxv-077	0	16.1	xxv-086	0	17.4
75	xxv-072	0	14.4	xxv-086	0	16.5	xxv-081	0	17.5
76	xxv-boese-hofmann1-1	1	14.5	xxv-059	0	16.6	xxv-050	0	17.6
77	xxv-091	0	14.5	xxv-083	0	16.7	xxv-090	0	17.6
78	xxv-069	0	14.6	xxv-elking-fustimolnar1-1	1	17.0	xxv-097	0	18.1
79	xxv-086	0	15.3	xxv-065	0	17.0	xxv-061	0	18.3
80	xxv-058	0	15.3	xxv-097	0	17.1	xxv-083	0	18.4
81	xxv-097	0	15.5	xxv-090	0	17.1	xxv-058	0	18.6
82	xxv-093	0	15.6	xxv-058	0	17.4	xxv-059	0	18.7
83	xxv-094	0	15.7	xxv-069	0	17.4	xxv-093	0	18.7
84	xxv-063	0	15.7	xxv-073	0	17.7	xxv-094	0	18.7
85	xxv-092	0	15.8	xxv-094	0	17.7	xxv-076	0	19.0
86	xxv-082	0	15.8	xxv-093	0	17.8	xxv-063	0	19.4
87	xxv-090	0	16.0	xxv-063	0	17.9	xxv-088	0	19.4
88	xxv-elking-fustimolnar1-1	1	16.3	xxv-092	0	18.0	xxv-092	0	19.6
89	xxv-088	0	16.3	xxv-088	0	18.2	xxv-065	0	19.8
90	xxv-076	0	16.6	xxv-076	0	18.3	xxv-078	0	19.8
91	xxv-073	0	16.9	xxv-082	0	18.5	xxv-069	0	19.9
92	xxv-071	0	17.1	xxv-078	0	19.0	xxv-082	0	20.4
93	xxv-facelli1-3	0	17.1	xxv-071	0	19.2	xxv-071	0	20.9
94	xxv-078	0	17.1	xxv-087	0	19.6	xxv-098	0	21.0
95	xxv-vandenende-cuppen2-1	0	17.3	xxv-098	0	20.2	xxv-087	0	21.0
96	xxv-087	0	18.0	xxv-facelli1-3	0	20.3	xxv-vandenende-cuppen1-3	0	21.4
97	xxv-098	0	19.0	xxv-vandenende-cuppen2-1	0	20.5	xxv-mohamed1-1	0	21.5
98	xxv-095	0	19.0	xxv-mohamed1-1	0	21.0	xxv-goto-obata2-3	0	21.9
99	xxv-084	0	19.1	xxv-vandenende-cuppen1-3	0	21.5	xxv-facelli1-3	0	22.1
100	xxv-mohamed1-1	0	20.3	xxv-084	0	21.6	xxv-084	0	22.3
101	xxv-vandenende-cuppen1-3	0	20.8	xxv-095	0	22.6	xxv-vandenende-cuppen2-1	0	22.7
102	xxv-vandenende-cuppen1-1	0	21.1	xxv-goto-obata2-3	0	22.8	xxv-goto-obata2-1	0	22.8
103	xxv-goto-obata2-3	0	22.8	xxv-vandenende-cuppen1-1	0	23.1	xxv-cole-1	0	23.7
104	xxv-cole-1	0	24.1	xxv-cole-1	0	24.7	xxv-day2-3	0	24.3
105	xxv-goto-obata2-1	0	26.0	xxv-goto-obata2-1	0	25.0	xxv-vandenende-cuppen1-1	0	25.0
106	xxv-boese-hofmann1-2	0	26.2	xxv-day2-3	0	27.7	xxv-095	0	25.3
107	xxv-cole-2	0	29.4	xxv-boese-hofmann1-2	0	28.7	xxv-cole-2	0	28.5
108	xxv-day2-3	0	30.8	xxv-cole-2	0	29.4	xxv-dzyabchenko-1	0	28.5
109	xxv-dzyabchenko-3	0	31.8	xxv-dzyabchenko-1	0	30.9	xxv-boese-hofmann1-2	0	31.0
110	xxv-boese-hofmann1-3	0	31.9	xxv-dzyabchenko-3	0	32.0	xxv-dzyabchenko-3	0	31.7
111	xxv-dzyabchenko-1	0	32.8	xxv-dzyabchenko-2	0	33.0	xxv-dzyabchenko-2	0	32.5
112	xxv-dzyabchenko-2	0	33.4	xxv-boese-hofmann1-3	0	33.2	xxv-boese-hofmann1-3	0	33.3
113	xxv-goto-obata2-2	0	34.5	xxv-goto-obata2-2	0	36.3	xxv-goto-obata2-2	0	36.3
114	xxv-vandenende-cuppen2-2	0	35.6	xxv-vandenende-cuppen2-2	0	38.1	xxv-vandenende-cuppen2-2	0	40.1
115	xxv-cole-3	0	39.9	xxv-cole-3	0	44.4	xxv-cole-3	0	46.1
116	xxv-hofmann1-1	0	48.4	xxv-hofmann1-1	0	50.7	xxv-hofmann1-1	0	51.9
117	xxv-hofmann1-2	0	60.0	xxv-hofmann1-2	0	61.6	xxv-hofmann1-2	0	62.7
118	xxv-hofmann1-3	0	61.0	xxv-hofmann1-3	0	62.9	xxv-hofmann1-3	0	64.3

TABLE XXVII: Computed energy ranking for unique candidate structures of compound XXVI, N,N'-([1,1'-Binaphthalene]-2,2'-diyl)bis(2-cholorobenzamide). Energies are expressed relative to the experimental form, in kJ/mol.

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
1	xxvi-expt	8	0.0	xxvi-expt	8	0.0	xxvi-expt	8	0.0
2	xxvi-neumann1-3	1	1.3	xxvi-004	1	0.9	xxvi-004	1	0.5
3	xxvi-002	8	2.0	xxvi-025	0	1.9	xxvi-025	0	0.9
4	xxvi-005	0	2.3	xxvi-zhu1-1	6	2.0	xxvi-zhu1-1	6	0.9
5	xxvi-neumann2-3	1	2.4	xxvi-neumann2-3	1	2.5	xxvi-neumann2-3	1	2.6
6	xxvi-010	0	2.5	xxvi-005	0	2.5	xxvi-005	0	2.8
7	xxvi-025	0	3.0	xxvi-neumann1-2	8	3.0	xxvi-007	4	3.5
8	xxvi-013	1	3.3	xxvi-010	0	3.2	xxvi-010	0	4.1
9	xxvi-006	0	3.4	xxvi-007	4	3.6	xxvi-neumann1-2	8	4.2
10	xxvi-018	0	3.6	xxvi-101	3	4.0	xxvi-101	3	4.3
11	xxvi-brandenburg-grimme1-2	6	3.7	xxvi-021	1	4.2	xxvi-015	0	4.6
12	xxvi-011	3	3.8	xxvi-006	0	4.3	xxvi-poly59-26-5	1	4.7
13	xxvi-109	4	3.8	xxvi-015	0	4.6	xxvi-099	0	5.1
14	xxvi-036	1	3.9	xxvi-099	0	4.7	xxvi-021	1	5.1
15	xxvi-030	1	3.9	xxvi-036	1	4.8	xxvi-072	0	5.4
16	xxvi-041	0	4.1	xxvi-028	1	4.9	xxvi-044	1	5.4
17	xxvi-016	0	4.2	xxvi-018	0	5.0	xxvi-006	0	5.4
18	xxvi-012	0	4.2	xxvi-023	0	5.0	xxvi-023	0	5.5
19	xxvi-099	0	4.3	xxvi-012	0	5.1	xxvi-065	0	5.5
20	xxvi-008	0	4.3	xxvi-016	0	5.1	xxvi-036	1	5.5
21	xxvi-032	0	4.4	xxvi-072	0	5.1	xxvi-017	0	5.7
22	xxvi-034	0	4.5	xxvi-008	0	5.1	xxvi-028	1	5.7
23	xxvi-014	0	4.5	xxvi-065	0	5.2	xxvi-008	0	5.8
24	xxvi-054	0	4.5	xxvi-044	1	5.3	xxvi-026	0	5.9
25	xxvi-042	0	4.6	xxvi-041	0	5.3	xxvi-047	0	5.9
26	xxvi-040	0	4.6	xxvi-034	0	5.4	xxvi-052	0	6.0
27	xxvi-020	0	4.6	xxvi-026	0	5.4	xxvi-034	0	6.1
28	xxvi-058	0	4.6	xxvi-017	0	5.4	xxvi-012	0	6.2
29	xxvi-023	0	4.7	xxvi-032	0	5.4	xxvi-016	0	6.2
30	xxvi-078	0	4.8	xxvi-078	0	5.5	xxvi-039	0	6.2
31	xxvi-015	0	4.8	xxvi-054	0	5.6	xxvi-018	0	6.2
32	xxvi-072	0	4.8	xxvi-042	0	5.6	xxvi-032	0	6.3
33	xxvi-074	0	4.9	xxvi-014	0	5.6	xxvi-078	0	6.3
34	xxvi-065	0	4.9	xxvi-040	0	5.7	xxvi-041	0	6.3
35	xxvi-027	0	4.9	xxvi-027	0	5.7	xxvi-042	0	6.4
36	xxvi-026	0	5.0	xxvi-058	0	5.8	xxvi-054	0	6.4
37	xxvi-082	0	5.0	xxvi-020	0	5.8	xxvi-068	0	6.4
38	xxvi-067	0	5.0	xxvi-poly59-26-5	1	5.8	xxvi-050	0	6.6
39	xxvi-022	0	5.0	xxvi-052	0	5.9	xxvi-014	0	6.6
40	xxvi-017	0	5.1	xxvi-047	0	6.0	xxvi-096	0	6.6
41	xxvi-019	0	5.2	xxvi-019	0	6.0	xxvi-019	0	6.7
42	xxvi-044	1	5.2	xxvi-039	0	6.1	xxvi-040	0	6.7
43	xxvi-adjiman-pantelides1-1	8	5.2	xxvi-074	0	6.1	xxvi-027	0	6.7
44	xxvi-075	0	5.3	xxvi-082	0	6.2	xxvi-056	0	6.7
45	xxvi-024	0	5.3	xxvi-075	0	6.3	xxvi-077	0	6.8
46	xxvi-035	0	5.3	xxvi-067	0	6.3	xxvi-091	0	6.8
47	xxvi-037	0	5.4	xxvi-022	0	6.3	xxvi-049	0	6.8
48	xxvi-092	0	5.5	xxvi-056	0	6.4	xxvi-071	0	6.8
49	xxvi-043	0	5.6	xxvi-049	0	6.4	xxvi-057	0	6.9
50	xxvi-038	0	5.6	xxvi-068	0	6.4	xxvi-058	0	6.9
51	xxvi-045	0	5.7	xxvi-024	0	6.4	xxvi-089	0	6.9
52	xxvi-031	0	5.8	xxvi-050	0	6.4	xxvi-020	0	7.0
53	xxvi-063	0	5.9	xxvi-057	0	6.4	xxvi-031	0	7.0
54	xxvi-039	0	5.9	xxvi-031	0	6.5	xxvi-088	0	7.1
55	xxvi-051	0	5.9	xxvi-096	0	6.5	xxvi-074	0	7.1
56	xxvi-052	0	5.9	xxvi-091	0	6.5	xxvi-075	0	7.2
57	xxvi-061	0	6.0	xxvi-035	0	6.6	xxvi-024	0	7.2
58	xxvi-056	0	6.0	xxvi-071	0	6.6	xxvi-084	0	7.3
59	xxvi-064	0	6.0	xxvi-037	0	6.7	xxvi-070	0	7.3
60	xxvi-049	0	6.0	xxvi-092	0	6.7	xxvi-085	0	7.3

Continued

Rank	GGA			25X			50X		
	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE	Structure	# Duplicates	ΔE
61	xxvi-057	0	6.0	xxvi-070	0	6.8	xxvi-082	0	7.3
62	xxvi-047	0	6.1	xxvi-048	0	6.8	xxvi-048	0	7.3
63	xxvi-081	0	6.1	xxvi-077	0	6.8	xxvi-067	0	7.5
64	xxvi-060	0	6.2	xxvi-089	0	6.9	xxvi-029	0	7.5
65	xxvi-048	0	6.2	xxvi-088	0	6.9	xxvi-092	0	7.6
66	xxvi-090	0	6.2	xxvi-085	0	6.9	xxvi-035	0	7.6
67	xxvi-091	0	6.2	xxvi-090	0	7.0	xxvi-080	0	7.7
68	xxvi-070	0	6.3	xxvi-060	0	7.0	xxvi-037	0	7.7
69	xxvi-096	0	6.3	xxvi-029	0	7.0	xxvi-090	0	7.7
70	xxvi-080	0	6.3	xxvi-063	0	7.0	xxvi-060	0	7.8
71	xxvi-059	0	6.3	xxvi-084	0	7.0	xxvi-022	0	7.8
72	xxvi-050	0	6.4	xxvi-080	0	7.1	xxvi-093	0	8.0
73	xxvi-071	0	6.4	xxvi-045	0	7.2	xxvi-062	0	8.0
74	xxvi-068	0	6.4	xxvi-062	0	7.2	xxvi-095	0	8.0
75	xxvi-062	0	6.4	xxvi-adjiman-pantelides1-2	8	7.2	xxvi-063	0	8.0
76	xxvi-085	0	6.4	xxvi-038	0	7.3	xxvi-086	0	8.4
77	xxvi-029	0	6.5	xxvi-061	0	7.3	xxvi-059	0	8.5
78	xxvi-088	0	6.6	xxvi-059	0	7.4	xxvi-097	0	8.5
79	xxvi-084	0	6.7	xxvi-043	0	7.4	xxvi-083	0	8.7
80	xxvi-089	0	6.8	xxvi-064	0	7.5	xxvi-098	0	8.7
81	xxvi-100	0	6.8	xxvi-093	0	7.6	xxvi-061	0	8.8
82	xxvi-079	0	6.9	xxvi-086	0	7.7	xxvi-045	0	8.9
83	xxvi-077	0	6.9	xxvi-051	0	7.8	xxvi-038	0	9.2
84	xxvi-086	0	7.0	xxvi-083	0	7.9	xxvi-064	0	9.2
85	xxvi-083	0	7.1	xxvi-097	0	7.9	xxvi-dzyabchenko-1	1	9.2
86	xxvi-094	0	7.1	xxvi-098	0	8.0	xxvi-adjiman-pantelides1-2	8	9.2
87	xxvi-087	0	7.1	xxvi-095	0	8.1	xxvi-043	0	9.3
88	xxvi-098	0	7.1	xxvi-100	0	8.2	xxvi-079	0	9.4
89	xxvi-093	0	7.1	xxvi-079	0	8.2	xxvi-100	0	9.5
90	xxvi-053	0	7.2	xxvi-081	0	8.2	xxvi-051	0	9.8
91	xxvi-069	0	7.3	xxvi-094	0	8.7	xxvi-046	0	10.1
92	xxvi-097	0	7.3	xxvi-087	0	8.8	xxvi-081	0	10.4
93	xxvi-poly59-26-5	1	7.4	xxvi-046	0	9.0	xxvi-094	0	10.4
94	xxvi-046	0	8.0	xxvi-069	0	9.2	xxvi-087	0	10.5
95	xxvi-095	0	8.7	xxvi-053	0	9.5	xxvi-zhu1-2	0	10.7
96	xxvi-zhu1-2	0	10.8	xxvi-zhu1-2	0	10.5	xxvi-069	0	11.3
97	xxvi-day1-2	0	11.3	xxvi-day1-2	0	12.1	xxvi-053	0	11.7
98	xxvi-poly59-26-10	1	13.4	xxvi-dzyabchenko-1	1	12.2	xxvi-poly59-26-10	1	11.8
99	xxvi-poly59-26-7	1	13.5	xxvi-poly59-26-10	1	12.4	xxvi-dzyabchenko-2	0	12.0
100	xxvi-zhu1-3	0	14.0	xxvi-dzyabchenko-2	0	14.6	xxvi-day1-2	0	12.6
101	xxvi-day1-1	0	14.2	xxvi-day1-1	0	14.6	xxvi-dzyabchenko-3	0	14.6
102	xxvi-poly59-26-8	1	15.1	xxvi-poly59-26-8	1	14.9	xxvi-poly59-26-8	1	15.0
103	xxvi-vaneijck1-1	1	16.2	xxvi-zhu1-3	0	15.1	xxvi-vaneijck1-2	0	15.5
104	xxvi-dzyabchenko-2	0	18.0	xxvi-107	1	15.4	xxvi-day1-1	0	15.6
105	xxvi-dzyabchenko-3	0	20.5	xxvi-dzyabchenko-3	0	17.1	xxvi-zhu1-3	0	16.0
106	xxvi-hofmann1-3	0	21.7	xxvi-vaneijck1-2	0	18.5	xxvi-vaneijck1-3	0	16.9
107	xxvi-vaneijck1-2	0	22.1	xxvi-vaneijck1-3	0	19.7	xxvi-107	1	17.7
108	xxvi-boese-hofmann1-1	0	22.7	xxvi-boese-hofmann1-1	0	22.5	xxvi-boese-hofmann1-1	0	22.5
109	xxvi-vaneijck1-3	0	23.1	xxvi-chadha-singh-1	1	23.6	xxvi-cole-3	0	22.9
110	xxvi-chadha-singh-1	1	24.7	xxvi-cole-3	0	23.7	xxvi-chadha-singh-1	1	23.7
111	xxvi-cole-3	0	24.9	xxvi-hofmann1-3	0	24.7	xxvi-boese-hofmann1-2	0	25.3
112	xxvi-cole-1	0	25.3	xxvi-cole-1	0	25.4	xxvi-cole-1	0	26.0
113	xxvi-boese-hofmann1-2	0	26.4	xxvi-boese-hofmann1-2	0	25.8	xxvi-mohamed1-1	0	26.8
114	xxvi-chadha-singh-3	0	28.2	xxvi-mohamed1-1	0	27.5	xxvi-hofmann1-3	0	27.5
115	xxvi-mohamed1-1	0	28.3	xxvi-chadha-singh-3	0	28.4	xxvi-chadha-singh-3	0	29.2
116	xxvi-mohamed1-3	0	28.5	xxvi-mohamed1-3	0	29.5	xxvi-boese-hofmann1-3	0	29.4
117	xxvi-boese-hofmann1-3	0	31.2	xxvi-boese-hofmann1-3	0	30.1	xxvi-mohamed1-3	0	30.6
118	xxvi-mohamed1-2	0	32.5	xxvi-cole-2	0	32.5	xxvi-cole-2	0	32.4
119	xxvi-cole-2	0	33.5	xxvi-mohamed1-2	0	35.0	xxvi-mohamed1-2	0	37.9
120	xxvi-hofmann1-2	0	39.8	xxvi-hofmann1-2	0	42.8	xxvi-hofmann1-2	0	45.4
121	xxvi-hofmann1-1	0	56.2	xxvi-hofmann1-1	0	58.1	xxvi-hofmann1-1	0	59.8