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Chemistry

Benzoic acid derivatives (1 mmol) and 2-amino-3-hydroxypyridine (1 mmol) were refluxed at 150°C for approximately 2 h in the presence of polyphosphoric acid (PPA). At the end of the period, the reaction contents were poured into ice and alkalized with 10% NaOH solution and filtered. The products were finally recrystallized from ethanol. The chemicals used in the synthesis and purification of the compounds were obtained from Sigma-Aldrich, Acros Organics, Fluka, and Riedel de Haen and were used without purification. Compounds are not original, analysis data are given in the relevant literature by us and their purity checked.

Table S1. Calculated bond length (°) of **P5, P6 and P7**

P5		**P6**		**P7**	
Bond Length	**B3LYP**	**Bond length**	**B3LYP**	**Bond length**	**B3LYP**
C1,C2	1.3967	C1,C2	1.3967	C1,C2	1.3967
C1,C6	1.396	C1,C6	1.396	C1,C6	1.396
C1,H18	1.1	C1,H20	1.1	C1,H21	1.1
C2,N3	1.3547	C2,C3	1.3547	C2,N3	1.3547
C2,H19	1.1	C2,H21	1.1	C2,H22	1.1
N3,C4	1.3528	N3,C4	1.3528	N3,C4	1.3528
C4,C5	1.3864	C4,C5	1.3864	C4,C5	1.3864
C4,N7	1.366	C4,N7	1.366	C4,7	1.366
C5,C6	1.3848	C5,C6	1.3848	C5,C6	1.3848
C5,O9	1.3634	C5,O9	1.3634	C5,O9	1.3634
C6,H20	1.1	C6,H22	1.1	C6,H23	1.1
N7,C8	1.3159	N7,C8	1.3159	N7,C8	1.3159
C8,O9	1.3662	C8,O9	1.3662	C8,O9	1.3662
C8,C10	1.337	C8,C10	1.337	C8,C10	1.337
C10,C11	1.3948	C10,C11	1.3948	C10,C11	1.3948
C10,C14	1.3949	C10,C14	1.3949	C10,C14	1.3949
C11,C12	1.3949	C11,C12	1.3949	C11,C12	1.3949
C11,H21	1.1001	C11,H23	1.1001	C11,H24	1.1001
C12,C15	1.3949	C12,C15	1.3949	C12,C15	1.3949
C12,H22	1.1	C12,H24	1.1	C12,H25	1.1
C13,C14	1.3948	C13,C14	1.3948	C13,C14	1.3948
C13,C15	1.3947	C13,C15	1.3947	C13,C15	1.3947
C13,H23	1.1001	C13,H25	1.1001	C13,H26	1.1001
C14,H24	1.1	C14,H26	1.1	C14,H27	1.1
C15,O16	1.3549	C15,C16	1.497	C15,O16	1.3549
O16,C17	1.402	C16,F17	1.3921	O16,C17	1.402
C17,H25	1.113	C16,F18	1.3919	C17,F18	1.392
C17,H26	1.113	C16,F19	1.392	C17,F19	1.392
C17,H27	1.113			C17,F20	1.3919

Table S2. Calculated bond angles (°) of **P5, P6 and P7**

P5		P6		P7	
Bond Angle	**B3LYP**	**Bond Angle**	**B3LYP**	**Bond Angle**	**B3LYP**
C2,C1,C6	119.8391	C2,C1,C6	119.8391	C2,C1,C6	119.8391
C2,1,H18	120.0795	C2,C1,H20	120.0795	C2,C1,H21	120.0795
C6,1,H18	120.0814	C6,C1,H20	120.0814	C6,C1,H21	120.0814
C1,C2,C3	125.9088	C1,C2,N3	125.9088	C1,C2,N3	125.9088
C1,C2,H19	117.0452	C1,C2,H21	117.0452	C1,C2,H22	117.0452
C3,C2,H19	117.046	N3,C2,H21	117.046	N3,C2,H22	117.046
C2,C3,C4	113.641	C2,N3,C4	113.641	C2,N3,C4	113.641
C3,C4,C5	123.2087	N3,C4,C5	123.2087	N3,C4,C5	123.2087
C3,C4,N7	126.6528	N3,C4,N	126.6528	N3,C4,N7	126.6528
C5,C4,N7	110.1384	C5,C4,N7	110.1384	C5,C4,N7	110.1384
C4,C5,C6	123.3159	C4,C5,6	123.3159	C4,C5,C6	123.3159
C4,C5,O9	107.8553	C4,C5,O9	107.8553	C4,C5,O9	107.8553
C6,C5,O9	128.8288	C6,C5,O9	128.8288	C6,C5,O9	128.8288
C1,C6,C5	114.0865	C1,C6,C5	114.0865	C1,C6,C5	114.0865
C1,6,H20	122.9566	C1,C6,H22	122.9566	C1,C6,H23	122.9566
C5,C6,H20	122.9569	C5,C6,H22	122.9569	C5,C6,H23	122.9569
C4,N7,C8	102.9166	C4,N7,C8	102.9166	C4,N7,C8	102.9166
N7,C8,O9	116.0044	N7,C8,O9	116.0044	N7,C8,O9	116.0044
N7,C8,C10	121.9963	N7,C8,C10	121.9963	N7,C8,C10	121.9963
O9,C8,10	121.9994	O9,C8,C10	121.9994	O9,C8,C10	121.9994
C5,O9,C8	103.0853	C5,O9,C8	103.0853	C5,O9,C8	103.0853
C8,C10,C11	120.0014	C8,C10,C11	120.0014	C8,C10,11	120.0014
C8,C10,C14	120.0012	C8,C10,C14	120.0012	C8,C10,14	120.0012
C11,C10,C14	119.9974	C11,C10,C14	119.9974	C11,C10,C14	119.9974
C10,C11,C12	120.0024	C10,C11,C12	120.0024	C10,C11,C12	120.0024
C10,C11,H21	119.9974	C10,C11,H23	119.9974	C10,C11,H24	119.9974
C12,C11,H21	120.0002	C12,C11,H23	120.0002	C12,C11,H24	120.0002
C11,C12,C15	119.9949	C11,C12,C15	119.9949	C11,C12,C15	119.9949
C11,C12,H22	119.9988	C11,C12,H24	119.9988	C11,C12,H25	119.9988
C15,C12,H22	120.0062	C15,C12,H24	120.0062	C15,C12,H25	120.0062
C14,C13,C15	120.0015	C14,C13,C15	120.0015	C14,C13,C15	120.0015
C14,C13,H23	120.0026	C14,C13,H25	120.0026	C14,C13,H26	120.0026
C15,C13,H23	119.9959	C15,C13,H25	119.9959	C15,13,H26	119.9959
C10,C14,C13	120.0014	C10,C14,C13	120.0014	C10,C14,C13	120.0014
C10,C14,H24	119.9961	C10,C14,H26	119.9961	C10,C14,H27	119.9961
C13,C14,H24	120.0025	C13,C14,H26	120.0025	C13,C14,H27	120.0025
C12,C15,C13	120.0024	C12,C15,C13	120.0024	C12,C15,C13	120.0024
C12,C15,O16	119.9947	C12,C15,C16	119.9947	C12,C15,O16	119.9947
C13,C15,O16	120.0029	C13,C15,C16	120.0029	C13,C15,O16	120.0029
C15,O16,C17	110.8009	C15,C16,F17	110.8009	C15,O16,C17	110.8009
O16,C17,H25	109.5009	C15,C16,F18	109.4441	O16,C17,F18	109.503
O16,C17,H26	109.4405	C15,C16,F19	109.4626	O16,C17,F19	109.4409
O16,C17,H27	109.4625	F17,C16,F18	109.4381	O16,C17,F20	109.4589
H25,C17,H26	109.4412	F17,C16,F19	109.4599	F18,C17,F19	109.4402
H25,C17,H27	109.4598	F18,C16,F19	109.5218	F18,C17,F20	109.4626
H26,C17,H27	109.5225			F19,C17,F20	109.5218

Table S3. Summary of Natural Population Analysis

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.23714	1.99915	4.22325	0.01474	6.23714
C	2	0.05487	1.99918	3.92104	0.02492	5.94513
N	3	-0.43502	1.99935	5.41965	0.01602	7.43502
C	4	0.32359	1.99888	3.64599	0.03155	5.67641
C	5	0.24846	1.99866	3.72820	0.02468	5.75154
C	6	-0.21015	1.99902	4.19651	0.01461	6.21015
N	7	-0.48832	1.99932	5.47490	0.01410	7.48832
C	8	0.57278	1.99901	3.39206	0.03615	5.42722
O	9	-0.48363	1.99970	6.47520	0.00872	8.48363
C	10	-0.13942	1.99890	4.12467	0.01585	6.13942
C	11	-0.14779	1.99905	4.13459	0.01415	6.14779
C	12	-0.22923	1.99901	4.21440	0.01582	6.22923
C	13	-0.25944	1.99899	4.24645	0.01399	6.25944
C	14	-0.12667	1.99905	4.11299	0.01462	6.12667
C	15	0.32040	1.99868	3.65879	0.02213	5.67960
O	16	-0.55181	1.99963	6.54204	0.01014	8.55181
C	17	1.32015	1.99962	2.60694	0.07329	4.67985
F	18	-0.33703	1.99991	7.33250	0.00462	9.33703
F	19	-0.36160	1.99992	7.35732	0.00436	9.36160
F	20	-0.35676	1.99992	7.35245	0.00440	9.35676
H	21	0.21034	0.00000	0.78757	0.00209	0.78966
H	22	0.18564	0.00000	0.81227	0.00209	0.81436
H	23	0.22116	0.00000	0.77607	0.00277	0.77884
H	24	0.22136	0.00000	0.77592	0.00272	0.77864
H	25	0.22460	0.00000	0.77257	0.00283	0.77540
H	26	0.22858	0.00000	0.76833	0.00309	0.77142
H	27	0.23209	0.00000	0.76492	0.00299	0.76791

Table S4. Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis of P7

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
1. BD (1) C 1 - C 2	/100. RY*(2) N 3	1.30	2.07	0.046
1. BD (1) C 1 - C 2	/138. RY*(1) C 6	0.62	2.05	0.032
1. BD (1) C 1 - C 2	/139. RY*(2) C 6	1.61	2.16	0.053
1. BD (1) C 1 - C 2	/369. BD*(1) C 1 - C 6	2.47	1.26	0.050
1. BD (1) C 1 - C 2	/371. BD*(1) C 1 - H 21	1.11	1.15	0.032
1. BD (1) C 1 - C 2	/372. BD*(1) C 2 - N 3	1.49	1.25	0.038
1. BD (1) C 1 - C 2	/374. BD*(1) C 2 - H 22	1.06	1.15	0.031
1. BD (1) C 1 - C 2	/381. BD*(1) C 6 - H 23	2.71	1.14	0.049
2. BD (1) C 1 - C 6	/ 86. RY*(1) C 2	1.65	1.91	0.050
2. BD (1) C 1 - C 6	/ 90. RY*(5) C 2	0.63	3.65	0.043
2. BD (1) C 1 - C 6	/125. RY*(1) C 5	1.67	2.28	0.055
2. BD (1) C 1 - C 6	/368. BD*(1) C 1 - C 2	2.27	1.26	0.048
2. BD (1) C 1 - C 6	/371. BD*(1) C 1 - H 21	1.02	1.15	0.031
2. BD (1) C 1 - C 6	/374. BD*(1) C 2 - H 22	1.90	1.15	0.042
2. BD (1) C 1 - C 6	/379. BD*(1) C 5 - C 6	3.17	1.27	0.057
2. BD (1) C 1 - C 6	/380. BD*(1) C 5 - O 9	7.66	1.05	0.080
2. BD (1) C 1 - C 6	/381. BD*(1) C 6 - H 23	1.27	1.14	0.034
3. BD (2) C 1 - C 6	/ 89. RY*(4) C 2	1.59	1.20	0.043
3. BD (2) C 1 - C 6	/129. RY*(5) C 5	1.48	1.17	0.041
3. BD (2) C 1 - C 6	/373. BD*(2) C 2 - N 3	25.39	0.27	0.075
3. BD (2) C 1 - C 6	/377. BD*(2) C 4 - C 5	19.92	0.28	0.068
4. BD (1) C 1 - H 21	/ 87. RY*(2) C 2	1.26	1.60	0.040
4. BD (1) C 1 - H 21	/138. RY*(1) C 6	1.41	1.86	0.046
4. BD (1) C 1 - H 21	/368. BD*(1) C 1 - C 2	0.57	1.08	0.022
4. BD (1) C 1 - H 21	/369. BD*(1) C 1 - C 6	0.59	1.08	0.023
4. BD (1) C 1 - H 21	/372. BD*(1) C 2 - N 3	4.54	1.07	0.062
4. BD (1) C 1 - H 21	/374. BD*(1) C 2 - H 22	0.64	0.97	0.022
4. BD (1) C 1 - H 21	/379. BD*(1) C 5 - C 6	3.47	1.09	0.055
4. BD (1) C 1 - H 21	/381. BD*(1) C 6 - H 23	0.52	0.95	0.020
5. BD (1) C 2 - N 3	/ 74. RY*(2) C 1	1.12	2.33	0.046
5. BD (1) C 2 - N 3	/112. RY*(1) C 4	1.54	1.85	0.048
5. BD (1) C 2 - N 3	/113. RY*(2) C 4	1.46	2.27	0.052
5. BD (1) C 2 - N 3	/368. BD*(1) C 1 - C 2	1.70	1.37	0.043
5. BD (1) C 2 - N 3	/371. BD*(1) C 1 - H 21	1.29	1.26	0.036
5. BD (1) C 2 - N 3	/375. BD*(1) N 3 - C 4	1.08	1.36	0.034
5. BD (1) C 2 - N 3	/378. BD*(1) C 4 - N 7	6.00	1.27	0.078
6. BD (2) C 2 - N 3	/ 77. RY*(5) C 1	0.56	1.73	0.030
6. BD (2) C 2 - N 3	/115. RY*(4) C 4	1.18	1.91	0.045
6. BD (2) C 2 - N 3	/116. RY*(5) C 4	1.15	1.26	0.036
6. BD (2) C 2 - N 3	/370. BD*(2) C 1 - C 6	13.91	0.31	0.060
6. BD (2) C 2 - N 3	/377. BD*(2) C 4 - C 5	26.38	0.31	0.084
7. BD (1) C 2 - H 22	/ 73. RY*(1) C 1	0.97	1.81	0.037
7. BD (1) C 2 - H 22	/ 99. RY*(1) N 3	1.16	1.37	0.036
7. BD (1) C 2 - H 22	/369. BD*(1) C 1 - C 6	4.07	1.07	0.059
7. BD (1) C 2 - H 22	/371. BD*(1) C 1 - H 21	0.67	0.96	0.023
7. BD (1) C 2 - H 22	/375. BD*(1) N 3 - C 4	5.04	1.06	0.065
8. BD (1) N 3 - C 4	/ 87. RY*(2) C 2	3.34	1.91	0.071
8. BD (1) N 3 - C 4	/372. BD*(1) C 2 - N 3	0.93	1.38	0.032

8. BD (1) N 3 - C 4	/374. BD*(1) C 2 - H 22	2.09	1.28	0.046
8. BD (1) N 3 - C 4	/376. BD*(1) C 4 - C 5	2.59	1.36	0.053
8. BD (1) N 3 - C 4	/378. BD*(1) C 4 - N 7	1.88	1.29	0.044
8. BD (1) N 3 - C 4	/380. BD*(1) C 5 - O 9	0.92	1.17	0.029
8. BD (1) N 3 - C 4	/382. BD*(1) N 7 - C 8	1.13	1.41	0.036
9. BD (1) C 4 - C 5	/100. RY*(2) N 3	1.13	2.06	0.043
9. BD (1) C 4 - C 5	/138. RY*(1) C 6	1.00	2.04	0.040
9. BD (1) C 4 - C 5	/139. RY*(2) C 6	1.12	2.16	0.044
9. BD (1) C 4 - C 5	/152. RY*(2) N 7	0.76	2.11	0.036
9. BD (1) C 4 - C 5	/165. RY*(2) C 8	0.75	2.10	0.035
9. BD (1) C 4 - C 5	/169. RY*(6) C 8	0.60	2.14	0.032
9. BD (1) C 4 - C 5	/375. BD*(1) N 3 - C 4	2.89	1.25	0.054
9. BD (1) C 4 - C 5	/378. BD*(1) C 4 - N 7	0.81	1.16	0.027
9. BD (1) C 4 - C 5	/379. BD*(1) C 5 - C 6	5.17	1.27	0.072
9. BD (1) C 4 - C 5	/381. BD*(1) C 6 - H 23	2.88	1.13	0.051
9. BD (1) C 4 - C 5	/385. BD*(1) C 8 - C 10	1.45	1.17	0.037
10. BD (2) C 4 - C 5	/101. RY*(3) N 3	1.38	1.08	0.039
10. BD (2) C 4 - C 5	/141. RY*(4) C 6	1.90	0.82	0.040
10. BD (2) C 4 - C 5	/153. RY*(3) N 7	0.86	1.15	0.032
10. BD (2) C 4 - C 5	/178. RY*(2) O 9	0.85	1.26	0.033
10. BD (2) C 4 - C 5	/370. BD*(2) C 1 - C 6	21.30	0.29	0.072
10. BD (2) C 4 - C 5	/373. BD*(2) C 2 - N 3	16.24	0.28	0.061
10. BD (2) C 4 - C 5	/383. BD*(2) N 7 - C 8	9.65	0.28	0.048
11. BD (1) C 4 - N 7	/ 99. RY*(1) N 3	0.56	1.62	0.027
11. BD (1) C 4 - N 7	/164. RY*(1) C 8	0.63	1.96	0.031
11. BD (1) C 4 - N 7	/165. RY*(2) C 8	1.37	2.16	0.049
11. BD (1) C 4 - N 7	/372. BD*(1) C 2 - N 3	2.15	1.31	0.048
11. BD (1) C 4 - N 7	/375. BD*(1) N 3 - C 4	1.92	1.31	0.045
11. BD (1) C 4 - N 7	/376. BD*(1) C 4 - C 5	0.96	1.29	0.032
11. BD (1) C 4 - N 7	/379. BD*(1) C 5 - C 6	2.71	1.33	0.054
11. BD (1) C 4 - N 7	/380. BD*(1) C 5 - O 9	0.92	1.10	0.029
11. BD (1) C 4 - N 7	/382. BD*(1) N 7 - C 8	0.71	1.34	0.028
11. BD (1) C 4 - N 7	/384. BD*(1) C 8 - O 9	1.72	1.07	0.039
11. BD (1) C 4 - N 7	/385. BD*(1) C 8 - C 10	7.62	1.23	0.087
12. BD (1) C 5 - C 6	/ 73. RY*(1) C 1	1.34	2.03	0.047
12. BD (1) C 5 - C 6	/ 74. RY*(2) C 1	0.81	2.25	0.038
12. BD (1) C 5 - C 6	/113. RY*(2) C 4	0.57	2.19	0.032
12. BD (1) C 5 - C 6	/369. BD*(1) C 1 - C 6	2.66	1.29	0.052
12. BD (1) C 5 - C 6	/371. BD*(1) C 1 - H 21	2.59	1.18	0.050
12. BD (1) C 5 - C 6	/376. BD*(1) C 4 - C 5	4.60	1.25	0.068
12. BD (1) C 5 - C 6	/378. BD*(1) C 4 - N 7	1.15	1.19	0.033
12. BD (1) C 5 - C 6	/380. BD*(1) C 5 - O 9	1.50	1.07	0.036
12. BD (1) C 5 - C 6	/381. BD*(1) C 6 - H 23	1.36	1.16	0.036
12. BD (1) C 5 - C 6	/384. BD*(1) C 8 - O 9	2.00	1.04	0.041
13. BD (1) C 5 - O 9	/138. RY*(1) C 6	0.51	2.25	0.030
13. BD (1) C 5 - O 9	/164. RY*(1) C 8	1.11	2.11	0.043
13. BD (1) C 5 - O 9	/369. BD*(1) C 1 - C 6	0.72	1.47	0.029
13. BD (1) C 5 - O 9	/375. BD*(1) N 3 - C 4	2.38	1.46	0.053
13. BD (1) C 5 - O 9	/376. BD*(1) C 4 - C 5	0.51	1.44	0.024
13. BD (1) C 5 - O 9	/379. BD*(1) C 5 - C 6	1.44	1.48	0.041
13. BD (1) C 5 - O 9	/385. BD*(1) C 8 - C 10	3.19	1.38	0.060
14. BD (1) C 6 - H 23	/ 73. RY*(1) C 1	1.19	1.83	0.042

14. BD (1) C 6 - H 23 /126. RY*(2) C 5 0.77 1.84 0.034
14. BD (1) C 6 - H 23 /128. RY*(4) C 5 0.69 2.39 0.037
14. BD (1) C 6 - H 23 /368. BD*(1) C 1 - C 2 3.32 1.09 0.054
14. BD (1) C 6 - H 23 /369. BD*(1) C 1 - C 6 0.99 1.10 0.030
14. BD (1) C 6 - H 23 /371. BD*(1) C 1 - H 21 0.54 0.99 0.021
14. BD (1) C 6 - H 23 /376. BD*(1) C 4 - C 5 3.76 1.06 0.057
14. BD (1) C 6 - H 23 /379. BD*(1) C 5 - C 6 0.73 1.11 0.025
15. BD (1) N 7 - C 8 /112. RY*(1) C 4 1.32 1.91 0.045
15. BD (1) N 7 - C 8 /114. RY*(3) C 4 1.51 2.69 0.057
15. BD (1) N 7 - C 8 /164. RY*(1) C 8 0.76 2.07 0.035
15. BD (1) N 7 - C 8 /191. RY*(2) C 10 1.58 2.50 0.056
15. BD (1) N 7 - C 8 /375. BD*(1) N 3 - C 4 5.53 1.42 0.079
15. BD (1) N 7 - C 8 /378. BD*(1) C 4 - N 7 0.78 1.33 0.029
15. BD (1) N 7 - C 8 /385. BD*(1) C 8 - C 10 4.03 1.34 0.066
15. BD (1) N 7 - C 8 /386. BD*(1) C 10 - C 11 1.54 1.42 0.042
16. BD (2) N 7 - C 8 / 60. LP (1) C 10 15.20 0.21 0.068
16. BD (2) N 7 - C 8 /115. RY*(4) C 4 1.48 1.94 0.050
16. BD (2) N 7 - C 8 /116. RY*(5) C 4 0.61 1.29 0.026
16. BD (2) N 7 - C 8 /192. RY*(3) C 10 1.08 0.97 0.030
16. BD (2) N 7 - C 8 /377. BD*(2) C 4 - C 5 17.13 0.34 0.074
16. BD (2) N 7 - C 8 /383. BD*(2) N 7 - C 8 0.53 0.34 0.012
17. BD (1) C 8 - O 9 /125. RY*(1) C 5 1.70 2.47 0.058
17. BD (1) C 8 - O 9 /128. RY*(4) C 5 1.19 2.74 0.051
17. BD (1) C 8 - O 9 /164. RY*(1) C 8 0.58 2.09 0.031
17. BD (1) C 8 - O 9 /191. RY*(2) C 10 1.41 2.52 0.053
17. BD (1) C 8 - O 9 /375. BD*(1) N 3 - C 4 0.68 1.44 0.028
17. BD (1) C 8 - O 9 /379. BD*(1) C 5 - C 6 4.86 1.46 0.075
17. BD (1) C 8 - O 9 /385. BD*(1) C 8 - C 10 0.53 1.36 0.024
17. BD (1) C 8 - O 9 /387. BD*(1) C 10 - C 14 1.67 1.45 0.044
18. BD (1) C 8 - C 10 /151. RY*(1) N 7 0.91 1.64 0.035
18. BD (1) C 8 - C 10 /177. RY*(1) O 9 0.54 1.86 0.028
18. BD (1) C 8 - C 10 /203. RY*(1) C 11 1.51 2.06 0.050
18. BD (1) C 8 - C 10 /242. RY*(1) C 14 1.45 2.05 0.049
18. BD (1) C 8 - C 10 /378. BD*(1) C 4 - N 7 2.60 1.15 0.049
18. BD (1) C 8 - C 10 /380. BD*(1) C 5 - O 9 2.26 1.03 0.043
18. BD (1) C 8 - C 10 /382. BD*(1) N 7 - C 8 3.52 1.27 0.060
18. BD (1) C 8 - C 10 /386. BD*(1) C 10 - C 11 3.12 1.24 0.056
18. BD (1) C 8 - C 10 /387. BD*(1) C 10 - C 14 2.82 1.25 0.053
18. BD (1) C 8 - C 10 /388. BD*(1) C 11 - C 12 1.90 1.27 0.044
18. BD (1) C 8 - C 10 /393. BD*(1) C 13 - C 14 2.17 1.27 0.047
19. BD (1) C 10 - C 11 /164. RY*(1) C 8 1.07 1.90 0.040
19. BD (1) C 10 - C 11 /165. RY*(2) C 8 0.63 2.10 0.033
19. BD (1) C 10 - C 11 /217. RY*(2) C 12 1.92 2.10 0.057
19. BD (1) C 10 - C 11 /242. RY*(1) C 14 0.56 2.06 0.030
19. BD (1) C 10 - C 11 /382. BD*(1) N 7 - C 8 2.52 1.28 0.051
19. BD (1) C 10 - C 11 /385. BD*(1) C 8 - C 10 2.95 1.17 0.053
19. BD (1) C 10 - C 11 /387. BD*(1) C 10 - C 14 4.67 1.26 0.068
19. BD (1) C 10 - C 11 /388. BD*(1) C 11 - C 12 2.97 1.28 0.055
19. BD (1) C 10 - C 11 /390. BD*(1) C 11 - H 24 1.17 1.15 0.033
19. BD (1) C 10 - C 11 /392. BD*(1) C 12 - H 25 2.38 1.14 0.047
19. BD (1) C 10 - C 11 /397. BD*(1) C 14 - H 27 2.14 1.16 0.045
20. BD (1) C 10 - C 14 /164. RY*(1) C 8 1.67 1.89 0.050

20. BD (1) C 10 - C 14	/203. RY*(1) C 11	0.51	2.07	0.029
20. BD (1) C 10 - C 14	/229. RY*(1) C 13	0.79	2.08	0.037
20. BD (1) C 10 - C 14	/230. RY*(2) C 13	1.35	2.10	0.048
20. BD (1) C 10 - C 14	/384. BD*(1) C 8 - O 9	3.13	1.00	0.050
20. BD (1) C 10 - C 14	/385. BD*(1) C 8 - C 10	3.17	1.17	0.054
20. BD (1) C 10 - C 14	/386. BD*(1) C 10 - C 11	4.69	1.25	0.068
20. BD (1) C 10 - C 14	/390. BD*(1) C 11 - H 24	2.34	1.15	0.046
20. BD (1) C 10 - C 14	/393. BD*(1) C 13 - C 14	2.88	1.28	0.054
20. BD (1) C 10 - C 14	/396. BD*(1) C 13 - H 26	2.23	1.14	0.045
20. BD (1) C 10 - C 14	/397. BD*(1) C 14 - H 27	1.16	1.15	0.033
21. BD (1) C 11 - C 12	/190. RY*(1) C 10	1.08	2.46	0.046
21. BD (1) C 11 - C 12	/191. RY*(2) C 10	1.01	2.34	0.044
21. BD (1) C 11 - C 12	/255. RY*(1) C 15	0.89	2.09	0.039
21. BD (1) C 11 - C 12	/256. RY*(2) C 15	1.05	2.19	0.043
21. BD (1) C 11 - C 12	/385. BD*(1) C 8 - C 10	3.70	1.18	0.059
21. BD (1) C 11 - C 12	/386. BD*(1) C 10 - C 11	3.50	1.26	0.059
21. BD (1) C 11 - C 12	/390. BD*(1) C 11 - H 24	1.09	1.16	0.032
21. BD (1) C 11 - C 12	/391. BD*(1) C 12 - C 15	3.15	1.26	0.056
21. BD (1) C 11 - C 12	/392. BD*(1) C 12 - H 25	1.40	1.15	0.036
21. BD (1) C 11 - C 12	/398. BD*(1) C 15 - O 16	3.68	1.01	0.055
22. BD (2) C 11 - C 12	/ 60. LP (1) C 10	44.11	0.14	0.090
22. BD (2) C 11 - C 12	/ 61. LP*(1) C 15	60.90	0.12	0.095
22. BD (2) C 11 - C 12	/192. RY*(3) C 10	0.50	0.91	0.021
22. BD (2) C 11 - C 12	/259. RY*(5) C 15	0.92	1.05	0.030
23. BD (1) C 11 - H 24	/190. RY*(1) C 10	2.21	2.27	0.063
23. BD (1) C 11 - H 24	/216. RY*(1) C 12	1.44	1.91	0.047
23. BD (1) C 11 - H 24	/386. BD*(1) C 10 - C 11	0.70	1.08	0.024
23. BD (1) C 11 - H 24	/387. BD*(1) C 10 - C 14	4.44	1.08	0.062
23. BD (1) C 11 - H 24	/388. BD*(1) C 11 - C 12	0.82	1.10	0.027
23. BD (1) C 11 - H 24	/391. BD*(1) C 12 - C 15	3.96	1.08	0.058
23. BD (1) C 11 - H 24	/392. BD*(1) C 12 - H 25	0.68	0.96	0.023
24. BD (1) C 12 - C 15	/203. RY*(1) C 11	0.58	2.09	0.031
24. BD (1) C 12 - C 15	/204. RY*(2) C 11	1.57	1.97	0.050
24. BD (1) C 12 - C 15	/229. RY*(1) C 13	0.81	2.10	0.037
24. BD (1) C 12 - C 15	/230. RY*(2) C 13	0.55	2.12	0.031
24. BD (1) C 12 - C 15	/268. RY*(1) O 16	0.85	1.87	0.036
24. BD (1) C 12 - C 15	/388. BD*(1) C 11 - C 12	3.05	1.30	0.056
24. BD (1) C 12 - C 15	/390. BD*(1) C 11 - H 24	2.24	1.17	0.046
24. BD (1) C 12 - C 15	/392. BD*(1) C 12 - H 25	1.26	1.16	0.034
24. BD (1) C 12 - C 15	/395. BD*(1) C 13 - C 15	4.71	1.27	0.069
24. BD (1) C 12 - C 15	/396. BD*(1) C 13 - H 26	2.28	1.17	0.046
24. BD (1) C 12 - C 15	/399. BD*(1) O 16 - C 17	3.10	1.02	0.051
25. BD (1) C 12 - H 25	/203. RY*(1) C 11	1.34	1.89	0.045
25. BD (1) C 12 - H 25	/255. RY*(1) C 15	1.02	1.90	0.039
25. BD (1) C 12 - H 25	/386. BD*(1) C 10 - C 11	3.96	1.08	0.058
25. BD (1) C 12 - H 25	/388. BD*(1) C 11 - C 12	1.00	1.10	0.030
25. BD (1) C 12 - H 25	/390. BD*(1) C 11 - H 24	0.68	0.97	0.023
25. BD (1) C 12 - H 25	/391. BD*(1) C 12 - C 15	0.68	1.08	0.024
25. BD (1) C 12 - H 25	/395. BD*(1) C 13 - C 15	4.52	1.07	0.062
25. BD (1) C 12 - H 25	/398. BD*(1) C 15 - O 16	1.48	0.82	0.031
26. BD (1) C 13 - C 14	/190. RY*(1) C 10	1.28	2.46	0.050
26. BD (1) C 13 - C 14	/191. RY*(2) C 10	0.85	2.34	0.040

26. BD (1) C 13 - C 14	/256. RY*(2) C 15	1.68	2.18	0.054
26. BD (1) C 13 - C 14	/385. BD*(1) C 8 - C 10	3.32	1.18	0.056
26. BD (1) C 13 - C 14	/387. BD*(1) C 10 - C 14	3.37	1.27	0.058
26. BD (1) C 13 - C 14	/395. BD*(1) C 13 - C 15	3.62	1.26	0.060
26. BD (1) C 13 - C 14	/396. BD*(1) C 13 - H 26	1.46	1.15	0.037
26. BD (1) C 13 - C 14	/397. BD*(1) C 14 - H 27	1.05	1.17	0.031
26. BD (1) C 13 - C 14	/398. BD*(1) C 15 - O 16	5.37	1.00	0.066
27. BD (2) C 13 - C 14	/ 60. LP (1) C 10	43.82	0.14	0.088
27. BD (2) C 13 - C 14	/ 61. LP*(1) C 15	64.91	0.12	0.097
27. BD (2) C 13 - C 14	/192. RY*(3) C 10	0.60	0.90	0.023
27. BD (2) C 13 - C 14	/259. RY*(5) C 15	0.76	1.05	0.028
28. BD (1) C 13 - C 15	/216. RY*(1) C 12	1.23	2.11	0.046
28. BD (1) C 13 - C 15	/217. RY*(2) C 12	0.64	2.13	0.033
28. BD (1) C 13 - C 15	/242. RY*(1) C 14	0.60	2.09	0.032
28. BD (1) C 13 - C 15	/243. RY*(2) C 14	1.55	1.97	0.050
28. BD (1) C 13 - C 15	/391. BD*(1) C 12 - C 15	4.91	1.28	0.071
28. BD (1) C 13 - C 15	/392. BD*(1) C 12 - H 25	1.88	1.17	0.042
28. BD (1) C 13 - C 15	/393. BD*(1) C 13 - C 14	3.30	1.31	0.059
28. BD (1) C 13 - C 15	/396. BD*(1) C 13 - H 26	1.37	1.17	0.036
28. BD (1) C 13 - C 15	/397. BD*(1) C 14 - H 27	2.12	1.19	0.045
29. BD (1) C 13 - H 26	/242. RY*(1) C 14	1.41	1.89	0.046
29. BD (1) C 13 - H 26	/255. RY*(1) C 15	1.59	1.91	0.049
29. BD (1) C 13 - H 26	/387. BD*(1) C 10 - C 14	4.02	1.09	0.059
29. BD (1) C 13 - H 26	/391. BD*(1) C 12 - C 15	4.17	1.08	0.060
29. BD (1) C 13 - H 26	/393. BD*(1) C 13 - C 14	1.18	1.11	0.032
29. BD (1) C 13 - H 26	/395. BD*(1) C 13 - C 15	0.65	1.08	0.024
29. BD (1) C 13 - H 26	/397. BD*(1) C 14 - H 27	0.65	0.99	0.023
29. BD (1) C 13 - H 26	/398. BD*(1) C 15 - O 16	0.90	0.82	0.024
30. BD (1) C 14 - H 27	/190. RY*(1) C 10	2.17	2.26	0.063
30. BD (1) C 14 - H 27	/229. RY*(1) C 13	1.37	1.90	0.046
30. BD (1) C 14 - H 27	/386. BD*(1) C 10 - C 11	4.62	1.07	0.063
30. BD (1) C 14 - H 27	/387. BD*(1) C 10 - C 14	0.74	1.07	0.025
30. BD (1) C 14 - H 27	/393. BD*(1) C 13 - C 14	0.82	1.09	0.027
30. BD (1) C 14 - H 27	/395. BD*(1) C 13 - C 15	4.17	1.06	0.060
30. BD (1) C 14 - H 27	/396. BD*(1) C 13 - H 26	0.75	0.96	0.024
31. BD (1) C 15 - O 16	/216. RY*(1) C 12	0.74	2.30	0.037
31. BD (1) C 15 - O 16	/281. RY*(1) C 17	1.30	1.92	0.045
31. BD (1) C 15 - O 16	/289. RY*(9) C 17	1.10	3.32	0.054
31. BD (1) C 15 - O 16	/388. BD*(1) C 11 - C 12	1.49	1.49	0.042
31. BD (1) C 15 - O 16	/393. BD*(1) C 13 - C 14	1.11	1.49	0.036
31. BD (1) C 15 - O 16	/395. BD*(1) C 13 - C 15	0.65	1.46	0.028
31. BD (1) C 15 - O 16	/400. BD*(1) C 17 - F 18	1.43	1.16	0.037
32. BD (1) O 16 - C 17	/256. RY*(2) C 15	2.50	2.43	0.070
32. BD (1) O 16 - C 17	/391. BD*(1) C 12 - C 15	1.67	1.50	0.045
33. BD (1) C 17 - F 18	/283. RY*(3) C 17	0.63	2.11	0.033
33. BD (1) C 17 - F 18	/398. BD*(1) C 15 - O 16	2.33	1.35	0.050
34. BD (1) C 17 - F 19	/282. RY*(2) C 17	0.66	2.06	0.033
34. BD (1) C 17 - F 19	/398. BD*(1) C 15 - O 16	0.63	1.32	0.026
34. BD (1) C 17 - F 19	/402. BD*(1) C 17 - F 20	0.70	1.25	0.027
35. BD (1) C 17 - F 20	/282. RY*(2) C 17	0.61	2.06	0.032
35. BD (1) C 17 - F 20	/398. BD*(1) C 15 - O 16	0.58	1.33	0.025
35. BD (1) C 17 - F 20	/401. BD*(1) C 17 - F 19	0.69	1.25	0.027

36. CR (1) C 1	/ 87. RY*(2) C 2	1.39	11.12	0.111
36. CR (1) C 1	/139. RY*(2) C 6	0.87	11.51	0.089
36. CR (1) C 1	/142. RY*(5) C 6	0.59	11.19	0.072
36. CR (1) C 1	/335. RY*(3) H 21	0.63	12.08	0.078
36. CR (1) C 1	/372. BD*(1) C 2 - N 3	0.68	10.59	0.076
36. CR (1) C 1	/379. BD*(1) C 5 - C 6	0.71	10.62	0.078
37. CR (1) C 2	/ 74. RY*(2) C 1	1.41	11.59	0.114
37. CR (1) C 2	/100. RY*(2) N 3	0.84	11.44	0.088
37. CR (1) C 2	/369. BD*(1) C 1 - C 6	0.87	10.63	0.086
37. CR (1) C 2	/375. BD*(1) N 3 - C 4	1.51	10.62	0.114
38. CR (1) N 3	/ 86. RY*(1) C 2	1.67	15.33	0.143
38. CR (1) N 3	/ 87. RY*(2) C 2	0.52	15.19	0.079
38. CR (1) N 3	/ 91. RY*(6) C 2	0.56	15.14	0.082
38. CR (1) N 3	/112. RY*(1) C 4	1.76	15.15	0.146
38. CR (1) N 3	/113. RY*(2) C 4	0.87	15.58	0.104
38. CR (1) N 3	/117. RY*(6) C 4	0.62	16.81	0.091
38. CR (1) N 3	/368. BD*(1) C 1 - C 2	0.81	14.67	0.098
38. CR (1) N 3	/376. BD*(1) C 4 - C 5	0.91	14.64	0.104
38. CR (1) N 3	/378. BD*(1) C 4 - N 7	0.85	14.57	0.100
39. CR (1) C 4	/100. RY*(2) N 3	0.72	11.47	0.081
39. CR (1) C 4	/125. RY*(1) C 5	1.25	11.68	0.108
39. CR (1) C 4	/372. BD*(1) C 2 - N 3	1.38	10.65	0.109
39. CR (1) C 4	/376. BD*(1) C 4 - C 5	0.67	10.63	0.076
39. CR (1) C 4	/379. BD*(1) C 5 - C 6	1.16	10.67	0.100
39. CR (1) C 4	/382. BD*(1) N 7 - C 8	0.96	10.68	0.091
40. CR (1) C 5	/112. RY*(1) C 4	1.44	11.15	0.113
40. CR (1) C 5	/114. RY*(3) C 4	0.58	11.93	0.074
40. CR (1) C 5	/139. RY*(2) C 6	1.58	11.57	0.121
40. CR (1) C 5	/369. BD*(1) C 1 - C 6	0.56	10.67	0.069
40. CR (1) C 5	/375. BD*(1) N 3 - C 4	0.85	10.66	0.086
40. CR (1) C 5	/376. BD*(1) C 4 - C 5	0.98	10.64	0.092
40. CR (1) C 5	/379. BD*(1) C 5 - C 6	0.76	10.68	0.081
40. CR (1) C 5	/380. BD*(1) C 5 - O 9	0.88	10.45	0.086
40. CR (1) C 5	/381. BD*(1) C 6 - H 23	0.57	10.54	0.069
40. CR (1) C 5	/384. BD*(1) C 8 - O 9	1.22	10.42	0.102
41. CR (1) C 6	/ 74. RY*(2) C 1	1.30	11.57	0.109
41. CR (1) C 6	/ 76. RY*(4) C 1	0.56	11.06	0.071
41. CR (1) C 6	/128. RY*(4) C 5	1.73	11.91	0.128
41. CR (1) C 6	/131. RY*(7) C 5	0.53	12.12	0.071
41. CR (1) C 6	/344. RY*(2) H 23	0.59	12.32	0.076
41. CR (1) C 6	/368. BD*(1) C 1 - C 2	0.76	10.61	0.080
41. CR (1) C 6	/376. BD*(1) C 4 - C 5	0.95	10.58	0.091
41. CR (1) C 6	/380. BD*(1) C 5 - O 9	1.54	10.40	0.114
42. CR (1) N 7	/112. RY*(1) C 4	0.93	15.15	0.106
42. CR (1) N 7	/113. RY*(2) C 4	0.67	15.58	0.091
42. CR (1) N 7	/164. RY*(1) C 8	3.52	15.31	0.208
42. CR (1) N 7	/375. BD*(1) N 3 - C 4	0.75	14.66	0.094
42. CR (1) N 7	/385. BD*(1) C 8 - C 10	1.38	14.59	0.128
43. CR (1) C 8	/152. RY*(2) N 7	0.67	11.57	0.079
43. CR (1) C 8	/190. RY*(1) C 10	0.89	11.90	0.092
43. CR (1) C 8	/194. RY*(5) C 10	0.64	11.66	0.077
43. CR (1) C 8	/378. BD*(1) C 4 - N 7	1.21	10.61	0.102

43. CR (1) C 8 /380. BD*(1) C 5 - O 9 1.20 10.50 0.101
43. CR (1) C 8 /384. BD*(1) C 8 - O 9 0.87 10.46 0.087
43. CR (1) C 8 /386. BD*(1) C 10 - C 11 0.83 10.71 0.085
43. CR (1) C 8 /387. BD*(1) C 10 - C 14 0.70 10.71 0.078
44. CR (1) O 9 /126. RY*(2) C 5 1.97 20.29 0.179
44. CR (1) O 9 /164. RY*(1) C 8 1.56 20.18 0.159
44. CR (1) O 9 /165. RY*(2) C 8 0.77 20.38 0.112
44. CR (1) O 9 /379. BD*(1) C 5 - C 6 0.68 19.55 0.103
45. CR (1) C 10 /169. RY*(6) C 8 1.63 11.50 0.122
45. CR (1) C 10 /204. RY*(2) C 11 1.51 11.31 0.117
45. CR (1) C 10 /243. RY*(2) C 14 1.48 11.30 0.115
45. CR (1) C 10 /382. BD*(1) N 7 - C 8 0.85 10.63 0.085
45. CR (1) C 10 /388. BD*(1) C 11 - C 12 0.77 10.64 0.081
45. CR (1) C 10 /393. BD*(1) C 13 - C 14 0.80 10.64 0.083
46. CR (1) C 11 /190. RY*(1) C 10 0.68 11.80 0.080
46. CR (1) C 11 /191. RY*(2) C 10 1.40 11.68 0.114
46. CR (1) C 11 /216. RY*(1) C 12 0.50 11.44 0.068
46. CR (1) C 11 /217. RY*(2) C 12 0.92 11.45 0.092
46. CR (1) C 11 /220. RY*(5) C 12 0.50 11.12 0.067
46. CR (1) C 11 /349. RY*(2) H 24 0.51 12.36 0.071
46. CR (1) C 11 /385. BD*(1) C 8 - C 10 1.03 10.52 0.094
46. CR (1) C 11 /387. BD*(1) C 10 - C 14 0.96 10.61 0.091
46. CR (1) C 11 /391. BD*(1) C 12 - C 15 0.91 10.60 0.088
47. CR (1) C 12 /204. RY*(2) C 11 0.68 11.30 0.078
47. CR (1) C 12 /207. RY*(5) C 11 0.85 11.54 0.089
47. CR (1) C 12 /256. RY*(2) C 15 2.01 11.52 0.136
47. CR (1) C 12 /354. RY*(2) H 25 0.55 12.35 0.073
47. CR (1) C 12 /386. BD*(1) C 10 - C 11 0.98 10.60 0.092
47. CR (1) C 12 /395. BD*(1) C 13 - C 15 1.22 10.59 0.102
47. CR (1) C 12 /398. BD*(1) C 15 - O 16 0.57 10.34 0.069
48. CR (1) C 13 /243. RY*(2) C 14 0.86 11.29 0.088
48. CR (1) C 13 /246. RY*(5) C 14 0.56 11.38 0.071
48. CR (1) C 13 /255. RY*(1) C 15 0.97 11.43 0.094
48. CR (1) C 13 /256. RY*(2) C 15 1.54 11.52 0.119
48. CR (1) C 13 /387. BD*(1) C 10 - C 14 0.98 10.61 0.092
48. CR (1) C 13 /391. BD*(1) C 12 - C 15 1.04 10.60 0.094
48. CR (1) C 13 /398. BD*(1) C 15 - O 16 0.92 10.34 0.088
49. CR (1) C 14 /190. RY*(1) C 10 0.53 11.80 0.071
49. CR (1) C 14 /191. RY*(2) C 10 1.53 11.68 0.119
49. CR (1) C 14 /230. RY*(2) C 13 0.95 11.45 0.093
49. CR (1) C 14 /232. RY*(4) C 13 0.67 11.13 0.077
49. CR (1) C 14 /385. BD*(1) C 8 - C 10 0.95 10.52 0.090
49. CR (1) C 14 /386. BD*(1) C 10 - C 11 1.01 10.60 0.093
49. CR (1) C 14 /395. BD*(1) C 13 - C 15 0.97 10.60 0.091
50. CR (1) C 15 /217. RY*(2) C 12 1.57 11.54 0.120
50. CR (1) C 15 /230. RY*(2) C 13 1.44 11.54 0.115
50. CR (1) C 15 /388. BD*(1) C 11 - C 12 0.78 10.71 0.082
50. CR (1) C 15 /391. BD*(1) C 12 - C 15 0.94 10.69 0.090
50. CR (1) C 15 /393. BD*(1) C 13 - C 14 0.69 10.71 0.077
50. CR (1) C 15 /395. BD*(1) C 13 - C 15 0.72 10.68 0.079
50. CR (1) C 15 /398. BD*(1) C 15 - O 16 1.30 10.43 0.105
50. CR (1) C 15 /399. BD*(1) O 16 - C 17 1.02 10.44 0.094

51. CR (1) O 16 /255. RY*(1) C 15 1.64 20.38 0.164
51. CR (1) O 16 /281. RY*(1) C 17 1.52 20.01 0.156
51. CR (1) O 16 /283. RY*(3) C 17 0.95 20.05 0.124
51. CR (1) O 16 /289. RY*(9) C 17 0.88 21.40 0.122
51. CR (1) O 16 /395. BD*(1) C 13 - C 15 0.56 19.55 0.094
52. CR (1) C 17 /398. BD*(1) C 15 - O 16 1.67 10.70 0.120
53. CR (1) F 18 /281. RY*(1) C 17 0.88 25.47 0.134
53. CR (1) F 18 /283. RY*(3) C 17 2.49 25.52 0.226
54. CR (1) F 19 /281. RY*(1) C 17 0.98 25.48 0.142
54. CR (1) F 19 /282. RY*(2) C 17 1.85 25.49 0.195
55. CR (1) F 20 /281. RY*(1) C 17 1.13 25.47 0.152
55. CR (1) F 20 /282. RY*(2) C 17 1.80 25.49 0.192
56. LP (1) N 3 / 86. RY*(1) C 2 3.02 1.54 0.062
56. LP (1) N 3 /107. RY*(9) N 3 0.54 3.05 0.037
56. LP (1) N 3 /112. RY*(1) C 4 2.14 1.37 0.049
56. LP (1) N 3 /113. RY*(2) C 4 1.81 1.79 0.052
56. LP (1) N 3 /368. BD*(1) C 1 - C 2 9.33 0.89 0.083
56. LP (1) N 3 /374. BD*(1) C 2 - H 22 4.34 0.78 0.053
56. LP (1) N 3 /376. BD*(1) C 4 - C 5 11.08 0.86 0.088
56. LP (1) N 3 /378. BD*(1) C 4 - N 7 3.06 0.79 0.044
56. LP (1) N 3 /380. BD*(1) C 5 - O 9 0.50 0.68 0.017
57. LP (1) N 7 /112. RY*(1) C 4 1.04 1.40 0.035
57. LP (1) N 7 /113. RY*(2) C 4 0.99 1.83 0.039
57. LP (1) N 7 /114. RY*(3) C 4 1.00 2.18 0.043
57. LP (1) N 7 /164. RY*(1) C 8 5.15 1.56 0.082
57. LP (1) N 7 /165. RY*(2) C 8 0.96 1.76 0.038
57. LP (1) N 7 /375. BD*(1) N 3 - C 4 1.39 0.91 0.032
57. LP (1) N 7 /376. BD*(1) C 4 - C 5 5.82 0.89 0.065
57. LP (1) N 7 /384. BD*(1) C 8 - O 9 13.96 0.67 0.087
57. LP (1) N 7 /385. BD*(1) C 8 - C 10 0.80 0.84 0.023
58. LP (1) O 9 /126. RY*(2) C 5 3.18 1.90 0.070
58. LP (1) O 9 /164. RY*(1) C 8 1.55 1.79 0.047
58. LP (1) O 9 /165. RY*(2) C 8 2.10 2.00 0.058
58. LP (1) O 9 /376. BD*(1) C 4 - C 5 3.62 1.12 0.057
58. LP (1) O 9 /382. BD*(1) N 7 - C 8 4.28 1.17 0.063
59. LP (2) O 9 /127. RY*(3) C 5 2.66 1.80 0.066
59. LP (2) O 9 /166. RY*(3) C 8 1.44 1.93 0.051
59. LP (2) O 9 /167. RY*(4) C 8 0.59 0.92 0.022
59. LP (2) O 9 /168. RY*(5) C 8 0.60 1.85 0.032
59. LP (2) O 9 /377. BD*(2) C 4 - C 5 23.46 0.36 0.086
59. LP (2) O 9 /383. BD*(2) N 7 - C 8 32.35 0.36 0.097
60. LP (1) C 10 /168. RY*(5) C 8 1.44 1.63 0.059
60. LP (1) C 10 /192. RY*(3) C 10 2.07 0.76 0.049
60. LP (1) C 10 /205. RY*(3) C 11 3.13 0.90 0.065
60. LP (1) C 10 /244. RY*(3) C 14 2.99 0.97 0.066
60. LP (1) C 10 /383. BD*(2) N 7 - C 8 66.75 0.13 0.101
60. LP (1) C 10 /389. BD*(2) C 11 - C 12 68.73 0.14 0.107
60. LP (1) C 10 /394. BD*(2) C 13 - C 14 69.57 0.14 0.108
61. LP*(1) C 15 / 60. LP (1) C 10 0.53 0.02 0.003
61. LP*(1) C 15 /218. RY*(3) C 12 3.01 0.71 0.058
61. LP*(1) C 15 /231. RY*(3) C 13 1.91 0.74 0.047
61. LP*(1) C 15 /233. RY*(5) C 13 0.79 1.80 0.048

61. LP*(1) C 15	/259. RY*(5) C 15	1.69	0.93	0.050
61. LP*(1) C 15	/269. RY*(2) O 16	1.11	1.22	0.046
61. LP*(1) C 15	/389. BD*(2) C 11 - C 12	54.55	0.16	0.105
61. LP*(1) C 15	/394. BD*(2) C 13 - C 14	53.86	0.17	0.104
62. LP (1) O 16	/255. RY*(1) C 15	1.60	1.95	0.050
62. LP (1) O 16	/281. RY*(1) C 17	2.85	1.58	0.060
62. LP (1) O 16	/285. RY*(5) C 17	2.01	2.26	0.061
62. LP (1) O 16	/289. RY*(9) C 17	1.41	2.97	0.059
62. LP (1) O 16	/292. RY*(12) C 17	0.55	3.47	0.040
62. LP (1) O 16	/391. BD*(1) C 12 - C 15	0.55	1.12	0.022
62. LP (1) O 16	/395. BD*(1) C 13 - C 15	6.28	1.12	0.075
62. LP (1) O 16	/400. BD*(1) C 17 - F 18	6.47	0.81	0.065
62. LP (1) O 16	/401. BD*(1) C 17 - F 19	2.59	0.79	0.041
62. LP (1) O 16	/402. BD*(1) C 17 - F 20	2.36	0.79	0.039
63. LP (2) O 16	/ 61. LP*(1) C 15	39.38	0.22	0.109
63. LP (2) O 16	/257. RY*(3) C 15	1.16	1.66	0.041
63. LP (2) O 16	/258. RY*(4) C 15	1.22	1.90	0.045
63. LP (2) O 16	/282. RY*(2) C 17	0.81	1.39	0.031
63. LP (2) O 16	/284. RY*(4) C 17	2.09	1.96	0.059
63. LP (2) O 16	/401. BD*(1) C 17 - F 19	14.19	0.57	0.081
63. LP (2) O 16	/402. BD*(1) C 17 - F 20	13.35	0.58	0.079
64. LP (1) F 18	/281. RY*(1) C 17	2.43	2.09	0.064
64. LP (1) F 18	/283. RY*(3) C 17	6.43	2.14	0.105
64. LP (1) F 18	/286. RY*(6) C 17	1.66	3.45	0.068
64. LP (1) F 18	/288. RY*(8) C 17	1.44	2.92	0.058
65. LP (2) F 18	/281. RY*(1) C 17	1.00	1.45	0.034
65. LP (2) F 18	/283. RY*(3) C 17	0.79	1.50	0.031
65. LP (2) F 18	/285. RY*(5) C 17	1.58	2.13	0.053
65. LP (2) F 18	/398. BD*(1) C 15 - O 16	0.78	0.74	0.021
65. LP (2) F 18	/399. BD*(1) O 16 - C 17	10.97	0.75	0.081
65. LP (2) F 18	/401. BD*(1) C 17 - F 19	4.63	0.66	0.050
65. LP (2) F 18	/402. BD*(1) C 17 - F 20	3.70	0.66	0.045
66. LP (3) F 18	/282. RY*(2) C 17	1.79	1.47	0.046
66. LP (3) F 18	/284. RY*(4) C 17	1.65	2.04	0.052
66. LP (3) F 18	/401. BD*(1) C 17 - F 19	10.65	0.66	0.076
66. LP (3) F 18	/402. BD*(1) C 17 - F 20	11.63	0.66	0.079
67. LP (1) F 19	/281. RY*(1) C 17	2.75	2.10	0.068
67. LP (1) F 19	/282. RY*(2) C 17	4.27	2.12	0.085
67. LP (1) F 19	/286. RY*(6) C 17	1.07	3.46	0.054
67. LP (1) F 19	/287. RY*(7) C 17	1.83	3.44	0.071
67. LP (1) F 19	/288. RY*(8) C 17	0.84	2.93	0.044
67. LP (1) F 19	/290. RY*(10) C 17	0.65	2.90	0.039
68. LP (2) F 19	/281. RY*(1) C 17	0.56	1.45	0.026
68. LP (2) F 19	/284. RY*(4) C 17	1.04	2.04	0.042
68. LP (2) F 19	/285. RY*(5) C 17	0.55	2.13	0.031
68. LP (2) F 19	/399. BD*(1) O 16 - C 17	10.91	0.75	0.081
68. LP (2) F 19	/400. BD*(1) C 17 - F 18	2.01	0.68	0.033
68. LP (2) F 19	/402. BD*(1) C 17 - F 20	5.74	0.66	0.056
69. LP (3) F 19	/281. RY*(1) C 17	0.75	1.45	0.030
69. LP (3) F 19	/283. RY*(3) C 17	1.01	1.50	0.035
69. LP (3) F 19	/284. RY*(4) C 17	0.57	2.04	0.031
69. LP (3) F 19	/285. RY*(5) C 17	0.63	2.13	0.033

69. LP (3) F 19	/400. BD*(1) C 17 - F 18	11.78	0.68	0.081
69. LP (3) F 19	/402. BD*(1) C 17 - F 20	8.00	0.66	0.066
70. LP (1) F 20	/281. RY*(1) C 17	3.16	2.10	0.073
70. LP (1) F 20	/282. RY*(2) C 17	4.09	2.12	0.083
70. LP (1) F 20	/286. RY*(6) C 17	0.60	3.45	0.041
70. LP (1) F 20	/287. RY*(7) C 17	2.20	3.44	0.078
70. LP (1) F 20	/288. RY*(8) C 17	0.89	2.93	0.046
70. LP (1) F 20	/290. RY*(10) C 17	0.69	2.90	0.040
71. LP (2) F 20	/281. RY*(1) C 17	0.61	1.45	0.027
71. LP (2) F 20	/284. RY*(4) C 17	0.83	2.04	0.037
71. LP (2) F 20	/285. RY*(5) C 17	0.75	2.13	0.036
71. LP (2) F 20	/399. BD*(1) O 16 - C 17	10.88	0.75	0.081
71. LP (2) F 20	/400. BD*(1) C 17 - F 18	1.52	0.68	0.029
71. LP (2) F 20	/401. BD*(1) C 17 - F 19	6.70	0.66	0.060
72. LP (3) F 20	/281. RY*(1) C 17	0.63	1.45	0.027
72. LP (3) F 20	/283. RY*(3) C 17	0.97	1.50	0.034
72. LP (3) F 20	/284. RY*(4) C 17	0.76	2.04	0.036
72. LP (3) F 20	/285. RY*(5) C 17	0.51	2.13	0.030
72. LP (3) F 20	/399. BD*(1) O 16 - C 17	0.51	0.75	0.018
72. LP (3) F 20	/400. BD*(1) C 17 - F 18	12.61	0.69	0.084
72. LP (3) F 20	/401. BD*(1) C 17 - F 19	7.38	0.66	0.063
370. BD*(2) C 1 - C 6	/ 75. RY*(3) C 1	2.29	0.81	0.093
370. BD*(2) C 1 - C 6	/ 89. RY*(4) C 2	0.52	0.92	0.047
370. BD*(2) C 1 - C 6	/141. RY*(4) C 6	2.50	0.53	0.079
373. BD*(2) C 2 - N 3	/ 88. RY*(3) C 2	2.12	1.34	0.110
373. BD*(2) C 2 - N 3	/101. RY*(3) N 3	1.23	0.80	0.065
377. BD*(2) C 4 - C 5	/101. RY*(3) N 3	0.62	0.79	0.042
377. BD*(2) C 4 - C 5	/118. RY*(7) C 4	1.39	1.21	0.078
377. BD*(2) C 4 - C 5	/130. RY*(6) C 5	1.15	1.39	0.076
377. BD*(2) C 4 - C 5	/141. RY*(4) C 6	0.68	0.53	0.036
377. BD*(2) C 4 - C 5	/153. RY*(3) N 7	0.56	0.86	0.042
383. BD*(2) N 7 - C 8	/153. RY*(3) N 7	0.75	0.87	0.059
383. BD*(2) N 7 - C 8	/166. RY*(3) C 8	1.11	1.58	0.096
383. BD*(2) N 7 - C 8	/167. RY*(4) C 8	1.61	0.57	0.070
383. BD*(2) N 7 - C 8	/394. BD*(2) C 13 - C 14	0.87	0.01	0.006
389. BD*(2) C 11 - C 12	/205. RY*(3) C 11	0.65	0.76	0.051
389. BD*(2) C 11 - C 12	/206. RY*(4) C 11	0.93	1.43	0.083
389. BD*(2) C 11 - C 12	/218. RY*(3) C 12	2.16	0.54	0.078
394. BD*(2) C 13 - C 14	/231. RY*(3) C 13	2.48	0.57	0.086
394. BD*(2) C 13 - C 14	/245. RY*(4) C 14	0.70	1.36	0.071
401. BD*(1) C 17 - F 19	/282. RY*(2) C 17	1.31	0.81	0.110
401. BD*(1) C 17 - F 19	/286. RY*(6) C 17	0.83	2.15	0.149
401. BD*(1) C 17 - F 19	/287. RY*(7) C 17	1.66	2.13	0.210
401. BD*(1) C 17 - F 19	/291. RY*(11) C 17	0.58	8.56	0.253
401. BD*(1) C 17 - F 19	/313. RY*(7) F 19	0.53	3.77	0.161
402. BD*(1) C 17 - F 20	/282. RY*(2) C 17	1.20	0.81	0.107
402. BD*(1) C 17 - F 20	/287. RY*(7) C 17	1.97	2.13	0.233
402. BD*(1) C 17 - F 20	/291. RY*(11) C 17	0.58	8.56	0.258

(Occupancy) Bond orbital/ Coefficients/ Hybrids of P7

1. (1.98537) BD (1) C 1 - C 2
   (50.97%) 0.7139* C 1 s(35.68%)p 1.80(64.27%)d 0.00(0.05%)
   0.0000 0.5972 0.0119 0.0005 -0.0791
   -0.0392 0.0000 -0.7963 0.0230 0.0022
   -0.0142 -0.0004 0.0000 0.0075 0.0002
   0.0008 -0.0165 -0.0126
   (49.03%) 0.7002* C 2 s(39.01%)p 1.56(60.95%)d 0.00(0.04%)
   0.0001 0.6244 0.0114 -0.0001 0.0829
   -0.0420 0.0015 0.7750 -0.0056 -0.0020
   0.0139 -0.0009 0.0000 0.0013 0.0000
   0.0006 -0.0185 -0.0099
2. (1.97239) BD (1) C 1 - C 6
   (49.06%) 0.7004* C 1 s(35.62%)p 1.81(64.33%)d 0.00(0.05%)
   0.0002 0.5967 0.0125 0.0006 -0.6187
   -0.0128 0.0004 0.5085 -0.0410 -0.0005
   -0.0041 -0.0009 0.0000 -0.0159 0.0003
   -0.0001 0.0072 -0.0125
   (50.94%) 0.7137* C 6 s(35.96%)p 1.78(64.00%)d 0.00(0.04%)
   -0.0001 0.5995 0.0156 -0.0003 0.6642
   -0.0324 0.0008 -0.4439 -0.0260 0.0023
   0.0062 -0.0010 0.0001 -0.0170 0.0001
   0.0000 -0.0003 -0.0109
3. (1.67612) BD (2) C 1 - C 6
   (51.39%) 0.7169* C 1 s(0.00%)p 1.00(99.95%)d 0.00(0.05%)
   0.0000 0.0000 0.0000 0.0000 -0.0197
   -0.0002 0.0000 -0.0159 -0.0002 0.0000
   0.9994 0.0100 -0.0002 0.0004 -0.0221
   -0.0001 0.0004 -0.0008
   (48.61%) 0.6972* C 6 s(0.00%)p 1.00(99.94%)d 0.00(0.06%)
   0.0000 0.0000 0.0000 0.0000 -0.0198
   -0.0002 -0.0001 -0.0158 -0.0001 -0.0001
   0.9993 0.0093 0.0058 0.0004 0.0072
   -0.0243 -0.0005 -0.0004
4. (1.97809) BD (1) C 1 - H 21
   (60.56%) 0.7782* C 1 s(28.66%)p 2.49(71.29%)d 0.00(0.05%)
   -0.0004 0.5350 -0.0204 -0.0010 0.7799
   0.0138 0.0026 0.3226 0.0067 0.0013
   0.0205 0.0004 0.0001 0.0135 0.0008
   0.0003 0.0136 -0.0094
   (39.44%) 0.6280* H 21 s(99.95%)p 0.00(0.05%)
   0.9998 -0.0003 0.0007 -0.0200 -0.0083
   -0.0005
5. (1.98321) BD (1) C 2 - N 3
   (40.37%) 0.6354* C 2 s(32.15%)p 2.11(67.75%)d 0.00(0.10%)
   0.0001 0.5664 0.0272 0.0002 -0.7277
   0.0145 0.0048 -0.3771 0.0711 0.0007
   -0.0202 0.0014 0.0001 0.0197 0.0012
   0.0006 0.0170 -0.0165
   (59.63%) 0.7722* N 3 s(35.48%)p 1.82(64.43%)d 0.00(0.09%)
   -0.0002 0.5956 0.0106 -0.0004 0.7329
   0.0287 0.0017 0.3250 -0.0189 -0.0018

0.0195 0.0003 0.0000 0.0262 0.0009
0.0009 0.0023 -0.0144

6. (1.73789) BD (2) C   2 - N   3
(41.93%) 0.6475* C   2 s(0.00%)p 1.00(99.86%)d 0.00(0.14%)
0.0000 0.0000 0.0000 0.0000 -0.0196
-0.0002 -0.0001 -0.0159 -0.0002 -0.0001
0.9989 0.0115 0.0035 0.0007 -0.0373
-0.0032 0.0007 -0.0014
(58.07%) 0.7621* N   3 s(0.00%)p 1.00(99.84%)d 0.00(0.16%)
0.0000 0.0000 0.0000 0.0000 -0.0196
-0.0002 0.0001 -0.0158 -0.0002 0.0001
0.9988 0.0106 -0.0044 -0.0009 0.0099
0.0388 0.0004 0.0014

7. (1.98042) BD (1) C   2 - H 22
(59.69%) 0.7726* C   2 s(28.84%)p 2.47(71.11%)d 0.00(0.06%)
-0.0006 0.5362 -0.0288 -0.0001 0.6766
0.0251 0.0025 -0.5027 -0.0043 -0.0019
0.0053 0.0004 0.0000 -0.0203 0.0002
-0.0002 0.0067 -0.0102
(40.31%) 0.6349* H 22 s(99.95%)p 0.00(0.05%)
0.9997 0.0017 0.0017 -0.0163 0.0158
-0.0001

8. (1.98440) BD (1) N   3 - C   4
(58.15%) 0.7626* N   3 s(35.53%)p 1.81(64.37%)d 0.00(0.09%)
-0.0001 0.5961 0.0066 -0.0003 -0.6751
-0.0216 -0.0030 0.4328 -0.0129 -0.0011
-0.0064 -0.0006 -0.0001 -0.0267 0.0000
-0.0001 -0.0030 -0.0146
(41.85%) 0.6469* C   4 s(34.49%)p 1.90(65.44%)d 0.00(0.07%)
-0.0001 0.5868 0.0238 0.0008 0.6178
0.0095 -0.0062 -0.5193 0.0542 0.0035
0.0040 0.0010 -0.0001 -0.0214 0.0003
-0.0001 0.0066 -0.0145

9. (1.98167) BD (1) C   4 - C   5
(48.87%) 0.6991* C   4 s(35.57%)p 1.81(64.37%)d 0.00(0.05%)
0.0001 0.5959 -0.0242 -0.0004 0.1024
-0.0035 0.0019 0.7955 0.0135 0.0022
0.0145 0.0001 0.0001 0.0007 -0.0001
0.0006 -0.0211 -0.0098
(51.13%) 0.7151* C   5 s(34.77%)p 1.87(65.18%)d 0.00(0.05%)
0.0000 0.5893 -0.0215 -0.0003 -0.0249
-0.0088 0.0049 -0.8067 -0.0079 -0.0016
-0.0132 -0.0003 0.0001 0.0055 0.0001
0.0007 -0.0184 -0.0109

10. (1.56697) BD (2) C   4 - C   5
(47.76%) 0.6911* C   4 s(0.00%)p 1.00(99.97%)d 0.00(0.03%)
0.0000 0.0000 0.0000 0.0000 -0.0197
-0.0003 -0.0002 -0.0157 -0.0003 -0.0002
0.9993 0.0180 0.0102 -0.0004 0.0047
0.0176 0.0002 0.0006
(52.24%) 0.7228* C   5 s(0.00%)p 1.00(99.97%)d 0.00(0.03%)
0.0000 0.0000 0.0000 0.0000 -0.0199

-0.0003 -0.0002 -0.0157 -0.0002 -0.0002
0.9994 0.0145 0.0099 0.0003 0.0020
-0.0158 -0.0003 -0.0004

11. (1.97244) BD (1) C 4 - N 7
(41.15%) 0.6415* C 4 s(29.48%)p 2.39(70.43%)d 0.00(0.09%)
-0.0002 0.5428 0.0125 -0.0008 -0.7787
-0.0077 0.0084 -0.3064 0.0600 -0.0005
-0.0202 0.0008 0.0002 0.0115 0.0012
0.0003 0.0220 -0.0164
(58.85%) 0.7671* N 7 s(30.94%)p 2.23(68.96%)d 0.00(0.10%)
-0.0002 0.5562 0.0034 -0.0004 0.8240
-0.0101 -0.0004 0.0977 0.0259 -0.0031
0.0180 0.0002 -0.0001 0.0231 0.0012
0.0006 0.0146 -0.0151

12. (1.97589) BD (1) C 5 - C 6
(50.83%) 0.7130* C 5 s(40.82%)p 1.45(59.16%)d 0.00(0.03%)
-0.0002 0.6387 0.0140 0.0002 0.6247
0.0252 -0.0022 0.4466 -0.0280 -0.0006
0.0194 0.0001 -0.0001 0.0124 0.0006
0.0004 0.0053 -0.0091
(49.17%) 0.7012* C 6 s(34.48%)p 1.90(65.46%)d 0.00(0.05%)
0.0001 0.5871 0.0110 0.0011 -0.7425
0.0254 -0.0018 -0.3185 -0.0291 -0.0005
-0.0197 0.0000 0.0000 0.0160 0.0009
0.0005 0.0107 -0.0133

13. (1.98853) BD (1) C 5 - O 9
(31.67%) 0.5627* C 5 s(24.16%)p 3.13(75.61%)d 0.01(0.24%)
-0.0002 0.4907 0.0272 -0.0002 -0.7785
0.0164 0.0141 0.3819 -0.0603 -0.0022
-0.0095 -0.0006 0.0002 -0.0273 0.0011
-0.0003 0.0305 -0.0262
(68.33%) 0.8266* O 9 s(31.69%)p 2.15(68.24%)d 0.00(0.07%)
-0.0001 0.5629 0.0006 -0.0002 0.8011
-0.0064 0.0006 -0.2006 -0.0121 0.0023
0.0128 -0.0003 0.0000 -0.0209 0.0004
-0.0002 0.0109 -0.0136

14. (1.97963) BD (1) C 6 - H 23
(61.25%) 0.7826* C 6 s(29.53%)p 2.39(70.43%)d 0.00(0.04%)
-0.0003 0.5430 -0.0219 -0.0005 0.0693
-0.0037 -0.0002 0.8361 0.0130 -0.0056
0.0146 0.0001 -0.0001 0.0014 0.0001
0.0006 -0.0172 -0.0114
(38.75%) 0.6225* H 23 s(99.95%)p 0.00(0.05%)
0.9998 0.0002 0.0017 -0.0019 -0.0216
-0.0004

15. (1.98505) BD (1) N 7 - C 8
(58.81%) 0.7669* N 7 s(36.62%)p 1.73(63.28%)d 0.00(0.11%)
-0.0001 0.6051 0.0071 -0.0004 -0.4825
0.0224 -0.0023 0.6320 -0.0021 0.0007
0.0005 0.0004 0.0000 -0.0181 -0.0002
0.0004 -0.0224 -0.0152
(41.19%) 0.6418* C 8 s(35.90%)p 1.78(64.02%)d 0.00(0.08%)

0.0001 0.5991 0.0089 0.0000 0.3875
-0.0144 -0.0043 -0.6984 -0.0453 0.0002
-0.0029 -0.0010 -0.0001 -0.0224 0.0000
0.0001 -0.0102 -0.0141

16. (1.85604) BD (2) N 7 - C 8
(59.75%) 0.7730* N 7 s(0.00%)p 1.00(99.81%)d 0.00(0.19%)
0.0000 -0.0002 0.0000 0.0000 -0.0198
0.0002 0.0001 -0.0157 0.0002 0.0001
0.9987 -0.0113 -0.0036 -0.0009 0.0050
0.0434 0.0006 0.0013
(40.25%) 0.6344* C 8 s(0.00%)p 1.00(99.79%)d 0.00(0.21%)
0.0000 -0.0001 0.0000 0.0000 -0.0201
0.0002 -0.0003 -0.0153 0.0002 -0.0002
0.9985 -0.0089 0.0130 0.0003 0.0296
-0.0354 -0.0011 0.0001

17. (1.98845) BD (1) C 8 - O 9
(30.57%) 0.5529* C 8 s(24.82%)p 3.02(74.91%)d 0.01(0.27%)
0.0001 -0.4982 0.0039 0.0019 -0.5025
0.0136 0.0058 -0.7025 -0.0489 0.0095
-0.0210 -0.0005 0.0003 -0.0432 -0.0013
-0.0018 0.0145 0.0259
(69.43%) 0.8333* O 9 s(30.05%)p 2.33(69.88%)d 0.00(0.07%)
0.0001 -0.5482 0.0043 0.0001 0.5434
-0.0071 0.0014 0.6348 0.0034 -0.0025
0.0209 -0.0001 0.0000 -0.0166 -0.0004
-0.0010 0.0167 0.0134

18. (1.97020) BD (1) C 8 - C 10
(49.42%) 0.7030* C 8 s(39.22%)p 1.55(60.75%)d 0.00(0.03%)
0.0003 -0.6262 0.0066 -0.0003 0.7710
-0.0322 -0.0020 -0.1090 0.0021 0.0013
0.0138 -0.0006 0.0000 0.0073 -0.0004
0.0002 -0.0135 0.0065
(50.58%) 0.7112* C 10 s(30.97%)p 2.23(68.98%)d 0.00(0.05%)
-0.0001 -0.5565 -0.0025 -0.0007 -0.8241
0.0054 0.0004 0.1022 -0.0028 -0.0004
-0.0155 0.0000 0.0000 0.0043 -0.0007
0.0000 -0.0183 0.0127

19. (1.97256) BD (1) C 10 - C 11
(51.40%) 0.7169* C 10 s(34.61%)p 1.89(65.35%)d 0.00(0.04%)
0.0000 0.5883 -0.0001 -0.0004 -0.3044
0.0108 -0.0002 0.7488 0.0071 0.0003
0.0032 0.0003 0.0000 -0.0107 0.0000
0.0001 -0.0111 -0.0113
(48.60%) 0.6972* C 11 s(35.61%)p 1.81(64.35%)d 0.00(0.04%)
0.0001 0.5967 0.0036 0.0013 0.3506
-0.0222 0.0003 -0.7211 -0.0085 -0.0019
-0.0020 -0.0006 0.0000 -0.0111 0.0000
0.0001 -0.0116 -0.0115

20. (1.96956) BD (1) C 10 - C 14
(51.54%) 0.7179* C 10 s(34.37%)p 1.91(65.60%)d 0.00(0.04%)
-0.0001 0.5863 -0.0002 -0.0003 -0.4767
0.0092 -0.0007 -0.6544 -0.0092 -0.0006

-0.0180 0.0001 0.0000 0.0143 0.0005
0.0006 -0.0045 -0.0114
(48.46%) 0.6961* C 14 s(35.49%)p 1.82(64.47%)d 0.00(0.04%)
0.0002 0.5957 0.0044 0.0013 0.5002
-0.0189 0.0008 0.6274 0.0130 0.0021
0.0201 -0.0002 0.0001 0.0150 0.0005
0.0007 -0.0060 -0.0115
21. (1.97383) BD (1) C 11 - C 12
(49.76%) 0.7054* C 11 s(36.06%)p 1.77(63.90%)d 0.00(0.04%)
0.0001 0.6002 0.0181 0.0005 -0.7900
0.0062 -0.0012 0.1129 -0.0427 0.0012
-0.0160 -0.0005 0.0000 -0.0003 0.0008
0.0000 0.0175 -0.0112
(50.24%) 0.7088* C 12 s(36.59%)p 1.73(63.37%)d 0.00(0.04%)
0.0000 0.6047 0.0152 0.0005 0.7925
-0.0151 0.0008 -0.0606 -0.0399 0.0006
0.0115 -0.0009 0.0000 -0.0078 0.0004
-0.0001 0.0149 -0.0113
22. (1.67759) BD (2) C 11 - C 12
(47.99%) 0.6927* C 11 s(0.00%)p 1.00(99.95%)d 0.00(0.05%)
0.0000 0.0002 0.0000 -0.0001 -0.0219
-0.0002 0.0000 -0.0132 0.0001 0.0000
0.9994 0.0035 0.0043 0.0005 -0.0209
-0.0088 0.0003 -0.0009
(52.01%) 0.7212* C 12 s(0.00%)p 1.00(99.95%)d 0.00(0.05%)
0.0000 0.0025 -0.0005 0.0001 -0.0177
-0.0002 0.0000 -0.0159 -0.0006 -0.0003
0.9994 0.0089 0.0062 0.0001 0.0157
-0.0159 -0.0007 0.0000
23. (1.97825) BD (1) C 11 - H 24
(61.17%) 0.7821* C 11 s(28.29%)p 2.53(71.66%)d 0.00(0.05%)
-0.0004 0.5315 -0.0194 -0.0013 0.5003
0.0106 -0.0038 0.6825 0.0055 -0.0035
0.0199 0.0003 -0.0001 0.0176 0.0006
0.0008 -0.0050 -0.0124
(38.83%) 0.6232* H 24 s(99.95%)p 0.00(0.05%)
0.9998 0.0003 0.0014 -0.0131 -0.0175
-0.0005
24. (1.97390) BD (1) C 12 - C 15
(49.42%) 0.7030* C 12 s(34.94%)p 1.86(65.01%)d 0.00(0.05%)
0.0002 0.5910 0.0134 0.0004 -0.4990
0.0346 -0.0004 -0.6320 -0.0111 0.0002
-0.0204 0.0008 0.0000 0.0170 0.0007
0.0009 -0.0060 -0.0120
(50.58%) 0.7112* C 15 s(37.69%)p 1.65(62.27%)d 0.00(0.04%)
-0.0001 0.6139 0.0008 0.0005 0.4371
-0.0374 0.0034 0.6556 0.0143 0.0009
0.0164 0.0004 0.0003 0.0148 0.0005
0.0004 -0.0086 -0.0096
25. (1.97558) BD (1) C 12 - H 25
(61.27%) 0.7828* C 12 s(28.45%)p 2.51(71.50%)d 0.00(0.04%)
-0.0003 0.5328 -0.0241 -0.0007 -0.3471

-0.0105 0.0031 0.7709 0.0089 -0.0049
 0.0047 -0.0001 0.0000 -0.0138 0.0001
 0.0002 -0.0101 -0.0125
(38.73%) 0.6223* H 25 s(99.95%)p 0.00(0.05%)
 0.9998 0.0003 0.0013 0.0094 -0.0192
-0.0001
26. (1.97156) BD (1) C 13 - C 14
(50.55%) 0.7110* C 13 s(36.58%)p 1.73(63.38%)d 0.00(0.04%)
-0.0001 0.6046 0.0156 0.0009 0.7880
-0.0057 0.0009 -0.1040 0.0396 -0.0013
 0.0195 0.0003 0.0000 0.0011 0.0010
 0.0001 0.0167 -0.0113
(49.45%) 0.7032* C 14 s(35.98%)p 1.78(63.98%)d 0.00(0.04%)
 0.0001 0.5995 0.0201 0.0004 -0.7959
 0.0157 -0.0013 0.0654 0.0409 -0.0006
-0.0140 0.0011 0.0000 -0.0074 0.0006
-0.0001 0.0158 -0.0110
27. (1.66929) BD (2) C 13 - C 14
(53.15%) 0.7290* C 13 s(0.00%)p 1.00(99.95%)d 0.00(0.05%)
 0.0000 -0.0030 -0.0003 -0.0001 -0.0251
-0.0015 -0.0002 -0.0203 -0.0001 -0.0002
 0.9992 0.0061 0.0047 -0.0005 0.0181
 0.0125 0.0000 0.0014
(46.85%) 0.6845* C 14 s(0.00%)p 1.00(99.94%)d 0.00(0.06%)
 0.0000 -0.0007 -0.0003 0.0000 -0.0195
-0.0002 -0.0001 -0.0158 0.0002 0.0000
 0.9994 0.0012 0.0038 0.0001 -0.0192
 0.0140 0.0007 -0.0004
28. (1.97998) BD (1) C 13 - C 15
(49.60%) 0.7043* C 13 s(34.67%)p 1.88(65.28%)d 0.00(0.05%)
 0.0000 0.5887 0.0106 0.0007 -0.3564
 0.0288 -0.0002 0.7245 0.0044 -0.0001
 0.0076 0.0012 -0.0001 -0.0133 -0.0002
 0.0006 -0.0121 -0.0124
(50.40%) 0.7099* C 15 s(39.25%)p 1.55(60.71%)d 0.00(0.04%)
 0.0000 0.6264 -0.0099 0.0001 0.2336
-0.0141 0.0021 -0.7432 -0.0032 -0.0024
-0.0005 -0.0020 0.0000 -0.0093 -0.0001
 0.0000 -0.0139 -0.0098
29. (1.97561) BD (1) C 13 - H 26
(61.54%) 0.7845* C 13 s(28.72%)p 2.48(71.24%)d 0.00(0.05%)
 0.0003 -0.5354 0.0217 0.0014 0.4996
 0.0138 -0.0024 0.6797 0.0028 -0.0038
 0.0247 -0.0003 -0.0002 -0.0169 -0.0006
-0.0009 0.0040 0.0125
(38.46%) 0.6202* H 26 s(99.95%)p 0.00(0.05%)
-0.9998 -0.0004 -0.0016 -0.0117 -0.0181
-0.0012
30. (1.97711) BD (1) C 14 - H 27
(61.70%) 0.7855* C 14 s(28.51%)p 2.51(71.45%)d 0.00(0.05%)
 0.0004 -0.5335 0.0211 0.0012 -0.3374
-0.0077 0.0035 0.7748 0.0098 -0.0035

0.0053 0.0001 0.0000 0.0139 0.0000
-0.0002 0.0117 0.0122
(38.30%) 0.6189* H 27 s(99.95%)p 0.00(0.05%)
-0.9998 -0.0008 -0.0014 0.0102 -0.0195
-0.0001
31. (1.98572) BD (1) C 15 - O 16
(30.89%) 0.5558* C 15 s(22.83%)p 3.37(76.94%)d 0.01(0.24%)
0.0000 0.4773 0.0210 -0.0015 -0.8666
-0.0201 0.0097 0.1298 0.0293 -0.0057
-0.0141 -0.0050 0.0001 -0.0125 0.0010
-0.0006 0.0402 -0.0244
(69.11%) 0.8313* O 16 s(34.53%)p 1.89(65.41%)d 0.00(0.06%)
-0.0002 0.5876 -0.0034 -0.0001 0.7813
-0.0032 0.0002 -0.2066 -0.0030 0.0033
0.0305 0.0019 -0.0007 -0.0173 0.0030
-0.0026 0.0097 -0.0128
32. (1.99354) BD (1) O 16 - C 17
(67.70%) 0.8228* O 16 s(28.70%)p 2.48(71.21%)d 0.00(0.09%)
0.0000 0.5357 0.0014 -0.0004 -0.5687
0.0185 -0.0015 -0.6095 -0.0070 0.0014
0.1300 -0.0006 -0.0003 0.0219 -0.0043
-0.0078 -0.0109 -0.0145
(32.30%) 0.5683* C 17 s(28.75%)p 2.47(70.96%)d 0.01(0.29%)
0.0001 0.5362 -0.0061 0.0027 0.6173
0.0053 0.0002 0.5587 -0.0340 0.0016
-0.1232 0.0063 0.0001 0.0440 -0.0101
-0.0090 0.0065 -0.0266
33. (1.99465) BD (1) C 17 - F 18
(27.94%) 0.5286* C 17 s(23.76%)p 3.19(75.79%)d 0.02(0.45%)
-0.0003 0.4873 0.0132 -0.0024 -0.7768
0.0279 0.0127 0.3915 -0.0129 -0.0089
-0.0002 -0.0004 0.0004 -0.0470 0.0003
-0.0005 0.0340 -0.0339
(72.06%) 0.8489* F 18 s(26.98%)p 2.70(72.93%)d 0.00(0.09%)
0.0000 0.5193 -0.0091 -0.0004 0.7611
-0.0099 -0.0038 -0.3870 0.0058 0.0020
0.0018 -0.0002 0.0000 -0.0215 0.0001
-0.0001 0.0155 -0.0152
34. (1.99573) BD (1) C 17 - F 19
(27.50%) 0.5244* C 17 s(23.65%)p 3.21(75.86%)d 0.02(0.49%)
-0.0001 0.4862 -0.0036 -0.0007 -0.0003
0.0113 -0.0052 -0.6017 0.0234 0.0072
-0.6287 0.0237 0.0088 -0.0009 -0.0003
0.0616 -0.0288 0.0177
(72.50%) 0.8515* F 19 s(26.00%)p 2.84(73.91%)d 0.00(0.09%)
0.0000 0.5098 -0.0087 -0.0003 0.0060
0.0007 -0.0002 0.5976 -0.0071 -0.0030
0.6180 -0.0076 -0.0032 0.0004 0.0006
0.0255 -0.0122 0.0081
35. (1.99596) BD (1) C 17 - F 20
(27.58%) 0.5251* C 17 s(23.80%)p 3.18(75.71%)d 0.02(0.49%)
-0.0001 0.4878 -0.0045 -0.0007 0.0990

0.0082 -0.0074 -0.4060 0.0167 0.0051
0.7622 -0.0309 -0.0094 -0.0078 0.0124
-0.0511 -0.0114 0.0438
(72.42%) 0.8510* F 20 s(26.18%)p 2.82(73.73%)d 0.00(0.09%)
0.0000 0.5116 -0.0088 -0.0004 -0.0946
0.0021 0.0004 0.4039 -0.0048 -0.0020
-0.7517 0.0093 0.0038 -0.0026 0.0047
-0.0212 -0.0053 0.0193
36. (1.99915) CR (1) C 1 s(100.00%)p 0.00(0.00%)
1.0000 0.0001 0.0000 0.0000 0.0004
0.0000 0.0000 0.0001 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
37. (1.99918) CR (1) C 2 s(100.00%)p 0.00(0.00%)
1.0000 0.0001 0.0000 0.0000 0.0005
0.0000 0.0000 -0.0003 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
38. (1.99935) CR (1) N 3 s(100.00%)
1.0000 0.0002 0.0000 0.0000 0.0001
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
39. (1.99888) CR (1) C 4 s(100.00%)p 0.00(0.00%)
1.0000 0.0001 0.0000 0.0000 -0.0001
0.0000 0.0000 -0.0002 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
40. (1.99867) CR (1) C 5 s(100.00%)p 0.00(0.00%)
1.0000 0.0002 0.0000 0.0000 0.0000
0.0000 0.0000 0.0002 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
41. (1.99902) CR (1) C 6 s(100.00%)p 0.00(0.00%)
1.0000 0.0001 0.0000 0.0000 0.0002
0.0000 0.0000 0.0002 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
42. (1.99932) CR (1) N 7 s(100.00%)p 0.00(0.00%)
1.0000 0.0002 0.0000 0.0000 0.0001
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
43. (1.99901) CR (1) C 8 s(100.00%)p 0.00(0.00%)
1.0000 0.0001 0.0000 0.0000 -0.0002
0.0000 0.0000 0.0001 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
44. (1.99970) CR (1) O 9 s(100.00%)
1.0000 0.0002 0.0000 0.0000 -0.0001
0.0000 0.0000 0.0001 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000

0.0000 0.0000 0.0000
45. (1.99890) CR (1) C 10 s(100.00%)p 0.00(0.00%)
1.0000 -0.0001 0.0000 0.0000 -0.0001
0.0000 0.0000 -0.0001 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
46. (1.99905) CR (1) C 11 s(100.00%)p 0.00(0.00%)
1.0000 0.0000 0.0000 0.0000 0.0002
0.0000 0.0000 0.0003 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
47. (1.99901) CR (1) C 12 s(100.00%)p 0.00(0.00%)
1.0000 0.0001 0.0000 0.0000 0.0000
0.0000 0.0000 0.0004 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
48. (1.99899) CR (1) C 13 s(100.00%)p 0.00(0.00%)
1.0000 0.0002 0.0000 0.0000 -0.0001
0.0000 0.0000 -0.0002 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
49. (1.99905) CR (1) C 14 s(100.00%)p 0.00(0.00%)
1.0000 0.0000 0.0000 0.0000 0.0001
0.0000 0.0000 -0.0004 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
50. (1.99868) CR (1) C 15 s(100.00%)p 0.00(0.00%)
1.0000 0.0001 0.0000 0.0000 0.0000
0.0000 0.0000 0.0001 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
51. (1.99963) CR (1) O 16 s(100.00%)
1.0000 0.0002 0.0000 0.0000 0.0001
0.0000 0.0000 0.0001 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
52. (1.99962) CR (1) C 17 s(100.00%)p 0.00(0.00%)
1.0000 0.0002 0.0000 0.0000 -0.0003
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
53. (1.99991) CR (1) F 18 s(100.00%)p 0.00(0.00%)
1.0000 0.0002 0.0000 0.0000 -0.0001
0.0000 0.0000 0.0001 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
54. (1.99992) CR (1) F 19 s(100.00%)
1.0000 0.0002 0.0000 0.0000 0.0000
0.0000 0.0000 -0.0001 0.0000 0.0000
-0.0001 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
55. (1.99992) CR (1) F 20 s(100.00%)

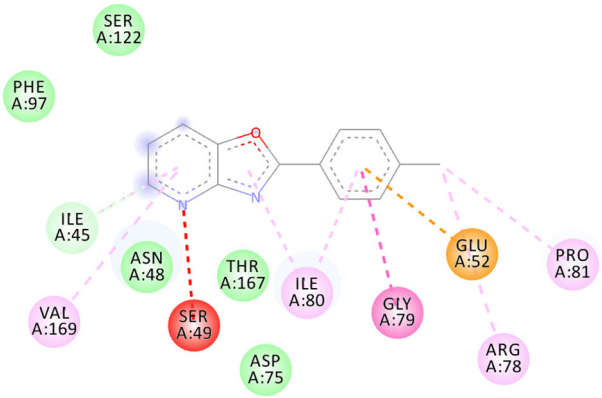
1.0000 0.0002 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
0.0001 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000
56. (1.91122) LP (1) N 3 s(28.98%)p 2.45(70.94%)d 0.00(0.08%)
-0.0001 0.5382 -0.0103 0.0006 -0.0637
0.0020 0.0004 -0.8394 0.0242 -0.0021
-0.0145 0.0004 0.0000 -0.0030 -0.0001
-0.0009 0.0239 0.0151
57. (1.90622) LP (1) N 7 s(32.43%)p 2.08(67.49%)d 0.00(0.08%)
-0.0001 0.5694 -0.0055 0.0006 -0.2923
-0.0145 -0.0009 -0.7672 -0.0168 -0.0028
-0.0178 -0.0005 -0.0001 -0.0150 -0.0003
-0.0010 0.0203 0.0137
58. (1.97146) LP (1) O 9 s(38.25%)p 1.61(61.72%)d 0.00(0.03%)
-0.0002 0.6185 0.0042 0.0002 -0.2477
-0.0019 -0.0010 0.7455 0.0045 0.0025
0.0067 0.0000 0.0000 0.0096 0.0001
-0.0002 0.0136 0.0079
59. (1.73882) LP (2) O 9 s(0.00%)p 1.00(99.93%)d 0.00(0.07%)
0.0000 0.0001 0.0000 0.0000 -0.0200
0.0000 0.0000 -0.0156 0.0000 0.0000
0.9993 -0.0004 -0.0011 0.0004 0.0072
-0.0246 -0.0005 -0.0004
60. (1.05958) LP (1) C 10 s(0.00%)p 1.00(100.00%)d 0.00(0.00%)
0.0000 0.0000 0.0001 0.0000 -0.0204
-0.0001 0.0000 -0.0126 0.0001 0.0000
0.9997 -0.0035 0.0014 0.0000 -0.0046
0.0008 0.0001 -0.0002
61. (1.00156) LP*(1) C 15 s(0.00%)p 1.00(99.99%)d 0.00(0.01%)
0.0000 0.0029 0.0033 0.0000 0.0193
-0.0052 0.0005 0.0092 -0.0017 0.0000
-0.9997 0.0094 -0.0031 0.0000 -0.0072
0.0008 0.0004 -0.0003
62. (1.94340) LP (1) O 16 s(36.57%)p 1.73(63.39%)d 0.00(0.04%)
-0.0002 0.6047 0.0041 0.0003 -0.2531
-0.0036 0.0005 0.7509 0.0029 0.0022
-0.0771 -0.0004 -0.0005 0.0089 -0.0019
0.0041 0.0155 0.0072
63. (1.84122) LP (2) O 16 s(0.17%)p99.99(99.78%)d 0.31(0.05%)
0.0000 0.0415 -0.0004 0.0000 -0.0311
0.0000 -0.0001 -0.1453 -0.0012 0.0002
-0.9878 -0.0027 0.0001 0.0006 -0.0026
0.0214 -0.0031 -0.0071
64. (1.99084) LP (1) F 18 s(73.02%)p 0.37(26.98%)d 0.00(0.00%)
-0.0002 0.8545 0.0030 0.0002 -0.4608
0.0066 -0.0027 0.2397 -0.0036 0.0013
-0.0021 0.0001 0.0000 0.0040 0.0000
0.0000 -0.0027 0.0028
65. (1.94339) LP (2) F 18 s(0.00%)p 1.00(99.97%)d 0.00(0.03%)
0.0000 0.0042 -0.0003 0.0000 -0.4523
-0.0022 -0.0002 -0.8834 -0.0042 -0.0008

0.1207 0.0005 0.0001 -0.0097 0.0017
-0.0012 -0.0143 -0.0004
66. (1.93655) LP (3) F 18 s(0.00%)p 1.00(99.97%)d 0.00(0.03%)
0.0000 0.0003 -0.0001 0.0000 0.0527
0.0003 0.0001 0.1086 0.0007 0.0001
0.9925 0.0057 0.0010 0.0014 0.0161
-0.0077 0.0017 0.0000
67. (1.99077) LP (1) F 19 s(73.99%)p 0.35(26.01%)d 0.00(0.00%)
-0.0002 0.8602 0.0027 0.0002 0.0009
0.0005 -0.0002 -0.3534 0.0054 -0.0020
-0.3675 0.0058 -0.0021 -0.0002 -0.0001
-0.0044 0.0022 -0.0016
68. (1.94821) LP (2) F 19 s(0.00%)p 1.00(99.97%)d 0.00(0.03%)
0.0000 0.0035 -0.0007 0.0001 -0.6775
-0.0034 -0.0006 -0.5267 -0.0021 -0.0005
0.5131 0.0015 0.0006 -0.0077 -0.0081
-0.0005 0.0058 0.0107
69. (1.94052) LP (3) F 19 s(0.00%)p 1.00(99.97%)d 0.00(0.03%)
0.0000 -0.0020 0.0022 0.0000 0.7353
0.0044 0.0007 -0.4898 -0.0025 -0.0007
0.4681 0.0029 0.0005 0.0083 0.0095
-0.0005 0.0065 0.0096
70. (1.99068) LP (1) F 20 s(73.81%)p 0.35(26.18%)d 0.00(0.00%)
-0.0002 0.8591 0.0027 0.0002 0.0596
-0.0007 0.0002 -0.2461 0.0036 -0.0014
0.4446 -0.0070 0.0026 0.0004 -0.0009
0.0038 0.0011 -0.0035
71. (1.94700) LP (2) F 20 s(0.00%)p 1.00(99.97%)d 0.00(0.03%)
0.0000 0.0020 0.0004 -0.0001 0.6919
0.0033 0.0006 0.6681 0.0029 0.0006
0.2732 0.0007 0.0004 0.0041 -0.0107
-0.0077 -0.0065 -0.0069
72. (1.93962) LP (3) F 20 s(0.00%)p 1.00(99.97%)d 0.00(0.03%)
0.0000 0.0058 -0.0018 0.0000 -0.7130
-0.0041 -0.0006 0.5740 0.0031 0.0007
0.4022 0.0028 0.0005 -0.0066 0.0104
-0.0055 -0.0038 -0.0103
73. (0.00470) RY*(1) C 1 s(1.71%)p54.17(92.61%)d 3.33(5.68%)
0.0000 0.0213 0.1290 0.0029 -0.0330
0.8306 0.0314 -0.0080 0.4831 0.0115
-0.0008 0.0239 0.0008 0.1314 0.0072
0.0005 0.1952 -0.0377
74. (0.00150) RY*(2) C 1 s(1.17%)p84.16(98.60%)d 0.19(0.22%)
0.0000 -0.0068 0.1073 -0.0127 -0.0096
-0.4924 0.1458 0.0444 0.8115 -0.2485
0.0005 0.0033 -0.0011 -0.0260 0.0012
0.0001 0.0186 -0.0350
75. (0.00099) RY*(3) C 1 s(0.00%)p 1.00(69.40%)d 0.44(30.60%)
0.0000 0.0000 0.0001 0.0000 0.0000
-0.0162 -0.0020 0.0000 -0.0132 -0.0015
0.0021 0.8269 0.0992 -0.0017 0.4685
-0.2937 -0.0138 0.0079

76. (0.00042) RY*(4) C 1   s(91.33%)p 0.04(3.53%)d 0.06(5.14%)
 0.0000 -0.0099 0.9502 -0.1011 0.0309
-0.0662 0.0028 0.0020 -0.1678 0.0425
 0.0006 -0.0041 0.0007 -0.0933 0.0066
 0.0013 0.1024 -0.1794
77. (0.00039) RY*(5) C 1   s(0.00%)p 1.00(19.53%)d 4.12(80.47%)
 0.0000 0.0000 0.0001 0.0000 0.0002
-0.0086 -0.0006 0.0002 -0.0070 -0.0005
-0.0097 0.4402 0.0365 -0.0132 -0.2442
 0.8627 0.0185 0.0153
78. (0.00010) RY*(6) C 1   s(4.24%)p 6.90(29.27%)d15.67(66.49%)
 0.0000 0.0010 0.1010 0.1795 -0.0088
-0.1627 -0.5127 0.0053 -0.0069 -0.0557
-0.0001 -0.0033 -0.0110 0.6710 0.0063
-0.0008 0.3349 0.3200
79. (0.00007) RY*(7) C 1   s(1.80%)p12.54(22.60%)d41.94(75.59%)
80. (0.00003) RY*(8) C 1   s(17.35%)p 1.96(33.99%)d 2.80(48.66%)
81. (0.00003) RY*(9) C 1   s(2.97%)p26.34(78.19%)d 6.35(18.84%)
82. (0.00001) RY*(10) C 1   s(0.02%)p99.99(11.23%)d99.99(88.75%)
83. (0.00000) RY*(11) C 1   s(0.01%)p 1.00(99.87%)d 0.00(0.13%)
84. (0.00000) RY*(12) C 1   s(74.31%)p 0.32(23.44%)d 0.03(2.24%)
85. (0.00001) RY*(13) C 1   s(5.13%)p 3.49(17.87%)d15.02(77.00%)
86. (0.00692) RY*(1) C 2   s(0.84%)p96.77(81.71%)d20.66(17.45%)
 0.0000 -0.0062 0.0897 0.0191 0.0067
 0.8656 0.0277 0.0569 0.2310 -0.0997
 0.0010 0.0207 -0.0010 -0.3370 0.0011
-0.0090 0.2415 -0.0500
87. (0.00501) RY*(2) C 2   s(0.58%)p99.99(98.52%)d 1.57(0.90%)
 0.0000 0.0331 0.0615 -0.0296 -0.0539
 0.2227 0.0611 -0.0171 -0.9617 0.0613
-0.0013 -0.0108 0.0022 -0.0890 -0.0004
-0.0008 -0.0043 -0.0330
88. (0.00173) RY*(3) C 2   s(0.00%)p 1.00(25.36%)d 2.94(74.64%)
 0.0000 0.0000 0.0000 0.0000 -0.0005
-0.0099 -0.0002 -0.0004 -0.0079 -0.0002
 0.0233 0.5027 0.0105 -0.0205 0.7395
 0.4446 -0.0074 0.0373
89. (0.00078) RY*(4) C 2   s(0.00%)p 1.00(60.62%)d 0.65(39.38%)
 0.0000 0.0000 0.0001 0.0000 -0.0003
 0.0152 0.0016 -0.0003 0.0123 0.0012
 0.0172 -0.7742 -0.0785 -0.0144 0.1615
 0.6058 0.0064 0.0222
90. (0.00049) RY*(5) C 2   s(1.92%)p13.30(25.55%)d37.75(72.53%)
 0.0000 -0.0043 0.1132 0.0799 0.0028
-0.3477 0.2622 0.0013 -0.0116 0.2561
 0.0001 -0.0070 0.0092 -0.3652 0.0102
-0.0186 0.7686 -0.0281
91. (0.00034) RY*(6) C 2   s(83.22%)p 0.01(0.71%)d 0.19(16.07%)
 0.0000 -0.0139 0.9085 -0.0810 0.0460
-0.0151 -0.0520 -0.0114 0.0330 -0.0284
 0.0007 0.0003 -0.0014 0.2791 0.0145
 0.0130 0.0175 -0.2866

92. (0.00010) RY*(7) C 2   s(13.31%)p 0.44(5.86%)d 6.07(80.82%)
93. (0.00005) RY*(8) C 2   s(5.26%)p12.86(67.62%)d 5.16(27.12%)
94. (0.00000) RY*(9) C 2   s(90.50%)p 0.05(4.47%)d 0.06(5.03%)
95. (0.00001) RY*(10) C 2   s(0.94%)p92.81(87.01%)d12.86(12.06%)
96. (0.00001) RY*(11) C 2   s(0.00%)p 1.00(14.36%)d 5.96(85.64%)
97. (0.00000) RY*(12) C 2   s(0.00%)p 1.00(99.80%)d 0.00(0.20%)
98. (0.00001) RY*(13) C 2   s(3.44%)p 8.37(28.75%)d19.74(67.82%)
99. (0.00380) RY*(1) N 3   s(1.94%)p48.10(93.40%)d 2.40(4.66%)
0.0000 -0.0087 0.1390 0.0036 -0.0022
-0.0603 -0.0198 -0.0292 -0.9629 0.0394
-0.0005 -0.0164 0.0002 -0.0806 0.0030
-0.0045 0.2000 -0.0094
100. (0.00169) RY*(2) N 3   s(0.02%)p99.99(98.69%)d78.39(1.29%)
0.0000 0.0054 0.0112 0.0030 0.0316
-0.9877 -0.0770 0.0009 0.0628 0.0141
0.0006 -0.0183 -0.0013 0.1094 0.0022
0.0016 0.0298 0.0054
101. (0.00062) RY*(3) N 3   s(0.00%)p 1.00(97.63%)d 0.02(2.37%)
0.0000 0.0000 0.0003 0.0000 0.0002
-0.0192 0.0004 0.0002 -0.0156 0.0005
-0.0122 0.9873 -0.0287 0.0007 -0.1338
0.0761 0.0037 -0.0025
102. (0.00038) RY*(4) N 3   s(78.36%)p 0.14(10.98%)d 0.14(10.66%)
0.0000 0.0007 0.8837 0.0525 -0.0116
0.0541 -0.2291 -0.0123 0.0756 0.2199
-0.0005 0.0028 -0.0013 0.2175 0.0012
0.0038 -0.2087 0.1255
103. (0.00037) RY*(5) N 3   s(0.00%)p 1.00(1.98%)d49.47(98.02%)
0.0000 0.0000 0.0055 0.0003 -0.0003
0.0029 -0.0021 -0.0002 0.0026 0.0008
0.0100 -0.1357 0.0356 0.0162 -0.9885
0.0371 0.0188 -0.0318
104. (0.00011) RY*(6) N 3   s(3.79%)p 2.39(9.07%)d22.99(87.14%)
0.0000 -0.0032 0.1934 -0.0221 0.0379
-0.0733 -0.2573 -0.0030 0.1145 -0.0674
0.0007 0.0004 -0.0061 -0.9243 -0.0101
-0.0147 0.0041 -0.1293
105. (0.00004) RY*(7) N 3   s(5.02%)p 5.29(26.52%)d13.65(68.47%)
106. (0.00002) RY*(8) N 3   s(0.00%)p 1.00(1.46%)d67.35(98.54%)
107. (0.00001) RY*(9) N 3   s(0.44%)p26.18(11.63%)d99.99(87.93%)
108. (0.00001) RY*(10) N 3   s(1.08%)p59.06(63.80%)d32.52(35.12%)
109. (0.00002) RY*(11) N 3   s(10.64%)p 8.05(85.64%)d 0.35(3.72%)
110. (0.00000) RY*(12) N 3   s(98.71%)p 0.01(0.54%)d 0.01(0.75%)
111. (0.00000) RY*(13) N 3   s(0.00%)p 1.00(99.09%)d 0.01(0.91%)
112. (0.00813) RY*(1) C 4   s(15.50%)p 5.03(78.00%)d 0.42(6.50%)
0.0000 -0.0678 0.3850 0.0474 0.0120
0.0767 -0.0122 0.0530 0.8771 -0.0389
0.0011 0.0154 -0.0009 -0.0223 0.0053
-0.0040 0.2532 -0.0181
113. (0.00611) RY*(2) C 4   s(17.03%)p 3.83(65.19%)d 1.04(17.77%)
0.0000 0.0091 0.4109 -0.0374 0.0168
-0.7845 -0.0176 0.0095 -0.1879 -0.0109

0.0005 -0.0185 -0.0005 0.2928 0.0133
0.0038 0.2878 -0.0948
114. (0.00480) RY*(3) C 4 s(45.75%)p 0.66(30.16%)d 0.53(24.09%)
0.0000 0.0194 0.6760 -0.0129 -0.0175
0.3733 -0.0420 0.0212 -0.3988 0.0260
0.0000 0.0012 -0.0004 -0.4367 0.0007
-0.0091 0.2005 -0.0994
115. (0.00270) RY*(4) C 4 s(0.00%)p 1.00(0.72%)d99.99(99.28%)
0.0000 0.0000 0.0001 -0.0001 -0.0001
0.0018 0.0006 0.0000 0.0012 0.0006
0.0032 -0.0764 -0.0368 0.0117 -0.9787
0.1831 0.0220 -0.0284
116. (0.00102) RY*(5) C 4 s(0.00%)p 1.00(63.29%)d 0.58(36.71%)
0.0000 0.0000 0.0002 -0.0001 -0.0005
0.0155 0.0012 -0.0004 0.0125 0.0009
0.0258 -0.7919 -0.0691 0.0124 -0.0479
-0.6035 -0.0090 -0.0181
117. (0.00065) RY*(6) C 4 s(4.78%)p 4.70(22.48%)d15.20(72.73%)
0.0000 -0.0107 0.1965 -0.0955 -0.0151
-0.3559 -0.0027 -0.0057 0.1323 -0.2835
-0.0004 -0.0056 -0.0046 -0.4627 -0.0208
0.0040 -0.7161 -0.0039
118. (0.00057) RY*(7) C 4 s(0.00%)p 1.00(36.13%)d 1.77(63.87%)
0.0000 0.0000 -0.0002 0.0002 0.0001
0.0126 0.0009 0.0001 0.0092 0.0010
-0.0035 -0.5998 -0.0361 -0.0173 0.1924
0.7749 0.0097 0.0277
119. (0.00024) RY*(8) C 4 s(14.12%)p 1.26(17.84%)d 4.82(68.04%)
0.0000 0.0075 0.3681 -0.0746 0.0048
0.3297 0.0024 -0.0043 -0.0587 -0.2573
0.0000 0.0058 -0.0040 0.7085 0.0044
0.0216 -0.4197 -0.0423
120. (0.00008) RY*(9) C 4 s(0.67%)p99.99(98.11%)d 1.83(1.22%)
121. (0.00004) RY*(10) C 4 s(17.18%)p 3.88(66.73%)d 0.94(16.08%)
122. (0.00001) RY*(11) C 4 s(84.57%)p 0.18(14.97%)d 0.01(0.46%)
123. (0.00001) RY*(12) C 4 s(0.84%)p 7.45(6.27%)d99.99(92.89%)
124. (0.00000) RY*(13) C 4 s(0.01%)p 1.00(99.88%)d 0.00(0.11%)
125. (0.00524) RY*(1) C 5 s(47.27%)p 0.92(43.55%)d 0.19(9.18%)
0.0000 0.0244 0.6869 -0.0164 -0.0061
-0.0937 0.0072 -0.0095 0.6530 -0.0059
-0.0003 0.0084 0.0001 0.0813 0.0107
0.0006 0.2672 -0.1167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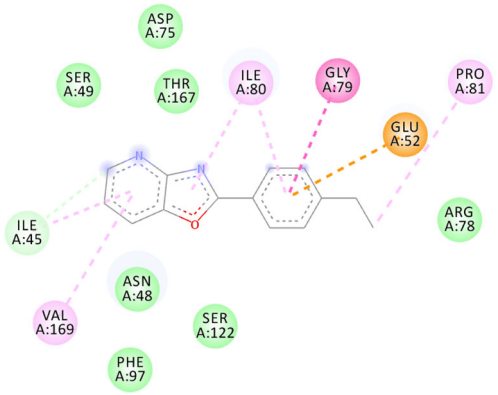
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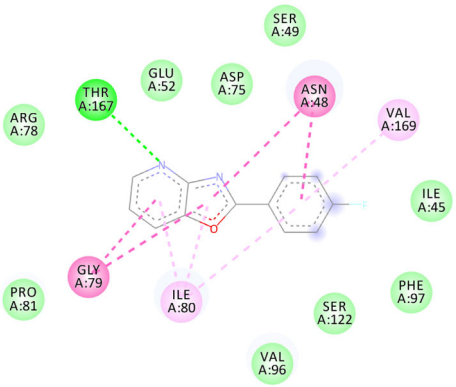
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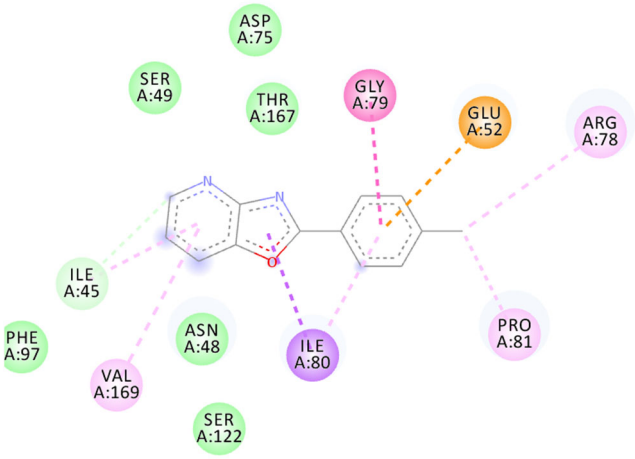
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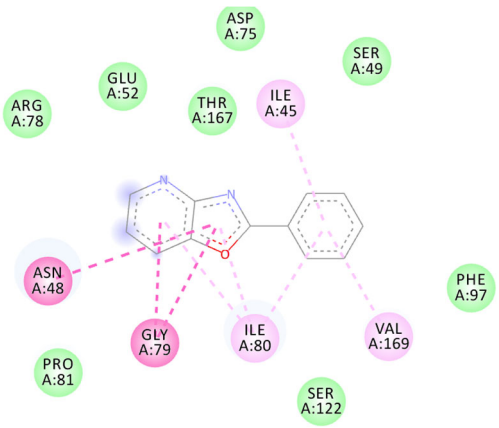
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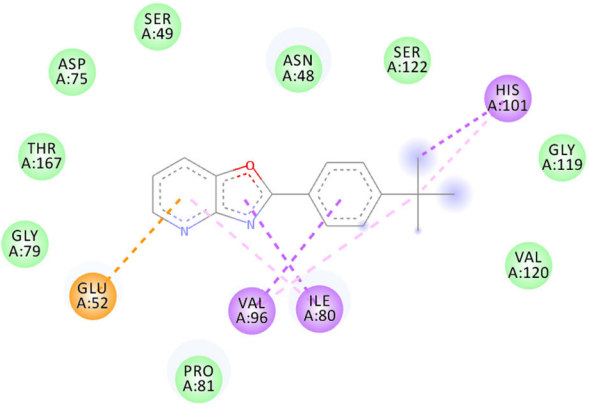
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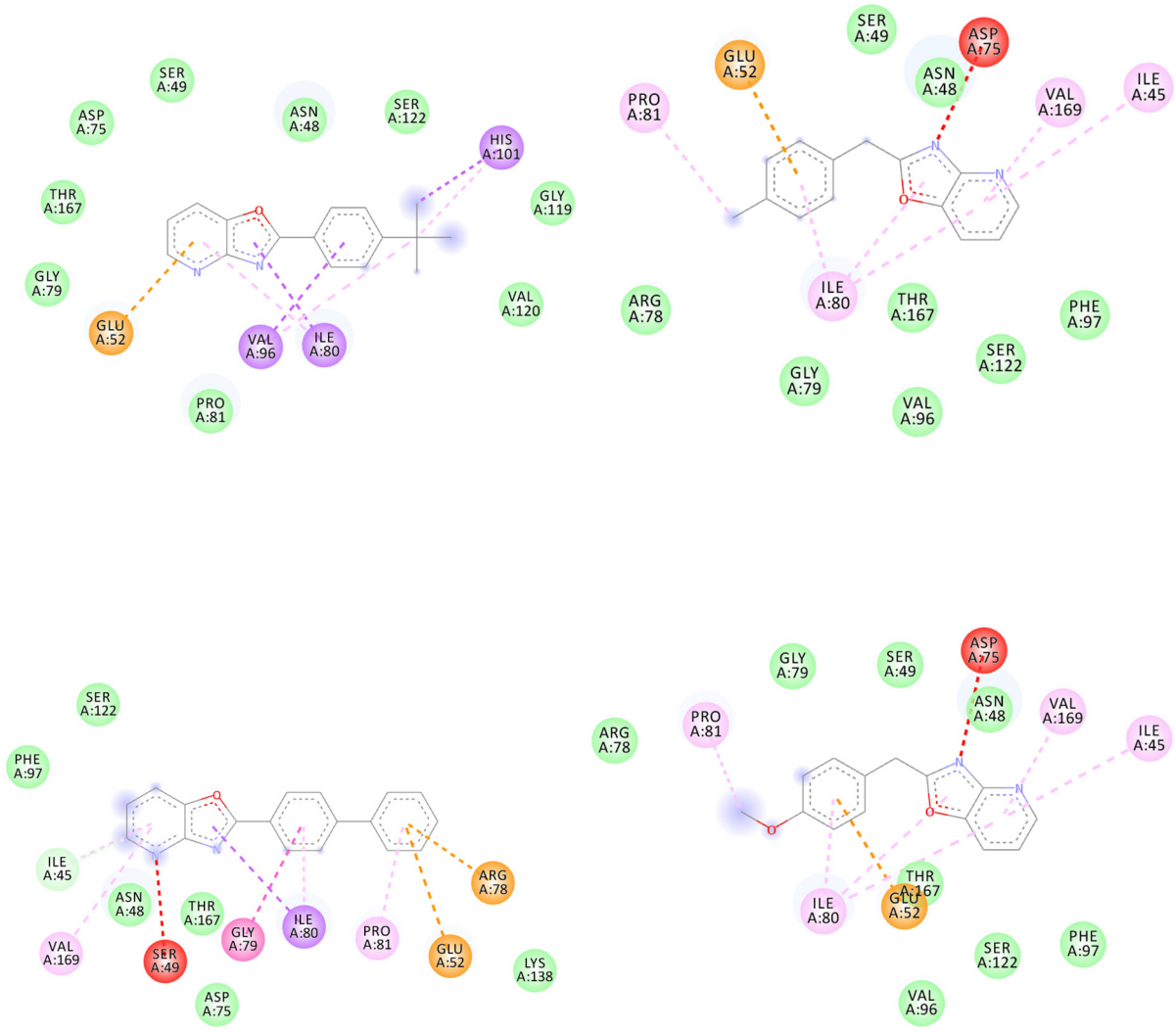

Figure S1. 2D diagram of the interactions of compounds at the DNA gyrase active site.