

Interaction, Dynamics and Stability analysis of some minor groove binders with B-DNA dodecamer 5'-(CGCAAATTTGCG)-3'

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Supporting Information

Table SI 1: The second-order perturbative estimates of donor-acceptor interactions in the NBO basis of the molecule 1.

Donor NBO (i)		Acceptor NBO (j)		E(2) kcal/mol	E(j) -E(i) a.u.	F(i,j) a.u.
BD(1)	C1-C2	RY*(1)	C3	1.95	1.8	0.053
BD(1)	C1-C2	RY*(1)	C5	0.66	1.99	0.033
BD(1)	C1-C2	RY*(2)	C5	0.9	1.84	0.036
BD(1)	C1-C2	BD*(1)	C1-C5	4.87	1.23	0.069
BD(1)	C1-C2	BD*(1)	C2-C3	2.36	1.23	0.048
BD(1)	C1-C2	BD*(1)	C2-H42	2.09	1.21	0.045
BD(1)	C1-C2	BD*(1)	C3-C11	4.24	1.23	0.065
BD(1)	C1-C2	BD*(1)	C5-C6	1.66	1.28	0.041
BD(2)	C1-C2	RY*(3)	C5	1.07	1.53	0.038
BD(2)	C1-C2	RY*(2)	O17	0.5	1.4	0.025
BD(2)	C1-C2	BD*(2)	C3-C4	16.09	0.3	0.064
BD(2)	C1-C2	BD*(1)	C5-C6	0.51	0.84	0.019
BD(2)	C1-C2	BD*(2)	C5-C10	11.15	0.3	0.054
BD(1)	C1-C5	RY*(1)	C2	0.67	1.93	0.032
BD(1)	C1-C5	RY*(1)	C6	1.27	1.94	0.044
BD(1)	C1-C5	RY*(1)	C10	0.99	1.94	0.039
BD(1)	C1-C5	RY*(1)	O17	0.51	1.88	0.028
BD(1)	C1-C5	BD*(1)	C1-C2	4.25	1.3	0.066
BD(1)	C1-C5	BD*(1)	C2-C3	0.83	1.21	0.028
BD(1)	C1-C5	BD*(1)	C4-O17	1.68	1.01	0.037
BD(1)	C1-C5	BD*(1)	C5-C6	3.05	1.25	0.055

BD(1)	C1-C5	BD*(1)	C5-C10	2.7	1.25	0.052
BD(1)	C1-C5	BD*(1)	C6-C7	1.66	1.29	0.041
BD(1)	C1-C5	BD*(1)	C9-C10	1.71	1.28	0.042
BD(1)	C1-O17	RY*(2)	C4	1.86	1.78	0.052
BD(1)	C1-O17	RY*(2)	C5	0.69	1.98	0.033
BD(1)	C1-O17	BD*(1)	C1-C2	0.58	1.48	0.026
BD(1)	C1-O17	BD*(1)	C2-H42	2.28	1.35	0.05
BD(1)	C1-O17	BD*(1)	C4-H43	2.65	1.35	0.053
BD(1)	C1-O17	BD*(1)	C5-C10	1.5	1.43	0.041
BD(1)	C2-C3	RY*(1)	C1	1.8	1.6	0.048
BD(1)	C2-C3	RY*(2)	C11	1.01	1.79	0.038
BD(1)	C2-C3	BD*(1)	C1-C2	2.58	1.26	0.051
BD(1)	C2-C3	BD*(1)	C1-C5	6.13	1.16	0.075
BD(1)	C2-C3	BD*(1)	C1-O17	1.87	0.95	0.038
BD(1)	C2-C3	BD*(1)	C2-H42	1.22	1.14	0.033
BD(1)	C2-C3	BD*(1)	C3-C4	2.52	1.25	0.05
BD(1)	C2-C3	BD*(1)	C3-C11	2.61	1.16	0.049
BD(1)	C2-C3	BD*(1)	C4-O17	1.49	0.97	0.034
BD(1)	C2-C3	BD*(1)	C4-H43	3.65	1.13	0.058
BD(1)	C2-C3	BD*(1)	C11-C12	1.86	1.23	0.043
BD(1)	C2-H42	RY*(2)	C1	0.99	1.78	0.038
BD(1)	C2-H42	RY*(2)	C3	0.87	1.78	0.035
BD(1)	C2-H42	BD*(1)	C1-C2	2.16	1.16	0.045
BD(1)	C2-H42	BD*(1)	C1-O17	3.42	0.85	0.048
BD(1)	C2-H42	BD*(1)	C2-C3	1.14	1.06	0.031
BD(1)	C2-H42	BD*(1)	C3-C4	1.56	1.15	0.038
BD(1)	C3-C4	RY*(2)	C1	0.67	1.94	0.032
BD(1)	C3-C4	RY*(2)	C11	1.32	1.85	0.044
BD(1)	C3-C4	BD*(1)	C2-C3	2.68	1.23	0.051
BD(1)	C3-C4	BD*(1)	C2-H42	3.07	1.2	0.054
BD(1)	C3-C4	BD*(1)	C3-C11	4	1.22	0.063
BD(1)	C3-C4	BD*(1)	C4-H43	1.75	1.2	0.041
BD(1)	C3-C4	BD*(1)	C11-C16	1.73	1.28	0.042
BD(2)	C3-C4	RY*(3)	C2	1.17	1.53	0.04
BD(2)	C3-C4	RY*(3)	C11	1	1.33	0.034
BD(2)	C3-C4	RY*(2)	O17	0.88	1.4	0.033
BD(2)	C3-C4	BD*(2)	C1-C2	14.24	0.3	0.06
BD(2)	C3-C4	BD*(2)	C3-C4	0.97	0.3	0.016
BD(2)	C3-C4	BD*(2)	C11-C12	9.72	0.31	0.051
BD(2)	C3-C4	BD*(1)	C11-C16	0.55	0.84	0.02
BD(1)	C3-C11	RY*(1)	C2	0.75	1.9	0.034

BD(1)	C3-C11	RY*(1)	C12	1.05	1.93	0.04
BD(1)	C3-C11	RY*(1)	C16	1.01	1.93	0.04
BD(1)	C3-C11	BD*(1)	C1-C2	0.64	1.27	0.026
BD(1)	C3-C11	BD*(1)	C2-C3	2.65	1.18	0.05
BD(1)	C3-C11	BD*(1)	C3-C4	3.59	1.26	0.06
BD(1)	C3-C11	BD*(1)	C4-O17	1.24	0.99	0.031
BD(1)	C3-C11	BD*(1)	C11-C12	2.78	1.24	0.052
BD(1)	C3-C11	BD*(1)	C11-C16	2.7	1.23	0.052
BD(1)	C3-C11	BD*(1)	C12-C13	1.79	1.26	0.042
BD(1)	C3-C11	BD*(1)	C15-C16	1.72	1.26	0.042
BD(1)	C4-O17	RY*(2)	C1	1.55	2.1	0.051
BD(1)	C4-O17	RY*(1)	C3	0.63	1.95	0.031
BD(1)	C4-O17	BD*(1)	C1-C5	2.59	1.38	0.054
BD(1)	C4-O17	BD*(1)	C3-C11	3.14	1.38	0.059
BD(1)	C4-H43	RY*(2)	C3	1.22	1.8	0.042
BD(1)	C4-H43	RY*(1)	O17	0.51	1.76	0.027
BD(1)	C4-H43	BD*(1)	C1-O17	2.16	0.88	0.039
BD(1)	C4-H43	BD*(1)	C2-C3	2.49	1.09	0.046
BD(1)	C4-H43	BD*(1)	C3-C4	1.67	1.17	0.039
BD(1)	C5-C6	RY*(1)	C1	1.31	1.64	0.042
BD(1)	C5-C6	RY*(1)	C7	0.81	1.96	0.036
BD(1)	C5-C6	RY*(2)	C7	1.54	1.47	0.043
BD(1)	C5-C6	RY*(2)	C10	0.52	1.46	0.025
BD(1)	C5-C6	BD*(1)	C1-C2	2.39	1.3	0.05
BD(1)	C5-C6	BD*(1)	C1-C5	2.89	1.2	0.053
BD(1)	C5-C6	BD*(1)	C5-C10	3.84	1.25	0.062
BD(1)	C5-C6	BD*(1)	C6-C7	2.77	1.29	0.053
BD(1)	C5-C6	BD*(1)	C6-H54	1.31	1.19	0.035
BD(1)	C5-C6	BD*(1)	C7-H55	2.11	1.18	0.045
BD(1)	C5-C6	BD*(1)	C10-H53	2.05	1.18	0.044
BD(1)	C5-C10	RY*(1)	C1	0.86	1.64	0.034
BD(1)	C5-C10	RY*(1)	C6	0.52	1.94	0.028
BD(1)	C5-C10	RY*(1)	C9	0.93	1.96	0.038
BD(1)	C5-C10	RY*(2)	C9	1.34	1.47	0.04
BD(1)	C5-C10	BD*(1)	C1-C5	3.18	1.2	0.055
BD(1)	C5-C10	BD*(1)	C1-O17	2.74	0.99	0.047
BD(1)	C5-C10	BD*(1)	C5-C6	3.83	1.25	0.062
BD(1)	C5-C10	BD*(1)	C6-H54	1.98	1.19	0.044
BD(1)	C5-C10	BD*(1)	C9-C10	2.79	1.28	0.053
BD(1)	C5-C10	BD*(1)	C9-H52	2.09	1.18	0.044
BD(1)	C5-C10	BD*(1)	C10-H53	1.28	1.18	0.035

BD(2)	C5-C10	RY*(3)	C6	1.22	1.53	0.043
BD(2)	C5-C10	RY*(4)	C9	1.42	1.12	0.039
BD(2)	C5-C10	BD*(2)	C1-C2	14.22	0.28	0.058
BD(2)	C5-C10	BD*(1)	C1-O17	1.19	0.56	0.025
BD(2)	C5-C10	BD*(2)	C6-C7	18.11	0.28	0.065
BD(2)	C5-C10	BD*(2)	C8-C9	21.08	0.28	0.069
BD(1)	C6-C7	RY*(1)	C5	1.82	1.97	0.054
BD(1)	C6-C7	RY*(2)	C8	2.08	1.97	0.057
BD(1)	C6-C7	BD*(1)	C1-C5	3.2	1.21	0.056
BD(1)	C6-C7	BD*(1)	C5-C6	3.17	1.26	0.056
BD(1)	C6-C7	BD*(1)	C6-H54	1.53	1.2	0.038
BD(1)	C6-C7	BD*(1)	C7-C8	3.38	1.27	0.059
BD(1)	C6-C7	BD*(1)	C7-H55	1.6	1.19	0.039
BD(1)	C6-C7	BD*(1)	C8-C18	2.91	1.16	0.052
BD(2)	C6-C7	RY*(6)	C5	0.66	1.67	0.032
BD(2)	C6-C7	BD*(2)	C5-C10	19.77	0.28	0.067
BD(2)	C6-C7	BD*(2)	C8-C9	19.25	0.28	0.067
BD(1)	C6-H54	RY*(1)	C5	1.13	1.8	0.04
BD(1)	C6-H54	RY*(1)	C7	0.93	1.8	0.037
BD(1)	C6-H54	BD*(1)	C5-C6	1.09	1.09	0.031
BD(1)	C6-H54	BD*(1)	C5-C10	3.82	1.09	0.058
BD(1)	C6-H54	BD*(1)	C6-C7	1.22	1.13	0.033
BD(1)	C6-H54	BD*(1)	C7-C8	3.69	1.1	0.057
BD(1)	C7-C8	RY*(1)	C6	0.67	1.93	0.032
BD(1)	C7-C8	RY*(2)	C6	1.68	1.46	0.044
BD(1)	C7-C8	RY*(1)	C18	0.53	1.55	0.026
BD(1)	C7-C8	RY*(2)	C18	0.92	1.58	0.034
BD(1)	C7-C8	BD*(1)	C6-C7	2.99	1.28	0.056
BD(1)	C7-C8	BD*(1)	C6-H54	2	1.19	0.044
BD(1)	C7-C8	BD*(1)	C7-H55	1.41	1.18	0.037
BD(1)	C7-C8	BD*(1)	C8-C9	3.93	1.26	0.063
BD(1)	C7-C8	BD*(1)	C8-C18	2.26	1.15	0.046
BD(1)	C7-C8	BD*(1)	C9-H52	2.19	1.18	0.045
BD(1)	C7-C8	BD*(1)	C18-N21	1.69	1.18	0.04
BD(1)	C7-H55	RY*(1)	C6	0.94	1.78	0.037
BD(1)	C7-H55	RY*(2)	C8	1.08	1.8	0.039
BD(1)	C7-H55	BD*(1)	C5-C6	3.58	1.1	0.056
BD(1)	C7-H55	BD*(1)	C6-C7	1.07	1.13	0.031
BD(1)	C7-H55	BD*(1)	C7-C8	1.25	1.11	0.033
BD(1)	C7-H55	BD*(1)	C8-C9	3.81	1.11	0.058
BD(1)	C7-H55	BD*(1)	N19-H20	1.1	1.02	0.03

BD(1)	C8-C9	RY*(1)	C10	1	1.94	0.04
BD(1)	C8-C9	RY*(2)	C10	1.19	1.46	0.037
BD(1)	C8-C9	RY*(2)	C18	1.21	1.58	0.039
BD(1)	C8-C9	BD*(1)	C7-C8	3.99	1.27	0.064
BD(1)	C8-C9	BD*(1)	C7-H55	2.03	1.19	0.044
BD(1)	C8-C9	BD*(1)	C8-C18	2.32	1.16	0.047
BD(1)	C8-C9	BD*(1)	C9-C10	3.06	1.28	0.056
BD(1)	C8-C9	BD*(1)	C9-H52	1.49	1.18	0.038
BD(1)	C8-C9	BD*(1)	C10-H53	2.02	1.18	0.044
BD(1)	C8-C9	BD*(1)	C18-N19	1.97	1.29	0.045
BD(2)	C8-C9	RY*(3)	C7	0.81	1.96	0.039
BD(2)	C8-C9	RY*(4)	C10	1.48	1.32	0.044
BD(2)	C8-C9	BD*(2)	C5-C10	20.45	0.28	0.067
BD(2)	C8-C9	BD*(2)	C6-C7	18.86	0.28	0.066
BD(2)	C8-C9	BD*(2)	C18-N19	16.39	0.29	0.064
BD(1)	C8-C18	RY*(1)	C7	1.16	1.92	0.042
BD(1)	C8-C18	RY*(1)	C9	1.04	1.92	0.04
BD(1)	C8-C18	RY*(1)	N19	0.91	1.69	0.035
BD(1)	C8-C18	RY*(1)	N21	0.77	1.62	0.032
BD(1)	C8-C18	BD*(1)	C6-C7	2.07	1.25	0.045
BD(1)	C8-C18	BD*(1)	C7-C8	2.3	1.22	0.047
BD(1)	C8-C18	BD*(1)	C8-C9	2.56	1.22	0.05
BD(1)	C8-C18	BD*(1)	C9-C10	1.81	1.24	0.042
BD(1)	C8-C18	BD*(1)	C18-N19	1.83	1.25	0.043
BD(1)	C8-C18	BD*(1)	C18-N21	0.71	1.14	0.025
BD(1)	C8-C18	BD*(1)	N21-C23	2.7	1.02	0.047
BD(1)	C9-C10	RY*(2)	C5	2	1.82	0.054
BD(1)	C9-C10	RY*(1)	C8	2.33	1.86	0.059
BD(1)	C9-C10	BD*(1)	C1-C5	3.11	1.21	0.055
BD(1)	C9-C10	BD*(1)	C5-C10	3.21	1.26	0.057
BD(1)	C9-C10	BD*(1)	C8-C9	3.43	1.27	0.059
BD(1)	C9-C10	BD*(1)	C8-C18	3.22	1.16	0.055
BD(1)	C9-C10	BD*(1)	C9-H52	1.58	1.19	0.039
BD(1)	C9-C10	BD*(1)	C10-H53	1.5	1.19	0.038
BD(1)	C9-H52	RY*(2)	C8	1.13	1.81	0.04
BD(1)	C9-H52	RY*(1)	C10	1.02	1.79	0.038
BD(1)	C9-H52	BD*(1)	C5-C10	3.56	1.1	0.056
BD(1)	C9-H52	BD*(1)	C7-C8	3.77	1.11	0.058
BD(1)	C9-H52	BD*(1)	C8-C9	1.24	1.11	0.033
BD(1)	C9-H52	BD*(1)	C9-C10	1.11	1.13	0.032
BD(1)	C10-H53	RY*(1)	C5	1.22	1.81	0.042

BD(1)	C10-H53	RY*(1)	C9	0.96	1.81	0.037
BD(1)	C10-H53	BD*(1)	C5-C6	3.71	1.1	0.057
BD(1)	C10-H53	BD*(1)	C5-C10	1.03	1.1	0.03
BD(1)	C10-H53	BD*(1)	C8-C9	3.62	1.11	0.057
BD(1)	C10-H53	BD*(1)	C9-C10	1.16	1.13	0.032
BD(1)	C11-C12	RY*(1)	C3	1.39	1.76	0.044
BD(1)	C11-C12	RY*(1)	C13	0.85	1.95	0.037
BD(1)	C11-C12	RY*(2)	C13	1.48	1.43	0.041
BD(1)	C11-C12	BD*(1)	C2-C3	2.31	1.2	0.047
BD(1)	C11-C12	BD*(1)	C3-C11	3.09	1.19	0.054
BD(1)	C11-C12	BD*(1)	C11-C16	3.73	1.25	0.061
BD(1)	C11-C12	BD*(1)	C12-C13	2.94	1.28	0.055
BD(1)	C11-C12	BD*(1)	C12-H39	1.37	1.18	0.036
BD(1)	C11-C12	BD*(1)	C13-H38	1.93	1.19	0.043
BD(1)	C11-C12	BD*(1)	C16-H40	2.05	1.18	0.044
BD(2)	C11-C12	RY*(3)	C3	0.63	1.5	0.03
BD(2)	C11-C12	RY*(4)	C13	1.51	0.97	0.038
BD(2)	C11-C12	RY*(4)	C16	1.53	0.96	0.038
BD(2)	C11-C12	BD*(1)	C2-C3	0.68	0.76	0.022
BD(2)	C11-C12	BD*(2)	C3-C4	13.39	0.27	0.055
BD(2)	C11-C12	BD*(2)	C13-C14	20.39	0.29	0.068
BD(2)	C11-C12	BD*(2)	C15-C16	18.95	0.28	0.066
BD(1)	C11-C16	RY*(1)	C3	0.97	1.76	0.037
BD(1)	C11-C16	RY*(1)	C15	0.94	1.95	0.038
BD(1)	C11-C16	RY*(2)	C15	1.4	1.51	0.041
BD(1)	C11-C16	BD*(1)	C3-C4	2.09	1.28	0.046
BD(1)	C11-C16	BD*(1)	C3-C11	3.02	1.19	0.053
BD(1)	C11-C16	BD*(1)	C11-C12	3.75	1.26	0.061
BD(1)	C11-C16	BD*(1)	C12-H39	2.11	1.18	0.045
BD(1)	C11-C16	BD*(1)	C15-C16	2.97	1.28	0.055
BD(1)	C11-C16	BD*(1)	C15-H41	2.12	1.18	0.045
BD(1)	C11-C16	BD*(1)	C16-H40	1.32	1.18	0.035
BD(1)	C12-C13	RY*(1)	C11	1.63	1.98	0.051
BD(1)	C12-C13	RY*(2)	C11	0.65	1.83	0.031
BD(1)	C12-C13	RY*(1)	C14	1.83	1.89	0.053
BD(1)	C12-C13	RY*(3)	C14	0.72	1.58	0.03
BD(1)	C12-C13	BD*(1)	C3-C11	3.23	1.19	0.056
BD(1)	C12-C13	BD*(1)	C11-C12	3.34	1.27	0.058
BD(1)	C12-C13	BD*(1)	C12-H39	1.5	1.18	0.038
BD(1)	C12-C13	BD*(1)	C13-C14	3.24	1.27	0.057
BD(1)	C12-C13	BD*(1)	C13-H38	1.42	1.19	0.037

BD(1)	C12-C13	BD*(1)	C14-C28	3.31	1.14	0.055
BD(1)	C12-H39	RY*(1)	C11	1.26	1.82	0.043
BD(1)	C12-H39	RY*(1)	C13	0.97	1.79	0.037
BD(1)	C12-H39	BD*(1)	C11-C12	1.12	1.11	0.031
BD(1)	C12-H39	BD*(1)	C11-C16	3.8	1.1	0.058
BD(1)	C12-H39	BD*(1)	C12-C13	1.09	1.12	0.031
BD(1)	C12-H39	BD*(1)	C13-C14	3.54	1.11	0.056
BD(1)	C13-C14	RY*(1)	C12	0.9	1.95	0.038
BD(1)	C13-C14	RY*(2)	C12	1.3	1.47	0.039
BD(1)	C13-C14	RY*(2)	C15	0.51	1.52	0.025
BD(1)	C13-C14	RY*(2)	C28	0.57	1.5	0.026
BD(1)	C13-C14	BD*(1)	C12-C13	2.82	1.28	0.054
BD(1)	C13-C14	BD*(1)	C12-H39	2.03	1.18	0.044
BD(1)	C13-C14	BD*(1)	C13-H38	1.4	1.19	0.037
BD(1)	C13-C14	BD*(1)	C14-C15	3.83	1.26	0.062
BD(1)	C13-C14	BD*(1)	C14-C28	2.52	1.14	0.048
BD(1)	C13-C14	BD*(1)	C15-H41	2.14	1.19	0.045
BD(1)	C13-C14	BD*(2)	C28-N29	0.99	0.71	0.024
BD(1)	C13-C14	BD*(1)	C28-N31	0.9	1.15	0.029
BD(2)	C13-C14	RY*(4)	C12	1.62	1.17	0.043
BD(2)	C13-C14	RY*(4)	C15	1.45	1	0.038
BD(2)	C13-C14	BD*(2)	C11-C12	21.2	0.28	0.068
BD(2)	C13-C14	BD*(2)	C15-C16	19.85	0.27	0.067
BD(2)	C13-C14	BD*(1)	C28-N29	2.02	0.84	0.04
BD(2)	C13-C14	BD*(2)	C28-N29	4.94	0.27	0.035
BD(2)	C13-C14	BD*(1)	C28-N31	2.81	0.71	0.043
BD(1)	C13-H38	RY*(1)	C12	0.88	1.79	0.036
BD(1)	C13-H38	RY*(1)	C14	1.17	1.73	0.04
BD(1)	C13-H38	BD*(1)	C11-C12	3.67	1.1	0.057
BD(1)	C13-H38	BD*(1)	C12-C13	1.08	1.12	0.031
BD(1)	C13-H38	BD*(1)	C13-C14	1.17	1.11	0.032
BD(1)	C13-H38	BD*(1)	C14-C15	3.82	1.1	0.058
BD(1)	C14-C15	RY*(1)	C13	0.52	1.94	0.029
BD(1)	C14-C15	RY*(2)	C13	0.54	1.43	0.025
BD(1)	C14-C15	RY*(1)	C16	0.95	1.95	0.039
BD(1)	C14-C15	RY*(2)	C16	1.22	1.48	0.038
BD(1)	C14-C15	RY*(2)	C28	0.66	1.5	0.028
BD(1)	C14-C15	BD*(1)	C13-C14	3.62	1.26	0.061
BD(1)	C14-C15	BD*(1)	C13-H38	2.11	1.19	0.045
BD(1)	C14-C15	BD*(1)	C14-C28	1.96	1.13	0.042
BD(1)	C14-C15	BD*(1)	C15-C16	3.09	1.28	0.056

BD(1)	C14-C15	BD*(1)	C15-H41	1.47	1.19	0.037
BD(1)	C14-C15	BD*(1)	C16-H40	2.08	1.18	0.044
BD(1)	C14-C15	BD*(1)	C28-N29	0.95	1.28	0.031
BD(1)	C14-C15	BD*(2)	C28-N29	0.96	0.71	0.024
BD(1)	C14-C28	RY*(1)	C13	1.2	1.9	0.043
BD(1)	C14-C28	RY*(1)	C15	1.27	1.91	0.044
BD(1)	C14-C28	RY*(1)	N29	1.49	1.6	0.044
BD(1)	C14-C28	RY*(1)	N31	1.93	1.53	0.049
BD(1)	C14-C28	BD*(1)	C12-C13	1.89	1.23	0.043
BD(1)	C14-C28	BD*(1)	C13-C14	2.59	1.22	0.05
BD(1)	C14-C28	BD*(1)	C14-C15	2.36	1.22	0.048
BD(1)	C14-C28	BD*(1)	C15-C16	2.26	1.24	0.047
BD(1)	C14-C28	BD*(1)	C28-N29	1.68	1.23	0.041
BD(1)	C14-C28	BD*(1)	C28-N31	0.53	1.11	0.022
BD(1)	C14-C28	BD*(1)	N29-H30	3.73	1.1	0.057
BD(1)	C14-C28	BD*(1)	N31-H32	1.14	1.1	0.032
BD(1)	C14-C28	BD*(1)	N31-C33	0.8	1	0.025
BD(1)	C15-C16	RY*(2)	C11	1.87	1.83	0.052
BD(1)	C15-C16	RY*(2)	C14	1.71	1.68	0.048
BD(1)	C15-C16	RY*(3)	C14	0.65	1.59	0.029
BD(1)	C15-C16	BD*(1)	C3-C11	3.14	1.2	0.055
BD(1)	C15-C16	BD*(1)	C11-C16	3.3	1.26	0.058
BD(1)	C15-C16	BD*(1)	C14-C15	3.46	1.27	0.059
BD(1)	C15-C16	BD*(1)	C14-C28	2.85	1.14	0.051
BD(1)	C15-C16	BD*(1)	C15-H41	1.62	1.19	0.039
BD(1)	C15-C16	BD*(1)	C16-H40	1.56	1.19	0.038
BD(2)	C15-C16	BD*(2)	C11-C12	19.16	0.29	0.067
BD(2)	C15-C16	BD*(2)	C13-C14	19.23	0.29	0.067
BD(1)	C15-H41	RY*(1)	C14	1.28	1.73	0.042
BD(1)	C15-H41	RY*(1)	C16	1.03	1.8	0.039
BD(1)	C15-H41	BD*(1)	C11-C16	3.59	1.1	0.056
BD(1)	C15-H41	BD*(1)	C13-C14	3.64	1.11	0.057
BD(1)	C15-H41	BD*(1)	C14-C15	1.24	1.11	0.033
BD(1)	C15-H41	BD*(1)	C15-C16	1.17	1.13	0.033
BD(1)	C16-H40	RY*(1)	C11	1.29	1.82	0.043
BD(1)	C16-H40	RY*(1)	C15	0.96	1.81	0.037
BD(1)	C16-H40	BD*(1)	C11-C12	3.67	1.11	0.057
BD(1)	C16-H40	BD*(1)	C11-C16	1.07	1.1	0.031
BD(1)	C16-H40	BD*(1)	C14-C15	3.61	1.11	0.057
BD(1)	C16-H40	BD*(1)	C15-C16	1.14	1.13	0.032
BD(1)	C18-N19	RY*(1)	C8	0.63	2.01	0.032

BD(1)	C18-N19	RY*(1)	C18	0.7	1.71	0.031
BD(1)	C18-N19	BD*(1)	C8-C9	1.17	1.42	0.036
BD(1)	C18-N19	BD*(1)	C8-C18	2.36	1.31	0.05
BD(1)	C18-N19	BD*(1)	C18-N21	1.66	1.33	0.042
BD(1)	C18-N19	BD*(1)	N21-H22	1.42	1.31	0.039
BD(2)	C18-N19	BD*(2)	C8-C9	7.47	0.33	0.048
BD(2)	C18-N19	BD*(1)	N21-H22	1.27	0.77	0.028
BD(2)	C18-N19	BD*(1)	N21-C23	0.82	0.67	0.021
BD(1)	C18-N21	RY*(1)	C8	1.22	1.95	0.044
BD(1)	C18-N21	RY*(1)	C23	2.11	1.83	0.056
BD(1)	C18-N21	RY*(2)	C23	0.5	1.7	0.026
BD(1)	C18-N21	BD*(1)	C7-C8	1.67	1.36	0.043
BD(1)	C18-N21	BD*(1)	C8-C18	0.71	1.25	0.027
BD(1)	C18-N21	BD*(1)	C18-N19	1.53	1.39	0.041
BD(1)	C18-N21	BD*(1)	N19-H20	2.2	1.27	0.047
BD(1)	C18-N21	BD*(1)	N21-H22	0.72	1.25	0.027
BD(1)	C18-N21	BD*(1)	N21-C23	1.5	1.16	0.037
BD(1)	C18-N21	BD*(1)	C23-C24	0.6	1.15	0.023
BD(1)	N19-H20	RY*(1)	C18	1.76	1.44	0.045
BD(1)	N19-H20	RY*(4)	C18	0.72	2.62	0.039
BD(1)	N19-H20	BD*(1)	C7-H55	0.64	1.08	0.024
BD(1)	N19-H20	BD*(1)	C18-N21	9.05	1.07	0.088
BD(1)	N21-H22	RY*(1)	C18	0.6	1.5	0.027
BD(1)	N21-H22	RY*(2)	C18	1.04	1.53	0.036
BD(1)	N21-H22	RY*(1)	C23	1.41	1.68	0.044
BD(1)	N21-H22	BD*(1)	C18-N19	2.41	1.24	0.049
BD(1)	N21-H22	BD*(2)	C18-N19	2.1	0.68	0.036
BD(1)	N21-H22	BD*(1)	C23-H64	1.25	1.17	0.034
BD(1)	N21-C23	RY*(1)	C18	0.79	1.57	0.031
BD(1)	N21-C23	RY*(3)	C18	0.53	2.2	0.031
BD(1)	N21-C23	RY*(1)	C24	0.55	1.8	0.028
BD(1)	N21-C23	BD*(1)	C8-C18	1.72	1.18	0.041
BD(1)	N21-C23	BD*(2)	C18-N19	1.08	0.75	0.027
BD(1)	N21-C23	BD*(1)	C18-N21	1.58	1.2	0.039
BD(1)	N21-C23	BD*(1)	C26-C27	0.71	1.1	0.025
BD(1)	C23-C24	RY*(1)	N21	0.71	1.53	0.03
BD(1)	C23-C24	RY*(2)	N21	0.82	1.97	0.036
BD(1)	C23-C24	RY*(1)	C25	0.62	1.68	0.029
BD(1)	C23-C24	BD*(1)	C18-N21	1.52	1.05	0.036
BD(1)	C23-C24	BD*(1)	C23-H64	0.62	1.08	0.023
BD(1)	C23-C24	BD*(1)	C24-C25	0.54	0.94	0.02

BD(1)	C23-C24	BD*(1)	C24-H62	0.54	1.06	0.021
BD(1)	C23-C24	BD*(1)	C24-H63	0.71	1.06	0.025
BD(1)	C23-C24	BD*(1)	C25-H60	1.38	1.07	0.034
BD(1)	C23-C24	BD*(1)	C27-H56	0.87	1.08	0.028
BD(1)	C23-C27	RY*(1)	N21	1.13	1.53	0.037
BD(1)	C23-C27	RY*(2)	N21	0.57	1.96	0.03
BD(1)	C23-C27	BD*(1)	C18-N21	1.17	1.05	0.031
BD(1)	C23-C27	BD*(1)	C23-H64	0.84	1.08	0.027
BD(1)	C23-C27	BD*(1)	C24-H63	0.82	1.06	0.026
BD(1)	C23-C27	BD*(1)	C26-C27	0.5	0.94	0.019
BD(1)	C23-C27	BD*(1)	C26-H59	1.42	1.07	0.035
BD(1)	C23-C27	BD*(1)	C27-H56	0.79	1.08	0.026
BD(1)	C23-H64	RY*(1)	C27	0.61	1.6	0.028
BD(1)	C23-H64	BD*(1)	N21-H22	3.38	0.96	0.051
BD(1)	C23-H64	BD*(1)	C24-C25	1.09	0.88	0.028
BD(1)	C23-H64	BD*(1)	C27-H57	1.32	1.01	0.033
BD(1)	C24-C25	RY*(1)	C26	0.58	1.69	0.028
BD(1)	C24-C25	BD*(1)	C23-C27	0.59	0.94	0.021
BD(1)	C24-C25	BD*(1)	C23-H64	0.85	1.09	0.027
BD(1)	C24-C25	BD*(1)	C24-H62	0.59	1.07	0.022
BD(1)	C24-C25	BD*(1)	C24-H63	0.68	1.06	0.024
BD(1)	C24-C25	BD*(1)	C25-C26	0.58	0.94	0.021
BD(1)	C24-C25	BD*(1)	C25-H60	0.72	1.08	0.025
BD(1)	C24-C25	BD*(1)	C25-H61	0.52	1.07	0.021
BD(1)	C24-C25	BD*(1)	C26-H59	1.84	1.08	0.04
BD(1)	C24-H62	RY*(1)	C23	0.51	1.55	0.025
BD(1)	C24-H62	RY*(1)	C25	0.53	1.63	0.026
BD(1)	C24-H62	BD*(1)	N21-C23	2.01	0.88	0.038
BD(1)	C24-H62	BD*(1)	C25-H61	1.97	1.01	0.04
BD(1)	C24-H63	RY*(2)	C23	0.66	1.41	0.027
BD(1)	C24-H63	RY*(2)	C25	0.52	1.55	0.026
BD(1)	C24-H63	BD*(1)	N21-C23	0.91	0.88	0.025
BD(1)	C24-H63	BD*(1)	C23-C27	0.91	0.88	0.025
BD(1)	C24-H63	BD*(1)	C25-C26	1.83	0.88	0.036
BD(1)	C25-C26	RY*(1)	C27	0.57	1.65	0.028
BD(1)	C25-C26	BD*(1)	C23-C24	0.6	0.92	0.021
BD(1)	C25-C26	BD*(1)	C23-C27	0.58	0.93	0.021
BD(1)	C25-C26	BD*(1)	C24-C25	0.61	0.94	0.021
BD(1)	C25-C26	BD*(1)	C24-H63	1.8	1.06	0.039
BD(1)	C25-C26	BD*(1)	C25-H60	0.73	1.07	0.025
BD(1)	C25-C26	BD*(1)	C25-H61	0.54	1.06	0.021

BD(1)	C25-C26	BD*(1)	C26-C27	0.58	0.94	0.021
BD(1)	C25-C26	BD*(1)	C26-H58	0.5	1.07	0.021
BD(1)	C25-C26	BD*(1)	C26-H59	0.69	1.07	0.024
BD(1)	C25-C26	BD*(1)	C27-H56	1.72	1.08	0.039
BD(1)	C25-H60	RY*(2)	C26	0.54	1.55	0.026
BD(1)	C25-H60	BD*(1)	C23-C24	1.94	0.86	0.037
BD(1)	C25-H60	BD*(1)	C26-C27	1.88	0.89	0.036
BD(1)	C25-H61	RY*(1)	C24	0.69	1.59	0.03
BD(1)	C25-H61	BD*(1)	C24-H62	1.9	1.01	0.039
BD(1)	C25-H61	BD*(1)	C26-H58	2.15	1.01	0.042
BD(1)	C26-C27	RY*(1)	C25	0.56	1.68	0.027
BD(1)	C26-C27	BD*(1)	N21-C23	1.64	0.93	0.035
BD(1)	C26-C27	BD*(1)	C23-C24	0.52	0.91	0.02
BD(1)	C26-C27	BD*(1)	C25-C26	0.59	0.93	0.021
BD(1)	C26-C27	BD*(1)	C25-H60	1.89	1.07	0.04
BD(1)	C26-C27	BD*(1)	C26-H58	0.57	1.06	0.022
BD(1)	C26-C27	BD*(1)	C26-H59	0.76	1.07	0.025
BD(1)	C26-C27	BD*(1)	C27-H56	0.64	1.08	0.023
BD(1)	C26-C27	BD*(1)	C27-H57	0.52	1.06	0.021
BD(1)	C26-H58	RY*(1)	C27	0.61	1.59	0.028
BD(1)	C26-H58	BD*(1)	C25-H61	2.2	1	0.042
BD(1)	C26-H58	BD*(1)	C27-H57	1.92	1.01	0.039
BD(1)	C26-H59	RY*(2)	C25	0.5	1.55	0.025
BD(1)	C26-H59	BD*(1)	C23-C27	1.9	0.87	0.036
BD(1)	C26-H59	BD*(1)	C24-C25	1.96	0.87	0.037
BD(1)	C27-H56	RY*(1)	C23	0.71	1.53	0.029
BD(1)	C27-H56	BD*(1)	C23-C24	1.44	0.85	0.031
BD(1)	C27-H56	BD*(1)	C25-C26	1.95	0.87	0.037
BD(1)	C27-H56	BD*(1)	C27-H57	0.5	1	0.02
BD(1)	C27-H57	BD*(1)	N21-C23	1.09	0.86	0.028
BD(1)	C27-H57	BD*(1)	C23-H64	1.2	1.01	0.031
BD(1)	C27-H57	BD*(1)	C26-H58	2.07	1	0.041
BD(1)	C28-N29	RY*(2)	C14	0.66	1.86	0.031
BD(1)	C28-N29	RY*(1)	C28	0.54	1.69	0.027
BD(1)	C28-N29	BD*(1)	C14-C15	0.88	1.45	0.032
BD(1)	C28-N29	BD*(1)	C14-C28	1.64	1.33	0.042
BD(1)	C28-N29	BD*(1)	C28-N31	1.77	1.34	0.044
BD(1)	C28-N29	BD*(1)	N31-C33	0.99	1.24	0.031
BD(2)	C28-N29	RY*(3)	C14	0.57	1.21	0.024
BD(2)	C28-N29	BD*(1)	C13-C14	1.64	0.9	0.034
BD(2)	C28-N29	BD*(2)	C13-C14	2.5	0.36	0.029

BD(2)	C28-N29	BD*(1)	C14-C15	2.01	0.9	0.038
BD(2)	C28-N29	BD*(1)	N31-H32	2.34	0.78	0.038
BD(2)	C28-N29	BD*(1)	N31-C33	2.62	0.68	0.038
BD(1)	C28-N31	RY*(2)	C14	0.89	1.79	0.036
BD(1)	C28-N31	RY*(1)	C33	2.08	1.82	0.055
BD(1)	C28-N31	BD*(1)	C13-C14	1.01	1.38	0.033
BD(1)	C28-N31	BD*(2)	C13-C14	0.68	0.84	0.023
BD(1)	C28-N31	BD*(1)	C14-C28	0.85	1.25	0.029
BD(1)	C28-N31	BD*(1)	C28-N29	1.37	1.39	0.039
BD(1)	C28-N31	BD*(1)	N31-H32	0.77	1.26	0.028
BD(1)	C28-N31	BD*(1)	N31-C33	1.38	1.16	0.036
BD(1)	C28-N31	BD*(1)	C33-C37	0.57	1.14	0.023
BD(1)	N29-H30	RY*(1)	C28	1.61	1.42	0.043
BD(1)	N29-H30	RY*(4)	C28	0.86	2.44	0.041
BD(1)	N29-H30	BD*(1)	C14-C28	6.9	1.05	0.077
BD(1)	N29-H30	BD*(1)	C28-N31	0.83	1.07	0.027
BD(1)	N31-H32	RY*(1)	C28	0.95	1.45	0.033
BD(1)	N31-H32	RY*(2)	C28	0.57	1.45	0.026
BD(1)	N31-H32	RY*(1)	C33	1.17	1.65	0.04
BD(1)	N31-H32	BD*(1)	C14-C28	1.15	1.09	0.032
BD(1)	N31-H32	BD*(2)	C28-N29	4.48	0.66	0.049
BD(1)	N31-H32	BD*(1)	C33-H65	1.44	1.13	0.036
BD(1)	N31-C33	RY*(2)	C28	1.55	1.54	0.044
BD(1)	N31-C33	RY*(2)	C34	0.53	1.46	0.025
BD(1)	N31-C33	BD*(1)	C28-N29	1.27	1.32	0.037
BD(1)	N31-C33	BD*(2)	C28-N29	2.02	0.75	0.035
BD(1)	N31-C33	BD*(1)	C28-N31	1.29	1.19	0.035
BD(1)	N31-C33	BD*(1)	C34-C35	0.73	1.1	0.025
BD(1)	C33-C34	RY*(1)	N31	0.91	1.47	0.033
BD(1)	C33-C34	RY*(2)	N31	0.5	2.07	0.029
BD(1)	C33-C34	RY*(1)	C35	0.63	1.69	0.029
BD(1)	C33-C34	BD*(1)	C28-N31	1.41	1.05	0.035
BD(1)	C33-C34	BD*(1)	C33-H65	0.88	1.07	0.027
BD(1)	C33-C34	BD*(1)	C34-C35	0.59	0.95	0.021
BD(1)	C33-C34	BD*(1)	C34-H44	0.73	1.08	0.025
BD(1)	C33-C34	BD*(1)	C34-H45	0.58	1.06	0.022
BD(1)	C33-C34	BD*(1)	C35-H46	1.56	1.08	0.037
BD(1)	C33-C34	BD*(1)	C37-H50	0.83	1.07	0.027
BD(1)	C33-C37	RY*(1)	N31	0.99	1.46	0.034
BD(1)	C33-C37	BD*(1)	C28-N31	1.45	1.03	0.035
BD(1)	C33-C37	BD*(1)	C33-H65	0.67	1.06	0.024

BD(1)	C33-C37	BD*(1)	C34-H44	1.23	1.07	0.032
BD(1)	C33-C37	BD*(1)	C36-H49	1.01	1.07	0.029
BD(1)	C33-C37	BD*(1)	C37-H50	0.52	1.06	0.021
BD(1)	C33-C37	BD*(1)	C37-H51	0.65	1.07	0.024
BD(1)	C33-H65	RY*(2)	N31	0.53	2.01	0.029
BD(1)	C33-H65	RY*(1)	C34	0.64	1.63	0.029
BD(1)	C33-H65	RY*(1)	C37	0.66	1.56	0.029
BD(1)	C33-H65	BD*(1)	C15-H41	0.69	1.02	0.024
BD(1)	C33-H65	BD*(1)	N31-H32	3.59	0.98	0.053
BD(1)	C33-H65	BD*(1)	C34-H45	2	1	0.04
BD(1)	C33-H65	BD*(1)	C37-H51	1.09	1.02	0.03
BD(1)	C34-C35	RY*(1)	C36	0.5	1.67	0.026
BD(1)	C34-C35	BD*(1)	N31-C33	2.97	0.94	0.047
BD(1)	C34-C35	BD*(1)	C33-C34	0.52	0.93	0.02
BD(1)	C34-C35	BD*(1)	C34-H44	0.71	1.07	0.025
BD(1)	C34-C35	BD*(1)	C34-H45	0.58	1.06	0.022
BD(1)	C34-C35	BD*(1)	C35-C36	0.59	0.94	0.021
BD(1)	C34-C35	BD*(1)	C35-H46	0.71	1.08	0.025
BD(1)	C34-C35	BD*(1)	C35-H47	0.52	1.07	0.021
BD(1)	C34-C35	BD*(1)	C36-H49	1.74	1.08	0.039
BD(1)	C34-H44	RY*(1)	C33	0.78	1.53	0.031
BD(1)	C34-H44	RY*(2)	C35	0.53	1.56	0.026
BD(1)	C34-H44	BD*(1)	C33-C37	1.95	0.85	0.037
BD(1)	C34-H44	BD*(1)	C35-C36	1.97	0.88	0.037
BD(1)	C34-H45	RY*(2)	C33	0.58	1.58	0.027
BD(1)	C34-H45	BD*(1)	N31-C33	0.6	0.88	0.02
BD(1)	C34-H45	BD*(1)	C33-H65	1.63	1.01	0.036
BD(1)	C34-H45	BD*(1)	C35-H47	2.15	1.01	0.042
BD(1)	C35-C36	RY*(1)	C34	0.62	1.68	0.029
BD(1)	C35-C36	RY*(3)	C37	0.52	1.47	0.025
BD(1)	C35-C36	BD*(1)	C33-C37	0.68	0.91	0.022
BD(1)	C35-C36	BD*(1)	C34-C35	0.56	0.94	0.021
BD(1)	C35-C36	BD*(1)	C34-H44	1.85	1.07	0.04
BD(1)	C35-C36	BD*(1)	C35-H46	0.72	1.07	0.025
BD(1)	C35-C36	BD*(1)	C35-H47	0.53	1.06	0.021
BD(1)	C35-C36	BD*(1)	C36-C37	0.52	0.94	0.02
BD(1)	C35-C36	BD*(1)	C36-H48	0.51	1.07	0.021
BD(1)	C35-C36	BD*(1)	C36-H49	0.67	1.07	0.024
BD(1)	C35-C36	BD*(1)	C37-H51	1.34	1.07	0.034
BD(1)	C35-H46	RY*(2)	C36	0.51	1.5	0.025
BD(1)	C35-H46	BD*(1)	C33-C34	2.01	0.87	0.037

BD(1)	C35-H46	BD*(1)	C36-C37	1.91	0.88	0.037
BD(1)	C35-H47	RY*(1)	C34	0.51	1.62	0.026
BD(1)	C35-H47	RY*(1)	C36	0.53	1.6	0.026
BD(1)	C35-H47	BD*(1)	C34-H45	2.19	1	0.042
BD(1)	C35-H47	BD*(1)	C36-H48	2.01	1.01	0.04
BD(1)	C36-C37	BD*(1)	N31-C33	1.37	0.93	0.032
BD(1)	C36-C37	BD*(1)	C35-H46	1.6	1.07	0.037
BD(1)	C36-C37	BD*(1)	C36-H48	0.52	1.06	0.021
BD(1)	C36-C37	BD*(1)	C36-H49	0.72	1.07	0.025
BD(1)	C36-C37	BD*(1)	C37-H50	0.62	1.06	0.023
BD(1)	C36-C37	BD*(1)	C37-H51	0.59	1.07	0.022
BD(1)	C36-H48	RY*(1)	C35	0.51	1.62	0.026
BD(1)	C36-H48	RY*(1)	C37	0.76	1.56	0.031
BD(1)	C36-H48	BD*(1)	C35-H47	2.07	1	0.041
BD(1)	C36-H48	BD*(1)	C37-H50	1.47	1.01	0.034
BD(1)	C36-H49	BD*(1)	C33-C37	1.51	0.85	0.032
BD(1)	C36-H49	BD*(1)	C34-C35	1.9	0.88	0.037
BD(1)	C37-H50	RY*(1)	C33	0.69	1.53	0.029
BD(1)	C37-H50	RY*(1)	C36	0.66	1.6	0.029
BD(1)	C37-H50	BD*(1)	N31-C33	1.01	0.87	0.027
BD(1)	C37-H50	BD*(1)	C33-C34	1.05	0.87	0.027
BD(1)	C37-H50	BD*(1)	C36-H48	1.49	1.01	0.035
BD(1)	C37-H51	RY*(2)	C33	0.5	1.57	0.025
BD(1)	C37-H51	BD*(1)	N31-C33	0.9	0.87	0.025
BD(1)	C37-H51	BD*(1)	C33-H65	0.84	1	0.026
BD(1)	C37-H51	BD*(1)	C35-C36	1.54	0.87	0.033
CR(1)	C1	RY*(1)	C2	0.97	11.36	0.094
CR(1)	C1	RY*(2)	C2	0.92	10.88	0.089
CR(1)	C1	RY*(1)	C5	1.06	11.39	0.098
CR(1)	C1	RY*(5)	C5	0.65	11.2	0.076
CR(1)	C1	BD*(1)	C1-C2	1.17	10.73	0.1
CR(1)	C1	BD*(1)	C1-O17	1.16	10.42	0.099
CR(1)	C1	BD*(1)	C2-H42	0.91	10.61	0.088
CR(1)	C1	BD*(1)	C4-O17	0.82	10.44	0.083
CR(1)	C1	BD*(1)	C5-C6	0.67	10.68	0.076
CR(1)	C1	BD*(1)	C5-C10	0.64	10.68	0.074
CR(1)	C2	RY*(1)	C1	0.64	11	0.075
CR(1)	C2	RY*(2)	C1	1.99	11.28	0.134
CR(1)	C2	RY*(2)	C3	1.19	11.27	0.103
CR(1)	C2	RY*(1)	H42	0.73	10.6	0.079
CR(1)	C2	BD*(1)	C1-C2	0.78	10.66	0.082

CR(1)	C2	BD*(1)	C1-C5	1.75	10.56	0.122
CR(1)	C2	BD*(1)	C3-C11	1.02	10.55	0.093
CR(1)	C3	RY*(2)	C2	1.28	10.81	0.105
CR(1)	C3	RY*(2)	C4	1.5	10.97	0.115
CR(1)	C3	RY*(1)	C11	1.05	11.35	0.097
CR(1)	C3	BD*(1)	C2-H42	0.72	10.54	0.078
CR(1)	C3	BD*(1)	C3-C4	0.69	10.65	0.077
CR(1)	C3	BD*(1)	C4-H43	0.78	10.54	0.081
CR(1)	C3	BD*(1)	C11-C12	0.61	10.63	0.073
CR(1)	C3	BD*(1)	C11-C16	0.63	10.62	0.073
CR(1)	C4	RY*(1)	C3	2.46	11.2	0.148
CR(1)	C4	RY*(1)	H43	0.82	10.67	0.084
CR(1)	C4	BD*(1)	C1-O17	0.91	10.42	0.088
CR(1)	C4	BD*(1)	C3-C4	1.81	10.72	0.125
CR(1)	C4	BD*(1)	C3-C11	1.36	10.63	0.108
CR(1)	C4	BD*(1)	C4-O17	1.29	10.44	0.104
CR(1)	C5	RY*(2)	C1	0.54	11.3	0.07
CR(1)	C5	RY*(2)	C6	1.54	10.83	0.115
CR(1)	C5	RY*(2)	C10	1.26	10.83	0.104
CR(1)	C5	BD*(1)	C1-C2	1.06	10.68	0.095
CR(1)	C5	BD*(1)	C6-C7	0.58	10.66	0.07
CR(1)	C5	BD*(1)	C6-H54	0.53	10.57	0.067
CR(1)	C5	BD*(1)	C9-C10	0.57	10.65	0.07
CR(1)	C5	BD*(1)	C10-H53	0.54	10.55	0.068
CR(1)	C6	RY*(2)	C5	1.98	11.17	0.133
CR(1)	C6	RY*(2)	C7	1.6	10.83	0.117
CR(1)	C6	RY*(1)	H54	0.68	10.6	0.076
CR(1)	C6	BD*(1)	C1-C5	0.82	10.56	0.084
CR(1)	C6	BD*(1)	C5-C10	0.76	10.61	0.081
CR(1)	C6	BD*(1)	C7-C8	0.8	10.62	0.083
CR(1)	C6	BD*(1)	C7-H55	0.62	10.54	0.072
CR(1)	C7	RY*(2)	C6	1.32	10.82	0.107
CR(1)	C7	RY*(5)	C6	0.74	11.1	0.081
CR(1)	C7	RY*(1)	C8	2.06	11.21	0.136
CR(1)	C7	RY*(1)	H55	0.67	10.65	0.076
CR(1)	C7	BD*(1)	C5-C6	0.77	10.61	0.081
CR(1)	C7	BD*(1)	C6-H54	0.57	10.55	0.069
CR(1)	C7	BD*(1)	C8-C9	0.79	10.62	0.082
CR(1)	C7	BD*(1)	C8-C18	0.74	10.51	0.08
CR(1)	C8	RY*(2)	C7	1.39	10.84	0.11
CR(1)	C8	RY*(2)	C9	1.36	10.83	0.108

CR(1)	C8	RY*(1)	C18	1.16	10.92	0.101
CR(1)	C8	BD*(1)	C6-C7	0.62	10.65	0.073
CR(1)	C8	BD*(1)	C7-H55	0.55	10.55	0.068
CR(1)	C8	BD*(1)	C9-C10	0.63	10.64	0.074
CR(1)	C8	BD*(1)	C9-H52	0.58	10.55	0.07
CR(1)	C8	BD*(1)	C18-N19	0.64	10.65	0.074
CR(1)	C9	RY*(1)	C8	0.65	11.21	0.076
CR(1)	C9	RY*(2)	C8	1.63	11.32	0.121
CR(1)	C9	RY*(2)	C10	1.61	10.82	0.118
CR(1)	C9	RY*(5)	C10	0.59	11.1	0.073
CR(1)	C9	RY*(1)	H52	0.68	10.69	0.076
CR(1)	C9	BD*(1)	C5-C10	0.76	10.61	0.081
CR(1)	C9	BD*(1)	C7-C8	0.77	10.62	0.081
CR(1)	C9	BD*(1)	C8-C18	0.85	10.51	0.086
CR(1)	C9	BD*(1)	C10-H53	0.59	10.54	0.07
CR(1)	C10	RY*(1)	C5	1.31	11.32	0.109
CR(1)	C10	RY*(2)	C5	0.7	11.17	0.079
CR(1)	C10	RY*(2)	C9	1.68	10.83	0.121
CR(1)	C10	RY*(5)	C9	0.53	11.11	0.069
CR(1)	C10	RY*(1)	H53	0.63	10.61	0.073
CR(1)	C10	BD*(1)	C1-C5	0.83	10.57	0.084
CR(1)	C10	BD*(1)	C5-C6	0.75	10.62	0.08
CR(1)	C10	BD*(1)	C8-C9	0.81	10.63	0.083
CR(1)	C10	BD*(1)	C9-H52	0.6	10.54	0.071
CR(1)	C11	RY*(2)	C3	0.75	11.28	0.082
CR(1)	C11	RY*(5)	C3	0.64	11.36	0.076
CR(1)	C11	RY*(2)	C12	1.41	10.83	0.11
CR(1)	C11	RY*(2)	C16	1.27	10.85	0.105
CR(1)	C11	BD*(1)	C2-C3	0.71	10.57	0.078
CR(1)	C11	BD*(1)	C3-C4	0.74	10.65	0.08
CR(1)	C11	BD*(1)	C12-C13	0.61	10.65	0.072
CR(1)	C11	BD*(1)	C12-H39	0.55	10.55	0.068
CR(1)	C11	BD*(1)	C15-C16	0.6	10.65	0.072
CR(1)	C11	BD*(1)	C16-H40	0.54	10.55	0.068
CR(1)	C12	RY*(2)	C11	1.94	11.18	0.132
CR(1)	C12	RY*(2)	C13	1.57	10.79	0.116
CR(1)	C12	RY*(5)	C13	0.6	11.15	0.073
CR(1)	C12	RY*(1)	H39	0.62	10.62	0.072
CR(1)	C12	BD*(1)	C3-C11	0.86	10.55	0.086
CR(1)	C12	BD*(1)	C11-C16	0.75	10.61	0.08
CR(1)	C12	BD*(1)	C13-C14	0.76	10.63	0.081

CR(1)	C12	BD*(1)	C13-H38	0.56	10.55	0.069
CR(1)	C13	RY*(2)	C12	1.46	10.82	0.112
CR(1)	C13	RY*(5)	C12	0.67	11.11	0.077
CR(1)	C13	RY*(2)	C14	1.52	11.03	0.116
CR(1)	C13	RY*(3)	C14	0.68	10.94	0.077
CR(1)	C13	RY*(1)	H38	0.63	10.59	0.073
CR(1)	C13	BD*(1)	C11-C12	0.79	10.62	0.082
CR(1)	C13	BD*(1)	C12-H39	0.6	10.54	0.071
CR(1)	C13	BD*(1)	C14-C15	0.76	10.62	0.081
CR(1)	C13	BD*(1)	C14-C28	0.91	10.49	0.088
CR(1)	C14	RY*(2)	C13	1.52	10.8	0.114
CR(1)	C14	RY*(2)	C15	1.48	10.88	0.113
CR(1)	C14	RY*(3)	C28	0.79	11.99	0.087
CR(1)	C14	RY*(5)	C28	0.53	11.74	0.07
CR(1)	C14	BD*(1)	C12-C13	0.61	10.64	0.072
CR(1)	C14	BD*(1)	C13-H38	0.56	10.55	0.069
CR(1)	C14	BD*(1)	C15-C16	0.62	10.65	0.073
CR(1)	C14	BD*(1)	C15-H41	0.58	10.55	0.07
CR(1)	C15	RY*(1)	C14	1.09	11.24	0.099
CR(1)	C15	RY*(3)	C14	0.62	10.94	0.073
CR(1)	C15	RY*(4)	C14	0.54	11.11	0.069
CR(1)	C15	RY*(2)	C16	1.59	10.84	0.117
CR(1)	C15	RY*(5)	C16	0.63	11.11	0.074
CR(1)	C15	RY*(1)	H41	0.68	10.72	0.076
CR(1)	C15	BD*(1)	C11-C16	0.79	10.61	0.082
CR(1)	C15	BD*(1)	C13-C14	0.75	10.63	0.08
CR(1)	C15	BD*(1)	C14-C28	0.72	10.49	0.078
CR(1)	C15	BD*(1)	C16-H40	0.6	10.54	0.071
CR(1)	C16	RY*(1)	C11	1.12	11.34	0.101
CR(1)	C16	RY*(2)	C11	0.83	11.18	0.086
CR(1)	C16	RY*(2)	C15	1.51	10.88	0.115
CR(1)	C16	RY*(5)	C15	0.68	11.11	0.078
CR(1)	C16	RY*(1)	H40	0.62	10.62	0.072
CR(1)	C16	BD*(1)	C3-C11	0.85	10.55	0.085
CR(1)	C16	BD*(1)	C11-C12	0.73	10.62	0.079
CR(1)	C16	BD*(1)	C14-C15	0.78	10.62	0.082
CR(1)	C16	BD*(1)	C15-H41	0.63	10.55	0.073
CR(1)	O17	RY*(1)	C1	2.17	19.95	0.186
CR(1)	O17	RY*(1)	C4	1.66	20.09	0.163
CR(1)	C18	RY*(2)	C8	0.87	11.39	0.089
CR(1)	C18	RY*(3)	N19	0.94	11.08	0.091

CR(1)	C18	BD*(1)	C7-C8	0.53	10.69	0.067
CR(1)	C18	BD*(1)	C8-C9	0.62	10.69	0.073
CR(1)	C18	BD*(1)	N19-H20	0.78	10.6	0.081
CR(1)	C18	BD*(1)	N21-H22	0.7	10.58	0.077
CR(1)	C18	BD*(1)	N21-C23	1.04	10.49	0.094
CR(1)	N19	RY*(1)	C18	4.33	14.97	0.228
CR(1)	N19	RY*(2)	C18	1.05	15	0.112
CR(1)	N19	RY*(1)	H20	0.56	14.83	0.081
CR(1)	N19	BD*(1)	C8-C18	1.05	14.57	0.112
CR(1)	N19	BD*(1)	C18-N21	0.55	14.6	0.081
CR(1)	N21	RY*(2)	C18	2.44	15.05	0.171
CR(1)	N21	RY*(3)	C18	0.73	15.65	0.096
CR(1)	N21	RY*(1)	H22	0.55	14.82	0.081
CR(1)	N21	RY*(2)	C23	1.33	15.07	0.126
CR(1)	N21	RY*(5)	C23	0.61	15.7	0.088
CR(1)	C23	RY*(3)	C24	0.89	11.07	0.089
CR(1)	C23	RY*(3)	C27	0.98	11.08	0.093
CR(1)	C23	RY*(1)	H64	0.62	10.72	0.073
CR(1)	C23	BD*(1)	C18-N21	0.69	10.57	0.077
CR(1)	C23	BD*(1)	N21-H22	0.53	10.54	0.067
CR(1)	C24	RY*(2)	C23	0.52	10.95	0.067
CR(1)	C24	RY*(3)	C25	0.67	10.84	0.076
CR(1)	C24	RY*(1)	H62	0.6	10.66	0.071
CR(1)	C24	RY*(1)	H63	0.6	10.71	0.072
CR(1)	C25	RY*(4)	C24	0.54	11.38	0.07
CR(1)	C25	RY*(3)	C26	0.72	10.83	0.079
CR(1)	C25	RY*(1)	H60	0.58	10.66	0.07
CR(1)	C25	RY*(1)	H61	0.57	10.66	0.07
CR(1)	C26	RY*(3)	C25	0.7	10.84	0.077
CR(1)	C26	RY*(2)	C27	0.68	10.89	0.077
CR(1)	C26	RY*(4)	C27	0.59	11.39	0.073
CR(1)	C26	RY*(1)	H58	0.58	10.66	0.07
CR(1)	C26	RY*(1)	H59	0.58	10.65	0.07
CR(1)	C27	RY*(3)	C23	0.86	11.5	0.089
CR(1)	C27	RY*(3)	C26	0.66	10.82	0.075
CR(1)	C27	RY*(1)	H56	0.61	10.66	0.072
CR(1)	C27	RY*(1)	H57	0.61	10.67	0.072
CR(1)	C28	RY*(1)	C14	1.03	11.34	0.097
CR(1)	C28	RY*(3)	N29	0.81	11.11	0.085
CR(1)	C28	BD*(1)	C13-C14	0.63	10.72	0.074
CR(1)	C28	BD*(1)	C14-C15	0.53	10.71	0.067

CR(1)	C28	BD*(1)	N29-H30	0.87	10.6	0.086
CR(1)	C28	BD*(1)	N31-H32	0.62	10.6	0.073
CR(1)	C28	BD*(1)	N31-C33	1.11	10.5	0.097
CR(1)	N29	RY*(1)	C28	4.58	14.95	0.234
CR(1)	N29	RY*(3)	C28	0.77	16.08	0.1
CR(1)	N29	RY*(5)	C28	0.52	15.82	0.081
CR(1)	N29	BD*(1)	C14-C28	0.56	14.59	0.082
CR(1)	N29	BD*(1)	C28-N31	1.12	14.6	0.116
CR(1)	N31	RY*(1)	C28	1.97	14.98	0.154
CR(1)	N31	RY*(4)	C28	0.53	16	0.082
CR(1)	N31	RY*(5)	C28	0.55	15.85	0.084
CR(1)	N31	RY*(1)	H32	0.5	14.76	0.077
CR(1)	N31	RY*(2)	C33	1.31	15.23	0.126
CR(1)	N31	RY*(5)	C33	0.95	15.61	0.108
CR(1)	N31	BD*(1)	C28-N29	0.68	14.76	0.09
CR(1)	C33	RY*(3)	C34	0.96	10.97	0.092
CR(1)	C33	RY*(3)	C37	0.97	11	0.092
CR(1)	C33	RY*(1)	H65	0.56	10.79	0.07
CR(1)	C33	BD*(1)	C28-N31	0.78	10.56	0.082
CR(1)	C34	RY*(3)	C35	0.68	10.82	0.077
CR(1)	C34	RY*(1)	H44	0.59	10.66	0.071
CR(1)	C34	RY*(1)	H45	0.59	10.67	0.071
CR(1)	C35	RY*(2)	C34	0.85	10.78	0.085
CR(1)	C35	RY*(3)	C36	0.73	10.82	0.079
CR(1)	C35	RY*(1)	H46	0.59	10.66	0.071
CR(1)	C35	RY*(1)	H47	0.58	10.66	0.07
CR(1)	C36	RY*(3)	C35	0.72	10.82	0.079
CR(1)	C36	RY*(2)	C37	0.58	10.9	0.071
CR(1)	C36	RY*(1)	H48	0.58	10.66	0.07
CR(1)	C36	RY*(1)	H49	0.59	10.66	0.071
CR(1)	C37	RY*(3)	C33	0.72	11.61	0.082
CR(1)	C37	RY*(4)	C33	0.54	11.45	0.07
CR(1)	C37	RY*(3)	C36	0.67	10.82	0.076
CR(1)	C37	RY*(1)	H50	0.6	10.68	0.071
CR(1)	C37	RY*(1)	H51	0.62	10.67	0.073
LP(1)	O17	RY*(1)	C1	3.19	1.54	0.063
LP(1)	O17	RY*(1)	C4	2.67	1.68	0.06
LP(1)	O17	BD*(1)	C1-C2	2.85	1.2	0.052
LP(1)	O17	BD*(1)	C3-C4	2.79	1.19	0.051
LP(2)	O17	RY*(3)	C1	0.77	1.41	0.032
LP(2)	O17	RY*(4)	C1	1.17	2.14	0.048

LP(2)	O17	RY*(3)	C4	2.74	1.61	0.064
LP(2)	O17	BD*(2)	C1-C2	24.98	0.36	0.085
LP(2)	O17	BD*(2)	C3-C4	24.4	0.36	0.084
LP(1)	N19	RY*(1)	C18	5.5	1.21	0.074
LP(1)	N19	RY*(2)	C18	0.69	1.24	0.027
LP(1)	N19	BD*(1)	C8-C18	13.17	0.82	0.093
LP(1)	N19	BD*(1)	C18-N21	3.03	0.84	0.045
LP(1)	N21	RY*(3)	C18	1.38	1.72	0.046
LP(1)	N21	RY*(4)	C18	0.58	2.27	0.034
LP(1)	N21	RY*(4)	C23	1.21	1.76	0.044
LP(1)	N21	BD*(1)	C8-C18	3.85	0.7	0.048
LP(1)	N21	BD*(1)	C18-N19	5.11	0.83	0.061
LP(1)	N21	BD*(2)	C18-N19	28.6	0.27	0.079
LP(1)	N21	BD*(1)	C23-C24	4.17	0.59	0.046
LP(1)	N21	BD*(1)	C23-C27	6.15	0.6	0.057
LP(1)	N29	RY*(1)	C28	5.94	1.18	0.076
LP(1)	N29	BD*(1)	C14-C28	1.81	0.82	0.034
LP(1)	N29	BD*(1)	C28-N31	15.66	0.83	0.102
LP(1)	N31	RY*(3)	C28	0.71	2.18	0.036
LP(1)	N31	RY*(3)	C33	0.54	1.8	0.029
LP(1)	N31	RY*(4)	C33	1.14	1.64	0.04
LP(1)	N31	BD*(2)	C13-C14	1.15	0.27	0.017
LP(1)	N31	BD*(1)	C14-C28	8.36	0.69	0.069
LP(1)	N31	BD*(1)	C28-N29	10.64	0.83	0.086
LP(1)	N31	BD*(2)	C28-N29	4.4	0.26	0.03
LP(1)	N31	BD*(1)	C33-C34	6.25	0.59	0.056
LP(1)	N31	BD*(1)	C33-C37	6.96	0.58	0.058
LP(1)	N31	BD*(1)	C34-C35	0.55	0.61	0.017
BD*(2)	C1-C2	RY*(6)	C1	0.55	1.69	0.071
BD*(2)	C1-C2	RY*(4)	C2	1.34	1.27	0.096
BD*(2)	C3-C4	RY*(6)	C3	0.95	1.54	0.089
BD*(2)	C3-C4	RY*(4)	C4	1.4	1.31	0.1
BD*(2)	C5-C10	RY*(6)	C5	0.65	1.39	0.061
BD*(2)	C5-C10	RY*(4)	C9	0.51	0.84	0.042
BD*(2)	C5-C10	RY*(3)	C10	1.14	1.53	0.085
BD*(2)	C5-C10	BD*(1)	C1-O17	0.58	0.28	0.025
BD*(2)	C6-C7	RY*(4)	C6	1.31	1.3	0.097
BD*(2)	C6-C7	RY*(4)	C7	1.05	1	0.076
BD*(2)	C6-C7	RY*(5)	C7	0.81	0.95	0.065
BD*(2)	C6-C7	BD*(2)	C18-N19	0.75	0.01	0.005
BD*(2)	C8-C9	RY*(5)	C8	0.92	1.27	0.07

BD*(2)	C8-C9	RY*(3)	C9	0.76	1.75	0.075
BD*(2)	C8-C9	RY*(4)	C9	0.87	0.83	0.056
BD*(2)	C8-C9	RY*(4)	C10	0.56	1.04	0.049
BD*(2)	C8-C9	BD*(2)	C18-N19	120.35	0.02	0.07
BD*(2)	C11-C12	RY*(3)	C12	0.88	1.68	0.079
BD*(2)	C11-C12	RY*(4)	C12	0.84	0.89	0.056
BD*(2)	C11-C12	RY*(4)	C16	0.57	0.68	0.041
BD*(2)	C13-C14	RY*(4)	C12	0.55	0.89	0.047
BD*(2)	C13-C14	RY*(4)	C13	1.93	0.69	0.078
BD*(2)	C13-C14	RY*(4)	C15	0.52	0.72	0.041
BD*(2)	C13-C14	BD*(1)	C28-N29	1.07	0.56	0.05
BD*(2)	C13-C14	BD*(1)	C28-N31	1.25	0.43	0.046
BD*(2)	C15-C16	RY*(4)	C15	1.3	0.72	0.069
BD*(2)	C15-C16	RY*(3)	C16	0.5	1.87	0.069
BD*(2)	C15-C16	RY*(4)	C16	1.5	0.68	0.072
BD*(2)	C18-N19	RY*(6)	C18	0.6	1.76	0.086
BD*(2)	C18-N19	RY*(2)	N19	0.92	0.91	0.077
BD*(2)	C18-N19	BD*(1)	C18-N19	0.77	0.56	0.053
BD*(2)	C18-N19	BD*(1)	N21-C23	0.94	0.33	0.045

Table SI 2: The second-order perturbative estimates of donor-acceptor interactions in the NBO basis of the molecule 2.

Donor NBO (i)		Acceptor NBO (j)		E(2) kcal/mol	E(j) -E(i) a.u.	F(i,j) a.u.
BD(1)	C1-C2	RY*(1)	C3	2.01	1.8	0.054
BD(1)	C1-C2	RY*(1)	C5	0.64	1.99	0.032
BD(1)	C1-C2	RY*(2)	C5	0.94	1.84	0.037
BD(1)	C1-C2	BD*(1)	C1-C5	4.87	1.23	0.069
BD(1)	C1-C2	BD*(1)	C2-C3	2.37	1.23	0.048
BD(1)	C1-C2	BD*(1)	C2-H46	2.07	1.21	0.045
BD(1)	C1-C2	BD*(1)	C3-C11	4.25	1.23	0.065
BD(1)	C1-C2	BD*(1)	C5-C6	1.66	1.28	0.041
BD(2)	C1-C2	RY*(3)	C5	1.08	1.53	0.038
BD(2)	C1-C2	RY*(2)	O17	0.51	1.4	0.025
BD(2)	C1-C2	BD*(2)	C3-C4	16.07	0.3	0.064
BD(2)	C1-C2	BD*(2)	C5-C10	11.17	0.3	0.054
BD(1)	C1-C5	RY*(1)	C2	0.68	1.94	0.033
BD(1)	C1-C5	RY*(1)	C6	1.27	1.94	0.045
BD(1)	C1-C5	RY*(1)	C10	0.99	1.94	0.039
BD(1)	C1-C5	RY*(1)	O17	0.52	1.88	0.028
BD(1)	C1-C5	BD*(1)	C1-C2	4.24	1.3	0.066
BD(1)	C1-C5	BD*(1)	C2-C3	0.83	1.21	0.028

BD(1)	C1-C5	BD*(1)	C4-O17	1.67	1.02	0.037
BD(1)	C1-C5	BD*(1)	C5-C6	3.03	1.25	0.055
BD(1)	C1-C5	BD*(1)	C5-C10	2.75	1.26	0.052
BD(1)	C1-C5	BD*(1)	C6-C7	1.64	1.29	0.041
BD(1)	C1-C5	BD*(1)	C9-C10	1.71	1.28	0.042
BD(1)	C1-O17	RY*(2)	C4	1.88	1.78	0.052
BD(1)	C1-O17	RY*(2)	C5	0.69	1.98	0.033
BD(1)	C1-O17	BD*(1)	C1-C2	0.56	1.48	0.026
BD(1)	C1-O17	BD*(1)	C2-H46	2.28	1.35	0.05
BD(1)	C1-O17	BD*(1)	C4-H45	2.64	1.35	0.053
BD(1)	C1-O17	BD*(1)	C5-C10	1.51	1.43	0.042
BD(1)	C2-C3	RY*(1)	C1	1.83	1.6	0.049
BD(1)	C2-C3	RY*(2)	C11	1.02	1.79	0.039
BD(1)	C2-C3	BD*(1)	C1-C2	2.56	1.26	0.051
BD(1)	C2-C3	BD*(1)	C1-C5	6.08	1.16	0.075
BD(1)	C2-C3	BD*(1)	C1-O17	1.85	0.95	0.038
BD(1)	C2-C3	BD*(1)	C2-H46	1.22	1.14	0.033
BD(1)	C2-C3	BD*(1)	C3-C4	2.51	1.25	0.05
BD(1)	C2-C3	BD*(1)	C3-C11	2.62	1.16	0.049
BD(1)	C2-C3	BD*(1)	C4-O17	1.47	0.97	0.034
BD(1)	C2-C3	BD*(1)	C4-H45	3.63	1.14	0.058
BD(1)	C2-C3	BD*(1)	C11-C12	1.86	1.22	0.043
BD(1)	C2-H46	RY*(2)	C1	1	1.79	0.038
BD(1)	C2-H46	RY*(2)	C3	0.89	1.78	0.036
BD(1)	C2-H46	BD*(1)	C1-C2	2.13	1.16	0.044
BD(1)	C2-H46	BD*(1)	C1-O17	3.4	0.85	0.048
BD(1)	C2-H46	BD*(1)	C2-C3	1.15	1.06	0.031
BD(1)	C2-H46	BD*(1)	C3-C4	1.57	1.15	0.038
BD(1)	C3-C4	RY*(2)	C1	0.67	1.95	0.032
BD(1)	C3-C4	RY*(2)	C11	1.33	1.85	0.044
BD(1)	C3-C4	BD*(1)	C2-C3	2.68	1.23	0.051
BD(1)	C3-C4	BD*(1)	C2-H46	3.09	1.2	0.054
BD(1)	C3-C4	BD*(1)	C3-C11	3.98	1.22	0.062
BD(1)	C3-C4	BD*(1)	C4-H45	1.72	1.2	0.041
BD(1)	C3-C4	BD*(1)	C11-C16	1.72	1.29	0.042
BD(2)	C3-C4	RY*(3)	C2	1.16	1.58	0.04
BD(2)	C3-C4	RY*(3)	C11	1	1.39	0.035
BD(2)	C3-C4	RY*(2)	O17	0.85	1.4	0.032
BD(2)	C3-C4	BD*(2)	C1-C2	14.44	0.3	0.06
BD(2)	C3-C4	BD*(2)	C3-C4	1.02	0.3	0.016
BD(2)	C3-C4	BD*(2)	C11-C16	11.11	0.31	0.055

BD(1)	C3-C11	RY*(1)	C2	0.74	1.91	0.034
BD(1)	C3-C11	RY*(1)	C12	1.05	1.93	0.04
BD(1)	C3-C11	RY*(1)	C16	1.01	1.93	0.04
BD(1)	C3-C11	BD*(1)	C1-C2	0.64	1.27	0.025
BD(1)	C3-C11	BD*(1)	C2-C3	2.67	1.18	0.05
BD(1)	C3-C11	BD*(1)	C3-C4	3.57	1.26	0.06
BD(1)	C3-C11	BD*(1)	C4-O17	1.23	0.99	0.031
BD(1)	C3-C11	BD*(1)	C11-C12	2.65	1.24	0.051
BD(1)	C3-C11	BD*(1)	C11-C16	2.75	1.24	0.052
BD(1)	C3-C11	BD*(1)	C12-C13	1.72	1.27	0.042
BD(1)	C3-C11	BD*(1)	C15-C16	1.75	1.26	0.042
BD(1)	C4-O17	RY*(1)	C1	0.52	1.82	0.027
BD(1)	C4-O17	RY*(2)	C1	1.51	2.11	0.05
BD(1)	C4-O17	RY*(1)	C3	0.64	1.96	0.032
BD(1)	C4-O17	BD*(1)	C1-C5	2.59	1.38	0.054
BD(1)	C4-O17	BD*(1)	C3-C11	3.12	1.38	0.059
BD(1)	C4-H45	RY*(2)	C3	1.22	1.8	0.042
BD(1)	C4-H45	RY*(1)	O17	0.52	1.76	0.027
BD(1)	C4-H45	BD*(1)	C1-O17	2.17	0.87	0.039
BD(1)	C4-H45	BD*(1)	C2-C3	2.48	1.09	0.046
BD(1)	C4-H45	BD*(1)	C3-C4	1.64	1.17	0.039
BD(1)	C5-C6	RY*(1)	C1	1.33	1.64	0.042
BD(1)	C5-C6	RY*(1)	C7	0.8	1.95	0.035
BD(1)	C5-C6	RY*(2)	C7	1.54	1.47	0.043
BD(1)	C5-C6	RY*(2)	C10	0.53	1.46	0.025
BD(1)	C5-C6	BD*(1)	C1-C2	2.44	1.3	0.05
BD(1)	C5-C6	BD*(1)	C1-C5	2.88	1.2	0.053
BD(1)	C5-C6	BD*(1)	C5-C10	3.85	1.25	0.062
BD(1)	C5-C6	BD*(1)	C6-C7	2.71	1.28	0.053
BD(1)	C5-C6	BD*(1)	C6-H47	1.29	1.19	0.035
BD(1)	C5-C6	BD*(1)	C7-H48	2.1	1.18	0.045
BD(1)	C5-C6	BD*(1)	C10-H50	2.07	1.18	0.044
BD(1)	C5-C10	RY*(1)	C1	0.88	1.64	0.034
BD(1)	C5-C10	RY*(1)	C6	0.52	1.94	0.029
BD(1)	C5-C10	RY*(1)	C9	0.94	1.95	0.039
BD(1)	C5-C10	RY*(2)	C9	1.29	1.47	0.039
BD(1)	C5-C10	BD*(1)	C1-C5	3.23	1.21	0.056
BD(1)	C5-C10	BD*(1)	C1-O17	2.75	1	0.047
BD(1)	C5-C10	BD*(1)	C5-C6	3.84	1.25	0.062
BD(1)	C5-C10	BD*(1)	C6-H47	1.96	1.19	0.043
BD(1)	C5-C10	BD*(1)	C9-C10	2.83	1.28	0.054

BD(1)	C5-C10	BD*(1)	C9-H49	2.07	1.18	0.044
BD(1)	C5-C10	BD*(1)	C10-H50	1.29	1.18	0.035
BD(2)	C5-C10	RY*(5)	C1	0.54	1.7	0.03
BD(2)	C5-C10	RY*(3)	C6	1.26	1.48	0.043
BD(2)	C5-C10	RY*(4)	C9	1.48	1.19	0.042
BD(2)	C5-C10	BD*(2)	C1-C2	14.38	0.28	0.058
BD(2)	C5-C10	BD*(1)	C1-O17	1.13	0.56	0.025
BD(2)	C5-C10	BD*(2)	C6-C7	18.06	0.28	0.065
BD(2)	C5-C10	BD*(2)	C8-C9	21	0.28	0.069
BD(1)	C6-C7	RY*(1)	C5	1.78	1.97	0.053
BD(1)	C6-C7	RY*(2)	C8	2.24	1.94	0.059
BD(1)	C6-C7	BD*(1)	C1-C5	3.18	1.21	0.056
BD(1)	C6-C7	BD*(1)	C5-C6	3.12	1.26	0.056
BD(1)	C6-C7	BD*(1)	C6-H47	1.51	1.2	0.038
BD(1)	C6-C7	BD*(1)	C7-C8	3.37	1.27	0.058
BD(1)	C6-C7	BD*(1)	C7-H48	1.59	1.19	0.039
BD(1)	C6-C7	BD*(1)	C8-C18	2.94	1.16	0.053
BD(2)	C6-C7	RY*(6)	C5	0.68	1.71	0.033
BD(2)	C6-C7	BD*(2)	C5-C10	19.65	0.28	0.067
BD(2)	C6-C7	BD*(2)	C8-C9	19.4	0.28	0.067
BD(1)	C6-H47	RY*(1)	C5	1.13	1.8	0.04
BD(1)	C6-H47	RY*(1)	C7	0.93	1.8	0.037
BD(1)	C6-H47	BD*(1)	C5-C6	1.07	1.09	0.031
BD(1)	C6-H47	BD*(1)	C5-C10	3.79	1.1	0.058
BD(1)	C6-H47	BD*(1)	C6-C7	1.21	1.12	0.033
BD(1)	C6-H47	BD*(1)	C7-C8	3.67	1.1	0.057
BD(1)	C7-C8	RY*(1)	C6	0.66	1.93	0.032
BD(1)	C7-C8	RY*(2)	C6	1.69	1.46	0.045
BD(1)	C7-C8	RY*(2)	C18	0.94	1.57	0.035
BD(1)	C7-C8	BD*(1)	C6-C7	2.96	1.28	0.055
BD(1)	C7-C8	BD*(1)	C6-H47	1.99	1.19	0.044
BD(1)	C7-C8	BD*(1)	C7-H48	1.41	1.18	0.037
BD(1)	C7-C8	BD*(1)	C8-C9	3.93	1.26	0.063
BD(1)	C7-C8	BD*(1)	C8-C18	2.29	1.15	0.046
BD(1)	C7-C8	BD*(1)	C9-H49	2.17	1.18	0.045
BD(1)	C7-C8	BD*(1)	C18-N21	1.67	1.18	0.04
BD(1)	C7-H48	RY*(1)	C6	0.94	1.78	0.037
BD(1)	C7-H48	RY*(1)	C8	0.54	1.71	0.027
BD(1)	C7-H48	RY*(2)	C8	0.91	1.78	0.036
BD(1)	C7-H48	BD*(1)	C5-C6	3.57	1.1	0.056
BD(1)	C7-H48	BD*(1)	C6-C7	1.06	1.13	0.031

BD(1)	C7-H48	BD*(1)	C7-C8	1.25	1.11	0.033
BD(1)	C7-H48	BD*(1)	C8-C9	3.82	1.11	0.058
BD(1)	C7-H48	BD*(1)	N19-H20	1	1.02	0.029
BD(1)	C8-C9	RY*(1)	C10	1.02	1.94	0.04
BD(1)	C8-C9	RY*(2)	C10	1.19	1.46	0.037
BD(1)	C8-C9	RY*(2)	C18	1.17	1.58	0.039
BD(1)	C8-C9	BD*(1)	C7-C8	3.97	1.27	0.063
BD(1)	C8-C9	BD*(1)	C7-H48	2.03	1.19	0.044
BD(1)	C8-C9	BD*(1)	C8-C18	2.26	1.16	0.046
BD(1)	C8-C9	BD*(1)	C9-C10	3.07	1.28	0.056
BD(1)	C8-C9	BD*(1)	C9-H49	1.46	1.18	0.037
BD(1)	C8-C9	BD*(1)	C10-H50	2.02	1.18	0.044
BD(1)	C8-C9	BD*(1)	C18-N19	1.95	1.29	0.045
BD(2)	C8-C9	RY*(3)	C7	0.82	1.95	0.04
BD(2)	C8-C9	RY*(4)	C10	1.49	1.33	0.044
BD(2)	C8-C9	BD*(2)	C5-C10	20.54	0.28	0.068
BD(2)	C8-C9	BD*(2)	C6-C7	18.86	0.28	0.066
BD(2)	C8-C9	BD*(2)	C18-N19	16.18	0.3	0.064
BD(1)	C8-C18	RY*(1)	C7	1.18	1.91	0.043
BD(1)	C8-C18	RY*(1)	C9	1.03	1.91	0.04
BD(1)	C8-C18	RY*(1)	N19	0.9	1.72	0.035
BD(1)	C8-C18	RY*(1)	N21	0.58	1.62	0.028
BD(1)	C8-C18	BD*(1)	C6-C7	2.07	1.24	0.045
BD(1)	C8-C18	BD*(1)	C7-C8	2.28	1.22	0.047
BD(1)	C8-C18	BD*(1)	C8-C9	2.52	1.22	0.05
BD(1)	C8-C18	BD*(1)	C9-C10	1.83	1.24	0.043
BD(1)	C8-C18	BD*(1)	C18-N19	1.86	1.25	0.043
BD(1)	C8-C18	BD*(1)	C18-N21	0.71	1.14	0.026
BD(1)	C8-C18	BD*(1)	N21-C23	2.88	1.01	0.048
BD(1)	C9-C10	RY*(2)	C5	1.99	1.82	0.054
BD(1)	C9-C10	RY*(1)	C8	2.4	1.87	0.06
BD(1)	C9-C10	BD*(1)	C1-C5	3.13	1.21	0.055
BD(1)	C9-C10	BD*(1)	C5-C10	3.26	1.26	0.057
BD(1)	C9-C10	BD*(1)	C8-C9	3.45	1.27	0.059
BD(1)	C9-C10	BD*(1)	C8-C18	3.19	1.16	0.055
BD(1)	C9-C10	BD*(1)	C9-H49	1.59	1.19	0.039
BD(1)	C9-C10	BD*(1)	C10-H50	1.51	1.19	0.038
BD(1)	C9-H49	RY*(2)	C8	0.97	1.78	0.037
BD(1)	C9-H49	RY*(1)	C10	1.03	1.79	0.038
BD(1)	C9-H49	BD*(1)	C5-C10	3.56	1.1	0.056
BD(1)	C9-H49	BD*(1)	C7-C8	3.76	1.11	0.058

BD(1)	C9-H49	BD*(1)	C8-C9	1.21	1.11	0.033
BD(1)	C9-H49	BD*(1)	C9-C10	1.12	1.13	0.032
BD(1)	C9-H49	BD*(1)	N21-H22	0.63	1	0.023
BD(1)	C10-H50	RY*(1)	C5	1.23	1.81	0.042
BD(1)	C10-H50	RY*(1)	C9	0.96	1.8	0.037
BD(1)	C10-H50	BD*(1)	C5-C6	3.75	1.1	0.057
BD(1)	C10-H50	BD*(1)	C5-C10	1.04	1.1	0.03
BD(1)	C10-H50	BD*(1)	C8-C9	3.63	1.11	0.057
BD(1)	C10-H50	BD*(1)	C9-C10	1.16	1.13	0.032
BD(1)	C11-C12	RY*(1)	C3	1.41	1.77	0.045
BD(1)	C11-C12	RY*(1)	C13	0.68	1.95	0.033
BD(1)	C11-C12	RY*(2)	C13	1.75	1.47	0.046
BD(1)	C11-C12	RY*(2)	C16	0.52	1.48	0.025
BD(1)	C11-C12	BD*(1)	C2-C3	2.32	1.2	0.047
BD(1)	C11-C12	BD*(1)	C3-C11	3.01	1.19	0.053
BD(1)	C11-C12	BD*(1)	C11-C16	3.74	1.26	0.061
BD(1)	C11-C12	BD*(1)	C12-C13	2.91	1.29	0.055
BD(1)	C11-C12	BD*(1)	C12-H41	1.31	1.18	0.035
BD(1)	C11-C12	BD*(1)	C13-H42	1.85	1.2	0.042
BD(1)	C11-C12	BD*(1)	C16-H44	2.1	1.18	0.045
BD(1)	C11-C16	RY*(1)	C3	1.02	1.77	0.038
BD(1)	C11-C16	RY*(1)	C15	0.96	1.98	0.039
BD(1)	C11-C16	RY*(2)	C15	1.35	1.46	0.04
BD(1)	C11-C16	BD*(1)	C3-C4	2.13	1.28	0.047
BD(1)	C11-C16	BD*(1)	C3-C11	3.07	1.19	0.054
BD(1)	C11-C16	BD*(1)	C11-C12	3.75	1.26	0.061
BD(1)	C11-C16	BD*(1)	C12-H41	2.05	1.18	0.044
BD(1)	C11-C16	BD*(1)	C15-C16	2.94	1.28	0.055
BD(1)	C11-C16	BD*(1)	C15-H43	2.01	1.19	0.044
BD(1)	C11-C16	BD*(1)	C16-H44	1.37	1.18	0.036
BD(2)	C11-C16	RY*(3)	C3	0.63	1.52	0.031
BD(2)	C11-C16	RY*(3)	C12	0.8	1.93	0.039
BD(2)	C11-C16	RY*(4)	C15	1.39	0.94	0.036
BD(2)	C11-C16	BD*(1)	C3-C4	0.51	0.84	0.02
BD(2)	C11-C16	BD*(2)	C3-C4	14.36	0.27	0.057
BD(2)	C11-C16	BD*(2)	C12-C13	16.89	0.29	0.063
BD(2)	C11-C16	BD*(2)	C14-C15	21.68	0.28	0.07
BD(1)	C12-C13	RY*(1)	C11	1.59	1.98	0.05
BD(1)	C12-C13	RY*(2)	C11	0.66	1.83	0.031
BD(1)	C12-C13	RY*(1)	C14	1.37	1.83	0.045
BD(1)	C12-C13	RY*(2)	C14	0.95	1.98	0.039

BD(1)	C12-C13	BD*(1)	C3-C11	3.2	1.19	0.055
BD(1)	C12-C13	BD*(1)	C11-C12	3.33	1.26	0.058
BD(1)	C12-C13	BD*(1)	C12-H41	1.54	1.18	0.038
BD(1)	C12-C13	BD*(1)	C13-C14	3.14	1.27	0.057
BD(1)	C12-C13	BD*(1)	C13-H42	1.48	1.21	0.038
BD(1)	C12-C13	BD*(1)	C14-C26	2.91	1.15	0.052
BD(2)	C12-C13	BD*(2)	C11-C16	21.21	0.28	0.069
BD(2)	C12-C13	BD*(2)	C14-C15	18.36	0.28	0.065
BD(1)	C12-H41	RY*(1)	C11	1.24	1.82	0.043
BD(1)	C12-H41	RY*(1)	C13	0.95	1.79	0.037
BD(1)	C12-H41	BD*(1)	C11-C12	1.03	1.1	0.03
BD(1)	C12-H41	BD*(1)	C11-C16	3.73	1.1	0.057
BD(1)	C12-H41	BD*(1)	C12-C13	1.18	1.13	0.033
BD(1)	C12-H41	BD*(1)	C13-C14	3.5	1.11	0.056
BD(1)	C13-C14	RY*(1)	C12	0.9	1.95	0.038
BD(1)	C13-C14	RY*(2)	C12	1.28	1.46	0.039
BD(1)	C13-C14	RY*(1)	C26	1.24	1.55	0.039
BD(1)	C13-C14	BD*(1)	C12-C13	2.87	1.28	0.054
BD(1)	C13-C14	BD*(1)	C12-H41	2.16	1.17	0.045
BD(1)	C13-C14	BD*(1)	C13-H42	1.49	1.2	0.038
BD(1)	C13-C14	BD*(1)	C14-C15	3.91	1.26	0.063
BD(1)	C13-C14	BD*(1)	C14-C26	2.22	1.14	0.045
BD(1)	C13-C14	BD*(1)	C15-H43	2.21	1.18	0.046
BD(1)	C13-C14	BD*(1)	C26-N29	1.95	1.15	0.043
BD(1)	C13-H42	RY*(1)	C12	0.87	1.78	0.035
BD(1)	C13-H42	RY*(2)	C14	1.38	1.81	0.045
BD(1)	C13-H42	BD*(1)	C11-C12	3.87	1.09	0.058
BD(1)	C13-H42	BD*(1)	C12-C13	1.13	1.12	0.032
BD(1)	C13-H42	BD*(1)	C13-C14	1.36	1.1	0.035
BD(1)	C13-H42	BD*(1)	C14-C15	3.86	1.1	0.058
BD(1)	C14-C15	RY*(1)	C13	0.54	1.95	0.029
BD(1)	C14-C15	RY*(1)	C16	0.99	1.95	0.039
BD(1)	C14-C15	RY*(2)	C16	1.19	1.48	0.038
BD(1)	C14-C15	RY*(1)	C26	0.92	1.56	0.034
BD(1)	C14-C15	BD*(1)	C13-C14	4.01	1.27	0.064
BD(1)	C14-C15	BD*(1)	C13-H42	1.97	1.2	0.044
BD(1)	C14-C15	BD*(1)	C14-C26	2.4	1.15	0.047
BD(1)	C14-C15	BD*(1)	C15-C16	2.95	1.28	0.055
BD(1)	C14-C15	BD*(1)	C15-H43	1.56	1.19	0.039
BD(1)	C14-C15	BD*(1)	C16-H44	2.04	1.18	0.044
BD(1)	C14-C15	BD*(1)	C26-N27	1.32	1.28	0.037

BD(2)	C14-C15	RY*(3)	C13	0.87	1.92	0.04
BD(2)	C14-C15	RY*(4)	C16	1.26	1.54	0.044
BD(2)	C14-C15	BD*(2)	C11-C16	19.48	0.28	0.066
BD(2)	C14-C15	BD*(2)	C12-C13	19.48	0.28	0.068
BD(2)	C14-C15	BD*(2)	C26-N27	16.41	0.27	0.063
BD(1)	C14-C26	RY*(1)	C13	1.26	1.91	0.044
BD(1)	C14-C26	RY*(1)	C15	1.06	1.94	0.041
BD(1)	C14-C26	RY*(1)	N27	0.98	1.7	0.037
BD(1)	C14-C26	RY*(1)	N29	1.14	1.58	0.038
BD(1)	C14-C26	BD*(1)	C12-C13	1.89	1.25	0.043
BD(1)	C14-C26	BD*(1)	C13-C14	2.42	1.23	0.049
BD(1)	C14-C26	BD*(1)	C14-C15	2.47	1.23	0.049
BD(1)	C14-C26	BD*(1)	C15-C16	1.72	1.23	0.041
BD(1)	C14-C26	BD*(1)	C26-N27	1.73	1.24	0.041
BD(1)	C14-C26	BD*(1)	C26-N29	0.51	1.12	0.021
BD(1)	C14-C26	BD*(1)	N27-H28	3.43	1.11	0.055
BD(1)	C14-C26	BD*(1)	N29-C31	2.01	1	0.04
BD(1)	C15-C16	RY*(1)	C11	0.52	1.99	0.029
BD(1)	C15-C16	RY*(2)	C11	1.82	1.83	0.052
BD(1)	C15-C16	RY*(1)	C14	1.28	1.83	0.043
BD(1)	C15-C16	RY*(2)	C14	1.12	1.98	0.042
BD(1)	C15-C16	BD*(1)	C3-C11	3.23	1.19	0.056
BD(1)	C15-C16	BD*(1)	C11-C16	3.33	1.26	0.058
BD(1)	C15-C16	BD*(1)	C14-C15	3.34	1.27	0.058
BD(1)	C15-C16	BD*(1)	C14-C26	3.31	1.15	0.056
BD(1)	C15-C16	BD*(1)	C15-H43	1.52	1.2	0.038
BD(1)	C15-C16	BD*(1)	C16-H44	1.49	1.18	0.038
BD(1)	C15-H43	RY*(2)	C14	1.42	1.82	0.045
BD(1)	C15-H43	RY*(1)	C16	0.96	1.79	0.037
BD(1)	C15-H43	BD*(1)	C11-C16	3.63	1.1	0.057
BD(1)	C15-H43	BD*(1)	C13-C14	3.77	1.11	0.058
BD(1)	C15-H43	BD*(1)	C14-C15	1.28	1.11	0.034
BD(1)	C15-H43	BD*(1)	C15-C16	1.07	1.12	0.031
BD(1)	C16-H44	RY*(1)	C11	1.33	1.83	0.044
BD(1)	C16-H44	RY*(1)	C15	0.99	1.83	0.038
BD(1)	C16-H44	BD*(1)	C11-C12	3.75	1.1	0.057
BD(1)	C16-H44	BD*(1)	C11-C16	1.13	1.11	0.032
BD(1)	C16-H44	BD*(1)	C14-C15	3.54	1.12	0.056
BD(1)	C16-H44	BD*(1)	C15-C16	1.1	1.12	0.031
BD(1)	C18-N19	RY*(1)	C8	0.51	2.02	0.029
BD(1)	C18-N19	RY*(1)	C18	0.68	1.7	0.03

BD(1)	C18-N19	BD*(1)	C8-C9	1.18	1.41	0.037
BD(1)	C18-N19	BD*(1)	C8-C18	2.41	1.3	0.051
BD(1)	C18-N19	BD*(1)	C18-N21	1.65	1.33	0.042
BD(1)	C18-N19	BD*(1)	N21-H22	1.53	1.31	0.04
BD(2)	C18-N19	BD*(2)	C8-C9	7.19	0.33	0.047
BD(2)	C18-N19	BD*(1)	N21-H22	0.86	0.76	0.023
BD(2)	C18-N19	BD*(1)	N21-C23	0.55	0.66	0.017
BD(1)	C18-N21	RY*(1)	C8	0.94	1.96	0.038
BD(1)	C18-N21	RY*(1)	C23	1.49	1.77	0.046
BD(1)	C18-N21	RY*(2)	C23	0.51	1.67	0.026
BD(1)	C18-N21	BD*(1)	C7-C8	1.61	1.36	0.042
BD(1)	C18-N21	BD*(1)	C8-C18	0.7	1.25	0.027
BD(1)	C18-N21	BD*(1)	C18-N19	1.58	1.39	0.042
BD(1)	C18-N21	BD*(1)	N19-H20	2.22	1.28	0.048
BD(1)	C18-N21	BD*(1)	N21-H22	0.73	1.25	0.027
BD(1)	C18-N21	BD*(1)	N21-C23	1.33	1.15	0.035
BD(1)	C18-N21	BD*(1)	C23-C24	0.57	1.17	0.023
BD(1)	N19-H20	RY*(1)	C18	1.74	1.44	0.045
BD(1)	N19-H20	RY*(4)	C18	0.78	2.55	0.04
BD(1)	N19-H20	BD*(1)	C7-H48	0.58	1.08	0.022
BD(1)	N19-H20	BD*(1)	C18-N21	8.98	1.07	0.088
BD(1)	N21-H22	RY*(1)	C18	0.74	1.51	0.03
BD(1)	N21-H22	RY*(2)	C18	0.96	1.53	0.034
BD(1)	N21-H22	RY*(1)	C23	1.05	1.62	0.037
BD(1)	N21-H22	BD*(1)	C18-N19	2.75	1.25	0.052
BD(1)	N21-H22	BD*(2)	C18-N19	1.5	0.69	0.03
BD(1)	N21-H22	BD*(1)	C18-N21	0.5	1.14	0.021
BD(1)	N21-H22	BD*(1)	C23-H51	0.96	1.17	0.03
BD(1)	N21-C23	RY*(1)	C18	0.86	1.57	0.033
BD(1)	N21-C23	RY*(2)	C25	0.68	1.6	0.03
BD(1)	N21-C23	BD*(1)	C8-C18	1.92	1.17	0.043
BD(1)	N21-C23	BD*(2)	C18-N19	0.84	0.75	0.024
BD(1)	N21-C23	BD*(1)	C18-N21	1.54	1.2	0.039
BD(1)	N21-C23	BD*(1)	C24-H53	0.72	1.2	0.026
BD(1)	N21-C23	BD*(1)	C25-H55	1.16	1.21	0.034
BD(1)	C23-C24	RY*(2)	N21	0.83	1.98	0.036
BD(1)	C23-C24	RY*(1)	C25	0.96	1.48	0.034
BD(1)	C23-C24	BD*(1)	C18-N21	2.19	1.07	0.044
BD(1)	C23-C24	BD*(1)	C23-C25	0.57	0.97	0.021
BD(1)	C23-C24	BD*(1)	C23-H51	0.65	1.11	0.024
BD(1)	C23-C24	BD*(1)	C24-H52	0.74	1.08	0.025

BD(1)	C23-C24	BD*(1)	C24-H53	0.62	1.08	0.023
BD(1)	C23-C24	BD*(1)	C24-H54	0.71	1.06	0.025
BD(1)	C23-C24	BD*(1)	C25-H56	1.48	1.11	0.036
BD(1)	C23-C25	RY*(1)	N21	1.51	1.54	0.043
BD(1)	C23-C25	RY*(1)	C24	0.98	1.38	0.033
BD(1)	C23-C25	BD*(1)	C18-N21	0.74	1.06	0.025
BD(1)	C23-C25	BD*(1)	N21-H22	0.51	1.03	0.021
BD(1)	C23-C25	BD*(1)	C23-C24	0.61	0.95	0.021
BD(1)	C23-C25	BD*(1)	C23-H51	0.66	1.09	0.024
BD(1)	C23-C25	BD*(1)	C24-H52	1.11	1.06	0.031
BD(1)	C23-C25	BD*(1)	C25-H55	0.68	1.07	0.024
BD(1)	C23-C25	BD*(1)	C25-H56	0.82	1.1	0.027
BD(1)	C23-C25	BD*(1)	C25-H57	0.57	1.07	0.022
BD(1)	C23-H51	BD*(1)	N21-H22	2.52	0.97	0.044
BD(1)	C23-H51	BD*(1)	C24-H54	1.41	0.98	0.033
BD(1)	C23-H51	BD*(1)	C25-H57	2.21	1.01	0.042
BD(1)	C24-H52	RY*(1)	C23	0.63	1.48	0.027
BD(1)	C24-H52	BD*(1)	C23-C25	1.82	0.89	0.036
BD(1)	C24-H53	RY*(3)	C23	0.61	1.54	0.027
BD(1)	C24-H53	BD*(1)	N21-C23	2.03	0.87	0.038
BD(1)	C24-H54	RY*(2)	C23	0.65	1.39	0.027
BD(1)	C24-H54	BD*(1)	N21-H22	0.53	0.98	0.02
BD(1)	C24-H54	BD*(1)	N21-C23	1.14	0.87	0.028
BD(1)	C24-H54	BD*(1)	C23-H51	1.48	1.04	0.035
BD(1)	C25-H55	RY*(2)	C23	0.57	1.37	0.025
BD(1)	C25-H55	BD*(1)	N21-C23	3.46	0.85	0.049
BD(1)	C25-H56	RY*(1)	C23	0.56	1.46	0.026
BD(1)	C25-H56	BD*(1)	C23-C24	2.76	0.86	0.044
BD(1)	C25-H57	BD*(1)	N21-C23	0.6	0.85	0.02
BD(1)	C25-H57	BD*(1)	C23-H51	2.35	1.01	0.044
BD(1)	C26-N27	RY*(1)	C14	1.02	2.01	0.041
BD(1)	C26-N27	RY*(1)	C26	0.82	1.75	0.034
BD(1)	C26-N27	BD*(1)	C14-C15	1.52	1.46	0.042
BD(1)	C26-N27	BD*(1)	C14-C26	1.79	1.33	0.044
BD(1)	C26-N27	BD*(1)	C26-N29	1.82	1.35	0.045
BD(1)	C26-N27	BD*(1)	N29-H30	0.64	1.34	0.026
BD(2)	C26-N27	BD*(2)	C14-C15	7.71	0.35	0.05
BD(2)	C26-N27	BD*(1)	N29-H30	2.86	0.78	0.043
BD(2)	C26-N27	BD*(1)	N29-C31	1.88	0.67	0.032
BD(1)	C26-N29	RY*(1)	C14	1.63	1.94	0.05
BD(1)	C26-N29	RY*(1)	C31	0.63	1.75	0.03

BD(1)	C26-N29	RY*(2)	C31	0.61	1.89	0.03
BD(1)	C26-N29	BD*(1)	C13-C14	1.51	1.38	0.041
BD(1)	C26-N29	BD*(1)	C14-C26	0.89	1.26	0.03
BD(1)	C26-N29	BD*(1)	C26-N27	1.56	1.39	0.042
BD(1)	C26-N29	BD*(1)	N29-H30	0.79	1.27	0.028
BD(1)	C26-N29	BD*(1)	N29-C31	1.26	1.16	0.034
BD(1)	C26-N29	BD*(1)	C31-C33	0.54	1.17	0.023
BD(1)	N27-H28	RY*(1)	C26	1.66	1.47	0.044
BD(1)	N27-H28	BD*(1)	C14-C26	7.27	1.06	0.079
BD(1)	N27-H28	BD*(1)	C26-N29	0.85	1.07	0.027
BD(1)	N29-H30	RY*(1)	C26	0.52	1.51	0.025
BD(1)	N29-H30	RY*(2)	C26	1.14	1.65	0.039
BD(1)	N29-H30	RY*(1)	C31	0.89	1.59	0.034
BD(1)	N29-H30	BD*(1)	C26-N27	1.23	1.23	0.035
BD(1)	N29-H30	BD*(2)	C26-N27	4.52	0.67	0.051
BD(1)	N29-H30	BD*(1)	C31-C32	1.9	1.01	0.039
BD(1)	N29-C31	RY*(1)	C26	0.78	1.59	0.032
BD(1)	N29-C31	RY*(2)	C26	0.62	1.73	0.029
BD(1)	N29-C31	RY*(2)	C33	0.57	1.51	0.026
BD(1)	N29-C31	BD*(1)	C14-C26	1.18	1.17	0.033
BD(1)	N29-C31	BD*(2)	C26-N27	1.9	0.74	0.035
BD(1)	N29-C31	BD*(1)	C26-N29	1.32	1.19	0.036
BD(1)	N29-C31	BD*(1)	C32-H40	0.64	1.2	0.025
BD(1)	N29-C31	BD*(1)	C33-H35	0.79	1.2	0.028
BD(1)	C31-C32	RY*(2)	N29	0.56	2.14	0.031
BD(1)	C31-C32	RY*(1)	C33	0.92	1.45	0.033
BD(1)	C31-C32	BD*(1)	N29-H30	2.73	1.06	0.048
BD(1)	C31-C32	BD*(1)	C31-C33	0.69	0.96	0.023
BD(1)	C31-C32	BD*(1)	C31-H34	0.61	1.1	0.023
BD(1)	C31-C32	BD*(1)	C32-H38	0.69	1.08	0.024
BD(1)	C31-C32	BD*(1)	C32-H39	0.7	1.09	0.025
BD(1)	C31-C32	BD*(1)	C32-H40	0.63	1.08	0.023
BD(1)	C31-C32	BD*(1)	C33-H37	1.18	1.07	0.032
BD(1)	C31-C33	RY*(1)	N29	1.07	1.53	0.036
BD(1)	C31-C33	RY*(1)	C32	0.93	1.41	0.032
BD(1)	C31-C33	BD*(1)	C26-N29	2.36	1.06	0.045
BD(1)	C31-C33	BD*(1)	C31-C32	0.72	0.96	0.023
BD(1)	C31-C33	BD*(1)	C31-H34	0.53	1.1	0.022
BD(1)	C31-C33	BD*(1)	C32-H38	0.94	1.08	0.028
BD(1)	C31-C33	BD*(1)	C33-H35	0.65	1.08	0.024
BD(1)	C31-C33	BD*(1)	C33-H36	0.72	1.08	0.025

BD(1)	C31-C33	BD*(1)	C33-H37	0.78	1.08	0.026
BD(1)	C31-H34	RY*(1)	N29	0.92	1.45	0.033
BD(1)	C31-H34	BD*(1)	C26-N29	1.02	0.99	0.029
BD(1)	C31-H34	BD*(1)	C32-H39	1.28	1.01	0.032
BD(1)	C31-H34	BD*(1)	C33-H36	1.7	1	0.037
BD(1)	C32-H38	BD*(1)	C31-C33	1.66	0.88	0.034
BD(1)	C32-H39	BD*(2)	C26-N27	1.52	0.54	0.026
BD(1)	C32-H39	BD*(1)	N29-C31	1.48	0.87	0.032
BD(1)	C32-H39	BD*(1)	C31-H34	1.38	1.02	0.034
BD(1)	C32-H40	BD*(1)	N29-C31	1.85	0.87	0.036
BD(1)	C33-H35	BD*(1)	N29-C31	2.42	0.88	0.041
BD(1)	C33-H35	BD*(1)	C32-H40	0.52	1.01	0.02
BD(1)	C33-H36	BD*(1)	N29-C31	1.08	0.87	0.028
BD(1)	C33-H36	BD*(1)	C31-H34	1.68	1.02	0.037
BD(1)	C33-H37	BD*(1)	C31-C32	2.05	0.88	0.038
CR(1)	C1	RY*(1)	C2	0.94	11.37	0.092
CR(1)	C1	RY*(2)	C2	0.94	10.87	0.09
CR(1)	C1	RY*(1)	C5	1.08	11.39	0.099
CR(1)	C1	RY*(5)	C5	0.71	11.14	0.079
CR(1)	C1	BD*(1)	C1-C2	1.15	10.73	0.1
CR(1)	C1	BD*(1)	C1-O17	1.16	10.42	0.099
CR(1)	C1	BD*(1)	C2-H46	0.9	10.61	0.088
CR(1)	C1	BD*(1)	C4-O17	0.82	10.44	0.083
CR(1)	C1	BD*(1)	C5-C6	0.67	10.68	0.076
CR(1)	C1	BD*(1)	C5-C10	0.65	10.69	0.075
CR(1)	C2	RY*(1)	C1	0.66	11	0.076
CR(1)	C2	RY*(2)	C1	1.93	11.29	0.132
CR(1)	C2	RY*(2)	C3	1.19	11.27	0.103
CR(1)	C2	RY*(1)	H46	0.73	10.6	0.079
CR(1)	C2	BD*(1)	C1-C2	0.77	10.66	0.081
CR(1)	C2	BD*(1)	C1-C5	1.75	10.56	0.122
CR(1)	C2	BD*(1)	C3-C11	1.02	10.55	0.093
CR(1)	C3	RY*(2)	C2	1.28	10.81	0.105
CR(1)	C3	RY*(2)	C4	1.51	10.96	0.115
CR(1)	C3	RY*(1)	C11	1.06	11.35	0.098
CR(1)	C3	BD*(1)	C2-H46	0.73	10.54	0.078
CR(1)	C3	BD*(1)	C3-C4	0.68	10.65	0.076
CR(1)	C3	BD*(1)	C4-H45	0.77	10.54	0.081
CR(1)	C3	BD*(1)	C11-C12	0.61	10.63	0.072
CR(1)	C3	BD*(1)	C11-C16	0.63	10.63	0.073
CR(1)	C4	RY*(1)	C3	2.43	11.21	0.147

CR(1)	C4	RY*(1)	H45	0.83	10.67	0.084
CR(1)	C4	BD*(1)	C1-O17	0.91	10.42	0.088
CR(1)	C4	BD*(1)	C3-C4	1.79	10.72	0.124
CR(1)	C4	BD*(1)	C3-C11	1.36	10.63	0.108
CR(1)	C4	BD*(1)	C4-O17	1.29	10.45	0.104
CR(1)	C5	RY*(2)	C1	0.54	11.3	0.07
CR(1)	C5	RY*(2)	C6	1.54	10.83	0.115
CR(1)	C5	RY*(2)	C10	1.27	10.83	0.105
CR(1)	C5	BD*(1)	C1-C2	1.06	10.67	0.096
CR(1)	C5	BD*(1)	C6-C7	0.57	10.66	0.07
CR(1)	C5	BD*(1)	C6-H47	0.52	10.56	0.067
CR(1)	C5	BD*(1)	C9-C10	0.58	10.65	0.07
CR(1)	C5	BD*(1)	C10-H50	0.54	10.55	0.068
CR(1)	C6	RY*(2)	C5	1.95	11.17	0.132
CR(1)	C6	RY*(2)	C7	1.58	10.83	0.117
CR(1)	C6	RY*(1)	H47	0.68	10.6	0.076
CR(1)	C6	BD*(1)	C1-C5	0.82	10.56	0.083
CR(1)	C6	BD*(1)	C5-C10	0.76	10.62	0.081
CR(1)	C6	BD*(1)	C7-C8	0.8	10.62	0.083
CR(1)	C6	BD*(1)	C7-H48	0.61	10.54	0.072
CR(1)	C7	RY*(2)	C6	1.3	10.82	0.106
CR(1)	C7	RY*(5)	C6	0.71	11.09	0.079
CR(1)	C7	RY*(1)	C8	2.02	11.22	0.135
CR(1)	C7	RY*(1)	H48	0.67	10.65	0.075
CR(1)	C7	BD*(1)	C5-C6	0.77	10.61	0.081
CR(1)	C7	BD*(1)	C6-H47	0.57	10.55	0.069
CR(1)	C7	BD*(1)	C8-C9	0.79	10.62	0.082
CR(1)	C7	BD*(1)	C8-C18	0.75	10.51	0.08
CR(1)	C8	RY*(2)	C7	1.41	10.83	0.11
CR(1)	C8	RY*(2)	C9	1.33	10.83	0.107
CR(1)	C8	RY*(1)	C18	1.16	10.92	0.101
CR(1)	C8	BD*(1)	C6-C7	0.62	10.65	0.073
CR(1)	C8	BD*(1)	C7-H48	0.55	10.55	0.068
CR(1)	C8	BD*(1)	C9-C10	0.63	10.64	0.073
CR(1)	C8	BD*(1)	C9-H49	0.58	10.54	0.07
CR(1)	C8	BD*(1)	C18-N19	0.62	10.66	0.073
CR(1)	C9	RY*(2)	C8	1.88	11.29	0.13
CR(1)	C9	RY*(2)	C10	1.61	10.82	0.118
CR(1)	C9	RY*(5)	C10	0.6	11.1	0.073
CR(1)	C9	RY*(1)	H49	0.67	10.65	0.075
CR(1)	C9	BD*(1)	C5-C10	0.77	10.62	0.081

CR(1)	C9	BD*(1)	C7-C8	0.77	10.63	0.081
CR(1)	C9	BD*(1)	C8-C18	0.84	10.51	0.085
CR(1)	C9	BD*(1)	C10-H50	0.59	10.54	0.07
CR(1)	C10	RY*(1)	C5	1.29	11.33	0.108
CR(1)	C10	RY*(2)	C5	0.72	11.17	0.08
CR(1)	C10	RY*(2)	C9	1.69	10.83	0.121
CR(1)	C10	RY*(5)	C9	0.55	11.1	0.07
CR(1)	C10	RY*(1)	H50	0.63	10.61	0.073
CR(1)	C10	BD*(1)	C1-C5	0.84	10.57	0.085
CR(1)	C10	BD*(1)	C5-C6	0.75	10.62	0.08
CR(1)	C10	BD*(1)	C8-C9	0.81	10.63	0.083
CR(1)	C10	BD*(1)	C9-H49	0.61	10.54	0.072
CR(1)	C11	RY*(2)	C3	0.75	11.28	0.082
CR(1)	C11	RY*(5)	C3	0.87	11.13	0.088
CR(1)	C11	RY*(2)	C12	1.38	10.84	0.109
CR(1)	C11	RY*(2)	C16	1.33	10.85	0.107
CR(1)	C11	BD*(1)	C2-C3	0.71	10.57	0.078
CR(1)	C11	BD*(1)	C3-C4	0.74	10.65	0.08
CR(1)	C11	BD*(1)	C12-C13	0.59	10.66	0.071
CR(1)	C11	BD*(1)	C12-H41	0.54	10.55	0.068
CR(1)	C11	BD*(1)	C15-C16	0.6	10.65	0.072
CR(1)	C11	BD*(1)	C16-H44	0.55	10.55	0.068
CR(1)	C12	RY*(2)	C11	1.89	11.18	0.13
CR(1)	C12	RY*(2)	C13	1.46	10.83	0.112
CR(1)	C12	RY*(4)	C13	0.68	11.1	0.078
CR(1)	C12	RY*(1)	H41	0.62	10.62	0.072
CR(1)	C12	BD*(1)	C3-C11	0.85	10.55	0.085
CR(1)	C12	BD*(1)	C11-C16	0.74	10.62	0.08
CR(1)	C12	BD*(1)	C13-C14	0.76	10.63	0.081
CR(1)	C12	BD*(1)	C13-H42	0.54	10.56	0.068
CR(1)	C13	RY*(2)	C12	1.5	10.82	0.114
CR(1)	C13	RY*(4)	C12	0.6	11.08	0.073
CR(1)	C13	RY*(1)	C14	1.58	11.18	0.119
CR(1)	C13	RY*(2)	C14	0.67	11.33	0.078
CR(1)	C13	RY*(1)	H42	0.75	10.63	0.08
CR(1)	C13	BD*(1)	C11-C12	0.81	10.61	0.083
CR(1)	C13	BD*(1)	C12-H41	0.6	10.53	0.071
CR(1)	C13	BD*(1)	C14-C15	0.82	10.62	0.084
CR(1)	C13	BD*(1)	C14-C26	0.73	10.5	0.079
CR(1)	C14	RY*(2)	C13	1.57	10.84	0.117
CR(1)	C14	RY*(2)	C15	1.36	10.82	0.108

CR(1)	C14	RY*(5)	C26	0.62	11.92	0.077
CR(1)	C14	RY*(7)	C26	0.62	11.34	0.075
CR(1)	C14	BD*(1)	C12-C13	0.62	10.65	0.073
CR(1)	C14	BD*(1)	C13-H42	0.55	10.56	0.068
CR(1)	C14	BD*(1)	C15-C16	0.63	10.64	0.073
CR(1)	C14	BD*(1)	C15-H43	0.59	10.55	0.071
CR(1)	C15	RY*(1)	C14	1.79	11.18	0.127
CR(1)	C15	RY*(2)	C14	0.5	11.34	0.068
CR(1)	C15	RY*(2)	C16	1.53	10.84	0.115
CR(1)	C15	RY*(5)	C16	0.64	11.1	0.075
CR(1)	C15	RY*(1)	H43	0.73	10.73	0.079
CR(1)	C15	BD*(1)	C11-C16	0.78	10.62	0.082
CR(1)	C15	BD*(1)	C13-C14	0.77	10.63	0.081
CR(1)	C15	BD*(1)	C14-C26	0.89	10.5	0.088
CR(1)	C15	BD*(1)	C16-H44	0.59	10.54	0.071
CR(1)	C16	RY*(1)	C11	1.13	11.34	0.101
CR(1)	C16	RY*(2)	C11	0.89	11.18	0.089
CR(1)	C16	RY*(5)	C11	0.52	11.25	0.068
CR(1)	C16	RY*(2)	C15	1.72	10.82	0.122
CR(1)	C16	RY*(5)	C15	0.52	11.13	0.068
CR(1)	C16	RY*(1)	H44	0.62	10.62	0.072
CR(1)	C16	BD*(1)	C3-C11	0.87	10.55	0.086
CR(1)	C16	BD*(1)	C11-C12	0.75	10.62	0.08
CR(1)	C16	BD*(1)	C14-C15	0.79	10.63	0.082
CR(1)	C16	BD*(1)	C15-H43	0.58	10.55	0.07
CR(1)	O17	RY*(1)	C1	2.16	19.95	0.186
CR(1)	O17	RY*(1)	C4	1.66	20.1	0.163
CR(1)	C18	RY*(2)	C8	0.72	11.36	0.081
CR(1)	C18	RY*(3)	N19	0.95	11.06	0.092
CR(1)	C18	BD*(1)	C7-C8	0.52	10.69	0.067
CR(1)	C18	BD*(1)	C8-C9	0.61	10.69	0.073
CR(1)	C18	BD*(1)	N19-H20	0.78	10.61	0.081
CR(1)	C18	BD*(1)	N21-H22	0.7	10.58	0.077
CR(1)	C18	BD*(1)	N21-C23	1	10.48	0.092
CR(1)	N19	RY*(1)	C18	4.23	14.97	0.225
CR(1)	N19	RY*(2)	C18	1.11	14.99	0.115
CR(1)	N19	RY*(1)	H20	0.56	14.82	0.081
CR(1)	N19	BD*(1)	C8-C18	1.05	14.57	0.112
CR(1)	N19	BD*(1)	C18-N21	0.55	14.6	0.081
CR(1)	N21	RY*(2)	C18	2.39	15.05	0.169
CR(1)	N21	RY*(3)	C18	0.74	15.73	0.096

CR(1)	N21	RY*(1)	H22	0.62	14.85	0.086
CR(1)	N21	RY*(2)	C23	0.7	15.05	0.091
CR(1)	N21	RY*(3)	C23	0.87	15.19	0.103
CR(1)	C23	RY*(3)	C24	0.93	11.04	0.091
CR(1)	C23	RY*(3)	C25	0.76	11.11	0.082
CR(1)	C23	RY*(1)	H51	0.61	10.71	0.072
CR(1)	C23	BD*(1)	C18-N21	0.69	10.57	0.077
CR(1)	C24	RY*(1)	C23	0.7	11.01	0.078
CR(1)	C24	RY*(2)	C23	0.56	10.91	0.07
CR(1)	C24	RY*(1)	H52	0.63	10.66	0.073
CR(1)	C24	RY*(1)	H53	0.65	10.69	0.075
CR(1)	C24	RY*(1)	H54	0.62	10.69	0.073
CR(1)	C25	RY*(3)	C23	0.68	11.04	0.077
CR(1)	C25	RY*(1)	H55	0.59	10.68	0.071
CR(1)	C25	RY*(1)	H56	0.73	10.69	0.079
CR(1)	C25	RY*(1)	H57	0.61	10.66	0.072
CR(1)	C26	RY*(2)	C14	1.12	11.42	0.101
CR(1)	C26	RY*(3)	N27	0.6	11.18	0.073
CR(1)	C26	BD*(1)	C13-C14	0.51	10.71	0.066
CR(1)	C26	BD*(1)	C14-C15	0.67	10.71	0.076
CR(1)	C26	BD*(1)	N27-H28	0.86	10.59	0.085
CR(1)	C26	BD*(1)	N29-H30	0.67	10.6	0.076
CR(1)	C26	BD*(1)	N29-C31	1.02	10.49	0.093
CR(1)	N27	RY*(1)	C26	4.99	15	0.245
CR(1)	N27	RY*(4)	C26	0.57	15.49	0.084
CR(1)	N27	BD*(1)	C14-C26	0.62	14.59	0.086
CR(1)	N27	BD*(1)	C26-N29	1.03	14.6	0.111
CR(1)	N29	RY*(1)	C26	2.23	15.04	0.164
CR(1)	N29	RY*(4)	C26	0.68	15.53	0.091
CR(1)	N29	RY*(1)	H30	0.51	14.76	0.077
CR(1)	N29	RY*(4)	C31	1.11	15.63	0.117
CR(1)	N29	RY*(5)	C31	0.51	16.16	0.081
CR(1)	N29	BD*(1)	C26-N27	0.71	14.76	0.092
CR(1)	C31	RY*(3)	C32	0.97	11.07	0.092
CR(1)	C31	RY*(3)	C33	0.84	11.16	0.086
CR(1)	C31	RY*(1)	H34	0.53	10.69	0.067
CR(1)	C31	BD*(1)	C26-N29	0.74	10.57	0.08
CR(1)	C32	RY*(1)	C31	0.62	10.99	0.074
CR(1)	C32	RY*(2)	C31	0.57	11.12	0.071
CR(1)	C32	RY*(1)	H38	0.62	10.66	0.073
CR(1)	C32	RY*(1)	H39	0.78	10.77	0.082

CR(1)	C32	RY*(1)	H40	0.65	10.69	0.074
CR(1)	C33	RY*(3)	C31	0.54	11.1	0.069
CR(1)	C33	RY*(7)	C31	0.53	11.68	0.07
CR(1)	C33	RY*(1)	H35	0.66	10.69	0.075
CR(1)	C33	RY*(1)	H36	0.71	10.77	0.078
CR(1)	C33	RY*(1)	H37	0.61	10.66	0.072
LP(1)	O17	RY*(1)	C1	3.16	1.54	0.062
LP(1)	O17	RY*(1)	C4	2.67	1.68	0.06
LP(1)	O17	BD*(1)	C1-C2	2.85	1.2	0.052
LP(1)	O17	BD*(1)	C3-C4	2.8	1.18	0.051
LP(2)	O17	RY*(3)	C1	0.77	1.44	0.032
LP(2)	O17	RY*(4)	C1	1.18	2.14	0.048
LP(2)	O17	RY*(3)	C4	2.75	1.61	0.064
LP(2)	O17	BD*(2)	C1-C2	24.97	0.36	0.084
LP(2)	O17	BD*(2)	C3-C4	24.59	0.36	0.084
LP(1)	N19	RY*(1)	C18	5.29	1.21	0.072
LP(1)	N19	RY*(2)	C18	0.75	1.23	0.028
LP(1)	N19	BD*(1)	C8-C18	13.15	0.81	0.093
LP(1)	N19	BD*(1)	C18-N21	3.09	0.84	0.046
LP(1)	N21	RY*(3)	C18	1.54	1.8	0.05
LP(1)	N21	RY*(3)	C23	0.59	1.26	0.026
LP(1)	N21	RY*(4)	C23	0.66	2.05	0.035
LP(1)	N21	BD*(1)	C8-C18	2.66	0.7	0.04
LP(1)	N21	BD*(1)	C18-N19	3.82	0.83	0.053
LP(1)	N21	BD*(2)	C18-N19	35.26	0.28	0.088
LP(1)	N21	BD*(1)	C23-C24	1.5	0.61	0.029
LP(1)	N21	BD*(1)	C23-C25	6.28	0.62	0.059
LP(1)	N21	BD*(1)	C23-H51	1.88	0.76	0.036
LP(1)	N21	BD*(1)	C25-H55	0.9	0.74	0.024
LP(1)	N27	RY*(1)	C26	6.7	1.24	0.082
LP(1)	N27	BD*(1)	C13-H42	0.81	0.88	0.024
LP(1)	N27	BD*(1)	C14-C26	1.92	0.82	0.036
LP(1)	N27	BD*(1)	C26-N29	15.09	0.83	0.1
LP(1)	N29	RY*(3)	C26	0.69	2.51	0.038
LP(1)	N29	RY*(2)	C31	0.52	1.33	0.024
LP(1)	N29	RY*(4)	C31	0.74	1.7	0.033
LP(1)	N29	BD*(1)	C14-C26	7.69	0.7	0.067
LP(1)	N29	BD*(1)	C26-N27	11.25	0.83	0.089
LP(1)	N29	BD*(2)	C26-N27	5.59	0.26	0.034
LP(1)	N29	BD*(1)	C31-C33	3.72	0.61	0.044
LP(1)	N29	BD*(1)	C31-H34	6.45	0.75	0.063

BD*(2)	C1-C2	RY*(6)	C1	0.6	1.64	0.073
BD*(2)	C1-C2	RY*(4)	C2	1.33	1.16	0.092
BD*(2)	C3-C4	RY*(6)	C3	0.94	1.52	0.088
BD*(2)	C3-C4	RY*(4)	C4	1.4	1.31	0.1
BD*(2)	C3-C4	BD*(2)	C12-C13	0.63	0.01	0.005
BD*(2)	C5-C10	RY*(6)	C5	0.63	1.43	0.061
BD*(2)	C5-C10	RY*(3)	C6	0.51	1.2	0.05
BD*(2)	C5-C10	RY*(4)	C9	0.55	0.91	0.046
BD*(2)	C5-C10	RY*(3)	C10	1.15	1.52	0.085
BD*(2)	C5-C10	BD*(1)	C1-O17	0.58	0.28	0.025
BD*(2)	C6-C7	RY*(4)	C6	1.16	1.36	0.093
BD*(2)	C6-C7	RY*(4)	C7	1.25	1	0.083
BD*(2)	C6-C7	RY*(5)	C7	0.59	0.96	0.056
BD*(2)	C6-C7	BD*(2)	C18-N19	0.65	0.01	0.005
BD*(2)	C8-C9	RY*(5)	C8	0.93	1.26	0.07
BD*(2)	C8-C9	RY*(3)	C9	0.86	1.68	0.078
BD*(2)	C8-C9	RY*(4)	C9	0.63	0.91	0.049
BD*(2)	C8-C9	RY*(4)	C10	0.55	1.05	0.049
BD*(2)	C8-C9	BD*(2)	C18-N19	107.86	0.02	0.069
BD*(2)	C11-C16	RY*(3)	C16	1.55	1.3	0.093
BD*(2)	C12-C13	RY*(5)	C12	1.71	0.96	0.097
BD*(2)	C12-C13	RY*(5)	C13	1.85	0.97	0.102
BD*(2)	C14-C15	RY*(5)	C14	0.56	1.78	0.066
BD*(2)	C14-C15	RY*(4)	C15	2.15	0.66	0.078
BD*(2)	C18-N19	RY*(6)	C18	0.84	1.57	0.094
BD*(2)	C18-N19	RY*(2)	N19	1.15	0.85	0.081
BD*(2)	C18-N19	BD*(1)	C18-N19	0.95	0.56	0.057
BD*(2)	C18-N19	BD*(1)	N21-C23	0.87	0.32	0.04
BD*(2)	C26-N27	BD*(1)	N29-H30	0.72	0.44	0.056
BD*(2)	C26-N27	BD*(1)	N29-C31	0.94	0.33	0.053

Table SI 3: The second-order perturbative estimates of donor-acceptor interactions in the NBO basis of the molecule 3

Donor NBO (i)		Acceptor NBO (j)		E(2) kcal/mol	E(j) -E(i) a.u.	F(i,j) a.u.
BD(1)	C1-C2	RY*(1)	C3	1.02	1.88	0.039
BD(1)	C1-C2	RY*(2)	C4	0.5	2.01	0.029
BD(1)	C1-C2	RY*(2)	C5	0.93	1.68	0.035
BD(1)	C1-C2	BD*(1)	C1-C5	4.75	1.23	0.068
BD(1)	C1-C2	BD*(1)	C2-C3	2.1	1.24	0.046
BD(1)	C1-C2	BD*(1)	C2-H52	1.88	1.2	0.043
BD(1)	C1-C2	BD*(1)	C3-H53	2.99	1.2	0.054

BD(1)	C1-C2	BD*(1)	C5-C10	1.08	1.28	0.033
BD(2)	C1-C2	RY*(3)	C3	1.26	1.59	0.042
BD(2)	C1-C2	RY*(3)	C5	0.79	1.21	0.029
BD(2)	C1-C2	RY*(2)	O29	0.8	1.39	0.031
BD(2)	C1-C2	BD*(2)	C3-C4	15.55	0.3	0.063
BD(2)	C1-C2	BD*(1)	C5-C6	2.01	0.83	0.038
BD(2)	C1-C2	BD*(2)	C5-C6	5.38	0.3	0.038
BD(2)	C1-C2	BD*(1)	C5-C10	1.97	0.83	0.038
BD(1)	C1-C5	RY*(1)	C2	0.91	1.87	0.037
BD(1)	C1-C5	RY*(1)	C6	1.56	1.97	0.05
BD(1)	C1-C5	RY*(1)	C10	1.29	1.93	0.045
BD(1)	C1-C5	RY*(1)	O29	0.86	2.13	0.038
BD(1)	C1-C5	BD*(1)	C1-C2	4.2	1.28	0.066
BD(1)	C1-C5	BD*(1)	C2-C3	0.79	1.21	0.028
BD(1)	C1-C5	BD*(1)	C4-O29	1.89	0.99	0.039
BD(1)	C1-C5	BD*(1)	C5-C6	3.35	1.24	0.058
BD(1)	C1-C5	BD*(1)	C5-C10	2.95	1.25	0.054
BD(1)	C1-C5	BD*(1)	C6-C7	1.94	1.26	0.044
BD(1)	C1-C5	BD*(1)	C9-C10	1.84	1.29	0.044
BD(1)	C1-O29	RY*(1)	C4	0.62	1.81	0.03
BD(1)	C1-O29	RY*(2)	C4	1.46	2.15	0.05
BD(1)	C1-O29	RY*(2)	C5	0.64	1.82	0.031
BD(1)	C1-O29	BD*(1)	C2-H52	2.46	1.35	0.051
BD(1)	C1-O29	BD*(1)	C4-C17	2.2	1.37	0.049
BD(1)	C1-O29	BD*(1)	C5-C6	1.14	1.42	0.036
BD(1)	C1-O29	BD*(2)	C5-C6	0.64	0.89	0.024
BD(1)	C2-C3	RY*(1)	C1	1.16	1.57	0.038
BD(1)	C2-C3	RY*(1)	C4	1.36	1.61	0.042
BD(1)	C2-C3	BD*(1)	C1-C2	2.37	1.26	0.049
BD(1)	C2-C3	BD*(1)	C1-C5	6.24	1.17	0.076
BD(1)	C2-C3	BD*(1)	C1-O29	1.79	0.97	0.037
BD(1)	C2-C3	BD*(1)	C2-H52	1.26	1.15	0.034
BD(1)	C2-C3	BD*(1)	C3-C4	2.44	1.26	0.05
BD(1)	C2-C3	BD*(1)	C3-H53	1.31	1.15	0.035
BD(1)	C2-C3	BD*(1)	C4-C17	6.37	1.17	0.077
BD(1)	C2-C3	BD*(1)	C4-O29	1.85	0.97	0.038
BD(1)	C2-H52	RY*(2)	C1	0.98	1.77	0.037
BD(1)	C2-H52	RY*(1)	C3	0.72	1.72	0.032
BD(1)	C2-H52	BD*(1)	C1-C2	1.95	1.15	0.042
BD(1)	C2-H52	BD*(1)	C1-O29	3.07	0.87	0.046
BD(1)	C2-H52	BD*(1)	C2-C3	0.95	1.08	0.029

BD(1)	C2-H52	BD*(1)	C3-C4	1.57	1.15	0.038
BD(1)	C3-C4	RY*(1)	C2	0.93	1.9	0.038
BD(1)	C3-C4	RY*(1)	C17	1.14	2.02	0.043
BD(1)	C3-C4	BD*(1)	C2-C3	2.1	1.25	0.046
BD(1)	C3-C4	BD*(1)	C2-H52	2.98	1.21	0.054
BD(1)	C3-C4	BD*(1)	C3-H53	1.92	1.21	0.043
BD(1)	C3-C4	BD*(1)	C4-C17	4.92	1.23	0.07
BD(1)	C3-C4	BD*(1)	C17-C22	1.8	1.28	0.043
BD(2)	C3-C4	RY*(3)	C2	1.1	1.73	0.041
BD(2)	C3-C4	RY*(3)	C17	1.14	1.45	0.038
BD(2)	C3-C4	BD*(2)	C1-C2	15.99	0.3	0.063
BD(2)	C3-C4	BD*(2)	C17-C22	12.34	0.3	0.058
BD(1)	C3-H53	RY*(1)	C2	0.77	1.73	0.033
BD(1)	C3-H53	RY*(2)	C4	0.94	1.84	0.037
BD(1)	C3-H53	BD*(1)	C1-C2	1.57	1.15	0.038
BD(1)	C3-H53	BD*(1)	C2-C3	0.93	1.08	0.028
BD(1)	C3-H53	BD*(1)	C3-C4	1.92	1.15	0.042
BD(1)	C3-H53	BD*(1)	C4-O29	3.2	0.86	0.047
BD(1)	C4-C17	RY*(1)	C3	0.69	1.85	0.032
BD(1)	C4-C17	RY*(1)	C18	0.98	1.96	0.039
BD(1)	C4-C17	RY*(1)	C22	1.64	1.98	0.051
BD(1)	C4-C17	BD*(1)	C1-O29	1.89	1	0.039
BD(1)	C4-C17	BD*(1)	C2-C3	0.65	1.22	0.025
BD(1)	C4-C17	BD*(1)	C3-C4	4.22	1.29	0.066
BD(1)	C4-C17	BD*(1)	C17-C18	2.63	1.26	0.051
BD(1)	C4-C17	BD*(1)	C17-C22	3.56	1.25	0.06
BD(1)	C4-C17	BD*(1)	C18-C19	1.94	1.28	0.045
BD(1)	C4-C17	BD*(1)	C21-C22	1.61	1.28	0.04
BD(1)	C4-O29	RY*(1)	C1	0.52	1.77	0.027
BD(1)	C4-O29	RY*(2)	C1	1.31	2.08	0.047
BD(1)	C4-O29	RY*(3)	C1	0.72	1.64	0.031
BD(1)	C4-O29	RY*(2)	C17	0.72	2.12	0.035
BD(1)	C4-O29	BD*(1)	C1-C5	2.21	1.37	0.049
BD(1)	C4-O29	BD*(1)	C3-C4	0.54	1.46	0.025
BD(1)	C4-O29	BD*(1)	C3-H53	2.35	1.35	0.05
BD(1)	C4-O29	BD*(1)	C17-C18	1.71	1.43	0.044
BD(1)	C5-C6	RY*(1)	C7	0.61	1.93	0.031
BD(1)	C5-C6	RY*(2)	C7	0.79	1.45	0.03
BD(1)	C5-C6	RY*(1)	C10	0.61	1.93	0.031
BD(1)	C5-C6	RY*(1)	C30	0.56	1.49	0.026
BD(1)	C5-C6	BD*(2)	C1-C2	0.67	0.71	0.021

BD(1)	C5-C6	BD*(1)	C1-C5	3.42	1.2	0.057
BD(1)	C5-C6	BD*(1)	C1-O29	1.52	1	0.035
BD(1)	C5-C6	BD*(1)	C5-C10	3.71	1.24	0.061
BD(1)	C5-C6	BD*(1)	C6-C7	3.24	1.26	0.057
BD(1)	C5-C6	BD*(1)	C6-C30	1.65	1.09	0.038
BD(1)	C5-C6	BD*(1)	C7-H46	1.98	1.16	0.043
BD(1)	C5-C6	BD*(1)	C10-H47	1.81	1.18	0.042
BD(1)	C5-C6	BD*(1)	C30-H49	0.55	1.16	0.023
BD(2)	C5-C6	RY*(4)	C7	0.88	1.86	0.04
BD(2)	C5-C6	RY*(3)	C10	0.67	2.11	0.037
BD(2)	C5-C6	BD*(1)	C1-C2	1.56	0.84	0.036
BD(2)	C5-C6	BD*(2)	C1-C2	8.47	0.27	0.044
BD(2)	C5-C6	BD*(1)	C1-O29	5.07	0.56	0.052
BD(2)	C5-C6	BD*(2)	C5-C6	0.57	0.28	0.011
BD(2)	C5-C6	BD*(2)	C7-C8	17.51	0.27	0.062
BD(2)	C5-C6	BD*(2)	C9-C10	21.66	0.28	0.071
BD(2)	C5-C6	BD*(1)	C30-H50	1.47	0.72	0.032
BD(2)	C5-C6	BD*(1)	C30-H51	1.38	0.73	0.031
BD(1)	C5-C10	RY*(1)	C1	0.99	1.59	0.036
BD(1)	C5-C10	RY*(1)	C6	0.67	1.97	0.033
BD(1)	C5-C10	RY*(2)	C6	0.74	1.67	0.032
BD(1)	C5-C10	RY*(1)	C9	1	1.93	0.039
BD(1)	C5-C10	RY*(2)	C9	1.32	1.5	0.04
BD(1)	C5-C10	BD*(1)	C1-C2	2.33	1.28	0.049
BD(1)	C5-C10	BD*(2)	C1-C2	0.78	0.7	0.022
BD(1)	C5-C10	BD*(1)	C1-C5	2.83	1.19	0.052
BD(1)	C5-C10	BD*(1)	C5-C6	4.01	1.24	0.063
BD(1)	C5-C10	BD*(1)	C6-C30	3.26	1.09	0.053
BD(1)	C5-C10	BD*(1)	C9-C10	2.76	1.29	0.053
BD(1)	C5-C10	BD*(1)	C9-H48	1.97	1.19	0.043
BD(1)	C5-C10	BD*(1)	C10-H47	1.2	1.18	0.034
BD(1)	C6-C7	RY*(1)	C5	0.72	2.02	0.034
BD(1)	C6-C7	RY*(2)	C5	0.73	1.66	0.031
BD(1)	C6-C7	RY*(1)	C8	1.53	1.75	0.046
BD(1)	C6-C7	RY*(2)	C8	0.89	1.91	0.037
BD(1)	C6-C7	RY*(1)	C30	0.66	1.51	0.028
BD(1)	C6-C7	BD*(1)	C1-C5	3.32	1.21	0.057
BD(1)	C6-C7	BD*(1)	C5-C6	3.79	1.26	0.062
BD(1)	C6-C7	BD*(1)	C6-C30	1.47	1.1	0.036
BD(1)	C6-C7	BD*(1)	C7-C8	3.8	1.27	0.062
BD(1)	C6-C7	BD*(1)	C7-H46	1.67	1.17	0.04

BD(1)	C6-C7	BD*(1)	C8-N31	4.2	1.12	0.061
BD(1)	C6-C30	RY*(1)	C5	1.34	1.94	0.046
BD(1)	C6-C30	RY*(1)	C7	0.98	1.86	0.038
BD(1)	C6-C30	BD*(1)	C5-C6	2.1	1.18	0.045
BD(1)	C6-C30	BD*(1)	C5-C10	2.37	1.18	0.047
BD(1)	C6-C30	BD*(1)	C6-C7	2.07	1.2	0.045
BD(1)	C6-C30	BD*(1)	C7-C8	2.79	1.2	0.052
BD(1)	C6-C30	BD*(1)	C30-H49	0.74	1.1	0.026
BD(1)	C6-C30	BD*(1)	C30-H50	0.83	1.1	0.027
BD(1)	C6-C30	BD*(1)	C30-H51	0.82	1.1	0.027
BD(1)	C7-C8	RY*(1)	C6	0.95	2	0.039
BD(1)	C7-C8	RY*(2)	C6	2.18	1.7	0.055
BD(1)	C7-C8	RY*(1)	C9	0.53	1.95	0.029
BD(1)	C7-C8	RY*(2)	C9	0.63	1.52	0.028
BD(1)	C7-C8	RY*(1)	N31	0.59	1.6	0.028
BD(1)	C7-C8	RY*(2)	N31	0.54	2.15	0.031
BD(1)	C7-C8	BD*(1)	C6-C7	3.33	1.29	0.059
BD(1)	C7-C8	BD*(1)	C6-C30	2.5	1.11	0.047
BD(1)	C7-C8	BD*(1)	C7-H46	1.51	1.18	0.038
BD(1)	C7-C8	BD*(1)	C8-C9	4.07	1.27	0.064
BD(1)	C7-C8	BD*(1)	C8-N31	1.58	1.13	0.038
BD(1)	C7-C8	BD*(1)	C9-H48	1.9	1.22	0.043
BD(1)	C7-C8	BD*(1)	N31-C33	2.72	1.13	0.05
BD(2)	C7-C8	RY*(3)	C9	0.93	0.96	0.029
BD(2)	C7-C8	RY*(1)	N31	0.53	1.16	0.024
BD(2)	C7-C8	BD*(2)	C5-C6	23.31	0.29	0.075
BD(2)	C7-C8	BD*(2)	C9-C10	15.67	0.3	0.061
BD(2)	C7-C8	BD*(1)	N31-H32	0.58	0.68	0.02
BD(1)	C7-H46	RY*(1)	C6	1.35	1.83	0.044
BD(1)	C7-H46	RY*(2)	C8	1.2	1.76	0.041
BD(1)	C7-H46	BD*(1)	C5-C6	4	1.1	0.059
BD(1)	C7-H46	BD*(1)	C6-C7	1.49	1.12	0.036
BD(1)	C7-H46	BD*(1)	C7-C8	0.92	1.11	0.029
BD(1)	C7-H46	BD*(1)	C8-C9	3.75	1.11	0.058
BD(1)	C8-C9	RY*(1)	C7	0.7	1.93	0.033
BD(1)	C8-C9	RY*(2)	C7	0.52	1.46	0.025
BD(1)	C8-C9	RY*(1)	C10	0.61	1.93	0.031
BD(1)	C8-C9	RY*(2)	C10	1.65	1.48	0.044
BD(1)	C8-C9	RY*(2)	N31	0.51	2.13	0.03
BD(1)	C8-C9	BD*(1)	C7-C8	4.06	1.26	0.064
BD(1)	C8-C9	BD*(1)	C7-H46	2.18	1.17	0.045

BD(1)	C8-C9	BD*(1)	C8-N31	1.16	1.11	0.032
BD(1)	C8-C9	BD*(1)	C9-C10	2.97	1.3	0.056
BD(1)	C8-C9	BD*(1)	C9-H48	1.53	1.2	0.038
BD(1)	C8-C9	BD*(1)	C10-H47	1.97	1.19	0.043
BD(1)	C8-C9	BD*(1)	N31-H32	1.85	1.11	0.041
BD(1)	C8-N31	RY*(1)	C7	0.62	2.04	0.032
BD(1)	C8-N31	RY*(1)	C33	0.7	1.63	0.03
BD(1)	C8-N31	RY*(3)	C33	0.59	1.82	0.029
BD(1)	C8-N31	BD*(1)	C6-C7	1.2	1.38	0.036
BD(1)	C8-N31	BD*(1)	C7-C8	1.48	1.37	0.04
BD(1)	C8-N31	BD*(1)	C8-C9	1.35	1.37	0.038
BD(1)	C8-N31	BD*(1)	C9-C10	1.32	1.41	0.039
BD(1)	C8-N31	BD*(1)	C11-C33	1.33	1.22	0.036
BD(1)	C8-N31	BD*(1)	N31-H32	0.79	1.22	0.028
BD(1)	C8-N31	BD*(1)	N31-C33	1.75	1.22	0.042
BD(1)	C8-N31	BD*(2)	C33-N34	0.69	0.8	0.022
BD(1)	C9-C10	RY*(1)	C5	1.34	2.01	0.047
BD(1)	C9-C10	RY*(2)	C5	0.6	1.66	0.028
BD(1)	C9-C10	RY*(3)	C5	0.71	1.64	0.031
BD(1)	C9-C10	RY*(1)	C8	1.68	1.74	0.049
BD(1)	C9-C10	RY*(2)	C8	0.57	1.91	0.03
BD(1)	C9-C10	BD*(1)	C1-C5	2.96	1.21	0.053
BD(1)	C9-C10	BD*(1)	C5-C10	3.26	1.25	0.057
BD(1)	C9-C10	BD*(1)	C8-C9	3.19	1.26	0.057
BD(1)	C9-C10	BD*(1)	C8-N31	3.6	1.11	0.057
BD(1)	C9-C10	BD*(1)	C9-H48	1.78	1.21	0.041
BD(1)	C9-C10	BD*(1)	C10-H47	1.47	1.19	0.038
BD(2)	C9-C10	RY*(5)	C8	0.74	1.8	0.035
BD(2)	C9-C10	BD*(2)	C5-C6	16.04	0.28	0.062
BD(2)	C9-C10	BD*(2)	C7-C8	22.01	0.27	0.071
BD(1)	C9-H48	RY*(2)	C8	1.19	1.74	0.041
BD(1)	C9-H48	RY*(1)	C10	0.93	1.77	0.036
BD(1)	C9-H48	BD*(1)	C5-C10	3.86	1.08	0.058
BD(1)	C9-H48	BD*(1)	C7-C8	3.67	1.1	0.057
BD(1)	C9-H48	BD*(1)	C8-C9	1.26	1.09	0.033
BD(1)	C9-H48	BD*(1)	C8-N31	0.55	0.94	0.02
BD(1)	C9-H48	BD*(1)	C9-C10	1.52	1.13	0.037
BD(1)	C10-H47	RY*(1)	C5	1.3	1.85	0.044
BD(1)	C10-H47	RY*(1)	C9	1	1.78	0.038
BD(1)	C10-H47	BD*(1)	C5-C6	3.85	1.09	0.058
BD(1)	C10-H47	BD*(1)	C5-C10	0.95	1.09	0.029

BD(1)	C10-H47	BD*(1)	C8-C9	3.87	1.1	0.058
BD(1)	C10-H47	BD*(1)	C9-C10	1.26	1.14	0.034
BD(1)	C11-C12	RY*(1)	C13	0.91	1.94	0.038
BD(1)	C11-C12	RY*(2)	C13	1.25	1.4	0.037
BD(1)	C11-C12	RY*(2)	C33	1.37	1.58	0.042
BD(1)	C11-C12	BD*(1)	C11-N16	2.08	1.22	0.045
BD(1)	C11-C12	BD*(1)	C11-C33	2.36	1.16	0.047
BD(1)	C11-C12	BD*(1)	C12-C13	2.66	1.28	0.052
BD(1)	C11-C12	BD*(1)	C12-H42	1.58	1.2	0.039
BD(1)	C11-C12	BD*(1)	C13-H43	2.2	1.2	0.046
BD(1)	C11-C12	BD*(1)	C33-N34	1.53	1.32	0.04
BD(2)	C11-C12	RY*(5)	C13	1.2	1.01	0.035
BD(2)	C11-C12	RY*(3)	N16	0.79	1.71	0.036
BD(2)	C11-C12	BD*(2)	C13-C14	21.41	0.28	0.07
BD(2)	C11-C12	BD*(2)	C15-N16	17.08	0.26	0.06
BD(2)	C11-C12	BD*(2)	C33-N34	13.25	0.3	0.06
BD(1)	C11-N16	RY*(2)	C15	3.27	1.71	0.067
BD(1)	C11-N16	RY*(1)	C33	0.72	1.68	0.031
BD(1)	C11-N16	BD*(1)	C11-C12	2.43	1.38	0.052
BD(1)	C11-N16	BD*(1)	C11-C33	1.13	1.26	0.034
BD(1)	C11-N16	BD*(1)	C12-H42	1.46	1.31	0.039
BD(1)	C11-N16	BD*(1)	C15-N16	1.16	1.35	0.035
BD(1)	C11-N16	BD*(1)	C15-H45	2.04	1.32	0.046
BD(1)	C11-N16	BD*(1)	N31-C33	1.96	1.27	0.045
BD(1)	C11-C33	RY*(1)	C12	1.01	1.89	0.039
BD(1)	C11-C33	RY*(1)	N16	1.18	1.57	0.039
BD(1)	C11-C33	RY*(1)	N31	1.03	1.59	0.036
BD(1)	C11-C33	RY*(1)	N34	0.79	1.7	0.033
BD(1)	C11-C33	BD*(1)	C8-N31	2.33	1.11	0.045
BD(1)	C11-C33	BD*(1)	C11-C12	2.27	1.23	0.047
BD(1)	C11-C33	BD*(1)	C11-N16	1	1.17	0.031
BD(1)	C11-C33	BD*(1)	C12-C13	1.77	1.23	0.042
BD(1)	C11-C33	BD*(1)	C15-N16	3.08	1.19	0.054
BD(1)	C11-C33	BD*(1)	N31-C33	0.63	1.11	0.024
BD(1)	C11-C33	BD*(1)	C33-N34	1.77	1.28	0.042
BD(1)	C12-C13	RY*(1)	C11	1.59	1.66	0.046
BD(1)	C12-C13	RY*(1)	C14	1.14	1.93	0.042
BD(1)	C12-C13	RY*(2)	C14	0.72	1.39	0.028
BD(1)	C12-C13	BD*(1)	C11-C12	2.96	1.27	0.055
BD(1)	C12-C13	BD*(1)	C11-C33	3.41	1.15	0.057
BD(1)	C12-C13	BD*(1)	C12-H42	1.52	1.2	0.038

BD(1)	C12-C13	BD*(1)	C13-C14	2.57	1.27	0.051
BD(1)	C12-C13	BD*(1)	C13-H43	1.29	1.2	0.035
BD(1)	C12-C13	BD*(1)	C14-H44	2.22	1.2	0.046
BD(1)	C12-H42	RY*(2)	C11	1.31	1.67	0.042
BD(1)	C12-H42	RY*(1)	C13	0.97	1.78	0.037
BD(1)	C12-H42	BD*(1)	C11-C12	1.29	1.11	0.034
BD(1)	C12-H42	BD*(1)	C11-N16	4.68	1.05	0.063
BD(1)	C12-H42	BD*(1)	C12-C13	1.1	1.11	0.031
BD(1)	C12-H42	BD*(1)	C13-C14	3.14	1.11	0.053
BD(1)	C13-C14	RY*(1)	C12	1.02	1.93	0.04
BD(1)	C13-C14	RY*(2)	C12	0.93	1.43	0.033
BD(1)	C13-C14	RY*(1)	C15	1.66	1.67	0.047
BD(1)	C13-C14	BD*(1)	C12-C13	2.6	1.28	0.051
BD(1)	C13-C14	BD*(1)	C12-H42	2.25	1.2	0.046
BD(1)	C13-C14	BD*(1)	C13-H43	1.32	1.2	0.036
BD(1)	C13-C14	BD*(1)	C14-C15	2.26	1.27	0.048
BD(1)	C13-C14	BD*(1)	C14-H44	1.38	1.2	0.036
BD(1)	C13-C14	BD*(1)	C15-H45	2.01	1.21	0.044
BD(2)	C13-C14	RY*(3)	C12	1.11	1.63	0.042
BD(2)	C13-C14	RY*(5)	C14	0.56	1.37	0.027
BD(2)	C13-C14	RY*(5)	C15	1.54	1.24	0.043
BD(2)	C13-C14	BD*(2)	C11-C12	18.11	0.28	0.064
BD(2)	C13-C14	BD*(2)	C15-N16	28.06	0.26	0.076
BD(1)	C13-H43	RY*(1)	C12	0.93	1.77	0.036
BD(1)	C13-H43	RY*(1)	C14	0.94	1.77	0.037
BD(1)	C13-H43	BD*(1)	C11-C12	3.31	1.11	0.054
BD(1)	C13-H43	BD*(1)	C12-C13	0.99	1.12	0.03
BD(1)	C13-H43	BD*(1)	C13-C14	0.94	1.11	0.029
BD(1)	C13-H43	BD*(1)	C14-C15	3.07	1.11	0.052
BD(1)	C14-C15	RY*(1)	C13	0.73	1.94	0.034
BD(1)	C14-C15	RY*(2)	C13	1.33	1.39	0.039
BD(1)	C14-C15	RY*(1)	N16	0.62	1.62	0.028
BD(1)	C14-C15	RY*(2)	N16	1.17	1.92	0.043
BD(1)	C14-C15	BD*(1)	C13-C14	2.46	1.28	0.05
BD(1)	C14-C15	BD*(1)	C13-H43	2.41	1.2	0.048
BD(1)	C14-C15	BD*(1)	C14-H44	1.43	1.2	0.037
BD(1)	C14-C15	BD*(1)	C15-N16	1.19	1.24	0.034
BD(1)	C14-C15	BD*(1)	C15-H45	1.28	1.21	0.035
BD(1)	C14-H44	RY*(1)	C13	0.99	1.78	0.038
BD(1)	C14-H44	RY*(2)	C15	0.81	1.44	0.03
BD(1)	C14-H44	BD*(1)	C12-C13	3.18	1.12	0.053

BD(1)	C14-H44	BD*(1)	C13-C14	1.04	1.11	0.03
BD(1)	C14-H44	BD*(1)	C14-C15	0.93	1.11	0.029
BD(1)	C14-H44	BD*(1)	C15-N16	3.99	1.08	0.059
BD(1)	C15-N16	RY*(2)	C11	2.47	1.95	0.062
BD(1)	C15-N16	RY*(2)	C14	1.17	1.5	0.038
BD(1)	C15-N16	BD*(1)	C11-N16	1.33	1.33	0.038
BD(1)	C15-N16	BD*(1)	C11-C33	2.78	1.27	0.054
BD(1)	C15-N16	BD*(1)	C14-C15	1.49	1.38	0.041
BD(1)	C15-N16	BD*(1)	C14-H44	1.5	1.31	0.04
BD(1)	C15-N16	BD*(1)	C15-H45	0.67	1.32	0.027
BD(2)	C15-N16	RY*(4)	C11	1.3	2.09	0.05
BD(2)	C15-N16	RY*(5)	C14	1.06	1.41	0.037
BD(2)	C15-N16	BD*(2)	C11-C12	24.08	0.32	0.08
BD(2)	C15-N16	BD*(2)	C13-C14	13.54	0.32	0.059
BD(1)	C15-H45	RY*(1)	C14	0.81	1.77	0.034
BD(1)	C15-H45	RY*(1)	N16	1.11	1.45	0.036
BD(1)	C15-H45	BD*(1)	C11-N16	4.32	1.05	0.06
BD(1)	C15-H45	BD*(1)	C13-C14	3.47	1.11	0.055
BD(1)	C15-H45	BD*(1)	C14-C15	0.61	1.11	0.023
BD(1)	C17-C18	RY*(1)	C4	0.86	1.64	0.034
BD(1)	C17-C18	RY*(1)	C19	0.94	1.93	0.038
BD(1)	C17-C18	RY*(2)	C19	1.27	1.43	0.038
BD(1)	C17-C18	RY*(1)	C22	0.91	1.97	0.038
BD(1)	C17-C18	BD*(1)	C4-C17	3.02	1.2	0.054
BD(1)	C17-C18	BD*(1)	C4-O29	2.98	0.99	0.049
BD(1)	C17-C18	BD*(1)	C17-C22	4.21	1.25	0.065
BD(1)	C17-C18	BD*(1)	C18-C19	2.87	1.28	0.054
BD(1)	C17-C18	BD*(1)	C18-H54	1.27	1.18	0.035
BD(1)	C17-C18	BD*(1)	C19-H55	1.84	1.19	0.042
BD(1)	C17-C18	BD*(1)	C22-C36	3.14	1.1	0.053
BD(1)	C17-C22	RY*(1)	C4	1.12	1.63	0.038
BD(1)	C17-C22	RY*(1)	C21	0.69	1.93	0.033
BD(1)	C17-C22	RY*(2)	C21	0.62	1.48	0.027
BD(1)	C17-C22	BD*(1)	C3-C4	2.44	1.28	0.05
BD(1)	C17-C22	BD*(1)	C4-C17	3.19	1.2	0.055
BD(1)	C17-C22	BD*(1)	C17-C18	3.99	1.25	0.063
BD(1)	C17-C22	BD*(1)	C18-H54	1.84	1.18	0.042
BD(1)	C17-C22	BD*(1)	C21-C22	3.22	1.27	0.057
BD(1)	C17-C22	BD*(1)	C21-H56	2.06	1.16	0.044
BD(1)	C17-C22	BD*(1)	C22-C36	1.71	1.1	0.039
BD(2)	C17-C22	RY*(5)	C4	0.98	1.23	0.035

BD(2)	C17-C22	RY*(3)	C18	0.78	2.03	0.039
BD(2)	C17-C22	RY*(4)	C21	0.77	1.24	0.031
BD(2)	C17-C22	RY*(5)	C21	0.63	1.17	0.027
BD(2)	C17-C22	BD*(2)	C3-C4	19.73	0.27	0.066
BD(2)	C17-C22	BD*(2)	C18-C19	21.07	0.28	0.07
BD(2)	C17-C22	BD*(2)	C20-C21	20	0.27	0.065
BD(2)	C17-C22	BD*(1)	C36-H57	1.84	0.73	0.036
BD(2)	C17-C22	BD*(1)	C36-H58	2.06	0.73	0.038
BD(1)	C18-C19	RY*(2)	C17	2.43	1.95	0.062
BD(1)	C18-C19	RY*(1)	C20	2.14	1.71	0.054
BD(1)	C18-C19	BD*(1)	C4-C17	2.78	1.21	0.052
BD(1)	C18-C19	BD*(1)	C17-C18	3.43	1.26	0.059
BD(1)	C18-C19	BD*(1)	C18-H54	1.49	1.19	0.038
BD(1)	C18-C19	BD*(1)	C19-C20	3.03	1.27	0.055
BD(1)	C18-C19	BD*(1)	C19-H55	1.57	1.2	0.039
BD(1)	C18-C19	BD*(1)	C20-N37	4.66	1.12	0.065
BD(2)	C18-C19	RY*(6)	C17	0.71	1.76	0.034
BD(2)	C18-C19	RY*(5)	C20	0.77	1.84	0.037
BD(2)	C18-C19	BD*(2)	C17-C22	16.88	0.28	0.063
BD(2)	C18-C19	BD*(2)	C20-C21	20.62	0.27	0.069
BD(1)	C18-H54	RY*(1)	C17	0.78	1.83	0.034
BD(1)	C18-H54	RY*(2)	C17	0.6	1.79	0.029
BD(1)	C18-H54	RY*(1)	C19	1.02	1.78	0.038
BD(1)	C18-H54	BD*(1)	C17-C18	0.96	1.1	0.029
BD(1)	C18-H54	BD*(1)	C17-C22	3.98	1.1	0.059
BD(1)	C18-H54	BD*(1)	C18-C19	1.11	1.13	0.032
BD(1)	C18-H54	BD*(1)	C19-C20	3.68	1.1	0.057
BD(1)	C19-C20	RY*(1)	C18	0.96	1.97	0.039
BD(1)	C19-C20	RY*(2)	C18	1.22	1.5	0.038
BD(1)	C19-C20	RY*(1)	C21	0.55	1.94	0.029
BD(1)	C19-C20	RY*(2)	C21	0.53	1.49	0.025
BD(1)	C19-C20	RY*(1)	N37	0.72	1.66	0.031
BD(1)	C19-C20	BD*(1)	C18-C19	2.7	1.29	0.053
BD(1)	C19-C20	BD*(1)	C18-H54	2.01	1.19	0.044
BD(1)	C19-C20	BD*(1)	C19-H55	1.48	1.21	0.038
BD(1)	C19-C20	BD*(1)	C20-C21	3.99	1.26	0.063
BD(1)	C19-C20	BD*(1)	C20-N37	1.58	1.12	0.038
BD(1)	C19-C20	BD*(1)	C21-H56	1.93	1.17	0.043
BD(1)	C19-C20	BD*(1)	N37-H38	1.49	1.13	0.037
BD(1)	C19-H55	RY*(1)	C18	0.88	1.8	0.036
BD(1)	C19-H55	RY*(2)	C20	1.17	1.71	0.04

BD(1)	C19-H55	BD*(1)	C17-C18	3.92	1.09	0.058
BD(1)	C19-H55	BD*(1)	C18-C19	1.39	1.12	0.035
BD(1)	C19-H55	BD*(1)	C19-C20	1.18	1.1	0.032
BD(1)	C19-H55	BD*(1)	C20-C21	3.67	1.09	0.057
BD(1)	C20-C21	RY*(1)	C19	0.53	1.94	0.029
BD(1)	C20-C21	RY*(2)	C19	0.74	1.44	0.029
BD(1)	C20-C21	RY*(2)	C22	2.48	1.71	0.059
BD(1)	C20-C21	RY*(1)	N37	1.16	1.66	0.039
BD(1)	C20-C21	BD*(1)	C19-C20	3.88	1.27	0.063
BD(1)	C20-C21	BD*(1)	C19-H55	2.03	1.2	0.044
BD(1)	C20-C21	BD*(1)	C20-N37	1.19	1.12	0.033
BD(1)	C20-C21	BD*(1)	C21-C22	3.45	1.28	0.06
BD(1)	C20-C21	BD*(1)	C21-H56	1.37	1.17	0.036
BD(1)	C20-C21	BD*(1)	C22-C36	2.58	1.11	0.048
BD(1)	C20-C21	BD*(1)	N37-C39	2.67	1.14	0.05
BD(2)	C20-C21	RY*(3)	C19	1.54	1.01	0.039
BD(2)	C20-C21	BD*(2)	C17-C22	21.88	0.29	0.072
BD(2)	C20-C21	BD*(2)	C18-C19	17.29	0.29	0.064
BD(2)	C20-C21	BD*(1)	N37-H38	0.68	0.69	0.021
BD(2)	C20-C21	BD*(1)	N37-C39	1.41	0.7	0.03
BD(1)	C20-N37	RY*(1)	C19	0.58	2.04	0.031
BD(1)	C20-N37	RY*(1)	C21	0.71	2.04	0.034
BD(1)	C20-N37	RY*(1)	C39	1.37	1.65	0.042
BD(1)	C20-N37	BD*(1)	C18-C19	1.07	1.4	0.035
BD(1)	C20-N37	BD*(1)	C19-C20	1.68	1.37	0.043
BD(1)	C20-N37	BD*(1)	C20-C21	1.23	1.37	0.037
BD(1)	C20-N37	BD*(1)	C21-C22	1.45	1.39	0.04
BD(1)	C20-N37	BD*(1)	C23-C39	1.58	1.22	0.04
BD(1)	C20-N37	BD*(1)	N37-H38	0.85	1.23	0.029
BD(1)	C20-N37	BD*(1)	N37-C39	2.23	1.24	0.047
BD(1)	C21-C22	RY*(1)	C17	1.55	1.99	0.05
BD(1)	C21-C22	RY*(2)	C20	1.84	1.88	0.053
BD(1)	C21-C22	RY*(1)	C36	0.79	1.49	0.031
BD(1)	C21-C22	BD*(1)	C4-C17	3.52	1.21	0.058
BD(1)	C21-C22	BD*(1)	C17-C22	3.74	1.26	0.061
BD(1)	C21-C22	BD*(1)	C20-C21	3.53	1.26	0.06
BD(1)	C21-C22	BD*(1)	C20-N37	3.18	1.12	0.053
BD(1)	C21-C22	BD*(1)	C21-H56	1.62	1.17	0.039
BD(1)	C21-C22	BD*(1)	C22-C36	1.66	1.11	0.039
BD(1)	C21-C22	BD*(1)	C36-H59	0.58	1.24	0.024
BD(1)	C21-H56	RY*(2)	C20	0.91	1.72	0.035

BD(1)	C21-H56	RY*(1)	C22	1.3	1.83	0.044
BD(1)	C21-H56	BD*(1)	C17-C22	4.12	1.1	0.06
BD(1)	C21-H56	BD*(1)	C19-C20	3.7	1.11	0.057
BD(1)	C21-H56	BD*(1)	C20-C21	0.85	1.1	0.027
BD(1)	C21-H56	BD*(1)	C20-N37	0.56	0.96	0.021
BD(1)	C21-H56	BD*(1)	C21-C22	1.5	1.13	0.037
BD(1)	C22-C36	RY*(1)	C17	1.18	1.91	0.043
BD(1)	C22-C36	RY*(1)	C21	1.09	1.85	0.04
BD(1)	C22-C36	BD*(1)	C17-C18	2.51	1.18	0.049
BD(1)	C22-C36	BD*(1)	C17-C22	2.11	1.17	0.045
BD(1)	C22-C36	BD*(1)	C20-C21	2.88	1.18	0.052
BD(1)	C22-C36	BD*(1)	C21-C22	2.26	1.2	0.046
BD(1)	C22-C36	BD*(1)	C36-H57	0.74	1.09	0.025
BD(1)	C22-C36	BD*(1)	C36-H58	0.74	1.09	0.026
BD(1)	C22-C36	BD*(1)	C36-H59	1.08	1.16	0.032
BD(1)	C23-C24	RY*(1)	C25	0.91	1.94	0.038
BD(1)	C23-C24	RY*(2)	C25	1.22	1.4	0.037
BD(1)	C23-C24	RY*(2)	N28	0.51	1.94	0.028
BD(1)	C23-C24	RY*(2)	C39	1.36	1.57	0.041
BD(1)	C23-C24	BD*(1)	C23-N28	2.1	1.23	0.045
BD(1)	C23-C24	BD*(1)	C23-C39	2.22	1.16	0.046
BD(1)	C23-C24	BD*(1)	C24-C25	2.9	1.28	0.054
BD(1)	C23-C24	BD*(1)	C24-H60	1.6	1.2	0.039
BD(1)	C23-C24	BD*(1)	C25-H61	2.14	1.21	0.045
BD(1)	C23-C24	BD*(1)	C39-N40	1.42	1.34	0.039
BD(2)	C23-C24	RY*(5)	C25	1.12	0.99	0.033
BD(2)	C23-C24	RY*(3)	N28	0.97	1.19	0.034
BD(2)	C23-C24	BD*(2)	C25-C26	21.9	0.28	0.071
BD(2)	C23-C24	BD*(2)	C27-N28	16.52	0.26	0.059
BD(2)	C23-C24	BD*(2)	C39-N40	13.04	0.31	0.059
BD(1)	C23-N28	RY*(2)	C27	3.3	1.7	0.067
BD(1)	C23-N28	RY*(2)	C39	0.69	1.67	0.03
BD(1)	C23-N28	BD*(1)	C23-C24	2.45	1.38	0.052
BD(1)	C23-N28	BD*(1)	C23-C39	1.15	1.26	0.034
BD(1)	C23-N28	BD*(1)	C24-H60	1.54	1.3	0.04
BD(1)	C23-N28	BD*(1)	C27-N28	1.2	1.35	0.036
BD(1)	C23-N28	BD*(1)	C27-H63	2.02	1.32	0.046
BD(1)	C23-N28	BD*(1)	N37-C39	1.72	1.29	0.042
BD(1)	C23-C39	RY*(1)	C24	0.86	1.87	0.036
BD(1)	C23-C39	RY*(1)	N28	1.23	1.57	0.039
BD(1)	C23-C39	RY*(2)	N37	0.88	2.07	0.038

BD(1)	C23-C39	RY*(1)	N40	0.98	1.73	0.037
BD(1)	C23-C39	BD*(1)	C20-N37	3.55	1.1	0.056
BD(1)	C23-C39	BD*(1)	C23-C24	2.22	1.21	0.046
BD(1)	C23-C39	BD*(1)	C23-N28	0.95	1.16	0.03
BD(1)	C23-C39	BD*(1)	C24-C25	1.82	1.22	0.042
BD(1)	C23-C39	BD*(1)	C27-N28	3.21	1.18	0.055
BD(1)	C23-C39	BD*(1)	C39-N40	1.94	1.28	0.045
BD(1)	C24-C25	RY*(1)	C23	1.65	1.69	0.047
BD(1)	C24-C25	RY*(1)	C26	1.14	1.93	0.042
BD(1)	C24-C25	RY*(2)	C26	0.73	1.39	0.029
BD(1)	C24-C25	BD*(1)	C23-C24	3.21	1.27	0.057
BD(1)	C24-C25	BD*(1)	C23-C39	3.43	1.15	0.057
BD(1)	C24-C25	BD*(1)	C24-H60	1.66	1.19	0.04
BD(1)	C24-C25	BD*(1)	C25-C26	2.57	1.27	0.051
BD(1)	C24-C25	BD*(1)	C25-H61	1.3	1.2	0.035
BD(1)	C24-C25	BD*(1)	C26-H62	2.21	1.2	0.046
BD(1)	C24-H60	RY*(2)	C23	1.34	1.7	0.043
BD(1)	C24-H60	RY*(1)	C25	1.07	1.78	0.039
BD(1)	C24-H60	BD*(1)	C23-C24	1.29	1.12	0.034
BD(1)	C24-H60	BD*(1)	C23-N28	4.52	1.07	0.062
BD(1)	C24-H60	BD*(1)	C24-C25	1.03	1.12	0.03
BD(1)	C24-H60	BD*(1)	C25-C26	2.96	1.12	0.052
BD(1)	C24-H60	BD*(1)	N37-H38	1.81	1.02	0.038
BD(1)	C25-C26	RY*(1)	C24	1.2	1.93	0.043
BD(1)	C25-C26	RY*(2)	C24	0.68	1.47	0.028
BD(1)	C25-C26	RY*(1)	C27	1.66	1.68	0.047
BD(1)	C25-C26	BD*(1)	C24-C25	2.67	1.27	0.052
BD(1)	C25-C26	BD*(1)	C24-H60	2.37	1.19	0.047
BD(1)	C25-C26	BD*(1)	C25-H61	1.33	1.2	0.036
BD(1)	C25-C26	BD*(1)	C26-C27	2.27	1.27	0.048
BD(1)	C25-C26	BD*(1)	C26-H62	1.39	1.2	0.036
BD(1)	C25-C26	BD*(1)	C27-H63	2	1.21	0.044
BD(2)	C25-C26	RY*(3)	C24	1.44	1.07	0.039
BD(2)	C25-C26	RY*(5)	C26	0.56	1.43	0.028
BD(2)	C25-C26	RY*(5)	C27	1.5	1.25	0.043
BD(2)	C25-C26	BD*(2)	C23-C24	17.6	0.28	0.063
BD(2)	C25-C26	BD*(2)	C27-N28	27.92	0.26	0.077
BD(1)	C25-H61	RY*(1)	C24	0.93	1.77	0.036
BD(1)	C25-H61	RY*(1)	C26	0.95	1.77	0.037
BD(1)	C25-H61	BD*(1)	C23-C24	3.37	1.11	0.055
BD(1)	C25-H61	BD*(1)	C24-C25	0.98	1.12	0.03

BD(1)	C25-H61	BD*(1)	C25-C26	0.95	1.12	0.029
BD(1)	C25-H61	BD*(1)	C26-C27	3.05	1.11	0.052
BD(1)	C26-C27	RY*(1)	C25	0.71	1.94	0.033
BD(1)	C26-C27	RY*(2)	C25	1.36	1.39	0.039
BD(1)	C26-C27	RY*(1)	N28	0.65	1.63	0.029
BD(1)	C26-C27	RY*(2)	N28	1.18	1.93	0.043
BD(1)	C26-C27	BD*(1)	C25-C26	2.47	1.28	0.05
BD(1)	C26-C27	BD*(1)	C25-H61	2.45	1.2	0.048
BD(1)	C26-C27	BD*(1)	C26-H62	1.44	1.2	0.037
BD(1)	C26-C27	BD*(1)	C27-N28	1.2	1.24	0.034
BD(1)	C26-C27	BD*(1)	C27-H63	1.27	1.21	0.035
BD(1)	C26-H62	RY*(1)	C25	0.99	1.78	0.037
BD(1)	C26-H62	RY*(2)	C27	0.79	1.43	0.03
BD(1)	C26-H62	BD*(1)	C24-C25	3.21	1.11	0.053
BD(1)	C26-H62	BD*(1)	C25-C26	1.05	1.11	0.031
BD(1)	C26-H62	BD*(1)	C26-C27	0.93	1.11	0.029
BD(1)	C26-H62	BD*(1)	C27-N28	3.95	1.08	0.058
BD(1)	C27-N28	RY*(2)	C23	2.51	1.97	0.063
BD(1)	C27-N28	RY*(2)	C26	1.18	1.5	0.038
BD(1)	C27-N28	BD*(1)	C23-N28	1.35	1.33	0.038
BD(1)	C27-N28	BD*(1)	C23-C39	2.63	1.27	0.052
BD(1)	C27-N28	BD*(1)	C26-C27	1.5	1.38	0.041
BD(1)	C27-N28	BD*(1)	C26-H62	1.5	1.31	0.04
BD(1)	C27-N28	BD*(1)	C27-H63	0.68	1.32	0.027
BD(2)	C27-N28	RY*(4)	C23	1.23	2.23	0.05
BD(2)	C27-N28	RY*(5)	C26	1.03	1.46	0.037
BD(2)	C27-N28	BD*(2)	C23-C24	24.75	0.32	0.08
BD(2)	C27-N28	BD*(2)	C25-C26	13.47	0.31	0.059
BD(1)	C27-H63	RY*(1)	C26	0.8	1.77	0.034
BD(1)	C27-H63	RY*(1)	N28	1.14	1.46	0.037
BD(1)	C27-H63	BD*(1)	C23-N28	4.36	1.05	0.061
BD(1)	C27-H63	BD*(1)	C25-C26	3.46	1.11	0.055
BD(1)	C27-H63	BD*(1)	C26-C27	0.6	1.11	0.023
BD(1)	C27-H63	BD*(1)	C27-N28	0.51	1.08	0.021
BD(1)	C30-H49	RY*(2)	C6	0.51	1.52	0.025
BD(1)	C30-H49	BD*(1)	C5-C6	4.17	1.09	0.06
BD(1)	C30-H49	BD*(1)	C6-C30	0.68	0.93	0.023
BD(1)	C30-H50	RY*(3)	C6	0.78	1.43	0.03
BD(1)	C30-H50	BD*(2)	C5-C6	3.02	0.55	0.041
BD(1)	C30-H50	BD*(1)	C6-C7	1.54	1.1	0.037
BD(1)	C30-H50	BD*(1)	C6-C30	0.67	0.93	0.022

BD(1)	C30-H51	RY*(3)	C6	0.78	1.43	0.03
BD(1)	C30-H51	BD*(2)	C5-C6	2.92	0.55	0.04
BD(1)	C30-H51	BD*(1)	C6-C7	1.65	1.1	0.038
BD(1)	C30-H51	BD*(1)	C6-C30	0.69	0.93	0.023
BD(1)	N31-H32	RY*(1)	C8	1.21	1.71	0.041
BD(1)	N31-H32	RY*(3)	C33	0.91	1.68	0.035
BD(1)	N31-H32	BD*(2)	C7-C8	0.98	0.68	0.025
BD(1)	N31-H32	BD*(1)	C8-C9	2.65	1.22	0.051
BD(1)	N31-H32	BD*(1)	C33-N34	0.84	1.24	0.029
BD(1)	N31-H32	BD*(2)	C33-N34	5.4	0.66	0.055
BD(1)	N31-C33	RY*(1)	C8	2.52	1.87	0.061
BD(1)	N31-C33	RY*(1)	C11	0.88	1.74	0.035
BD(1)	N31-C33	RY*(1)	N34	0.55	1.83	0.028
BD(1)	N31-C33	BD*(1)	C7-C8	1.83	1.39	0.045
BD(1)	N31-C33	BD*(1)	C8-N31	1.9	1.24	0.043
BD(1)	N31-C33	BD*(1)	C11-N16	1.27	1.3	0.036
BD(1)	N31-C33	BD*(1)	N31-H32	0.75	1.24	0.027
BD(1)	N31-C33	BD*(1)	C33-N34	1.29	1.4	0.038
BD(1)	N31-C33	BD*(1)	N34-H35	2.47	1.27	0.05
BD(1)	C33-N34	RY*(1)	C11	0.81	1.83	0.034
BD(1)	C33-N34	RY*(1)	C33	0.79	1.73	0.033
BD(1)	C33-N34	BD*(1)	C11-C12	1.19	1.44	0.037
BD(1)	C33-N34	BD*(1)	C11-C33	2.17	1.32	0.048
BD(1)	C33-N34	BD*(1)	N31-H32	0.75	1.32	0.028
BD(1)	C33-N34	BD*(1)	N31-C33	1.13	1.32	0.035
BD(2)	C33-N34	BD*(1)	C8-N31	1.48	0.76	0.03
BD(2)	C33-N34	BD*(1)	C9-H48	0.74	0.85	0.023
BD(2)	C33-N34	BD*(2)	C11-C12	8.79	0.33	0.052
BD(2)	C33-N34	BD*(1)	N31-H32	2.43	0.76	0.039
BD(1)	N34-H35	RY*(1)	C33	1.58	1.44	0.043
BD(1)	N34-H35	RY*(4)	C33	1.03	2.59	0.046
BD(1)	N34-H35	BD*(1)	C11-C33	0.63	1.03	0.023
BD(1)	N34-H35	BD*(1)	N31-C33	9.33	1.04	0.088
BD(1)	C36-H57	RY*(3)	C22	0.72	1.41	0.029
BD(1)	C36-H57	BD*(1)	C17-C22	2.27	1.07	0.044
BD(1)	C36-H57	BD*(2)	C17-C22	2.98	0.54	0.04
BD(1)	C36-H57	BD*(1)	C22-C36	0.62	0.92	0.021
BD(1)	C36-H57	BD*(1)	C36-H59	0.57	1.05	0.022
BD(1)	C36-H58	RY*(3)	C22	0.78	1.41	0.03
BD(1)	C36-H58	BD*(1)	C17-C22	1.86	1.07	0.04
BD(1)	C36-H58	BD*(2)	C17-C22	3.47	0.53	0.043

BD(1)	C36-H58	BD*(1)	C22-C36	0.62	0.92	0.021
BD(1)	C36-H58	BD*(1)	C36-H59	0.58	1.05	0.022
BD(1)	C36-H59	RY*(2)	C22	0.78	1.52	0.031
BD(1)	C36-H59	BD*(1)	C1-O29	0.99	0.82	0.026
BD(1)	C36-H59	BD*(1)	C21-C22	3.67	1.09	0.057
BD(1)	C36-H59	BD*(1)	C22-C36	1.03	0.92	0.028
BD(1)	C36-H59	BD*(1)	C36-H57	0.86	0.99	0.026
BD(1)	C36-H59	BD*(1)	C36-H58	0.82	0.99	0.025
BD(1)	N37-H38	RY*(1)	C20	1.52	1.69	0.045
BD(1)	N37-H38	RY*(1)	C39	0.75	1.52	0.03
BD(1)	N37-H38	RY*(2)	C39	0.83	1.5	0.032
BD(1)	N37-H38	BD*(1)	C19-C20	2.9	1.24	0.054
BD(1)	N37-H38	BD*(2)	C20-C21	1.05	0.69	0.027
BD(1)	N37-H38	BD*(1)	C24-H60	0.55	1.13	0.022
BD(1)	N37-H38	BD*(1)	C39-N40	3.73	1.27	0.062
BD(1)	N37-C39	RY*(1)	C20	1.09	1.83	0.04
BD(1)	N37-C39	RY*(2)	C20	0.54	2	0.03
BD(1)	N37-C39	RY*(1)	C23	0.82	1.77	0.034
BD(1)	N37-C39	BD*(1)	C20-C21	1.02	1.38	0.034
BD(1)	N37-C39	BD*(1)	C20-N37	2.24	1.24	0.047
BD(1)	N37-C39	BD*(1)	C23-N28	1.29	1.3	0.037
BD(1)	N37-C39	BD*(1)	N37-H38	0.82	1.25	0.029
BD(1)	N37-C39	BD*(1)	C39-N40	1.73	1.42	0.044
BD(1)	N37-C39	BD*(1)	N40-H41	2.04	1.3	0.046
BD(1)	C39-N40	RY*(1)	C23	0.66	1.83	0.031
BD(1)	C39-N40	RY*(1)	C39	0.7	1.73	0.031
BD(1)	C39-N40	BD*(1)	C23-C24	1.2	1.42	0.037
BD(1)	C39-N40	BD*(1)	C23-C39	2.39	1.3	0.05
BD(1)	C39-N40	BD*(1)	N37-H38	1.47	1.31	0.039
BD(1)	C39-N40	BD*(1)	N37-C39	1.7	1.32	0.043
BD(2)	C39-N40	RY*(1)	N37	0.63	1.29	0.026
BD(2)	C39-N40	BD*(2)	C23-C24	8.91	0.31	0.051
BD(1)	N40-H41	RY*(1)	C39	1.84	1.44	0.046
BD(1)	N40-H41	RY*(4)	C39	0.93	2.44	0.043
BD(1)	N40-H41	BD*(1)	C23-C39	0.74	1.01	0.025
BD(1)	N40-H41	BD*(1)	N37-C39	10.95	1.04	0.096
CR(1)	C1	RY*(1)	C2	1.02	11.3	0.096
CR(1)	C1	RY*(2)	C2	1.02	10.84	0.094
CR(1)	C1	RY*(1)	C5	1.23	11.44	0.106
CR(1)	C1	BD*(1)	C1-C2	0.97	10.72	0.092
CR(1)	C1	BD*(1)	C1-O29	1	10.43	0.092

CR(1)	C1	BD*(1)	C2-H52	0.88	10.61	0.086
CR(1)	C1	BD*(1)	C4-O29	0.85	10.43	0.085
CR(1)	C1	BD*(1)	C5-C6	0.76	10.68	0.081
CR(1)	C1	BD*(1)	C5-C10	0.57	10.68	0.07
CR(1)	C2	RY*(2)	C1	1.63	11.27	0.121
CR(1)	C2	RY*(3)	C1	0.66	10.83	0.075
CR(1)	C2	RY*(2)	C3	1.49	10.81	0.113
CR(1)	C2	RY*(1)	H52	0.71	10.58	0.077
CR(1)	C2	BD*(1)	C1-C2	0.74	10.65	0.079
CR(1)	C2	BD*(1)	C1-C5	1.84	10.56	0.125
CR(1)	C2	BD*(1)	C3-H53	0.76	10.54	0.08
CR(1)	C3	RY*(2)	C2	1.54	10.77	0.115
CR(1)	C3	RY*(1)	C4	0.52	11	0.068
CR(1)	C3	RY*(2)	C4	2.06	11.34	0.137
CR(1)	C3	RY*(1)	H53	0.72	10.59	0.078
CR(1)	C3	BD*(1)	C2-H52	0.76	10.54	0.08
CR(1)	C3	BD*(1)	C3-C4	0.73	10.65	0.079
CR(1)	C3	BD*(1)	C4-C17	1.93	10.56	0.128
CR(1)	C4	RY*(1)	C3	1.17	11.29	0.103
CR(1)	C4	RY*(2)	C3	0.89	10.88	0.088
CR(1)	C4	RY*(1)	C17	0.73	11.42	0.082
CR(1)	C4	RY*(2)	C17	0.55	11.38	0.071
CR(1)	C4	RY*(5)	C17	0.71	11.14	0.079
CR(1)	C4	BD*(1)	C1-O29	0.84	10.44	0.084
CR(1)	C4	BD*(1)	C3-C4	0.95	10.72	0.091
CR(1)	C4	BD*(1)	C3-H53	0.86	10.61	0.086
CR(1)	C4	BD*(1)	C4-O29	0.97	10.43	0.09
CR(1)	C4	BD*(1)	C17-C18	0.57	10.69	0.07
CR(1)	C4	BD*(1)	C17-C22	0.75	10.69	0.081
CR(1)	C5	RY*(2)	C1	0.53	11.27	0.069
CR(1)	C5	RY*(6)	C1	0.64	11.53	0.077
CR(1)	C5	RY*(2)	C6	1.59	11.04	0.118
CR(1)	C5	RY*(5)	C6	0.57	11.13	0.071
CR(1)	C5	RY*(2)	C10	1.57	10.84	0.117
CR(1)	C5	BD*(1)	C1-C2	1.18	10.65	0.101
CR(1)	C5	BD*(1)	C6-C7	0.61	10.63	0.072
CR(1)	C5	BD*(1)	C6-C30	0.82	10.46	0.083
CR(1)	C5	BD*(1)	C9-C10	0.61	10.66	0.072
CR(1)	C5	BD*(1)	C10-H47	0.5	10.55	0.065
CR(1)	C6	RY*(1)	C5	0.56	11.39	0.071
CR(1)	C6	RY*(2)	C5	0.61	11.03	0.073

CR(1)	C6	RY*(3)	C5	0.63	11.01	0.074
CR(1)	C6	RY*(2)	C7	1.36	10.83	0.108
CR(1)	C6	RY*(3)	C30	1.18	10.75	0.1
CR(1)	C6	BD*(1)	C1-C5	0.91	10.58	0.088
CR(1)	C6	BD*(1)	C5-C10	0.61	10.63	0.072
CR(1)	C6	BD*(1)	C7-C8	0.84	10.64	0.085
CR(1)	C6	BD*(1)	C7-H46	0.56	10.54	0.069
CR(1)	C7	RY*(1)	C6	0.71	11.34	0.08
CR(1)	C7	RY*(2)	C6	1.76	11.04	0.124
CR(1)	C7	RY*(1)	C8	1.79	11.1	0.126
CR(1)	C7	RY*(1)	H46	0.58	10.59	0.07
CR(1)	C7	BD*(1)	C5-C6	0.89	10.61	0.088
CR(1)	C7	BD*(1)	C6-C30	0.67	10.45	0.075
CR(1)	C7	BD*(1)	C8-C9	0.77	10.62	0.081
CR(1)	C7	BD*(1)	C8-N31	0.98	10.47	0.091
CR(1)	C8	RY*(2)	C7	1.27	10.87	0.105
CR(1)	C8	RY*(5)	C7	0.78	11.23	0.084
CR(1)	C8	RY*(2)	C9	1.28	10.92	0.106
CR(1)	C8	RY*(5)	C9	0.54	11.18	0.069
CR(1)	C8	BD*(1)	C6-C7	0.66	10.69	0.075
CR(1)	C8	BD*(1)	C7-C8	0.61	10.68	0.072
CR(1)	C8	BD*(1)	C7-H46	0.59	10.58	0.071
CR(1)	C8	BD*(1)	C8-C9	0.66	10.67	0.076
CR(1)	C8	BD*(1)	C9-C10	0.56	10.71	0.07
CR(1)	C8	BD*(1)	C9-H48	0.55	10.62	0.068
CR(1)	C8	BD*(1)	N31-C33	1.01	10.53	0.093
CR(1)	C9	RY*(1)	C8	1.67	11.09	0.122
CR(1)	C9	RY*(2)	C8	0.74	11.25	0.082
CR(1)	C9	RY*(2)	C10	1.28	10.82	0.105
CR(1)	C9	RY*(1)	H48	0.83	10.68	0.084
CR(1)	C9	BD*(1)	C5-C10	0.85	10.6	0.085
CR(1)	C9	BD*(1)	C7-C8	0.81	10.61	0.083
CR(1)	C9	BD*(1)	C8-N31	0.63	10.46	0.073
CR(1)	C9	BD*(1)	C10-H47	0.57	10.54	0.069
CR(1)	C10	RY*(2)	C5	1.26	11.01	0.105
CR(1)	C10	RY*(2)	C9	1.65	10.87	0.12
CR(1)	C10	RY*(5)	C9	0.54	11.13	0.069
CR(1)	C10	RY*(1)	H47	0.63	10.6	0.073
CR(1)	C10	BD*(1)	C1-C5	0.76	10.56	0.08
CR(1)	C10	BD*(1)	C5-C6	0.78	10.61	0.082
CR(1)	C10	BD*(1)	C8-C9	0.79	10.62	0.082

CR(1)	C10	BD*(1)	C9-H48	0.59	10.56	0.071
CR(1)	C11	RY*(2)	C12	1.52	10.83	0.115
CR(1)	C11	RY*(2)	N16	0.66	11.31	0.077
CR(1)	C11	RY*(1)	C33	0.85	10.96	0.086
CR(1)	C11	BD*(1)	C12-C13	0.56	10.67	0.069
CR(1)	C11	BD*(1)	C12-H42	0.59	10.59	0.071
CR(1)	C11	BD*(1)	C15-N16	1.19	10.63	0.101
CR(1)	C11	BD*(1)	C33-N34	0.51	10.71	0.066
CR(1)	C12	RY*(1)	C11	1.1	11.01	0.098
CR(1)	C12	RY*(2)	C11	1.28	11.19	0.107
CR(1)	C12	RY*(2)	C13	1.8	10.74	0.124
CR(1)	C12	RY*(1)	H42	0.71	10.63	0.077
CR(1)	C12	BD*(1)	C11-N16	0.72	10.57	0.078
CR(1)	C12	BD*(1)	C11-C33	0.85	10.51	0.086
CR(1)	C12	BD*(1)	C13-C14	0.62	10.63	0.073
CR(1)	C12	BD*(1)	C13-H43	0.58	10.55	0.07
CR(1)	C13	RY*(2)	C12	1.5	10.8	0.114
CR(1)	C13	RY*(2)	C14	1.71	10.75	0.121
CR(1)	C13	RY*(4)	C14	0.62	11.01	0.074
CR(1)	C13	RY*(1)	H43	0.66	10.59	0.074
CR(1)	C13	BD*(1)	C11-C12	0.66	10.63	0.076
CR(1)	C13	BD*(1)	C12-H42	0.61	10.56	0.072
CR(1)	C13	BD*(1)	C14-C15	0.55	10.63	0.069
CR(1)	C13	BD*(1)	C14-H44	0.6	10.56	0.071
CR(1)	C14	RY*(2)	C13	1.61	10.75	0.118
CR(1)	C14	RY*(4)	C13	0.55	11.05	0.07
CR(1)	C14	RY*(1)	C15	0.54	11.03	0.069
CR(1)	C14	RY*(2)	C15	1.61	10.95	0.119
CR(1)	C14	RY*(1)	H44	0.67	10.59	0.075
CR(1)	C14	BD*(1)	C12-C13	0.62	10.63	0.073
CR(1)	C14	BD*(1)	C13-H43	0.6	10.55	0.071
CR(1)	C14	BD*(1)	C15-N16	0.56	10.59	0.069
CR(1)	C15	RY*(1)	C14	0.52	11.32	0.069
CR(1)	C15	RY*(2)	C14	1.54	10.78	0.115
CR(1)	C15	RY*(2)	N16	0.82	11.31	0.086
CR(1)	C15	RY*(1)	H45	0.66	10.64	0.075
CR(1)	C15	BD*(1)	C11-N16	1.33	10.61	0.107
CR(1)	C15	BD*(1)	C13-C14	0.6	10.66	0.072
CR(1)	C15	BD*(1)	C14-H44	0.6	10.59	0.072
CR(1)	N16	RY*(1)	C11	3.31	15.11	0.2
CR(1)	N16	RY*(1)	C15	2.49	15.12	0.173

CR(1)	N16	RY*(6)	C15	0.58	15.71	0.085
CR(1)	N16	BD*(1)	C11-C12	0.71	14.72	0.092
CR(1)	N16	BD*(1)	C14-C15	0.54	14.72	0.08
CR(1)	C17	RY*(2)	C4	0.54	11.35	0.07
CR(1)	C17	RY*(4)	C4	0.97	11.46	0.094
CR(1)	C17	RY*(2)	C18	1.37	10.86	0.109
CR(1)	C17	RY*(2)	C22	1.94	11.07	0.131
CR(1)	C17	BD*(1)	C3-C4	1.16	10.65	0.1
CR(1)	C17	BD*(1)	C18-C19	0.65	10.65	0.074
CR(1)	C17	BD*(1)	C21-C22	0.58	10.65	0.071
CR(1)	C17	BD*(1)	C22-C36	0.8	10.48	0.082
CR(1)	C18	RY*(1)	C17	1.72	11.35	0.125
CR(1)	C18	RY*(2)	C19	1.74	10.8	0.122
CR(1)	C18	RY*(5)	C19	0.51	11.11	0.067
CR(1)	C18	RY*(1)	H54	0.62	10.63	0.072
CR(1)	C18	BD*(1)	C4-C17	0.75	10.56	0.08
CR(1)	C18	BD*(1)	C17-C22	0.81	10.61	0.083
CR(1)	C18	BD*(1)	C19-C20	0.73	10.62	0.079
CR(1)	C18	BD*(1)	C19-H55	0.57	10.56	0.069
CR(1)	C19	RY*(2)	C18	1.4	10.85	0.11
CR(1)	C19	RY*(5)	C18	0.7	11.1	0.079
CR(1)	C19	RY*(1)	C20	0.62	11.06	0.074
CR(1)	C19	RY*(2)	C20	1.55	11.23	0.118
CR(1)	C19	RY*(1)	H55	0.74	10.63	0.079
CR(1)	C19	BD*(1)	C17-C18	0.89	10.61	0.087
CR(1)	C19	BD*(1)	C18-H54	0.55	10.54	0.068
CR(1)	C19	BD*(1)	C20-C21	0.77	10.61	0.081
CR(1)	C19	BD*(1)	C20-N37	0.94	10.47	0.089
CR(1)	C20	RY*(2)	C19	1.29	10.85	0.106
CR(1)	C20	RY*(5)	C19	0.64	11.16	0.075
CR(1)	C20	RY*(2)	C21	1.13	10.9	0.099
CR(1)	C20	BD*(1)	C18-C19	0.52	10.7	0.067
CR(1)	C20	BD*(1)	C19-C20	0.52	10.67	0.067
CR(1)	C20	BD*(1)	C19-H55	0.58	10.61	0.07
CR(1)	C20	BD*(1)	C20-C21	0.69	10.67	0.077
CR(1)	C20	BD*(1)	C21-C22	0.69	10.69	0.077
CR(1)	C20	BD*(1)	C21-H56	0.56	10.58	0.069
CR(1)	C20	BD*(1)	N37-H38	0.5	10.54	0.065
CR(1)	C20	BD*(1)	N37-C39	1.09	10.54	0.097
CR(1)	C21	RY*(1)	C20	1.87	11.06	0.129
CR(1)	C21	RY*(1)	C22	1.08	11.33	0.099

CR(1)	C21	RY*(2)	C22	1.17	11.06	0.101
CR(1)	C21	RY*(5)	C22	0.75	11.23	0.082
CR(1)	C21	RY*(1)	H56	0.58	10.58	0.07
CR(1)	C21	BD*(1)	C17-C22	0.9	10.61	0.088
CR(1)	C21	BD*(1)	C19-C20	0.8	10.61	0.083
CR(1)	C21	BD*(1)	C20-N37	0.63	10.47	0.073
CR(1)	C21	BD*(1)	C21-C22	0.5	10.63	0.066
CR(1)	C21	BD*(1)	C22-C36	0.68	10.46	0.076
CR(1)	C22	RY*(2)	C17	1.83	11.32	0.128
CR(1)	C22	RY*(2)	C21	1.49	10.85	0.113
CR(1)	C22	RY*(3)	C36	1.03	10.82	0.094
CR(1)	C22	BD*(1)	C4-C17	0.94	10.57	0.09
CR(1)	C22	BD*(1)	C17-C18	0.62	10.63	0.073
CR(1)	C22	BD*(1)	C20-C21	0.82	10.63	0.084
CR(1)	C22	BD*(1)	C21-C22	0.53	10.65	0.067
CR(1)	C22	BD*(1)	C21-H56	0.57	10.54	0.069
CR(1)	C23	RY*(1)	C24	0.52	11.32	0.069
CR(1)	C23	RY*(2)	C24	1.37	10.87	0.109
CR(1)	C23	RY*(2)	N28	0.67	11.33	0.078
CR(1)	C23	RY*(1)	C39	1.1	10.98	0.099
CR(1)	C23	BD*(1)	C24-C25	0.58	10.67	0.07
CR(1)	C23	BD*(1)	C24-H60	0.61	10.58	0.072
CR(1)	C23	BD*(1)	C27-N28	1.21	10.63	0.101
CR(1)	C24	RY*(1)	C23	1.07	11.04	0.097
CR(1)	C24	RY*(2)	C23	1.32	11.21	0.109
CR(1)	C24	RY*(2)	C25	1.85	10.74	0.126
CR(1)	C24	RY*(1)	H60	0.68	10.66	0.076
CR(1)	C24	BD*(1)	C23-N28	0.68	10.57	0.076
CR(1)	C24	BD*(1)	C23-C39	0.87	10.51	0.087
CR(1)	C24	BD*(1)	C25-C26	0.61	10.63	0.072
CR(1)	C24	BD*(1)	C25-H61	0.58	10.55	0.07
CR(1)	C25	RY*(2)	C24	1.45	10.84	0.112
CR(1)	C25	RY*(5)	C24	0.55	11.08	0.07
CR(1)	C25	RY*(2)	C26	1.71	10.75	0.121
CR(1)	C25	RY*(4)	C26	0.63	11.01	0.074
CR(1)	C25	RY*(1)	H61	0.65	10.59	0.074
CR(1)	C25	BD*(1)	C23-C24	0.7	10.63	0.077
CR(1)	C25	BD*(1)	C24-H60	0.67	10.55	0.075
CR(1)	C25	BD*(1)	C26-C27	0.55	10.63	0.068
CR(1)	C25	BD*(1)	C26-H62	0.6	10.56	0.071
CR(1)	C26	RY*(2)	C25	1.55	10.74	0.115

CR(1)	C26	RY*(4)	C25	0.55	11.04	0.07
CR(1)	C26	RY*(1)	C27	0.5	11.04	0.067
CR(1)	C26	RY*(2)	C27	1.64	10.94	0.12
CR(1)	C26	RY*(1)	H62	0.67	10.59	0.075
CR(1)	C26	BD*(1)	C24-C25	0.63	10.63	0.073
CR(1)	C26	BD*(1)	C25-H61	0.6	10.55	0.071
CR(1)	C26	BD*(1)	C27-N28	0.55	10.59	0.069
CR(1)	C27	RY*(1)	C26	0.53	11.32	0.069
CR(1)	C27	RY*(2)	C26	1.53	10.78	0.115
CR(1)	C27	RY*(2)	N28	0.83	11.32	0.086
CR(1)	C27	RY*(1)	H63	0.66	10.63	0.075
CR(1)	C27	BD*(1)	C23-N28	1.35	10.61	0.107
CR(1)	C27	BD*(1)	C25-C26	0.6	10.66	0.071
CR(1)	C27	BD*(1)	C26-H62	0.61	10.59	0.072
CR(1)	N28	RY*(1)	C23	3.28	15.13	0.199
CR(1)	N28	RY*(1)	C27	2.47	15.13	0.173
CR(1)	N28	RY*(6)	C27	0.6	15.68	0.086
CR(1)	N28	BD*(1)	C23-C24	0.72	14.71	0.092
CR(1)	N28	BD*(1)	C26-C27	0.55	14.72	0.081
CR(1)	O29	RY*(1)	C1	1.99	19.9	0.178
CR(1)	O29	RY*(1)	C4	2.28	19.94	0.191
CR(1)	O29	BD*(1)	C36-H59	0.52	19.53	0.091
CR(1)	C30	RY*(1)	C6	1.15	11.34	0.102
CR(1)	C30	RY*(1)	H49	0.61	10.69	0.072
CR(1)	C30	RY*(1)	H50	0.65	10.72	0.075
CR(1)	C30	RY*(1)	H51	0.65	10.68	0.075
CR(1)	C30	BD*(1)	C5-C6	0.63	10.61	0.074
CR(1)	C30	BD*(1)	C6-C7	0.51	10.63	0.066
CR(1)	N31	RY*(2)	C8	1.79	15.42	0.148
CR(1)	N31	RY*(6)	C8	1.01	15.22	0.11
CR(1)	N31	RY*(2)	C33	3.35	15.05	0.201
CR(1)	C33	RY*(2)	C11	1.05	11.26	0.097
CR(1)	C33	RY*(3)	C11	0.8	11.3	0.085
CR(1)	C33	RY*(3)	N34	1.08	11.03	0.098
CR(1)	C33	BD*(1)	C8-N31	1.13	10.58	0.098
CR(1)	C33	BD*(1)	C11-C12	0.68	10.69	0.076
CR(1)	C33	BD*(1)	N34-H35	0.76	10.61	0.081
CR(1)	N34	RY*(1)	C33	5.17	14.98	0.249
CR(1)	N34	RY*(1)	H35	0.64	14.82	0.087
CR(1)	N34	BD*(1)	C11-C33	0.97	14.56	0.108
CR(1)	C36	RY*(1)	C22	1.09	11.31	0.099

CR(1)	C36	RY*(1)	H57	0.59	10.66	0.071
CR(1)	C36	RY*(1)	H58	0.6	10.66	0.071
CR(1)	C36	RY*(1)	H59	1.28	10.79	0.105
CR(1)	C36	BD*(1)	C17-C22	0.64	10.58	0.074
CR(1)	C36	BD*(1)	C21-C22	0.53	10.61	0.067
CR(1)	N37	RY*(2)	C20	1.5	15.4	0.136
CR(1)	N37	RY*(6)	C20	0.94	15.39	0.107
CR(1)	N37	RY*(1)	H38	0.63	14.89	0.087
CR(1)	N37	RY*(2)	C39	3.15	15.03	0.194
CR(1)	N37	BD*(1)	C19-C20	0.57	14.78	0.082
CR(1)	C39	RY*(2)	C23	1.09	11.27	0.099
CR(1)	C39	RY*(3)	C23	0.72	11.26	0.08
CR(1)	C39	RY*(3)	N40	0.97	11.05	0.093
CR(1)	C39	BD*(1)	C20-N37	1.17	10.57	0.1
CR(1)	C39	BD*(1)	C23-C24	0.7	10.68	0.078
CR(1)	C39	BD*(1)	N37-H38	0.57	10.58	0.07
CR(1)	C39	BD*(1)	N40-H41	0.71	10.62	0.078
CR(1)	N40	RY*(1)	C39	4.43	14.97	0.23
CR(1)	N40	RY*(2)	C39	1.01	14.95	0.11
CR(1)	N40	RY*(1)	H41	0.66	14.82	0.088
CR(1)	N40	BD*(1)	C23-C39	0.97	14.54	0.108
CR(1)	N40	BD*(1)	N37-C39	0.72	14.57	0.092
LP(1)	N16	RY*(1)	C11	3.71	1.3	0.063
LP(1)	N16	RY*(1)	C15	2.94	1.31	0.056
LP(1)	N16	BD*(1)	C11-C12	9.17	0.91	0.083
LP(1)	N16	BD*(1)	C11-C33	2.43	0.79	0.039
LP(1)	N16	BD*(1)	C14-C15	8.79	0.91	0.081
LP(1)	N16	BD*(1)	C15-H45	2.65	0.85	0.043
LP(1)	N16	BD*(1)	N34-H35	2.25	0.83	0.039
LP(1)	N28	RY*(1)	C23	3.69	1.32	0.064
LP(1)	N28	RY*(1)	C27	2.91	1.32	0.056
LP(1)	N28	BD*(1)	C23-C24	9.1	0.91	0.082
LP(1)	N28	BD*(1)	C23-C39	2.42	0.79	0.039
LP(1)	N28	BD*(1)	C26-C27	8.89	0.91	0.081
LP(1)	N28	BD*(1)	C27-H63	2.71	0.85	0.043
LP(1)	N28	BD*(1)	N40-H41	2.71	0.85	0.043
LP(1)	O29	RY*(1)	C1	2.82	1.5	0.059
LP(1)	O29	RY*(3)	C1	0.54	1.37	0.025
LP(1)	O29	RY*(1)	C4	3.09	1.54	0.062
LP(1)	O29	BD*(1)	C1-C2	2.57	1.18	0.049
LP(1)	O29	BD*(1)	C3-C4	2.42	1.19	0.048

LP(1)	O29	BD*(1)	C36-H59	13.93	1.14	0.113
LP(2)	O29	RY*(4)	C1	1.29	2.24	0.052
LP(2)	O29	RY*(3)	C4	1.68	2.11	0.057
LP(2)	O29	BD*(2)	C1-C2	23.87	0.36	0.083
LP(2)	O29	BD*(2)	C3-C4	23.82	0.36	0.083
LP(1)	N31	RY*(3)	C8	1.98	1.92	0.058
LP(1)	N31	RY*(4)	C33	0.78	2.25	0.039
LP(1)	N31	BD*(1)	C7-C8	0.74	0.85	0.023
LP(1)	N31	BD*(2)	C7-C8	26.95	0.29	0.084
LP(1)	N31	BD*(1)	C8-C9	1.67	0.84	0.035
LP(1)	N31	BD*(1)	C11-C33	5.32	0.69	0.056
LP(1)	N31	BD*(1)	C33-N34	8.07	0.86	0.078
LP(1)	N31	BD*(2)	C33-N34	9.25	0.28	0.046
LP(1)	N34	RY*(1)	C33	6.07	1.23	0.078
LP(1)	N34	BD*(1)	C9-H48	1.48	0.91	0.033
LP(1)	N34	BD*(1)	C11-C33	12.81	0.81	0.091
LP(1)	N34	BD*(1)	N31-C33	3.3	0.82	0.047
LP(1)	N37	RY*(3)	C20	1.88	1.64	0.053
LP(1)	N37	RY*(3)	C39	1.72	1.98	0.056
LP(1)	N37	BD*(1)	C19-C20	3.07	0.84	0.049
LP(1)	N37	BD*(1)	C20-C21	2.66	0.83	0.045
LP(1)	N37	BD*(2)	C20-C21	19.86	0.29	0.07
LP(1)	N37	BD*(1)	C39-N40	0.59	0.87	0.022
LP(1)	N37	BD*(2)	C39-N40	46.06	0.29	0.104
LP(1)	N40	RY*(1)	C39	5.4	1.22	0.073
LP(1)	N40	RY*(4)	C39	0.52	2.22	0.031
LP(1)	N40	BD*(1)	C19-H55	0.5	0.88	0.019
LP(1)	N40	BD*(1)	C23-C39	13.55	0.79	0.092
LP(1)	N40	BD*(1)	N37-C39	2.85	0.81	0.043
BD*(2)	C1-C2	RY*(4)	C2	1.7	1.07	0.099
BD*(2)	C1-C2	BD*(1)	C5-C6	0.9	0.53	0.048
BD*(2)	C1-C2	BD*(1)	C5-C10	0.71	0.53	0.044
BD*(2)	C3-C4	RY*(4)	C3	1.63	1.21	0.1
BD*(2)	C3-C4	RY*(6)	C4	0.81	1.7	0.083
BD*(2)	C5-C6	RY*(3)	C5	0.65	0.91	0.048
BD*(2)	C5-C6	RY*(3)	C6	0.65	0.88	0.047
BD*(2)	C5-C6	RY*(7)	C6	0.58	1.66	0.061
BD*(2)	C5-C6	BD*(1)	C1-C2	0.8	0.57	0.041
BD*(2)	C5-C6	BD*(1)	C1-O29	2.57	0.29	0.051
BD*(2)	C5-C6	BD*(1)	C30-H50	1.28	0.45	0.047
BD*(2)	C5-C6	BD*(1)	C30-H51	1.26	0.45	0.047

BD*(2)	C7-C8	RY*(3)	C7	2.48	0.96	0.097
BD*(2)	C7-C8	RY*(4)	C8	1.33	1.33	0.083
BD*(2)	C7-C8	BD*(2)	C9-C10	202.48	0.01	0.081
BD*(2)	C7-C8	BD*(1)	N31-H32	0.75	0.4	0.034
BD*(2)	C9-C10	RY*(3)	C9	2.16	0.67	0.086
BD*(2)	C9-C10	RY*(4)	C10	0.9	0.96	0.067
BD*(2)	C9-C10	RY*(5)	C10	0.98	0.84	0.065
BD*(2)	C11-C12	RY*(7)	C11	0.78	1.54	0.076
BD*(2)	C11-C12	RY*(4)	C12	0.8	1.21	0.068
BD*(2)	C11-C12	RY*(5)	C12	0.94	0.95	0.065
BD*(2)	C11-C12	BD*(2)	C33-N34	98.52	0.01	0.066
BD*(2)	C13-C14	RY*(5)	C13	2.06	0.73	0.088
BD*(2)	C13-C14	RY*(3)	C14	0.99	1.5	0.088
BD*(2)	C15-N16	RY*(5)	C14	0.58	1.11	0.053
BD*(2)	C15-N16	RY*(3)	C15	1.42	1.8	0.106
BD*(2)	C15-N16	RY*(4)	N16	1.59	1.2	0.092
BD*(2)	C15-N16	BD*(2)	C11-C12	119.94	0.02	0.077
BD*(2)	C15-N16	BD*(2)	C13-C14	162.88	0.02	0.084
BD*(2)	C17-C22	RY*(4)	C17	0.61	1.81	0.066
BD*(2)	C17-C22	RY*(6)	C17	0.61	1.48	0.059
BD*(2)	C17-C22	RY*(7)	C22	0.53	1.66	0.059
BD*(2)	C17-C22	BD*(1)	C36-H57	1	0.45	0.042
BD*(2)	C17-C22	BD*(1)	C36-H58	1.18	0.45	0.045
BD*(2)	C18-C19	RY*(4)	C18	2.02	0.83	0.093
BD*(2)	C18-C19	RY*(3)	C19	1.31	0.72	0.07
BD*(2)	C18-C19	RY*(4)	C19	0.51	1.86	0.07
BD*(2)	C20-C21	RY*(3)	C19	0.64	0.73	0.043
BD*(2)	C20-C21	RY*(4)	C20	0.97	1.62	0.079
BD*(2)	C20-C21	RY*(3)	C21	0.74	1.79	0.073
BD*(2)	C20-C21	RY*(5)	C21	0.64	0.91	0.048
BD*(2)	C20-C21	BD*(2)	C17-C22	348.36	0.01	0.083
BD*(2)	C20-C21	BD*(2)	C18-C19	261.78	0.01	0.081
BD*(2)	C20-C21	BD*(1)	N37-H38	0.84	0.41	0.037
BD*(2)	C20-C21	BD*(1)	N37-C39	0.63	0.42	0.031
BD*(2)	C23-C24	RY*(7)	C23	1.42	0.99	0.082
BD*(2)	C23-C24	RY*(3)	C24	0.91	0.79	0.058
BD*(2)	C23-C24	BD*(2)	C39-N40	57.02	0.03	0.07
BD*(2)	C25-C26	RY*(5)	C25	2.25	0.71	0.091
BD*(2)	C25-C26	RY*(3)	C26	1.09	1.44	0.09
BD*(2)	C27-N28	RY*(5)	C26	0.57	1.16	0.054
BD*(2)	C27-N28	RY*(3)	C27	1.41	1.81	0.106

BD*(2)	C27-N28	RY*(3)	N28	1.19	0.92	0.07
BD*(2)	C27-N28	BD*(2)	C23-C24	141.19	0.02	0.078
BD*(2)	C27-N28	BD*(2)	C25-C26	181.04	0.02	0.084
BD*(2)	C39-N40	RY*(7)	C39	0.54	1.77	0.081
BD*(2)	C39-N40	RY*(2)	N40	1.47	0.8	0.089

Table SI 4: The second-order perturbative estimates of donor-acceptor interactions in the NBO basis of the molecule 4.

Donor NBO (i)		Acceptor NBO (j)		E(2) kcal/mol	E(j) -E(i) a.u.	F(i,j) a.u.
BD(1)	C1-C2	RY*(1)	C3	1.01	1.88	0.039
BD(1)	C1-C2	RY*(2)	C4	0.5	2	0.028
BD(1)	C1-C2	RY*(2)	C5	1	1.75	0.038
BD(1)	C1-C2	BD*(1)	C1-C5	4.84	1.23	0.069
BD(1)	C1-C2	BD*(1)	C2-C3	2.17	1.25	0.047
BD(1)	C1-C2	BD*(1)	C2-H62	1.92	1.21	0.043
BD(1)	C1-C2	BD*(1)	C3-H63	3	1.2	0.054
BD(1)	C1-C2	BD*(1)	C5-C10	1.26	1.28	0.036
BD(2)	C1-C2	RY*(3)	C3	1.28	1.58	0.042
BD(2)	C1-C2	RY*(3)	C5	1.05	1.32	0.035
BD(2)	C1-C2	RY*(2)	O37	0.79	1.43	0.032
BD(2)	C1-C2	BD*(2)	C3-C4	15.61	0.3	0.063
BD(2)	C1-C2	BD*(1)	C5-C6	1.17	0.84	0.029
BD(2)	C1-C2	BD*(2)	C5-C6	8.22	0.3	0.047
BD(2)	C1-C2	BD*(1)	C5-C10	1.19	0.83	0.029
BD(2)	C1-C2	BD*(1)	C38-H56	0.99	0.76	0.026
BD(1)	C1-C5	RY*(1)	C2	0.85	1.86	0.036
BD(1)	C1-C5	RY*(1)	C6	1.54	1.99	0.05
BD(1)	C1-C5	RY*(1)	C10	1.22	1.94	0.044
BD(1)	C1-C5	RY*(1)	O37	0.61	1.99	0.031
BD(1)	C1-C5	BD*(1)	C1-C2	4.22	1.28	0.066
BD(1)	C1-C5	BD*(1)	C2-C3	0.8	1.22	0.028
BD(1)	C1-C5	BD*(1)	C4-O37	1.82	1	0.038
BD(1)	C1-C5	BD*(1)	C5-C6	3.26	1.25	0.057
BD(1)	C1-C5	BD*(1)	C5-C10	2.9	1.25	0.054
BD(1)	C1-C5	BD*(1)	C6-C7	1.84	1.27	0.043
BD(1)	C1-C5	BD*(1)	C9-C10	1.73	1.3	0.042
BD(1)	C1-O37	RY*(1)	C4	0.71	1.81	0.032
BD(1)	C1-O37	RY*(2)	C4	1.4	2.14	0.049
BD(1)	C1-O37	RY*(2)	C5	0.69	1.89	0.032
BD(1)	C1-O37	BD*(1)	C1-C2	0.53	1.45	0.025
BD(1)	C1-O37	BD*(1)	C2-H62	2.48	1.35	0.052

BD(1)	C1-O37	BD*(1)	C4-C21	2.24	1.37	0.05
BD(1)	C1-O37	BD*(1)	C5-C6	1.47	1.42	0.041
BD(1)	C2-C3	RY*(1)	C1	1.22	1.57	0.039
BD(1)	C2-C3	RY*(1)	C4	1.36	1.61	0.042
BD(1)	C2-C3	BD*(1)	C1-C2	2.47	1.26	0.05
BD(1)	C2-C3	BD*(1)	C1-C5	6.24	1.17	0.076
BD(1)	C2-C3	BD*(1)	C1-O37	1.78	0.97	0.037
BD(1)	C2-C3	BD*(1)	C2-H62	1.3	1.15	0.035
BD(1)	C2-C3	BD*(1)	C3-C4	2.49	1.26	0.05
BD(1)	C2-C3	BD*(1)	C3-H63	1.32	1.15	0.035
BD(1)	C2-C3	BD*(1)	C4-C21	6.36	1.17	0.077
BD(1)	C2-C3	BD*(1)	C4-O37	1.82	0.97	0.038
BD(1)	C2-H62	RY*(2)	C1	1.06	1.81	0.039
BD(1)	C2-H62	RY*(1)	C3	0.74	1.72	0.032
BD(1)	C2-H62	BD*(1)	C1-C2	2	1.15	0.043
BD(1)	C2-H62	BD*(1)	C1-O37	3.09	0.86	0.046
BD(1)	C2-H62	BD*(1)	C2-C3	1.01	1.08	0.03
BD(1)	C2-H62	BD*(1)	C3-C4	1.56	1.15	0.038
BD(1)	C3-C4	RY*(1)	C2	0.95	1.89	0.038
BD(1)	C3-C4	RY*(1)	C21	1.17	1.99	0.043
BD(1)	C3-C4	BD*(1)	C2-C3	2.13	1.25	0.046
BD(1)	C3-C4	BD*(1)	C2-H62	3	1.21	0.054
BD(1)	C3-C4	BD*(1)	C3-H63	1.93	1.2	0.043
BD(1)	C3-C4	BD*(1)	C4-C21	4.91	1.23	0.07
BD(1)	C3-C4	BD*(1)	C21-C26	1.74	1.28	0.042
BD(2)	C3-C4	RY*(3)	C2	1.16	1.71	0.042
BD(2)	C3-C4	RY*(3)	C21	1.13	1.43	0.038
BD(2)	C3-C4	BD*(2)	C1-C2	15.9	0.3	0.063
BD(2)	C3-C4	BD*(2)	C21-C22	11.13	0.3	0.054
BD(1)	C3-H63	RY*(1)	C2	0.76	1.72	0.032
BD(1)	C3-H63	RY*(2)	C4	0.97	1.83	0.038
BD(1)	C3-H63	BD*(1)	C1-C2	1.58	1.15	0.038
BD(1)	C3-H63	BD*(1)	C2-C3	0.96	1.08	0.029
BD(1)	C3-H63	BD*(1)	C3-C4	1.92	1.15	0.042
BD(1)	C3-H63	BD*(1)	C4-O37	3.17	0.86	0.047
BD(1)	C4-C21	RY*(1)	C3	0.69	1.85	0.032
BD(1)	C4-C21	RY*(1)	C22	0.95	1.94	0.039
BD(1)	C4-C21	RY*(1)	C26	1.69	1.96	0.052
BD(1)	C4-C21	RY*(1)	O37	0.56	1.99	0.03
BD(1)	C4-C21	BD*(1)	C1-O37	1.9	1	0.039
BD(1)	C4-C21	BD*(1)	C2-C3	0.67	1.22	0.026

BD(1)	C4-C21	BD*(1)	C3-C4	4.22	1.29	0.066
BD(1)	C4-C21	BD*(1)	C21-C22	2.64	1.25	0.051
BD(1)	C4-C21	BD*(1)	C21-C26	3.54	1.25	0.06
BD(1)	C4-C21	BD*(1)	C22-C23	2.01	1.28	0.045
BD(1)	C4-C21	BD*(1)	C25-C26	1.59	1.29	0.041
BD(1)	C4-O37	RY*(1)	C1	0.71	1.77	0.032
BD(1)	C4-O37	RY*(2)	C1	1.36	2.11	0.048
BD(1)	C4-O37	RY*(2)	C21	0.71	2.1	0.034
BD(1)	C4-O37	BD*(1)	C1-C5	2.27	1.37	0.05
BD(1)	C4-O37	BD*(1)	C3-C4	0.55	1.46	0.025
BD(1)	C4-O37	BD*(1)	C3-H63	2.39	1.34	0.051
BD(1)	C4-O37	BD*(1)	C21-C22	1.71	1.42	0.044
BD(1)	C5-C6	RY*(1)	C1	0.59	1.59	0.027
BD(1)	C5-C6	RY*(1)	C7	0.74	1.94	0.034
BD(1)	C5-C6	RY*(2)	C7	0.55	1.47	0.026
BD(1)	C5-C6	RY*(1)	C10	0.61	1.93	0.031
BD(1)	C5-C6	RY*(1)	C38	0.51	1.48	0.025
BD(1)	C5-C6	BD*(1)	C1-C5	3.4	1.19	0.057
BD(1)	C5-C6	BD*(1)	C1-O37	1.92	0.99	0.039
BD(1)	C5-C6	BD*(1)	C5-C10	3.83	1.24	0.062
BD(1)	C5-C6	BD*(1)	C6-C7	3.23	1.27	0.057
BD(1)	C5-C6	BD*(1)	C6-C38	1.66	1.1	0.038
BD(1)	C5-C6	BD*(1)	C7-H61	1.88	1.17	0.042
BD(1)	C5-C6	BD*(1)	C10-H59	1.84	1.18	0.042
BD(2)	C5-C6	RY*(5)	C7	0.75	1.23	0.03
BD(2)	C5-C6	RY*(3)	C10	0.98	1.82	0.042
BD(2)	C5-C6	BD*(1)	C1-C2	0.93	0.84	0.027
BD(2)	C5-C6	BD*(2)	C1-C2	12.36	0.27	0.052
BD(2)	C5-C6	BD*(1)	C1-O37	2.92	0.56	0.039
BD(2)	C5-C6	BD*(2)	C7-C8	19.58	0.28	0.066
BD(2)	C5-C6	BD*(2)	C9-C10	19.57	0.28	0.068
BD(2)	C5-C6	BD*(1)	C38-H57	1.55	0.72	0.033
BD(2)	C5-C6	BD*(1)	C38-H58	2.36	0.72	0.041
BD(1)	C5-C10	RY*(1)	C1	1.06	1.59	0.037
BD(1)	C5-C10	RY*(1)	C6	0.69	1.98	0.033
BD(1)	C5-C10	RY*(2)	C6	0.68	1.67	0.03
BD(1)	C5-C10	RY*(1)	C9	0.78	1.96	0.035
BD(1)	C5-C10	RY*(2)	C9	1.72	1.47	0.045
BD(1)	C5-C10	BD*(1)	C1-C2	2.59	1.27	0.051
BD(1)	C5-C10	BD*(1)	C1-C5	2.79	1.19	0.051
BD(1)	C5-C10	BD*(1)	C5-C6	4.11	1.24	0.064

BD(1)	C5-C10	BD*(1)	C6-C38	3.21	1.09	0.053
BD(1)	C5-C10	BD*(1)	C9-C10	2.8	1.29	0.054
BD(1)	C5-C10	BD*(1)	C9-H60	1.98	1.2	0.044
BD(1)	C5-C10	BD*(1)	C10-H59	1.25	1.18	0.034
BD(1)	C6-C7	RY*(1)	C5	0.62	2.01	0.032
BD(1)	C6-C7	RY*(2)	C5	0.92	1.72	0.036
BD(1)	C6-C7	RY*(2)	C8	2.3	1.65	0.055
BD(1)	C6-C7	RY*(3)	C8	0.52	1.53	0.025
BD(1)	C6-C7	RY*(1)	C38	0.81	1.49	0.031
BD(1)	C6-C7	BD*(1)	C1-C5	3.32	1.2	0.056
BD(1)	C6-C7	BD*(1)	C5-C6	3.79	1.25	0.062
BD(1)	C6-C7	BD*(1)	C6-C38	1.52	1.1	0.037
BD(1)	C6-C7	BD*(1)	C7-C8	3.32	1.27	0.058
BD(1)	C6-C7	BD*(1)	C7-H61	1.45	1.18	0.037
BD(1)	C6-C7	BD*(1)	C8-N39	3.95	1.13	0.06
BD(1)	C6-C7	BD*(1)	C38-H56	0.64	1.18	0.025
BD(1)	C6-C38	RY*(1)	C5	1.27	1.94	0.045
BD(1)	C6-C38	RY*(1)	C7	1.15	1.87	0.042
BD(1)	C6-C38	BD*(1)	C5-C6	2.07	1.18	0.044
BD(1)	C6-C38	BD*(1)	C5-C10	2.42	1.18	0.048
BD(1)	C6-C38	BD*(1)	C6-C7	2.07	1.2	0.045
BD(1)	C6-C38	BD*(1)	C7-C8	2.65	1.2	0.051
BD(1)	C6-C38	BD*(1)	C38-H56	0.85	1.11	0.027
BD(1)	C6-C38	BD*(1)	C38-H57	0.79	1.1	0.026
BD(1)	C6-C38	BD*(1)	C38-H58	0.82	1.09	0.027
BD(1)	C7-C8	RY*(1)	C6	0.89	1.99	0.038
BD(1)	C7-C8	RY*(2)	C6	1.95	1.68	0.051
BD(1)	C7-C8	RY*(1)	C9	0.72	1.97	0.034
BD(1)	C7-C8	RY*(2)	C9	0.53	1.48	0.025
BD(1)	C7-C8	RY*(1)	N39	1.1	1.63	0.038
BD(1)	C7-C8	BD*(1)	C6-C7	3.43	1.28	0.059
BD(1)	C7-C8	BD*(1)	C6-C38	2.66	1.1	0.048
BD(1)	C7-C8	BD*(1)	C7-H61	1.5	1.18	0.038
BD(1)	C7-C8	BD*(1)	C8-C9	3.5	1.27	0.06
BD(1)	C7-C8	BD*(1)	C8-N39	1.51	1.13	0.037
BD(1)	C7-C8	BD*(1)	C9-H60	1.92	1.21	0.043
BD(1)	C7-C8	BD*(1)	N39-C41	1.5	1.13	0.037
BD(2)	C7-C8	RY*(3)	C9	1.11	1.46	0.039
BD(2)	C7-C8	BD*(2)	C5-C6	21.46	0.28	0.071
BD(2)	C7-C8	BD*(2)	C9-C10	17.96	0.29	0.065
BD(2)	C7-C8	BD*(1)	N39-H40	1.82	0.7	0.035

BD(2)	C7-C8	BD*(1)	N39-C41	2.75	0.69	0.042
BD(1)	C7-H61	RY*(1)	C6	1.23	1.83	0.042
BD(1)	C7-H61	RY*(1)	C8	1.19	1.74	0.041
BD(1)	C7-H61	BD*(1)	C5-C6	4.21	1.09	0.061
BD(1)	C7-H61	BD*(1)	C6-C7	1.34	1.11	0.034
BD(1)	C7-H61	BD*(1)	C7-C8	1.02	1.11	0.03
BD(1)	C7-H61	BD*(1)	C8-C9	3.66	1.11	0.057
BD(1)	C8-C9	RY*(1)	C7	0.58	1.93	0.03
BD(1)	C8-C9	RY*(2)	C7	0.7	1.46	0.029
BD(1)	C8-C9	RY*(1)	C10	0.62	1.93	0.031
BD(1)	C8-C9	RY*(2)	C10	1.66	1.47	0.044
BD(1)	C8-C9	RY*(1)	N39	1.16	1.62	0.039
BD(1)	C8-C9	BD*(1)	C7-C8	3.49	1.27	0.059
BD(1)	C8-C9	BD*(1)	C7-H61	2.11	1.17	0.045
BD(1)	C8-C9	BD*(1)	C8-N39	1.31	1.12	0.034
BD(1)	C8-C9	BD*(1)	C9-C10	2.91	1.29	0.055
BD(1)	C8-C9	BD*(1)	C9-H60	1.53	1.2	0.038
BD(1)	C8-C9	BD*(1)	C10-H59	2.1	1.18	0.045
BD(1)	C8-C9	BD*(1)	N39-H40	1.19	1.13	0.033
BD(1)	C8-C9	BD*(1)	N39-C41	0.84	1.12	0.028
BD(1)	C8-N39	RY*(1)	C7	0.65	2.03	0.032
BD(1)	C8-N39	RY*(1)	C9	0.81	2.06	0.037
BD(1)	C8-N39	RY*(3)	C41	1.33	1.66	0.042
BD(1)	C8-N39	BD*(1)	C6-C7	1.37	1.36	0.039
BD(1)	C8-N39	BD*(1)	C7-C8	1.56	1.36	0.041
BD(1)	C8-N39	BD*(1)	C8-C9	1.39	1.35	0.039
BD(1)	C8-N39	BD*(1)	C9-C10	1.44	1.39	0.04
BD(1)	C8-N39	BD*(1)	C11-C41	0.82	1.2	0.028
BD(1)	C8-N39	BD*(1)	N39-H40	0.68	1.23	0.026
BD(1)	C8-N39	BD*(1)	N39-C41	1.7	1.22	0.041
BD(1)	C8-N39	BD*(2)	C41-N42	1.2	0.78	0.028
BD(1)	C9-C10	RY*(1)	C5	1.42	2.02	0.048
BD(1)	C9-C10	RY*(2)	C5	0.74	1.72	0.032
BD(1)	C9-C10	RY*(1)	C8	1.71	1.91	0.051
BD(1)	C9-C10	RY*(3)	C8	0.74	1.54	0.03
BD(1)	C9-C10	BD*(1)	C1-C5	3.01	1.2	0.054
BD(1)	C9-C10	BD*(1)	C5-C10	3.36	1.25	0.058
BD(1)	C9-C10	BD*(1)	C8-C9	2.81	1.27	0.053
BD(1)	C9-C10	BD*(1)	C8-N39	3.67	1.13	0.058
BD(1)	C9-C10	BD*(1)	C9-H60	1.59	1.21	0.039
BD(1)	C9-C10	BD*(1)	C10-H59	1.54	1.19	0.038

BD(2)	C9-C10	BD*(2)	C5-C6	17.68	0.28	0.064
BD(2)	C9-C10	BD*(2)	C7-C8	20.06	0.28	0.068
BD(1)	C9-H60	RY*(1)	C8	1.14	1.73	0.04
BD(1)	C9-H60	RY*(1)	C10	0.84	1.77	0.034
BD(1)	C9-H60	BD*(1)	C5-C10	4	1.08	0.059
BD(1)	C9-H60	BD*(1)	C7-C8	3.6	1.1	0.056
BD(1)	C9-H60	BD*(1)	C8-C9	1.29	1.1	0.034
BD(1)	C9-H60	BD*(1)	C8-N39	0.51	0.96	0.02
BD(1)	C9-H60	BD*(1)	C9-C10	1.36	1.13	0.035
BD(1)	C10-H59	RY*(1)	C5	1.28	1.85	0.044
BD(1)	C10-H59	RY*(1)	C9	1	1.81	0.038
BD(1)	C10-H59	BD*(1)	C5-C6	3.86	1.09	0.058
BD(1)	C10-H59	BD*(1)	C5-C10	0.96	1.09	0.029
BD(1)	C10-H59	BD*(1)	C8-C9	3.72	1.1	0.057
BD(1)	C10-H59	BD*(1)	C9-C10	1.25	1.14	0.034
BD(1)	C11-C12	RY*(1)	C13	0.68	1.94	0.033
BD(1)	C11-C12	RY*(2)	C13	1.54	1.42	0.042
BD(1)	C11-C12	RY*(2)	N17	0.62	2.03	0.032
BD(1)	C11-C12	RY*(1)	C41	1.28	1.5	0.039
BD(1)	C11-C12	BD*(1)	C11-N17	2.14	1.25	0.046
BD(1)	C11-C12	BD*(1)	C11-C41	2.07	1.14	0.044
BD(1)	C11-C12	BD*(1)	C12-C13	2.81	1.3	0.054
BD(1)	C11-C12	BD*(1)	C12-H50	1.34	1.18	0.036
BD(1)	C11-C12	BD*(1)	C13-H51	2.47	1.18	0.048
BD(1)	C11-C12	BD*(1)	N39-C41	1.74	1.16	0.04
BD(1)	C11-N17	RY*(1)	C15	1.13	1.86	0.041
BD(1)	C11-N17	RY*(2)	C15	2.24	2.04	0.061
BD(1)	C11-N17	RY*(2)	C41	0.92	1.76	0.036
BD(1)	C11-N17	BD*(1)	C11-C12	2.38	1.37	0.051
BD(1)	C11-N17	BD*(1)	C11-C41	1.18	1.28	0.035
BD(1)	C11-N17	BD*(1)	C12-H50	1.27	1.32	0.037
BD(1)	C11-N17	BD*(1)	C15-N17	1.37	1.33	0.038
BD(1)	C11-N17	BD*(1)	C15-C18	2.59	1.39	0.054
BD(1)	C11-N17	BD*(1)	C41-N42	1.41	1.44	0.04
BD(2)	C11-N17	RY*(3)	C12	1.1	1.18	0.034
BD(2)	C11-N17	RY*(4)	C15	1.39	2.25	0.053
BD(2)	C11-N17	BD*(2)	C12-C13	11.72	0.32	0.055
BD(2)	C11-N17	BD*(2)	C14-C15	19.37	0.32	0.075
BD(2)	C11-N17	BD*(2)	C41-N42	10.77	0.33	0.056
BD(1)	C11-C41	RY*(1)	C12	0.95	1.9	0.038
BD(1)	C11-C41	RY*(1)	N17	1.33	1.67	0.042

BD(1)	C11-C41	RY*(1)	N39	1.33	1.62	0.042
BD(1)	C11-C41	RY*(1)	N42	0.86	1.65	0.034
BD(1)	C11-C41	BD*(1)	C8-N39	1.45	1.12	0.036
BD(1)	C11-C41	BD*(1)	C11-C12	1.56	1.19	0.039
BD(1)	C11-C41	BD*(1)	C11-N17	1.61	1.21	0.039
BD(1)	C11-C41	BD*(1)	C12-C13	1.71	1.26	0.041
BD(1)	C11-C41	BD*(1)	C15-N17	3.58	1.15	0.057
BD(1)	C11-C41	BD*(1)	N39-H40	0.59	1.13	0.023
BD(1)	C11-C41	BD*(1)	N39-C41	0.72	1.12	0.026
BD(1)	C11-C41	BD*(1)	C41-N42	1.25	1.26	0.035
BD(1)	C12-C13	RY*(1)	C11	1.4	1.65	0.043
BD(1)	C12-C13	RY*(2)	C11	0.58	1.93	0.03
BD(1)	C12-C13	RY*(1)	C14	2	1.96	0.056
BD(1)	C12-C13	RY*(2)	C14	0.56	2	0.03
BD(1)	C12-C13	BD*(1)	C11-C12	3.01	1.25	0.055
BD(1)	C12-C13	BD*(1)	C11-C41	2.96	1.16	0.053
BD(1)	C12-C13	BD*(1)	C12-H50	1.8	1.2	0.042
BD(1)	C12-C13	BD*(1)	C13-C14	2.99	1.26	0.055
BD(1)	C12-C13	BD*(1)	C13-H51	1.57	1.2	0.039
BD(1)	C12-C13	BD*(1)	C14-C16	3.02	1.27	0.055
BD(2)	C12-C13	BD*(2)	C11-N17	23.11	0.28	0.073
BD(2)	C12-C13	BD*(2)	C14-C15	14.27	0.29	0.061
BD(1)	C12-H50	RY*(2)	C11	1.26	1.76	0.042
BD(1)	C12-H50	RY*(1)	C13	0.99	1.79	0.038
BD(1)	C12-H50	BD*(1)	C11-C12	0.96	1.08	0.029
BD(1)	C12-H50	BD*(1)	C11-N17	4.29	1.1	0.061
BD(1)	C12-H50	BD*(1)	C12-C13	1.42	1.15	0.036
BD(1)	C12-H50	BD*(1)	C13-C14	3.59	1.09	0.056
BD(1)	C12-H50	BD*(1)	N42-H43	0.81	1.01	0.026
BD(1)	C13-C14	RY*(1)	C12	1.01	1.94	0.04
BD(1)	C13-C14	RY*(2)	C12	1.12	1.41	0.036
BD(1)	C13-C14	RY*(1)	C15	0.68	1.72	0.031
BD(1)	C13-C14	RY*(1)	C16	1.09	1.94	0.041
BD(1)	C13-C14	BD*(1)	C12-C13	2.88	1.29	0.055
BD(1)	C13-C14	BD*(1)	C12-H50	2.39	1.18	0.047
BD(1)	C13-C14	BD*(1)	C13-H51	1.14	1.18	0.033
BD(1)	C13-C14	BD*(1)	C14-C15	3.01	1.23	0.055
BD(1)	C13-C14	BD*(1)	C14-C16	3.31	1.24	0.057
BD(1)	C13-C14	BD*(1)	C15-C18	2.34	1.25	0.048
BD(1)	C13-C14	BD*(1)	C16-C20	1.4	1.3	0.038
BD(1)	C13-H51	RY*(1)	C12	0.93	1.79	0.037

BD(1)	C13-H51	RY*(2)	C14	1.05	1.83	0.039
BD(1)	C13-H51	BD*(1)	C11-C12	3.67	1.08	0.056
BD(1)	C13-H51	BD*(1)	C12-C13	1.3	1.15	0.035
BD(1)	C13-H51	BD*(1)	C13-C14	0.96	1.09	0.029
BD(1)	C13-H51	BD*(1)	C14-C15	3.61	1.08	0.056
BD(1)	C14-C15	RY*(1)	C13	0.6	1.92	0.031
BD(1)	C14-C15	RY*(1)	C16	0.61	1.93	0.031
BD(1)	C14-C15	RY*(2)	N17	0.73	2.01	0.034
BD(1)	C14-C15	RY*(1)	C18	1.07	1.87	0.04
BD(1)	C14-C15	BD*(1)	C13-C14	2.9	1.22	0.053
BD(1)	C14-C15	BD*(1)	C13-H51	2.08	1.16	0.044
BD(1)	C14-C15	BD*(1)	C14-C16	3.26	1.23	0.057
BD(1)	C14-C15	BD*(1)	C15-N17	1.38	1.18	0.036
BD(1)	C14-C15	BD*(1)	C15-C18	3.17	1.24	0.056
BD(1)	C14-C15	BD*(1)	C16-H52	1.86	1.17	0.042
BD(1)	C14-C15	BD*(1)	C18-H55	1.7	1.19	0.04
BD(2)	C14-C15	RY*(3)	C13	0.65	2.05	0.038
BD(2)	C14-C15	RY*(3)	C16	1.07	1.62	0.043
BD(2)	C14-C15	RY*(3)	N17	1.02	1.19	0.036
BD(2)	C14-C15	RY*(3)	C18	1.15	1.47	0.042
BD(2)	C14-C15	BD*(2)	C11-N17	15.01	0.26	0.058
BD(2)	C14-C15	BD*(2)	C12-C13	17.96	0.27	0.066
BD(2)	C14-C15	BD*(2)	C16-C20	16.19	0.28	0.064
BD(2)	C14-C15	BD*(2)	C18-C19	14.84	0.28	0.062
BD(1)	C14-C16	RY*(1)	C13	1.06	1.93	0.041
BD(1)	C14-C16	RY*(2)	C15	1.02	1.9	0.039
BD(1)	C14-C16	RY*(1)	C20	0.89	1.94	0.037
BD(1)	C14-C16	RY*(2)	C20	1.39	1.39	0.039
BD(1)	C14-C16	BD*(1)	C12-C13	1.42	1.29	0.038
BD(1)	C14-C16	BD*(1)	C13-C14	3.38	1.23	0.058
BD(1)	C14-C16	BD*(1)	C14-C15	3.33	1.23	0.057
BD(1)	C14-C16	BD*(1)	C15-N17	2.8	1.18	0.051
BD(1)	C14-C16	BD*(1)	C16-C20	2.78	1.29	0.054
BD(1)	C14-C16	BD*(1)	C16-H52	1.14	1.18	0.033
BD(1)	C14-C16	BD*(1)	C20-H53	2.17	1.19	0.045
BD(1)	C15-N17	RY*(1)	C11	0.74	1.73	0.032
BD(1)	C15-N17	RY*(2)	C11	2.2	2	0.059
BD(1)	C15-N17	RY*(1)	C18	0.91	1.98	0.038
BD(1)	C15-N17	BD*(1)	C11-N17	1.36	1.35	0.038
BD(1)	C15-N17	BD*(1)	C11-C41	2.97	1.24	0.055
BD(1)	C15-N17	BD*(1)	C14-C15	1.96	1.33	0.046

BD(1)	C15-N17	BD*(1)	C14-C16	1.58	1.34	0.041
BD(1)	C15-N17	BD*(1)	C15-C18	1.75	1.35	0.043
BD(1)	C15-N17	BD*(1)	C18-C19	1.26	1.41	0.038
BD(1)	C15-C18	RY*(2)	C14	1.44	1.97	0.048
BD(1)	C15-C18	RY*(1)	N17	1.09	1.7	0.039
BD(1)	C15-C18	RY*(1)	C19	0.86	1.94	0.037
BD(1)	C15-C18	RY*(2)	C19	1.36	1.39	0.039
BD(1)	C15-C18	BD*(1)	C11-N17	2.54	1.23	0.05
BD(1)	C15-C18	BD*(1)	C13-C14	2.26	1.23	0.047
BD(1)	C15-C18	BD*(1)	C14-C15	3.07	1.22	0.055
BD(1)	C15-C18	BD*(1)	C15-N17	1.91	1.18	0.042
BD(1)	C15-C18	BD*(1)	C18-C19	2.62	1.29	0.052
BD(1)	C15-C18	BD*(1)	C18-H55	1.28	1.19	0.035
BD(1)	C15-C18	BD*(1)	C19-H54	2.24	1.18	0.046
BD(1)	C16-C20	RY*(1)	C14	2.62	1.94	0.064
BD(1)	C16-C20	RY*(1)	C19	0.77	1.96	0.035
BD(1)	C16-C20	RY*(2)	C19	1.26	1.41	0.038
BD(1)	C16-C20	BD*(1)	C13-C14	3.15	1.25	0.056
BD(1)	C16-C20	BD*(1)	C14-C16	3.02	1.26	0.055
BD(1)	C16-C20	BD*(1)	C16-H52	1.65	1.2	0.04
BD(1)	C16-C20	BD*(1)	C19-C20	2.57	1.26	0.051
BD(1)	C16-C20	BD*(1)	C19-H54	1.86	1.21	0.042
BD(1)	C16-C20	BD*(1)	C20-H53	1.52	1.21	0.038
BD(2)	C16-C20	RY*(6)	C14	0.84	0.97	0.027
BD(2)	C16-C20	RY*(3)	C19	0.9	1.85	0.039
BD(2)	C16-C20	BD*(2)	C14-C15	16.5	0.28	0.064
BD(2)	C16-C20	BD*(2)	C18-C19	16.72	0.3	0.063
BD(1)	C16-H52	RY*(1)	C14	0.73	1.77	0.032
BD(1)	C16-H52	RY*(2)	C14	0.59	1.82	0.029
BD(1)	C16-H52	RY*(1)	C20	1.02	1.79	0.038
BD(1)	C16-H52	BD*(1)	C14-C15	3.94	1.08	0.058
BD(1)	C16-H52	BD*(1)	C14-C16	0.95	1.09	0.029
BD(1)	C16-H52	BD*(1)	C16-C20	1.28	1.14	0.034
BD(1)	C16-H52	BD*(1)	C19-C20	3.66	1.09	0.056
BD(1)	C18-C19	RY*(1)	C15	1.88	1.73	0.051
BD(1)	C18-C19	RY*(2)	C15	0.52	1.91	0.028
BD(1)	C18-C19	RY*(1)	C20	0.74	1.96	0.034
BD(1)	C18-C19	RY*(2)	C20	1.27	1.4	0.038
BD(1)	C18-C19	BD*(1)	C15-N17	3.14	1.2	0.055
BD(1)	C18-C19	BD*(1)	C15-C18	2.63	1.26	0.051
BD(1)	C18-C19	BD*(1)	C18-H55	1.62	1.21	0.04

BD(1)	C18-C19	BD*(1)	C19-C20	2.58	1.25	0.051
BD(1)	C18-C19	BD*(1)	C19-H54	1.51	1.21	0.038
BD(1)	C18-C19	BD*(1)	C20-H53	1.91	1.2	0.043
BD(2)	C18-C19	RY*(7)	C15	1.06	1.13	0.033
BD(2)	C18-C19	RY*(3)	C20	0.92	1.84	0.04
BD(2)	C18-C19	BD*(2)	C14-C15	17.43	0.28	0.065
BD(2)	C18-C19	BD*(2)	C16-C20	17.64	0.29	0.064
BD(1)	C18-H55	RY*(1)	C15	0.78	1.56	0.031
BD(1)	C18-H55	RY*(1)	C19	0.92	1.78	0.036
BD(1)	C18-H55	BD*(1)	C14-C15	3.89	1.07	0.058
BD(1)	C18-H55	BD*(1)	C15-C18	0.96	1.08	0.029
BD(1)	C18-H55	BD*(1)	C18-C19	1.29	1.14	0.034
BD(1)	C18-H55	BD*(1)	C19-C20	3.84	1.08	0.057
BD(1)	C19-C20	RY*(1)	C16	0.6	1.93	0.03
BD(1)	C19-C20	RY*(2)	C16	1.59	1.42	0.043
BD(1)	C19-C20	RY*(2)	C18	2.13	1.48	0.05
BD(1)	C19-C20	BD*(1)	C16-C20	2.71	1.29	0.053
BD(1)	C19-C20	BD*(1)	C16-H52	2.38	1.17	0.047
BD(1)	C19-C20	BD*(1)	C18-C19	2.63	1.29	0.052
BD(1)	C19-C20	BD*(1)	C18-H55	2.3	1.19	0.047
BD(1)	C19-C20	BD*(1)	C19-H54	1.17	1.18	0.033
BD(1)	C19-C20	BD*(1)	C20-H53	1.17	1.18	0.033
BD(1)	C19-H54	RY*(1)	C18	0.89	1.72	0.035
BD(1)	C19-H54	RY*(1)	C20	0.92	1.79	0.036
BD(1)	C19-H54	BD*(1)	C15-C18	3.81	1.09	0.058
BD(1)	C19-H54	BD*(1)	C16-C20	3.08	1.14	0.053
BD(1)	C19-H54	BD*(1)	C18-C19	1.26	1.14	0.034
BD(1)	C19-H54	BD*(1)	C19-C20	0.7	1.08	0.025
BD(1)	C20-H53	RY*(1)	C16	0.93	1.79	0.037
BD(1)	C20-H53	RY*(1)	C19	0.93	1.79	0.037
BD(1)	C20-H53	BD*(1)	C14-C16	3.9	1.08	0.058
BD(1)	C20-H53	BD*(1)	C16-C20	1.21	1.14	0.033
BD(1)	C20-H53	BD*(1)	C18-C19	3.02	1.15	0.053
BD(1)	C20-H53	BD*(1)	C19-C20	0.71	1.08	0.025
BD(1)	C21-C22	RY*(1)	C4	0.86	1.64	0.034
BD(1)	C21-C22	RY*(1)	C23	0.7	1.93	0.033
BD(1)	C21-C22	RY*(2)	C23	1.45	1.38	0.04
BD(1)	C21-C22	RY*(1)	C26	0.96	1.96	0.039
BD(1)	C21-C22	BD*(1)	C4-C21	2.96	1.2	0.053
BD(1)	C21-C22	BD*(1)	C4-O37	2.85	1	0.048
BD(1)	C21-C22	BD*(1)	C21-C26	4.19	1.25	0.065

BD(1)	C21-C22	BD*(1)	C22-C23	2.98	1.27	0.055
BD(1)	C21-C22	BD*(1)	C22-H67	1.28	1.17	0.035
BD(1)	C21-C22	BD*(1)	C23-H68	2.08	1.16	0.044
BD(1)	C21-C22	BD*(1)	C26-C44	3.12	1.11	0.053
BD(2)	C21-C22	RY*(5)	C4	0.71	1.43	0.031
BD(2)	C21-C22	RY*(4)	C23	1.31	1.51	0.044
BD(2)	C21-C22	BD*(2)	C3-C4	17.72	0.28	0.063
BD(2)	C21-C22	BD*(2)	C23-C24	19.14	0.27	0.065
BD(2)	C21-C22	BD*(2)	C25-C26	19.06	0.29	0.068
BD(1)	C21-C26	RY*(1)	C4	1.08	1.63	0.038
BD(1)	C21-C26	RY*(2)	C22	0.53	1.48	0.025
BD(1)	C21-C26	RY*(1)	C25	0.74	1.93	0.034
BD(1)	C21-C26	RY*(2)	C25	0.73	1.51	0.03
BD(1)	C21-C26	RY*(1)	C44	0.53	1.53	0.026
BD(1)	C21-C26	BD*(1)	C3-C4	2.42	1.28	0.05
BD(1)	C21-C26	BD*(1)	C4-C21	3.27	1.19	0.056
BD(1)	C21-C26	BD*(1)	C21-C22	3.91	1.25	0.062
BD(1)	C21-C26	BD*(1)	C22-H67	1.87	1.17	0.042
BD(1)	C21-C26	BD*(1)	C25-C26	3.09	1.28	0.056
BD(1)	C21-C26	BD*(1)	C25-H69	1.83	1.19	0.042
BD(1)	C21-C26	BD*(1)	C26-C44	1.68	1.1	0.039
BD(1)	C21-C26	BD*(1)	C44-H66	0.56	1.18	0.023
BD(1)	C22-C23	RY*(2)	C21	2.42	1.95	0.062
BD(1)	C22-C23	RY*(1)	C24	0.95	1.69	0.036
BD(1)	C22-C23	RY*(2)	C24	1.22	1.92	0.043
BD(1)	C22-C23	BD*(1)	C4-C21	2.68	1.21	0.051
BD(1)	C22-C23	BD*(1)	C21-C22	3.39	1.26	0.059
BD(1)	C22-C23	BD*(1)	C22-H67	1.48	1.19	0.038
BD(1)	C22-C23	BD*(1)	C23-C24	3.32	1.27	0.058
BD(1)	C22-C23	BD*(1)	C23-H68	1.63	1.18	0.039
BD(1)	C22-C23	BD*(1)	C24-N45	4.93	1.13	0.067
BD(1)	C22-H67	RY*(1)	C21	0.76	1.81	0.033
BD(1)	C22-H67	RY*(2)	C21	0.66	1.78	0.031
BD(1)	C22-H67	RY*(1)	C23	0.94	1.78	0.037
BD(1)	C22-H67	BD*(1)	C21-C22	0.99	1.1	0.029
BD(1)	C22-H67	BD*(1)	C21-C26	3.9	1.1	0.059
BD(1)	C22-H67	BD*(1)	C22-C23	1.05	1.12	0.031
BD(1)	C22-H67	BD*(1)	C23-C24	3.71	1.1	0.057
BD(1)	C23-C24	RY*(1)	C22	1.05	1.96	0.041
BD(1)	C23-C24	RY*(2)	C22	1.2	1.5	0.038
BD(1)	C23-C24	RY*(1)	C25	0.62	1.95	0.031

BD(1)	C23-C24	RY*(2)	C25	0.58	1.53	0.027
BD(1)	C23-C24	RY*(1)	N45	0.9	1.64	0.034
BD(1)	C23-C24	BD*(1)	C22-C23	2.86	1.29	0.054
BD(1)	C23-C24	BD*(1)	C22-H67	2	1.19	0.044
BD(1)	C23-C24	BD*(1)	C23-H68	1.42	1.18	0.037
BD(1)	C23-C24	BD*(1)	C24-C25	4	1.27	0.064
BD(1)	C23-C24	BD*(1)	C24-N45	1.64	1.13	0.038
BD(1)	C23-C24	BD*(1)	C25-H69	1.7	1.21	0.041
BD(1)	C23-C24	BD*(1)	N45-C47	2.31	1.15	0.046
BD(2)	C23-C24	RY*(4)	C22	1.76	1.03	0.042
BD(2)	C23-C24	RY*(4)	C23	0.51	1.52	0.027
BD(2)	C23-C24	RY*(3)	C25	1.35	1.01	0.036
BD(2)	C23-C24	BD*(2)	C21-C22	21.9	0.28	0.072
BD(2)	C23-C24	BD*(2)	C25-C26	16.45	0.3	0.064
BD(2)	C23-C24	BD*(1)	N45-H46	0.64	0.7	0.021
BD(2)	C23-C24	BD*(1)	N45-C47	1.29	0.71	0.029
BD(1)	C23-H68	RY*(1)	C22	0.97	1.8	0.037
BD(1)	C23-H68	RY*(2)	C24	1.28	1.76	0.043
BD(1)	C23-H68	BD*(1)	C21-C22	3.67	1.11	0.057
BD(1)	C23-H68	BD*(1)	C22-C23	1.33	1.13	0.035
BD(1)	C23-H68	BD*(1)	C23-C24	0.9	1.11	0.028
BD(1)	C23-H68	BD*(1)	C24-C25	3.54	1.12	0.056
BD(1)	C24-C25	RY*(1)	C23	0.58	1.93	0.03
BD(1)	C24-C25	RY*(2)	C23	0.56	1.38	0.025
BD(1)	C24-C25	RY*(2)	C26	2.5	1.71	0.059
BD(1)	C24-C25	RY*(1)	N45	0.92	1.62	0.035
BD(1)	C24-C25	BD*(1)	C23-C24	3.9	1.25	0.062
BD(1)	C24-C25	BD*(1)	C23-H68	2.26	1.16	0.046
BD(1)	C24-C25	BD*(1)	C24-N45	1.16	1.11	0.032
BD(1)	C24-C25	BD*(1)	C25-C26	3.33	1.29	0.059
BD(1)	C24-C25	BD*(1)	C25-H69	1.45	1.2	0.037
BD(1)	C24-C25	BD*(1)	C26-C44	2.67	1.11	0.049
BD(1)	C24-C25	BD*(1)	N45-H46	1.87	1.12	0.041
BD(1)	C24-N45	RY*(1)	C23	0.63	2.04	0.032
BD(1)	C24-N45	RY*(1)	C25	0.71	2.05	0.034
BD(1)	C24-N45	RY*(1)	C47	1.37	1.67	0.043
BD(1)	C24-N45	BD*(1)	C22-C23	0.96	1.39	0.033
BD(1)	C24-N45	BD*(1)	C23-C24	1.5	1.37	0.04
BD(1)	C24-N45	BD*(1)	C24-C25	1.41	1.37	0.039
BD(1)	C24-N45	BD*(1)	C25-C26	1.61	1.4	0.042
BD(1)	C24-N45	BD*(1)	C27-C47	1.56	1.22	0.039

BD(1)	C24-N45	BD*(1)	N45-H46	0.97	1.24	0.031
BD(1)	C24-N45	BD*(1)	N45-C47	2.19	1.25	0.047
BD(1)	C25-C26	RY*(1)	C21	1.55	1.96	0.05
BD(1)	C25-C26	RY*(1)	C24	1.63	1.68	0.047
BD(1)	C25-C26	RY*(1)	C44	0.74	1.54	0.03
BD(1)	C25-C26	BD*(1)	C4-C21	3.6	1.2	0.059
BD(1)	C25-C26	BD*(1)	C21-C26	3.82	1.25	0.062
BD(1)	C25-C26	BD*(1)	C24-C25	3.34	1.26	0.058
BD(1)	C25-C26	BD*(1)	C24-N45	2.9	1.12	0.051
BD(1)	C25-C26	BD*(1)	C25-H69	1.65	1.2	0.04
BD(1)	C25-C26	BD*(1)	C26-C44	1.66	1.11	0.038
BD(1)	C25-C26	BD*(1)	C44-H65	0.52	1.19	0.022
BD(2)	C25-C26	RY*(6)	C21	0.63	1.68	0.032
BD(2)	C25-C26	RY*(6)	C24	0.58	1.72	0.031
BD(2)	C25-C26	BD*(2)	C21-C22	18.41	0.27	0.064
BD(2)	C25-C26	BD*(2)	C23-C24	22.07	0.26	0.069
BD(2)	C25-C26	BD*(1)	C44-H64	2.55	0.73	0.042
BD(2)	C25-C26	BD*(1)	C44-H65	0.97	0.75	0.026
BD(1)	C25-H69	RY*(2)	C24	1.15	1.73	0.04
BD(1)	C25-H69	RY*(1)	C26	1.25	1.79	0.042
BD(1)	C25-H69	BD*(1)	C21-C26	4.36	1.08	0.061
BD(1)	C25-H69	BD*(1)	C23-C24	3.84	1.08	0.058
BD(1)	C25-H69	BD*(1)	C24-C25	1.19	1.09	0.032
BD(1)	C25-H69	BD*(1)	C24-N45	0.62	0.94	0.022
BD(1)	C25-H69	BD*(1)	C25-C26	1.65	1.12	0.038
BD(1)	C26-C44	RY*(1)	C21	1.16	1.88	0.042
BD(1)	C26-C44	RY*(1)	C25	1.11	1.86	0.041
BD(1)	C26-C44	BD*(1)	C21-C22	2.53	1.17	0.049
BD(1)	C26-C44	BD*(1)	C21-C26	2.1	1.17	0.044
BD(1)	C26-C44	BD*(1)	C24-C25	2.83	1.18	0.052
BD(1)	C26-C44	BD*(1)	C25-C26	2.32	1.21	0.047
BD(1)	C26-C44	BD*(1)	C44-H64	0.79	1.1	0.026
BD(1)	C26-C44	BD*(1)	C44-H65	0.85	1.11	0.028
BD(1)	C26-C44	BD*(1)	C44-H66	0.73	1.11	0.025
BD(1)	C27-C28	RY*(1)	C29	0.69	1.95	0.033
BD(1)	C27-C28	RY*(2)	C29	1.49	1.42	0.041
BD(1)	C27-C28	RY*(2)	N33	0.61	2.02	0.031
BD(1)	C27-C28	RY*(2)	C47	1.32	1.56	0.041
BD(1)	C27-C28	BD*(1)	C27-N33	2.22	1.25	0.047
BD(1)	C27-C28	BD*(1)	C27-C47	1.81	1.14	0.041
BD(1)	C27-C28	BD*(1)	C28-C29	2.96	1.3	0.055

BD(1)	C27-C28	BD*(1)	C28-H70	1.38	1.18	0.036
BD(1)	C27-C28	BD*(1)	C29-H71	2.4	1.18	0.048
BD(1)	C27-C28	BD*(1)	C47-N48	1.5	1.33	0.04
BD(1)	C27-N33	RY*(1)	C31	0.94	1.86	0.038
BD(1)	C27-N33	RY*(2)	C31	2.41	2.04	0.063
BD(1)	C27-N33	RY*(2)	C47	0.69	1.69	0.031
BD(1)	C27-N33	BD*(1)	C27-C28	2.44	1.37	0.052
BD(1)	C27-N33	BD*(1)	C27-C47	1.35	1.28	0.037
BD(1)	C27-N33	BD*(1)	C28-H70	1.3	1.31	0.037
BD(1)	C27-N33	BD*(1)	C31-N33	1.41	1.33	0.039
BD(1)	C27-N33	BD*(1)	C31-C34	2.51	1.39	0.053
BD(1)	C27-N33	BD*(1)	N45-C47	1.63	1.3	0.042
BD(2)	C27-N33	RY*(3)	C28	0.89	0.97	0.028
BD(2)	C27-N33	RY*(4)	C31	1.41	2.26	0.054
BD(2)	C27-N33	BD*(2)	C28-C29	11.59	0.32	0.055
BD(2)	C27-N33	BD*(2)	C30-C31	19.59	0.32	0.075
BD(2)	C27-N33	BD*(2)	C47-N48	10.3	0.35	0.054
BD(1)	C27-C47	RY*(1)	C28	0.75	1.88	0.034
BD(1)	C27-C47	RY*(1)	N33	1.27	1.57	0.04
BD(1)	C27-C47	RY*(2)	N45	1.12	2.1	0.043
BD(1)	C27-C47	RY*(1)	N48	0.94	1.74	0.036
BD(1)	C27-C47	BD*(1)	C24-N45	3.74	1.1	0.057
BD(1)	C27-C47	BD*(1)	C27-C28	1.72	1.18	0.04
BD(1)	C27-C47	BD*(1)	C27-N33	1.19	1.2	0.034
BD(1)	C27-C47	BD*(1)	C28-C29	1.63	1.25	0.04
BD(1)	C27-C47	BD*(1)	C31-N33	3.68	1.15	0.058
BD(1)	C27-C47	BD*(1)	C47-N48	1.93	1.28	0.045
BD(1)	C28-C29	RY*(1)	C27	1.57	1.69	0.046
BD(1)	C28-C29	RY*(1)	C30	2.05	1.96	0.057
BD(1)	C28-C29	RY*(2)	C30	0.53	2	0.029
BD(1)	C28-C29	BD*(1)	C27-C28	3.11	1.25	0.056
BD(1)	C28-C29	BD*(1)	C27-C47	3.02	1.16	0.053
BD(1)	C28-C29	BD*(1)	C28-H70	1.88	1.2	0.042
BD(1)	C28-C29	BD*(1)	C29-C30	2.99	1.27	0.055
BD(1)	C28-C29	BD*(1)	C29-H71	1.57	1.2	0.039
BD(1)	C28-C29	BD*(1)	C30-C32	3.04	1.27	0.056
BD(2)	C28-C29	RY*(6)	C30	0.51	0.98	0.021
BD(2)	C28-C29	BD*(2)	C27-N33	23.49	0.28	0.074
BD(2)	C28-C29	BD*(2)	C30-C31	14.06	0.29	0.06
BD(1)	C28-H70	RY*(2)	C27	1.26	1.77	0.042
BD(1)	C28-H70	RY*(1)	C29	1.05	1.8	0.039

BD(1)	C28-H70	BD*(1)	C27-C28	0.96	1.09	0.029
BD(1)	C28-H70	BD*(1)	C27-N33	4.11	1.1	0.06
BD(1)	C28-H70	BD*(1)	C28-C29	1.33	1.15	0.035
BD(1)	C28-H70	BD*(1)	C29-C30	3.47	1.1	0.055
BD(1)	C28-H70	BD*(1)	N45-H46	2.14	1.02	0.042
BD(1)	C29-C30	RY*(1)	C28	1.31	1.93	0.045
BD(1)	C29-C30	RY*(2)	C28	0.74	1.47	0.03
BD(1)	C29-C30	RY*(1)	C31	0.75	1.72	0.032
BD(1)	C29-C30	RY*(1)	C32	1.09	1.95	0.041
BD(1)	C29-C30	BD*(1)	C28-C29	2.91	1.29	0.055
BD(1)	C29-C30	BD*(1)	C28-H70	2.44	1.17	0.048
BD(1)	C29-C30	BD*(1)	C29-H71	1.16	1.18	0.033
BD(1)	C29-C30	BD*(1)	C30-C31	3.02	1.23	0.055
BD(1)	C29-C30	BD*(1)	C30-C32	3.38	1.24	0.058
BD(1)	C29-C30	BD*(1)	C31-C34	2.32	1.25	0.048
BD(1)	C29-C30	BD*(1)	C32-C36	1.4	1.3	0.038
BD(1)	C29-H71	RY*(1)	C28	0.92	1.78	0.036
BD(1)	C29-H71	RY*(2)	C30	1.05	1.83	0.039
BD(1)	C29-H71	BD*(1)	C27-C28	3.72	1.08	0.057
BD(1)	C29-H71	BD*(1)	C28-C29	1.28	1.15	0.034
BD(1)	C29-H71	BD*(1)	C29-C30	0.99	1.09	0.029
BD(1)	C29-H71	BD*(1)	C30-C31	3.64	1.08	0.056
BD(1)	C30-C31	RY*(1)	C29	0.61	1.93	0.031
BD(1)	C30-C31	RY*(1)	C32	0.61	1.93	0.031
BD(1)	C30-C31	RY*(2)	N33	0.62	2	0.032
BD(1)	C30-C31	RY*(1)	C34	1.08	1.87	0.04
BD(1)	C30-C31	BD*(1)	C29-C30	2.92	1.23	0.053
BD(1)	C30-C31	BD*(1)	C29-H71	2.1	1.16	0.044
BD(1)	C30-C31	BD*(1)	C30-C32	3.26	1.23	0.057
BD(1)	C30-C31	BD*(1)	C31-N33	1.41	1.18	0.037
BD(1)	C30-C31	BD*(1)	C31-C34	3.19	1.24	0.056
BD(1)	C30-C31	BD*(1)	C32-H72	1.87	1.17	0.042
BD(1)	C30-C31	BD*(1)	C34-H75	1.73	1.18	0.041
BD(2)	C30-C31	RY*(3)	C29	0.58	2.11	0.036
BD(2)	C30-C31	RY*(5)	C29	0.65	0.95	0.026
BD(2)	C30-C31	RY*(3)	C32	1.06	1.63	0.043
BD(2)	C30-C31	RY*(3)	N33	1.03	1.22	0.036
BD(2)	C30-C31	RY*(3)	C34	1.16	1.46	0.042
BD(2)	C30-C31	BD*(2)	C27-N33	14.88	0.26	0.057
BD(2)	C30-C31	BD*(2)	C28-C29	18.83	0.27	0.067
BD(2)	C30-C31	BD*(2)	C32-C36	16.28	0.28	0.064

BD(2)	C30-C31	BD*(2)	C34-C35	14.67	0.28	0.061
BD(1)	C30-C32	RY*(1)	C29	1.06	1.93	0.041
BD(1)	C30-C32	RY*(2)	C31	0.98	1.89	0.039
BD(1)	C30-C32	RY*(1)	C36	0.89	1.94	0.037
BD(1)	C30-C32	RY*(2)	C36	1.39	1.39	0.039
BD(1)	C30-C32	BD*(1)	C28-C29	1.44	1.29	0.039
BD(1)	C30-C32	BD*(1)	C29-C30	3.45	1.23	0.058
BD(1)	C30-C32	BD*(1)	C30-C31	3.34	1.22	0.057
BD(1)	C30-C32	BD*(1)	C31-N33	2.78	1.19	0.051
BD(1)	C30-C32	BD*(1)	C32-C36	2.82	1.29	0.054
BD(1)	C30-C32	BD*(1)	C32-H72	1.14	1.18	0.033
BD(1)	C30-C32	BD*(1)	C36-H73	2.17	1.19	0.045
BD(1)	C31-N33	RY*(1)	C27	0.51	1.77	0.027
BD(1)	C31-N33	RY*(2)	C27	2.34	2.02	0.061
BD(1)	C31-N33	RY*(1)	C34	0.91	1.98	0.038
BD(1)	C31-N33	BD*(1)	C27-N33	1.47	1.35	0.04
BD(1)	C31-N33	BD*(1)	C27-C47	2.88	1.24	0.054
BD(1)	C31-N33	BD*(1)	C30-C31	1.95	1.33	0.046
BD(1)	C31-N33	BD*(1)	C30-C32	1.56	1.35	0.041
BD(1)	C31-N33	BD*(1)	C31-C34	1.75	1.35	0.044
BD(1)	C31-N33	BD*(1)	C34-C35	1.25	1.41	0.037
BD(1)	C31-C34	RY*(2)	C30	1.42	1.96	0.047
BD(1)	C31-C34	RY*(1)	N33	1.14	1.6	0.038
BD(1)	C31-C34	RY*(1)	C35	0.87	1.94	0.037
BD(1)	C31-C34	RY*(2)	C35	1.38	1.39	0.039
BD(1)	C31-C34	BD*(1)	C27-N33	2.57	1.23	0.05
BD(1)	C31-C34	BD*(1)	C29-C30	2.23	1.23	0.047
BD(1)	C31-C34	BD*(1)	C30-C31	3.08	1.22	0.055
BD(1)	C31-C34	BD*(1)	C31-N33	1.93	1.18	0.043
BD(1)	C31-C34	BD*(1)	C34-C35	2.59	1.29	0.052
BD(1)	C31-C34	BD*(1)	C34-H75	1.27	1.19	0.035
BD(1)	C31-C34	BD*(1)	C35-H74	2.23	1.19	0.046
BD(1)	C32-C36	RY*(1)	C30	2.63	1.94	0.064
BD(1)	C32-C36	RY*(1)	C35	0.77	1.96	0.035
BD(1)	C32-C36	RY*(2)	C35	1.25	1.41	0.038
BD(1)	C32-C36	BD*(1)	C29-C30	3.17	1.25	0.056
BD(1)	C32-C36	BD*(1)	C30-C32	3.06	1.26	0.055
BD(1)	C32-C36	BD*(1)	C32-H72	1.67	1.2	0.04
BD(1)	C32-C36	BD*(1)	C35-C36	2.52	1.25	0.05
BD(1)	C32-C36	BD*(1)	C35-H74	1.83	1.21	0.042
BD(1)	C32-C36	BD*(1)	C36-H73	1.53	1.21	0.038

BD(2)	C32-C36	RY*(6)	C30	0.83	0.97	0.027
BD(2)	C32-C36	RY*(3)	C35	0.89	1.86	0.039
BD(2)	C32-C36	BD*(2)	C30-C31	16.41	0.28	0.064
BD(2)	C32-C36	BD*(2)	C34-C35	16.64	0.3	0.063
BD(1)	C32-H72	RY*(1)	C30	0.71	1.77	0.032
BD(1)	C32-H72	RY*(2)	C30	0.61	1.82	0.03
BD(1)	C32-H72	RY*(1)	C36	1.03	1.79	0.038
BD(1)	C32-H72	BD*(1)	C30-C31	3.98	1.07	0.059
BD(1)	C32-H72	BD*(1)	C30-C32	0.96	1.09	0.029
BD(1)	C32-H72	BD*(1)	C32-C36	1.3	1.14	0.034
BD(1)	C32-H72	BD*(1)	C35-C36	3.68	1.08	0.056
BD(1)	C34-C35	RY*(1)	C31	1.76	1.73	0.049
BD(1)	C34-C35	RY*(2)	C31	0.67	1.91	0.032
BD(1)	C34-C35	RY*(1)	C36	0.73	1.96	0.034
BD(1)	C34-C35	RY*(2)	C36	1.26	1.4	0.038
BD(1)	C34-C35	BD*(1)	C31-N33	3.18	1.2	0.055
BD(1)	C34-C35	BD*(1)	C31-C34	2.62	1.26	0.051
BD(1)	C34-C35	BD*(1)	C34-H75	1.62	1.21	0.04
BD(1)	C34-C35	BD*(1)	C35-C36	2.53	1.25	0.05
BD(1)	C34-C35	BD*(1)	C35-H74	1.5	1.21	0.038
BD(1)	C34-C35	BD*(1)	C36-H73	1.88	1.2	0.043
BD(2)	C34-C35	RY*(6)	C31	1.04	1.16	0.033
BD(2)	C34-C35	RY*(3)	C36	0.93	1.82	0.04
BD(2)	C34-C35	BD*(2)	C30-C31	17.62	0.28	0.066
BD(2)	C34-C35	BD*(2)	C32-C36	17.28	0.29	0.063
BD(1)	C34-H75	RY*(1)	C31	0.8	1.56	0.032
BD(1)	C34-H75	RY*(1)	C35	0.92	1.78	0.036
BD(1)	C34-H75	BD*(1)	C30-C31	3.9	1.06	0.058
BD(1)	C34-H75	BD*(1)	C31-C34	0.96	1.08	0.029
BD(1)	C34-H75	BD*(1)	C34-C35	1.31	1.14	0.035
BD(1)	C34-H75	BD*(1)	C35-C36	3.85	1.07	0.057
BD(1)	C35-C36	RY*(1)	C32	0.6	1.93	0.03
BD(1)	C35-C36	RY*(2)	C32	1.59	1.42	0.043
BD(1)	C35-C36	RY*(2)	C34	2.09	1.46	0.049
BD(1)	C35-C36	BD*(1)	C32-C36	2.68	1.29	0.052
BD(1)	C35-C36	BD*(1)	C32-H72	2.42	1.17	0.048
BD(1)	C35-C36	BD*(1)	C34-C35	2.58	1.29	0.052
BD(1)	C35-C36	BD*(1)	C34-H75	2.27	1.18	0.046
BD(1)	C35-C36	BD*(1)	C35-H74	1.14	1.18	0.033
BD(1)	C35-C36	BD*(1)	C36-H73	1.15	1.18	0.033
BD(1)	C35-H74	RY*(1)	C34	0.88	1.72	0.035

BD(1)	C35-H74	RY*(1)	C36	0.92	1.79	0.036
BD(1)	C35-H74	BD*(1)	C31-C34	3.78	1.09	0.057
BD(1)	C35-H74	BD*(1)	C32-C36	3.03	1.14	0.053
BD(1)	C35-H74	BD*(1)	C34-C35	1.25	1.14	0.034
BD(1)	C35-H74	BD*(1)	C35-C36	0.68	1.08	0.024
BD(1)	C36-H73	RY*(1)	C32	0.94	1.79	0.037
BD(1)	C36-H73	RY*(1)	C35	0.93	1.79	0.037
BD(1)	C36-H73	BD*(1)	C30-C32	3.92	1.09	0.058
BD(1)	C36-H73	BD*(1)	C32-C36	1.24	1.14	0.034
BD(1)	C36-H73	BD*(1)	C34-C35	2.98	1.14	0.052
BD(1)	C36-H73	BD*(1)	C35-C36	0.69	1.08	0.024
BD(1)	C38-H56	RY*(2)	C6	0.68	1.51	0.029
BD(1)	C38-H56	BD*(1)	C6-C7	3.52	1.1	0.056
BD(1)	C38-H56	BD*(1)	C6-C38	0.75	0.93	0.024
BD(1)	C38-H56	BD*(1)	C38-H57	0.53	1	0.02
BD(1)	C38-H57	RY*(3)	C6	0.55	1.41	0.025
BD(1)	C38-H57	BD*(1)	C5-C6	2.66	1.08	0.048
BD(1)	C38-H57	BD*(2)	C5-C6	2.29	0.55	0.035
BD(1)	C38-H57	BD*(1)	C6-C38	0.74	0.93	0.023
BD(1)	C38-H58	RY*(3)	C6	0.99	1.41	0.033
BD(1)	C38-H58	BD*(1)	C5-C6	1.3	1.08	0.034
BD(1)	C38-H58	BD*(2)	C5-C6	3.72	0.55	0.045
BD(1)	C38-H58	BD*(1)	C6-C38	0.67	0.93	0.022
BD(1)	N39-H40	RY*(1)	C8	0.85	1.84	0.036
BD(1)	N39-H40	RY*(2)	C41	1.14	1.53	0.038
BD(1)	N39-H40	BD*(2)	C7-C8	2.45	0.66	0.039
BD(1)	N39-H40	BD*(1)	C8-C9	1.62	1.21	0.04
BD(1)	N39-H40	BD*(1)	C11-C41	1.05	1.05	0.03
BD(1)	N39-H40	BD*(2)	C41-N42	5.85	0.64	0.055
BD(1)	N39-C41	RY*(2)	C8	0.72	1.76	0.032
BD(1)	N39-C41	RY*(3)	C8	1.01	1.64	0.036
BD(1)	N39-C41	RY*(1)	C11	1.04	1.7	0.038
BD(1)	N39-C41	RY*(1)	N42	0.75	1.77	0.033
BD(1)	N39-C41	BD*(1)	C7-C8	0.86	1.38	0.031
BD(1)	N39-C41	BD*(2)	C7-C8	1.01	0.82	0.028
BD(1)	N39-C41	BD*(1)	C8-N39	1.96	1.24	0.044
BD(1)	N39-C41	BD*(1)	C11-C12	1.46	1.3	0.039
BD(1)	N39-C41	BD*(1)	C11-C41	0.58	1.21	0.024
BD(1)	N39-C41	BD*(1)	N39-H40	0.5	1.24	0.022
BD(1)	N39-C41	BD*(1)	C41-N42	1.19	1.38	0.036
BD(1)	N39-C41	BD*(1)	N42-H43	2.55	1.23	0.05

BD(1)	C41-N42	RY*(1)	C11	0.63	1.81	0.03
BD(1)	C41-N42	RY*(1)	N39	0.66	1.84	0.031
BD(1)	C41-N42	RY*(1)	C41	0.81	1.68	0.033
BD(1)	C41-N42	BD*(1)	C8-N39	0.92	1.35	0.032
BD(1)	C41-N42	BD*(1)	C11-N17	0.91	1.43	0.032
BD(1)	C41-N42	BD*(1)	C11-C41	1.65	1.32	0.042
BD(1)	C41-N42	BD*(1)	N39-C41	1.25	1.34	0.037
BD(2)	C41-N42	BD*(1)	C8-N39	2.14	0.78	0.037
BD(2)	C41-N42	BD*(2)	C11-N17	8.42	0.33	0.051
BD(2)	C41-N42	BD*(1)	N39-H40	2.16	0.79	0.037
BD(1)	N42-H43	RY*(1)	C41	1.71	1.4	0.044
BD(1)	N42-H43	RY*(4)	C41	0.94	2.88	0.047
BD(1)	N42-H43	BD*(1)	C11-C41	0.62	1.04	0.023
BD(1)	N42-H43	BD*(1)	N39-C41	9.22	1.06	0.089
BD(1)	C44-H64	RY*(3)	C26	1.05	1.44	0.035
BD(1)	C44-H64	BD*(1)	C25-C26	0.52	1.1	0.021
BD(1)	C44-H64	BD*(2)	C25-C26	3.92	0.55	0.045
BD(1)	C44-H64	BD*(1)	C26-C44	0.59	0.92	0.021
BD(1)	C44-H65	RY*(2)	C26	0.54	1.52	0.026
BD(1)	C44-H65	BD*(1)	C25-C26	2.82	1.1	0.05
BD(1)	C44-H65	BD*(2)	C25-C26	1.51	0.54	0.028
BD(1)	C44-H65	BD*(1)	C26-C44	0.75	0.92	0.024
BD(1)	C44-H65	BD*(1)	C44-H66	0.6	1	0.022
BD(1)	C44-H66	BD*(1)	C21-C26	3.81	1.07	0.057
BD(1)	C44-H66	BD*(2)	C25-C26	0.64	0.55	0.018
BD(1)	C44-H66	BD*(1)	C26-C44	0.71	0.92	0.023
BD(1)	N45-H46	RY*(1)	C24	1.54	1.66	0.045
BD(1)	N45-H46	RY*(1)	C47	0.75	1.54	0.03
BD(1)	N45-H46	RY*(2)	C47	0.75	1.5	0.03
BD(1)	N45-H46	BD*(2)	C23-C24	1.04	0.69	0.027
BD(1)	N45-H46	BD*(1)	C24-C25	2.5	1.24	0.05
BD(1)	N45-H46	BD*(1)	C28-H70	0.62	1.13	0.024
BD(1)	N45-H46	BD*(1)	C47-N48	3.95	1.27	0.063
BD(1)	N45-C47	RY*(1)	C24	1.43	1.81	0.046
BD(1)	N45-C47	RY*(1)	C27	0.81	1.77	0.034
BD(1)	N45-C47	BD*(1)	C23-C24	1.48	1.39	0.04
BD(1)	N45-C47	BD*(1)	C24-N45	2.31	1.25	0.048
BD(1)	N45-C47	BD*(1)	C27-N33	1.21	1.35	0.036
BD(1)	N45-C47	BD*(1)	N45-H46	0.87	1.26	0.03
BD(1)	N45-C47	BD*(1)	C47-N48	1.7	1.42	0.044
BD(1)	N45-C47	BD*(1)	N48-H49	2.08	1.3	0.046

BD(1)	C47-N48	RY*(1)	C27	0.62	1.82	0.03
BD(1)	C47-N48	RY*(1)	C47	0.68	1.74	0.031
BD(1)	C47-N48	BD*(1)	C27-C28	1.18	1.38	0.036
BD(1)	C47-N48	BD*(1)	C27-C47	2.41	1.29	0.051
BD(1)	C47-N48	BD*(1)	N45-H46	1.52	1.31	0.04
BD(1)	C47-N48	BD*(1)	N45-C47	1.68	1.32	0.042
BD(2)	C47-N48	RY*(1)	N45	0.75	1.25	0.028
BD(2)	C47-N48	BD*(2)	C27-N33	8.03	0.3	0.047
BD(2)	C47-N48	BD*(2)	C47-N48	0.56	0.34	0.013
BD(1)	N48-H49	RY*(1)	C47	1.74	1.46	0.045
BD(1)	N48-H49	RY*(4)	C47	0.91	2.42	0.042
BD(1)	N48-H49	BD*(1)	C27-C47	0.73	1.01	0.024
BD(1)	N48-H49	BD*(1)	N45-C47	10.99	1.03	0.096
CR(1)	C1	RY*(1)	C2	1.1	11.29	0.099
CR(1)	C1	RY*(2)	C2	0.94	10.86	0.09
CR(1)	C1	RY*(1)	C5	1.25	11.44	0.107
CR(1)	C1	BD*(1)	C1-C2	1.02	10.72	0.094
CR(1)	C1	BD*(1)	C1-O37	1.04	10.43	0.094
CR(1)	C1	BD*(1)	C2-H62	0.89	10.61	0.087
CR(1)	C1	BD*(1)	C4-O37	0.85	10.43	0.084
CR(1)	C1	BD*(1)	C5-C6	0.76	10.68	0.081
CR(1)	C1	BD*(1)	C5-C10	0.58	10.68	0.071
CR(1)	C2	RY*(1)	C1	0.5	10.96	0.066
CR(1)	C2	RY*(2)	C1	1.78	11.31	0.127
CR(1)	C2	RY*(2)	C3	1.51	10.81	0.114
CR(1)	C2	RY*(1)	H62	0.72	10.59	0.078
CR(1)	C2	BD*(1)	C1-C2	0.76	10.65	0.081
CR(1)	C2	BD*(1)	C1-C5	1.85	10.56	0.126
CR(1)	C2	BD*(1)	C3-H63	0.76	10.54	0.08
CR(1)	C3	RY*(2)	C2	1.61	10.79	0.118
CR(1)	C3	RY*(1)	C4	0.59	11	0.072
CR(1)	C3	RY*(2)	C4	1.99	11.33	0.134
CR(1)	C3	RY*(1)	H63	0.71	10.58	0.077
CR(1)	C3	BD*(1)	C2-H62	0.77	10.54	0.08
CR(1)	C3	BD*(1)	C3-C4	0.74	10.65	0.08
CR(1)	C3	BD*(1)	C4-C21	1.91	10.56	0.128
CR(1)	C4	RY*(1)	C3	1.16	11.29	0.102
CR(1)	C4	RY*(2)	C3	0.9	10.88	0.088
CR(1)	C4	RY*(1)	C21	0.71	11.4	0.081
CR(1)	C4	RY*(2)	C21	0.58	11.37	0.072
CR(1)	C4	RY*(5)	C21	0.6	11.21	0.073

CR(1)	C4	BD*(1)	C1-O37	0.85	10.43	0.085
CR(1)	C4	BD*(1)	C3-C4	0.97	10.72	0.091
CR(1)	C4	BD*(1)	C3-H63	0.88	10.61	0.086
CR(1)	C4	BD*(1)	C4-O37	1	10.43	0.092
CR(1)	C4	BD*(1)	C21-C22	0.58	10.69	0.071
CR(1)	C4	BD*(1)	C21-C26	0.74	10.69	0.08
CR(1)	C5	RY*(2)	C1	0.56	11.31	0.071
CR(1)	C5	RY*(6)	C1	0.57	11.53	0.073
CR(1)	C5	RY*(2)	C6	1.72	11.05	0.123
CR(1)	C5	RY*(2)	C10	1.54	10.85	0.116
CR(1)	C5	BD*(1)	C1-C2	1.18	10.65	0.101
CR(1)	C5	BD*(1)	C6-C7	0.6	10.64	0.072
CR(1)	C5	BD*(1)	C6-C38	0.8	10.47	0.082
CR(1)	C5	BD*(1)	C9-C10	0.6	10.67	0.072
CR(1)	C5	BD*(1)	C10-H59	0.51	10.56	0.065
CR(1)	C6	RY*(1)	C5	0.68	11.38	0.078
CR(1)	C6	RY*(2)	C5	0.8	11.09	0.084
CR(1)	C6	RY*(2)	C7	1.67	10.84	0.12
CR(1)	C6	RY*(3)	C38	1.21	10.69	0.101
CR(1)	C6	BD*(1)	C1-C5	0.91	10.57	0.088
CR(1)	C6	BD*(1)	C5-C10	0.63	10.62	0.073
CR(1)	C6	BD*(1)	C7-C8	0.75	10.64	0.08
CR(1)	C6	BD*(1)	C7-H61	0.53	10.55	0.067
CR(1)	C7	RY*(1)	C6	0.73	11.34	0.081
CR(1)	C7	RY*(2)	C6	1.52	11.03	0.115
CR(1)	C7	RY*(5)	C6	0.67	11.16	0.077
CR(1)	C7	RY*(1)	C8	1.36	11.25	0.111
CR(1)	C7	RY*(3)	C8	0.85	10.88	0.086
CR(1)	C7	RY*(1)	H61	0.61	10.58	0.072
CR(1)	C7	BD*(1)	C5-C6	0.9	10.6	0.088
CR(1)	C7	BD*(1)	C6-C38	0.68	10.45	0.075
CR(1)	C7	BD*(1)	C8-C9	0.75	10.62	0.08
CR(1)	C7	BD*(1)	C8-N39	0.86	10.48	0.086
CR(1)	C8	RY*(2)	C7	1.09	10.87	0.097
CR(1)	C8	RY*(2)	C9	1.47	10.88	0.113
CR(1)	C8	BD*(1)	C6-C7	0.69	10.67	0.077
CR(1)	C8	BD*(1)	C7-C8	0.53	10.67	0.067
CR(1)	C8	BD*(1)	C7-H61	0.59	10.58	0.071
CR(1)	C8	BD*(1)	C8-C9	0.57	10.67	0.07
CR(1)	C8	BD*(1)	C9-C10	0.59	10.7	0.071
CR(1)	C8	BD*(1)	C9-H60	0.57	10.61	0.07

CR(1)	C8	BD*(1)	N39-H40	0.5	10.54	0.065
CR(1)	C8	BD*(1)	N39-C41	1.03	10.53	0.094
CR(1)	C9	RY*(2)	C8	2.14	11	0.137
CR(1)	C9	RY*(2)	C10	1.24	10.83	0.104
CR(1)	C9	RY*(5)	C10	0.83	11.1	0.086
CR(1)	C9	RY*(1)	H60	0.8	10.76	0.083
CR(1)	C9	BD*(1)	C5-C10	0.86	10.59	0.086
CR(1)	C9	BD*(1)	C7-C8	0.78	10.62	0.082
CR(1)	C9	BD*(1)	C8-N39	0.66	10.48	0.075
CR(1)	C9	BD*(1)	C10-H59	0.58	10.53	0.07
CR(1)	C10	RY*(2)	C5	1.51	11.08	0.116
CR(1)	C10	RY*(2)	C9	1.71	10.83	0.121
CR(1)	C10	RY*(1)	H59	0.65	10.62	0.074
CR(1)	C10	BD*(1)	C1-C5	0.77	10.56	0.081
CR(1)	C10	BD*(1)	C5-C6	0.79	10.61	0.082
CR(1)	C10	BD*(1)	C8-C9	0.73	10.62	0.079
CR(1)	C10	BD*(1)	C9-H60	0.57	10.56	0.07
CR(1)	C11	RY*(2)	C12	1.35	10.82	0.108
CR(1)	C11	RY*(2)	N17	0.7	11.43	0.08
CR(1)	C11	RY*(1)	C41	0.85	10.9	0.086
CR(1)	C11	RY*(5)	C41	0.69	11.74	0.081
CR(1)	C11	BD*(1)	C12-C13	0.52	10.7	0.066
CR(1)	C11	BD*(1)	C12-H50	0.55	10.58	0.069
CR(1)	C11	BD*(1)	C15-N17	1.38	10.6	0.108
CR(1)	C11	BD*(1)	C41-N42	0.52	10.71	0.067
CR(1)	C12	RY*(1)	C11	1.12	10.99	0.099
CR(1)	C12	RY*(2)	C11	0.95	11.27	0.092
CR(1)	C12	RY*(2)	C13	1.52	10.78	0.114
CR(1)	C12	RY*(4)	C13	0.71	11.07	0.079
CR(1)	C12	RY*(1)	H50	0.68	10.63	0.076
CR(1)	C12	BD*(1)	C11-N17	0.69	10.61	0.077
CR(1)	C12	BD*(1)	C11-C41	0.74	10.5	0.08
CR(1)	C12	BD*(1)	C12-C13	0.5	10.66	0.066
CR(1)	C12	BD*(1)	C13-C14	0.77	10.6	0.081
CR(1)	C12	BD*(1)	C13-H51	0.63	10.54	0.073
CR(1)	C13	RY*(2)	C12	1.66	10.79	0.119
CR(1)	C13	RY*(4)	C12	0.63	11.06	0.074
CR(1)	C13	RY*(1)	C14	0.66	11.3	0.077
CR(1)	C13	RY*(2)	C14	0.82	11.35	0.086
CR(1)	C13	RY*(3)	C14	0.59	11.17	0.072
CR(1)	C13	RY*(1)	H51	0.63	10.59	0.073

CR(1)	C13	BD*(1)	C11-C12	0.74	10.6	0.08
CR(1)	C13	BD*(1)	C12-H50	0.68	10.55	0.076
CR(1)	C13	BD*(1)	C14-C15	0.66	10.6	0.075
CR(1)	C13	BD*(1)	C14-C16	0.88	10.61	0.087
CR(1)	C14	RY*(2)	C13	1.44	10.78	0.111
CR(1)	C14	RY*(1)	C15	1.42	11.09	0.112
CR(1)	C14	RY*(2)	C15	0.76	11.27	0.083
CR(1)	C14	RY*(2)	C16	1.47	10.8	0.113
CR(1)	C14	BD*(1)	C12-C13	0.55	10.66	0.069
CR(1)	C14	BD*(1)	C13-H51	0.51	10.54	0.066
CR(1)	C14	BD*(1)	C15-N17	0.6	10.56	0.071
CR(1)	C14	BD*(1)	C15-C18	0.64	10.61	0.074
CR(1)	C14	BD*(1)	C16-C20	0.55	10.66	0.068
CR(1)	C14	BD*(1)	C16-H52	0.5	10.55	0.065
CR(1)	C15	RY*(1)	C14	1.93	11.33	0.132
CR(1)	C15	RY*(2)	N17	0.52	11.42	0.069
CR(1)	C15	RY*(2)	C18	1.54	10.88	0.116
CR(1)	C15	BD*(1)	C11-N17	1.2	10.64	0.101
CR(1)	C15	BD*(1)	C13-C14	0.6	10.63	0.072
CR(1)	C15	BD*(1)	C14-C16	0.68	10.64	0.076
CR(1)	C15	BD*(1)	C18-C19	0.56	10.7	0.069
CR(1)	C15	BD*(1)	C18-H55	0.51	10.59	0.066
CR(1)	C16	RY*(2)	C14	1.65	11.33	0.122
CR(1)	C16	RY*(3)	C14	0.64	11.16	0.075
CR(1)	C16	RY*(2)	C20	1.89	10.75	0.127
CR(1)	C16	RY*(5)	C20	0.52	11.13	0.068
CR(1)	C16	RY*(1)	H52	0.62	10.59	0.073
CR(1)	C16	BD*(1)	C13-C14	0.9	10.6	0.087
CR(1)	C16	BD*(1)	C14-C15	0.75	10.59	0.081
CR(1)	C16	BD*(1)	C19-C20	0.72	10.6	0.078
CR(1)	C16	BD*(1)	C20-H53	0.59	10.55	0.071
CR(1)	N17	RY*(1)	C11	3.44	15.07	0.204
CR(1)	N17	RY*(1)	C15	2.6	15.17	0.178
CR(1)	N17	BD*(1)	C11-C12	0.78	14.68	0.096
CR(1)	N17	BD*(1)	C14-C15	0.69	14.68	0.091
CR(1)	C18	RY*(2)	C15	1.42	11.26	0.113
CR(1)	C18	RY*(3)	C15	0.94	11.61	0.093
CR(1)	C18	RY*(2)	C19	1.85	10.75	0.126
CR(1)	C18	RY*(1)	H55	0.67	10.63	0.075
CR(1)	C18	BD*(1)	C14-C15	0.83	10.58	0.085
CR(1)	C18	BD*(1)	C15-N17	0.66	10.54	0.075

CR(1)	C18	BD*(1)	C19-C20	0.74	10.59	0.079
CR(1)	C18	BD*(1)	C19-H54	0.6	10.55	0.071
CR(1)	C19	RY*(1)	C18	0.92	11.24	0.091
CR(1)	C19	RY*(2)	C18	1.12	10.85	0.098
CR(1)	C19	RY*(4)	C18	0.62	11.15	0.074
CR(1)	C19	RY*(2)	C20	1.47	10.75	0.112
CR(1)	C19	RY*(5)	C20	0.54	11.13	0.069
CR(1)	C19	RY*(1)	H54	0.63	10.59	0.073
CR(1)	C19	BD*(1)	C15-C18	0.74	10.61	0.08
CR(1)	C19	BD*(1)	C16-C20	0.62	10.66	0.073
CR(1)	C19	BD*(1)	C18-H55	0.6	10.56	0.071
CR(1)	C19	BD*(1)	C20-H53	0.53	10.55	0.067
CR(1)	C20	RY*(2)	C16	1.36	10.8	0.108
CR(1)	C20	RY*(5)	C16	0.8	11.11	0.084
CR(1)	C20	RY*(2)	C19	1.5	10.76	0.114
CR(1)	C20	RY*(5)	C19	0.58	11.19	0.072
CR(1)	C20	RY*(1)	H53	0.63	10.59	0.073
CR(1)	C20	BD*(1)	C14-C16	0.78	10.6	0.082
CR(1)	C20	BD*(1)	C16-H52	0.64	10.55	0.074
CR(1)	C20	BD*(1)	C18-C19	0.6	10.67	0.072
CR(1)	C20	BD*(1)	C19-H54	0.53	10.56	0.067
CR(1)	C21	RY*(2)	C4	0.54	11.34	0.07
CR(1)	C21	RY*(2)	C22	1.31	10.86	0.106
CR(1)	C21	RY*(2)	C26	1.94	11.08	0.131
CR(1)	C21	BD*(1)	C3-C4	1.15	10.65	0.099
CR(1)	C21	BD*(1)	C22-C23	0.67	10.64	0.075
CR(1)	C21	BD*(1)	C25-C26	0.56	10.66	0.069
CR(1)	C21	BD*(1)	C26-C44	0.79	10.48	0.081
CR(1)	C22	RY*(1)	C21	1.72	11.33	0.125
CR(1)	C22	RY*(2)	C23	1.58	10.75	0.116
CR(1)	C22	RY*(1)	H67	0.61	10.63	0.072
CR(1)	C22	BD*(1)	C4-C21	0.74	10.57	0.079
CR(1)	C22	BD*(1)	C21-C26	0.8	10.62	0.083
CR(1)	C22	BD*(1)	C23-C24	0.76	10.62	0.08
CR(1)	C22	BD*(1)	C23-H68	0.64	10.53	0.073
CR(1)	C23	RY*(2)	C22	1.49	10.85	0.114
CR(1)	C23	RY*(5)	C22	0.8	11.14	0.084
CR(1)	C23	RY*(1)	C24	1.52	11.04	0.116
CR(1)	C23	RY*(1)	H68	0.6	10.57	0.071
CR(1)	C23	BD*(1)	C21-C22	0.86	10.62	0.086
CR(1)	C23	BD*(1)	C22-H67	0.56	10.54	0.069

CR(1)	C23	BD*(1)	C24-C25	0.71	10.62	0.078
CR(1)	C23	BD*(1)	C24-N45	1.07	10.48	0.095
CR(1)	C24	RY*(2)	C23	1.34	10.79	0.107
CR(1)	C24	RY*(5)	C23	0.65	11.18	0.076
CR(1)	C24	RY*(2)	C25	1.28	10.93	0.105
CR(1)	C24	RY*(5)	C25	0.68	11.19	0.078
CR(1)	C24	BD*(1)	C22-C23	0.51	10.69	0.066
CR(1)	C24	BD*(1)	C23-H68	0.62	10.58	0.073
CR(1)	C24	BD*(1)	C24-C25	0.72	10.67	0.078
CR(1)	C24	BD*(1)	C25-C26	0.69	10.7	0.077
CR(1)	C24	BD*(1)	C25-H69	0.52	10.61	0.066
CR(1)	C24	BD*(1)	N45-H46	0.52	10.53	0.066
CR(1)	C24	BD*(1)	N45-C47	1.08	10.54	0.096
CR(1)	C25	RY*(1)	C24	1.25	11.02	0.105
CR(1)	C25	RY*(2)	C24	0.85	11.25	0.087
CR(1)	C25	RY*(1)	C26	1.17	11.31	0.103
CR(1)	C25	RY*(2)	C26	1.16	11.06	0.101
CR(1)	C25	RY*(1)	H69	0.74	10.66	0.079
CR(1)	C25	BD*(1)	C21-C26	0.93	10.6	0.089
CR(1)	C25	BD*(1)	C23-C24	0.85	10.6	0.085
CR(1)	C25	BD*(1)	C24-N45	0.53	10.46	0.067
CR(1)	C25	BD*(1)	C26-C44	0.69	10.45	0.076
CR(1)	C26	RY*(2)	C21	1.77	11.3	0.126
CR(1)	C26	RY*(2)	C25	1.43	10.89	0.112
CR(1)	C26	RY*(5)	C25	0.51	11.15	0.067
CR(1)	C26	RY*(2)	C44	0.58	11.13	0.071
CR(1)	C26	BD*(1)	C4-C21	0.95	10.57	0.09
CR(1)	C26	BD*(1)	C21-C22	0.63	10.62	0.073
CR(1)	C26	BD*(1)	C24-C25	0.81	10.63	0.083
CR(1)	C26	BD*(1)	C25-C26	0.54	10.66	0.068
CR(1)	C26	BD*(1)	C25-H69	0.52	10.57	0.066
CR(1)	C27	RY*(2)	C28	1.22	10.88	0.103
CR(1)	C27	RY*(2)	N33	0.64	11.42	0.076
CR(1)	C27	RY*(1)	C47	1.08	10.99	0.097
CR(1)	C27	BD*(1)	C28-C29	0.52	10.7	0.067
CR(1)	C27	BD*(1)	C28-H70	0.56	10.58	0.069
CR(1)	C27	BD*(1)	C31-N33	1.38	10.6	0.108
CR(1)	C28	RY*(1)	C27	0.96	11.03	0.092
CR(1)	C28	RY*(2)	C27	1.1	11.28	0.1
CR(1)	C28	RY*(2)	C29	1.55	10.78	0.115
CR(1)	C28	RY*(4)	C29	0.7	11.09	0.079

CR(1)	C28	RY*(1)	H70	0.67	10.67	0.076
CR(1)	C28	BD*(1)	C27-N33	0.66	10.61	0.075
CR(1)	C28	BD*(1)	C27-C47	0.75	10.5	0.081
CR(1)	C28	BD*(1)	C29-C30	0.76	10.61	0.08
CR(1)	C28	BD*(1)	C29-H71	0.63	10.55	0.073
CR(1)	C29	RY*(2)	C28	1.57	10.84	0.117
CR(1)	C29	RY*(4)	C28	0.61	11.19	0.074
CR(1)	C29	RY*(1)	C30	0.65	11.3	0.076
CR(1)	C29	RY*(2)	C30	0.85	11.35	0.088
CR(1)	C29	RY*(3)	C30	0.62	11.13	0.074
CR(1)	C29	RY*(1)	H71	0.64	10.59	0.073
CR(1)	C29	BD*(1)	C27-C28	0.76	10.6	0.081
CR(1)	C29	BD*(1)	C28-H70	0.7	10.55	0.077
CR(1)	C29	BD*(1)	C30-C31	0.66	10.6	0.076
CR(1)	C29	BD*(1)	C30-C32	0.89	10.62	0.087
CR(1)	C30	RY*(2)	C29	1.42	10.78	0.11
CR(1)	C30	RY*(1)	C31	1.26	11.09	0.106
CR(1)	C30	RY*(2)	C31	0.9	11.26	0.09
CR(1)	C30	RY*(2)	C32	1.48	10.8	0.113
CR(1)	C30	BD*(1)	C28-C29	0.57	10.66	0.07
CR(1)	C30	BD*(1)	C29-H71	0.52	10.54	0.066
CR(1)	C30	BD*(1)	C31-N33	0.6	10.56	0.071
CR(1)	C30	BD*(1)	C31-C34	0.64	10.61	0.074
CR(1)	C30	BD*(1)	C32-C36	0.55	10.67	0.069
CR(1)	C30	BD*(1)	C32-H72	0.5	10.55	0.065
CR(1)	C31	RY*(1)	C30	1.93	11.33	0.132
CR(1)	C31	RY*(2)	N33	0.52	11.41	0.069
CR(1)	C31	RY*(2)	C34	1.54	10.87	0.116
CR(1)	C31	BD*(1)	C27-N33	1.22	10.64	0.102
CR(1)	C31	BD*(1)	C29-C30	0.6	10.64	0.071
CR(1)	C31	BD*(1)	C30-C32	0.67	10.64	0.076
CR(1)	C31	BD*(1)	C34-C35	0.56	10.7	0.069
CR(1)	C31	BD*(1)	C34-H75	0.51	10.59	0.066
CR(1)	C32	RY*(2)	C30	1.64	11.33	0.122
CR(1)	C32	RY*(3)	C30	0.67	11.12	0.077
CR(1)	C32	RY*(2)	C36	1.91	10.75	0.128
CR(1)	C32	RY*(5)	C36	0.53	11.13	0.068
CR(1)	C32	RY*(1)	H72	0.62	10.59	0.072
CR(1)	C32	BD*(1)	C29-C30	0.9	10.6	0.088
CR(1)	C32	BD*(1)	C30-C31	0.76	10.59	0.081
CR(1)	C32	BD*(1)	C35-C36	0.72	10.6	0.078

CR(1)	C32	BD*(1)	C36-H73	0.6	10.55	0.071
CR(1)	N33	RY*(1)	C27	3.48	15.11	0.205
CR(1)	N33	RY*(1)	C31	2.75	15.17	0.182
CR(1)	N33	BD*(1)	C27-C28	0.76	14.67	0.095
CR(1)	N33	BD*(1)	C30-C31	0.68	14.68	0.09
CR(1)	C34	RY*(2)	C31	1.41	11.25	0.113
CR(1)	C34	RY*(3)	C31	0.99	11.58	0.096
CR(1)	C34	RY*(2)	C35	1.85	10.75	0.126
CR(1)	C34	RY*(1)	H75	0.67	10.59	0.075
CR(1)	C34	BD*(1)	C30-C31	0.84	10.58	0.085
CR(1)	C34	BD*(1)	C31-N33	0.66	10.54	0.075
CR(1)	C34	BD*(1)	C35-C36	0.74	10.59	0.079
CR(1)	C34	BD*(1)	C35-H74	0.59	10.55	0.071
CR(1)	C35	RY*(1)	C34	0.9	11.24	0.09
CR(1)	C35	RY*(2)	C34	1.11	10.83	0.098
CR(1)	C35	RY*(4)	C34	0.65	11.13	0.076
CR(1)	C35	RY*(2)	C36	1.44	10.75	0.111
CR(1)	C35	RY*(5)	C36	0.53	11.14	0.069
CR(1)	C35	RY*(1)	H74	0.64	10.59	0.073
CR(1)	C35	BD*(1)	C31-C34	0.74	10.61	0.08
CR(1)	C35	BD*(1)	C32-C36	0.6	10.66	0.072
CR(1)	C35	BD*(1)	C34-H75	0.6	10.56	0.071
CR(1)	C35	BD*(1)	C36-H73	0.52	10.55	0.067
CR(1)	C36	RY*(2)	C32	1.36	10.8	0.108
CR(1)	C36	RY*(5)	C32	0.81	11.11	0.085
CR(1)	C36	RY*(2)	C35	1.49	10.76	0.113
CR(1)	C36	RY*(5)	C35	0.57	11.19	0.071
CR(1)	C36	RY*(1)	H73	0.63	10.59	0.073
CR(1)	C36	BD*(1)	C30-C32	0.79	10.61	0.082
CR(1)	C36	BD*(1)	C32-H72	0.64	10.54	0.074
CR(1)	C36	BD*(1)	C34-C35	0.6	10.66	0.071
CR(1)	C36	BD*(1)	C35-H74	0.52	10.56	0.066
CR(1)	O37	RY*(1)	C1	2.1	19.89	0.183
CR(1)	O37	RY*(1)	C4	2.24	19.94	0.189
CR(1)	C38	RY*(1)	C6	1.14	11.34	0.101
CR(1)	C38	RY*(1)	H56	0.76	10.78	0.081
CR(1)	C38	RY*(1)	H57	0.62	10.67	0.073
CR(1)	C38	RY*(1)	H58	0.63	10.67	0.073
CR(1)	C38	BD*(1)	C5-C6	0.63	10.6	0.073
CR(1)	C38	BD*(1)	C6-C7	0.5	10.63	0.066
CR(1)	N39	RY*(1)	C8	1.34	15.39	0.128

CR(1)	N39	RY*(6)	C8	1.01	15.25	0.111
CR(1)	N39	RY*(2)	C41	1.5	15.07	0.134
CR(1)	N39	RY*(3)	C41	1.73	15.06	0.144
CR(1)	N39	BD*(1)	C7-C8	0.53	14.76	0.08
CR(1)	C41	RY*(2)	C11	1.05	11.34	0.098
CR(1)	C41	RY*(3)	C11	0.66	11.41	0.077
CR(1)	C41	RY*(3)	N42	1.12	11.01	0.099
CR(1)	C41	BD*(1)	C8-N39	1.13	10.6	0.098
CR(1)	C41	BD*(1)	C11-C12	0.59	10.67	0.071
CR(1)	C41	BD*(1)	N42-H43	0.8	10.59	0.082
CR(1)	N42	RY*(1)	C41	5.69	14.93	0.261
CR(1)	N42	RY*(1)	H43	0.53	14.83	0.079
CR(1)	N42	BD*(1)	C11-C41	0.85	14.57	0.101
CR(1)	C44	RY*(1)	C26	1.06	11.3	0.098
CR(1)	C44	RY*(1)	H64	0.64	10.69	0.074
CR(1)	C44	RY*(1)	H65	0.81	10.75	0.083
CR(1)	C44	RY*(1)	H66	0.6	10.68	0.071
CR(1)	C44	BD*(1)	C21-C26	0.65	10.59	0.074
CR(1)	C44	BD*(1)	C25-C26	0.52	10.63	0.067
CR(1)	N45	RY*(2)	C24	1.7	15.43	0.145
CR(1)	N45	RY*(5)	C24	0.71	15.47	0.094
CR(1)	N45	RY*(1)	H46	0.64	14.89	0.087
CR(1)	N45	RY*(2)	C47	3.1	15.04	0.193
CR(1)	N45	BD*(1)	C23-C24	0.51	14.77	0.078
CR(1)	C47	RY*(2)	C27	1.05	11.34	0.098
CR(1)	C47	RY*(3)	C27	0.7	11.28	0.079
CR(1)	C47	RY*(3)	N48	0.99	11.04	0.093
CR(1)	C47	BD*(1)	C24-N45	1.23	10.58	0.102
CR(1)	C47	BD*(1)	C27-C28	0.65	10.65	0.075
CR(1)	C47	BD*(1)	N45-H46	0.57	10.58	0.069
CR(1)	C47	BD*(1)	N48-H49	0.71	10.62	0.078
CR(1)	N48	RY*(1)	C47	4.37	14.98	0.229
CR(1)	N48	RY*(2)	C47	1	14.95	0.109
CR(1)	N48	RY*(1)	H49	0.64	14.82	0.087
CR(1)	N48	BD*(1)	C27-C47	0.98	14.54	0.108
CR(1)	N48	BD*(1)	N45-C47	0.71	14.56	0.092
LP(1)	N17	RY*(1)	C11	3.84	1.27	0.064
LP(1)	N17	RY*(1)	C15	2.47	1.37	0.053
LP(1)	N17	RY*(2)	C15	0.59	1.55	0.028
LP(1)	N17	RY*(3)	C15	0.52	1.9	0.029
LP(1)	N17	BD*(1)	C9-H60	1.83	0.88	0.036

LP(1)	N17	BD*(1)	C11-C12	9.9	0.87	0.084
LP(1)	N17	BD*(1)	C11-C41	2.9	0.78	0.043
LP(1)	N17	BD*(1)	C14-C15	9.6	0.88	0.083
LP(1)	N17	BD*(1)	C15-C18	1.77	0.89	0.036
LP(1)	N33	RY*(1)	C27	3.82	1.31	0.064
LP(1)	N33	RY*(1)	C31	2.63	1.37	0.055
LP(1)	N33	RY*(2)	C31	0.53	1.54	0.026
LP(1)	N33	RY*(3)	C31	0.53	1.87	0.029
LP(1)	N33	BD*(1)	C27-C28	9.98	0.87	0.084
LP(1)	N33	BD*(1)	C27-C47	2.71	0.78	0.041
LP(1)	N33	BD*(1)	C30-C31	9.6	0.88	0.083
LP(1)	N33	BD*(1)	C31-C34	1.78	0.89	0.036
LP(1)	N33	BD*(1)	N48-H49	2.28	0.84	0.04
LP(1)	O37	RY*(1)	C1	3.07	1.49	0.061
LP(1)	O37	RY*(1)	C4	3.08	1.54	0.062
LP(1)	O37	BD*(1)	C1-C2	2.65	1.18	0.05
LP(1)	O37	BD*(1)	C3-C4	2.57	1.19	0.049
LP(1)	O37	BD*(1)	C44-H65	1.37	1.09	0.035
LP(1)	O37	BD*(1)	C44-H66	1.04	1.08	0.03
LP(2)	O37	RY*(4)	C1	1.35	2.22	0.053
LP(2)	O37	RY*(3)	C4	1.26	1.8	0.046
LP(2)	O37	RY*(4)	C4	0.7	1.91	0.035
LP(2)	O37	BD*(2)	C1-C2	24.28	0.35	0.083
LP(2)	O37	BD*(2)	C3-C4	24.4	0.35	0.084
LP(2)	O37	BD*(1)	C44-H65	1.06	0.83	0.029
LP(1)	N39	RY*(3)	C8	0.51	1.09	0.022
LP(1)	N39	RY*(4)	C8	1.09	2.57	0.049
LP(1)	N39	RY*(4)	C41	0.78	2.5	0.041
LP(1)	N39	BD*(1)	C7-C8	7.42	0.83	0.071
LP(1)	N39	BD*(2)	C7-C8	5.38	0.27	0.036
LP(1)	N39	BD*(1)	C8-C9	5.72	0.82	0.063
LP(1)	N39	BD*(1)	C11-C41	8.28	0.66	0.067
LP(1)	N39	BD*(1)	C41-N42	10.42	0.83	0.085
LP(1)	N39	BD*(2)	C41-N42	0.96	0.25	0.014
LP(1)	N39	BD*(1)	N42-H43	0.59	0.68	0.018
LP(1)	N42	RY*(1)	C41	6.78	1.18	0.081
LP(1)	N42	BD*(1)	C11-C41	11.78	0.82	0.088
LP(1)	N42	BD*(1)	N39-C41	3.01	0.84	0.045
LP(1)	N45	RY*(3)	C24	1.94	1.66	0.055
LP(1)	N45	RY*(3)	C47	1.63	1.99	0.055
LP(1)	N45	BD*(1)	C23-C24	2.89	0.83	0.047

LP(1)	N45	BD*(2)	C23-C24	21.45	0.29	0.072
LP(1)	N45	BD*(1)	C24-C25	2.7	0.84	0.046
LP(1)	N45	BD*(2)	C47-N48	49.04	0.29	0.107
LP(1)	N48	RY*(1)	C47	5.4	1.23	0.074
LP(1)	N48	RY*(4)	C47	0.51	2.2	0.03
LP(1)	N48	BD*(1)	C25-H69	0.65	0.88	0.022
LP(1)	N48	BD*(1)	C27-C47	13.37	0.79	0.092
LP(1)	N48	BD*(1)	N45-C47	2.81	0.81	0.043
BD*(2)	C1-C2	RY*(4)	C2	1.71	1.09	0.098
BD*(2)	C1-C2	BD*(1)	C5-C6	0.57	0.54	0.038
BD*(2)	C3-C4	RY*(4)	C3	1.59	1.24	0.099
BD*(2)	C3-C4	RY*(6)	C4	0.75	1.69	0.079
BD*(2)	C5-C6	RY*(4)	C5	0.54	1.84	0.063
BD*(2)	C5-C6	RY*(3)	C6	0.51	0.86	0.042
BD*(2)	C5-C6	BD*(1)	C1-O37	1.54	0.28	0.04
BD*(2)	C5-C6	BD*(1)	C38-H57	0.76	0.45	0.037
BD*(2)	C5-C6	BD*(1)	C38-H58	1.28	0.44	0.047
BD*(2)	C7-C8	RY*(3)	C7	0.94	0.88	0.06
BD*(2)	C7-C8	RY*(5)	C7	0.54	0.95	0.048
BD*(2)	C7-C8	BD*(1)	N39-H40	1.3	0.42	0.048
BD*(2)	C7-C8	BD*(1)	N39-C41	1.4	0.41	0.048
BD*(2)	C9-C10	RY*(4)	C9	0.77	1.56	0.081
BD*(2)	C9-C10	RY*(5)	C9	0.62	0.94	0.056
BD*(2)	C9-C10	RY*(4)	C10	1.73	1.04	0.098
BD*(2)	C11-N17	RY*(4)	C11	0.96	2.04	0.096
BD*(2)	C11-N17	RY*(3)	C12	0.54	0.87	0.047
BD*(2)	C11-N17	RY*(3)	N17	0.82	0.93	0.06
BD*(2)	C11-N17	RY*(4)	N17	0.63	1.72	0.072
BD*(2)	C11-N17	BD*(2)	C12-C13	178.73	0.01	0.08
BD*(2)	C11-N17	BD*(2)	C14-C15	227.65	0.01	0.075
BD*(2)	C11-N17	BD*(2)	C41-N42	55.05	0.02	0.065
BD*(2)	C12-C13	RY*(5)	C12	0.64	1.7	0.087
BD*(2)	C12-C13	RY*(5)	C13	1.9	0.75	0.1
BD*(2)	C14-C15	RY*(6)	C14	1.65	0.69	0.063
BD*(2)	C14-C15	RY*(5)	C15	0.67	1.81	0.065
BD*(2)	C14-C15	RY*(7)	C15	0.84	0.85	0.05
BD*(2)	C14-C15	RY*(3)	C16	0.5	1.35	0.049
BD*(2)	C14-C15	RY*(3)	N17	0.64	0.92	0.045
BD*(2)	C14-C15	RY*(3)	C18	0.61	1.2	0.05
BD*(2)	C14-C15	BD*(2)	C18-C19	195.49	0.01	0.078
BD*(2)	C16-C20	RY*(4)	C16	1.4	1.19	0.103

BD*(2)	C16-C20	RY*(4)	C20	1.63	1	0.102
BD*(2)	C18-C19	RY*(5)	C18	1.14	1.32	0.1
BD*(2)	C18-C19	RY*(4)	C19	1.55	1.01	0.103
BD*(2)	C21-C22	RY*(6)	C21	0.71	1.41	0.063
BD*(2)	C21-C22	RY*(3)	C22	0.7	1.81	0.07
BD*(2)	C21-C22	RY*(4)	C22	1.57	0.75	0.068
BD*(2)	C21-C22	RY*(4)	C23	0.57	1.24	0.053
BD*(2)	C21-C22	BD*(2)	C25-C26	160.22	0.02	0.08
BD*(2)	C23-C24	RY*(4)	C22	0.62	0.75	0.043
BD*(2)	C23-C24	RY*(3)	C23	1.69	1.32	0.093
BD*(2)	C23-C24	RY*(4)	C24	1.06	1.59	0.081
BD*(2)	C23-C24	RY*(3)	C25	0.54	0.73	0.039
BD*(2)	C23-C24	BD*(2)	C25-C26	126.63	0.02	0.08
BD*(2)	C23-C24	BD*(1)	N45-H46	0.72	0.42	0.033
BD*(2)	C23-C24	BD*(1)	N45-C47	0.73	0.43	0.033
BD*(2)	C25-C26	RY*(3)	C25	1.58	0.71	0.076
BD*(2)	C25-C26	RY*(7)	C26	0.54	1.67	0.068
BD*(2)	C25-C26	BD*(1)	C44-H64	1.04	0.45	0.049
BD*(2)	C27-N33	RY*(4)	C27	1.04	2	0.099
BD*(2)	C27-N33	RY*(3)	N33	0.7	0.96	0.056
BD*(2)	C27-N33	RY*(4)	N33	0.72	1.68	0.076
BD*(2)	C27-N33	BD*(2)	C28-C29	216.71	0.01	0.08
BD*(2)	C27-N33	BD*(2)	C30-C31	224.29	0.01	0.075
BD*(2)	C27-N33	BD*(2)	C47-N48	50.41	0.04	0.073
BD*(2)	C28-C29	RY*(3)	C28	1.34	0.65	0.076
BD*(2)	C28-C29	RY*(5)	C29	2.1	0.68	0.097
BD*(2)	C30-C31	RY*(6)	C30	1.67	0.69	0.063
BD*(2)	C30-C31	RY*(5)	C31	0.7	1.8	0.066
BD*(2)	C30-C31	RY*(6)	C31	0.77	0.88	0.048
BD*(2)	C30-C31	RY*(3)	C32	0.5	1.37	0.049
BD*(2)	C30-C31	RY*(3)	N33	0.67	0.95	0.047
BD*(2)	C30-C31	RY*(3)	C34	0.62	1.19	0.051
BD*(2)	C30-C31	BD*(2)	C32-C36	257.85	0.01	0.077
BD*(2)	C30-C31	BD*(2)	C34-C35	188.03	0.01	0.078
BD*(2)	C32-C36	RY*(4)	C32	1.41	1.18	0.104
BD*(2)	C32-C36	RY*(4)	C36	1.58	1.02	0.102
BD*(2)	C34-C35	RY*(5)	C34	1.1	1.35	0.1
BD*(2)	C34-C35	RY*(4)	C35	1.55	1	0.102
BD*(2)	C47-N48	RY*(7)	C47	0.72	1.68	0.089
BD*(2)	C47-N48	RY*(2)	N48	1.52	0.79	0.089

'E2' denotes 'the hyper energy conjugated interaction (stabilization energy in kcal/mol) by energy difference between donor and acceptor i and j NBO orbitals. F(i, j) is the Fock matrix element between i and j NBO orbitals. 'LP' denotes 'lone-pair', 'LV' denotes

'lone vacant', 'RY' denotes 'Rydberg', 'BD' denotes 'bonding', and 'CR' denotes 'core' orbitals. Entries are included in this table only when the interaction energy exceeds a default threshold of 0.05 kcal/mol.