

Effect of *meso*-pentafluorophenyl group on two-photon absorption in heterocorroles and heterocorrins

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1. Oscillator strengths & Excitation energies of S0 → S1 and S0 → S2 transitions :

The table presents the oscillator strengths and excitation energies of first 2 singlet states (S1 and S2) of all the considered systems calculated at RICC2/cc-pVDZ level of theory as implemented in Turbomole 7.3 program.

ST1a : Heterocorroles

System	S1-Ex.Ene (eV)	S1-Osc.stgh	S2-Ex.Ene (eV)	S2-Osc.stgh
Corrole	2.43	0.049727	2.66	0.129657
PFPh-Corrole	2.34	0.050315	2.54	0.249763
10-NH-Cor	2.57	0.032543	2.78	0.014696
10-NH-PFPh-Cor	2.44	0.033384	2.64	0.031042
10-NMe-Cor	2.53	0.030474	2.75	0.003680
10-NMe-PFPh-Cor	2.40	0.031985	2.60	0.013977
10-O-Cor	2.58	0.106761	2.90	0.029154
10-O-PFPh-Cor	2.45	0.157800	2.70	0.060219
10-S-Cor	2.52	0.063456	2.78	0.022741
10-S-PFPh-Cor	2.39	0.075362	2.61	0.061736
10-Se-Cor	2.48	0.090948	2.76	0.028450
10-Se-PFPh-Cor	2.35	0.116790	2.59	0.063633
10-SiMe2-Cor	2.21	0.135410	3.17	0.012432
10-SiMe2-PFPh-Cor	2.07	0.200827	2.92	0.023084
20-O-Cor	2.45	0.038268	2.71	0.135031
20-O-PFPh-Cor	2.38	0.042282	2.63	0.237112
21-O-Cor	2.37	0.034561	2.73	0.061921
21-O-PFPh-Cor	2.30	0.042803	2.65	0.062467
21-S-Cor	2.27	0.034681	2.68	0.044813
21-S-PFPh-Cor	2.11	0.038193	2.44	0.141924
N1-Con-Cor	1.87	0.179844	2.32	0.034565
N1-Con-PFPh-Cor	1.80	0.337440	2.18	0.027282
N2-Con-Cor	2.30	0.245744	2.68	0.128024
N2-Con-PFPh-Cor	2.12	0.377529	2.42	0.159767
Neo-Con-Cor	2.25	0.222583	2.74	0.050071
Neo-Con-PFPh-Cor	2.11	0.352916	2.54	0.070744

ST1b : Heterocorrins

System	S1-Ex.Ene (eV)	S1-Osc.stgh	S2-Ex.Ene (eV)	S2-Osc.stgh
Corrin	3.11	0.329812	3.97	0.002740
PFPh-Corrin	2.91	0.505736	3.85	0.007662
10-NH-Corrin	4.14	0.000179	4.25	0.153559
10-NH-PFPh-Corrin	3.89	0.029378	4.01	0.402123
10-NMe-Corrin	4.02	0.155835	4.14	0.013080
10-NMe-PFPh-Corrin	3.83	0.341290	3.90	0.040637
10-O-Corrin	4.22	0.004125	4.72	0.095447
10-O-PFPh-Corrin	4.02	0.023079	4.52	0.259349
10-S-Corrin	4.11	0.000229	4.33	0.099594
10-S-PFPh-Corrin	3.91	0.002091	4.14	0.289874
10-Se-Corrin	4.13	0.001401	4.33	0.097472
10-Se-PFPh-Corrin	3.96	0.005912	4.15	0.271708
10-SiMe2-Corrin	3.96	0.002303	4.31	0.004380
10-SiMe2-PFPh-Corrin	3.97	0.008674	4.30	0.018997
20-O-Corrin	3.57	0.254970	3.86	0.028537
20-O-PFPh-Corrin	3.38	0.207120	3.81	0.100397
21-O-Corrin	4.25	0.209624	4.68	0.004836
21-O-PFPh-Corrin	3.92	0.504829	4.46	0.042603
21-S-Corrin	3.77	0.205610	4.04	0.003803
21-S-PFPh-Corrin	3.49	0.406016	3.73	0.019150
N1-Con-Corrin	3.11	0.158480	3.81	0.259189
N1-Con-PFPh-Corrin	2.87	0.343980	3.47	0.289667
N2-Con-Corrin	3.65	0.267508	3.82	0.025439
N2-Con-PFPh-Corrin	3.33	0.428823	3.62	0.018245
Neo-Con-Corrin	3.35	0.009083	3.63	0.252314
Neo-Con-PFPh-Corrin	3.33	0.428823	3.62	0.018245

2. TPA strengths [RICC2] of S0 → S1 and S0 → S2 transitions:

ST2 : The table presents the TPA strengths (in a.u.) first 2 singlet states (S1 and S2) of all the considered systems calculated at RICC2/cc-pVDZ level of theory as implemented in Turbomole 7.3 program.

System	S1-TPA	S2-TPA	System	S1-TPA	S2-TPA
Corrole	2019	457	Corrin	910	21
PFPh-Corrole	4490	1465	PFPh-Corrin	1912	829
10-NH-Cor	4500	7234	10-NH-Corrin	1	105
10-NH-PFPh-Cor	13199	10214	10-NH-PFPh-Corrin	37	281
10-NMe-Cor	4414	6738	10-NMe-Corrin	133	11
10-NMe-PFPh-Cor	12081	9958	10-NMe-PFPh-Corrin	244	17
10-O-Cor	3524	11523	10-O-Corrin	4	84
10-O-PFPh-Cor	10473	22007	10-O-PFPh-Corrin	26	276
10-S-Cor	4536	8458	10-S-Corrin	3	168
10-S-PFPh-Cor	12345	13549	10-S-PFPh-Corrin	7	424
10-Se-Cor	4590	9849	10-Se-Corrin	8	289
10-Se-PFPh-Cor	11955	16811	10-Se-PFPh-Corrin	23	645
10-SiMe2-Cor	2301	36155	10-SiMe2-Corrin	14	50
10-SiMe2-PFPh-Cor	3401	86032	10-SiMe2-PFPh-Corrin	48	9
20-O-Cor	1675	414	20-O-Corrin	273	163
20-O-PFPh-Cor	3421	1132	20-O-PFPh-Corrin	1567	1690
21-O-Cor	1907	2380	21-O-Corrin	112	60
21-O-PFPh-Cor	3748	4207	21-O-PFPh-Corrin	389	1695
21-S-Cor	1697	1802	21-S-Corrin	401	25
21-S-PFPh-Cor	4576	4296	21-S-PFPh-Corrin	645	92
N1-Con-Cor	3237	5477	N1-Con-Corrin	504	2869
N1-Con-PFPh-Cor	13235	16708	N1-Con-PFPh-Corrin	689	16319
N2-Con-Cor	447	13429	N2-Con-Corrin	128	16
N2-Con-PFPh-Cor	553	31591	N2-Con-PFPh-Corrin	1629	42
Neo-Con-Cor	2937	8312	Neo-Con-Corrin	432	168
Neo-Con-PFPh-Cor	8012	24318	Neo-Con-PFPh-Corrin	1629	42

3. TPA strengths [GFSM] of S0 → S1 and S0 → S2 transitions :

ST3 : The table presents the TPA strengths (in a.u.) of S2 state evaluated employing 3SM (S1 as intermediate), 3SM (S3 as intermediate), and 4SM for those PFPh-substituted corroles and corrins (and their respective unsubstituted analogues) having the top 5 highest TPA-RICC2 strengths.

System	3SM(i=1)	3SM(i=3)	4SM(i=1,3)
10-O-cor	1136	3190	6945
10-O-PFPh-cor	2161	11720	19210
10-Se-cor	584	6149	9222
10-Se-PFPh-cor	883	14570	18380
10-Sime2-cor	28720	225	27500
10-Sime2-PFPh-cor	69010	318	66000
N2-Con-cor	7406	750	8088
N2-Con-PFPh-cor	18060	422	17900
Neo-Con-cor	2565	365	3209
Neo-Con-PFPh-cor	9240	971	10360
Corrole	53	599	598
PFPh-Corrole	83	1442	1066
20-O-corrin	59	22	119
20-O-PFPh-corrin	1366	174	1441
21-O-corrin	27	1	27
21-O-PFPh-corrin	1673	163.2	1704
N1-Con-corrin	2598	861	2426
N1-Con-PFPh-corrin	21260	487	17930
N2-Con-corrin	45	19	68
N2-Con-PFPh-corrin	115	88	166
Neo-Con-corrin	261	393	386
Neo-Con-PFPh-corrin	3092	3465	3479
Corrin	16	1	15
PFPh-Corrin	746	6	810

4. Magnitudes of different dipole moments and transition dipole moments :

The following tables presents the state dipole strengths (in a.u.) of S0, S1, S2, S3 states and transition dipole strengths between the said states for those PFPh-substituted corroles and corrins (and their respective unsubstituted analogues) having the top 5 larger TPA-RICC2 strengths, which are evaluated RICC2/cc-pVDZ level of theory.

ST4a : Dipole strengths of considered corroles

System	μ_{00}	μ_{11}	μ_{22}	μ_{33}
Corrole	0.698	0.655	0.876	1.064
PFPh-Corrole	1.428	1.241	1.562	1.814
10-O-Cor	0.226	0.828	0.703	0.451
10-O-PFPh-Cor	0.317	1.305	1.058	0.652
10-Se-Cor	0.11	0.845	0.576	0.872
10-Se-PFPh-Cor	0.35	1.221	0.874	1.092
10-SiMe2-Cor	0.072	0.63	0.68	0.498
10-SiMe2-PFPh-Cor	0.37	0.827	0.778	0.794
N2-Con-Cor	1.435	1.747	2.172	2.085
N2-Con-PFPh-Cor	2.058	2.351	2.656	2.702
Neo-Con-Cor	0.545	1.069	0.47	0.795
Neo-Con-PFPh-Cor	0.487	1.121	0.744	0.978

ST4b : Transition dipole strengths of considered corroles

System	μ_{01}	μ_{02}	μ_{03}	μ_{10}	μ_{12}	μ_{13}	μ_{20}	μ_{22}	μ_{23}	μ_{30}	μ_{31}	μ_{32}
Corrole	1.05	1.68	3.88	0.80	0.28	1.28	1.19	0.39	0.82	2.51	1.17	0.78
PFPh-Corrole	1.06	2.42	4.46	0.84	0.31	0.60	1.66	0.49	1.40	2.92	0.84	1.00
10-O-Cor	1.59	0.71	3.08	1.06	1.19	1.14	0.58	0.88	2.54	1.94	1.18	2.58
10-O-PFPh-Cor	2.00	1.07	3.59	1.31	1.07	1.67	0.85	0.68	2.85	2.16	1.69	2.97
10-Se-Cor	1.47	0.78	3.02	0.99	0.87	1.35	0.56	0.58	2.78	1.85	1.51	2.83
10-Se-PFPh-Cor	1.75	1.15	3.84	1.16	0.68	1.89	0.88	0.36	2.84	2.32	1.97	2.89
10-SiMe2-Cor	2.03	0.48	4.26	1.23	2.94	1.34	0.33	2.50	0.47	2.61	1.17	0.40
10-SiMe2-PFPh-Cor	2.56	0.68	3.98	1.55	3.54	1.39	0.47	2.94	0.48	2.46	1.13	0.44
N2-Con-Cor	2.57	1.75	3.25	1.70	1.65	1.61	1.12	1.29	0.30	2.07	0.78	0.25
N2-Con-PFPh-Cor	3.32	2.03	3.99	2.19	1.96	2.18	1.33	1.51	0.17	2.55	1.03	0.04
Neo-Con-Cor	2.45	1.00	2.85	1.65	1.15	0.52	0.75	0.77	1.35	2.05	0.34	1.15
Neo-Con-PFPh-Cor	3.23	1.21	3.45	2.11	1.41	0.52	0.94	0.91	1.45	2.63	0.37	1.10

ST4c : Dipole strengths of considered corrins

System	μ_{00}	μ_{11}	μ_{22}	μ_{33}
Corrin	0.896	1.722	0.687	0.596
PFPh-Corrin	1.207	2.211	0.889	1.48
20-O-Corrin	1.246	1.546	1.203	0.704
20-O-PFPh-Corrin	1.139	2.414	1.967	1.97
21-O-Corrin	2.09	1.875	1.481	1.096
21-O-PFPh-Corrin	1.858	1.192	1.233	1.852
N1-Con-Corrin	1.029	1.292	1.96	0.927
N1-Con-PFPh-Corrin	1.1	1.44	1.762	1.629
N2-Con-Corrin	1.661	1.395	1.599	1.636
N2-Con-PFPh-Corrin	1.417	1.07	1.081	3.047
Neo-Con-Corrin	1.411	3.045	1.128	1.236
Neo-Con-PFPh-Corrin	1.338	3.686	0.922	1.014

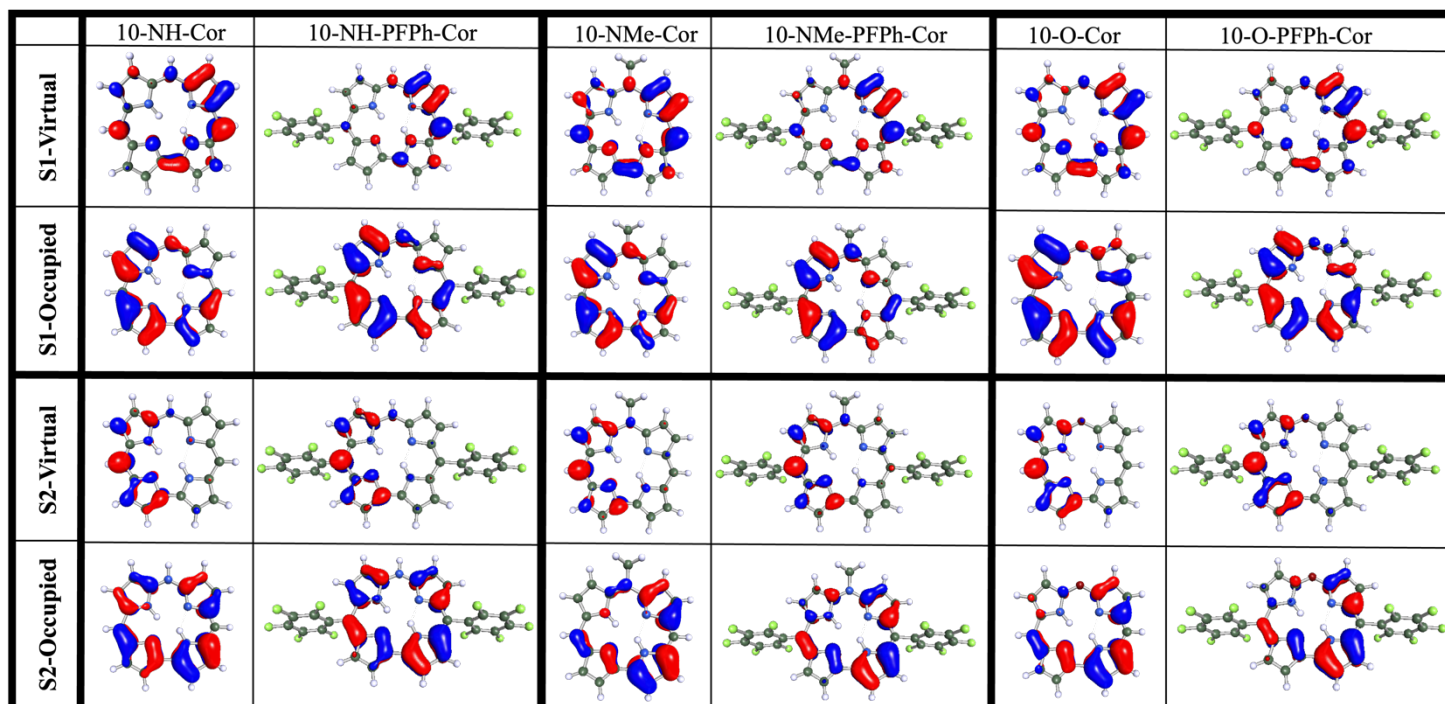
ST4d : Transition dipole strengths of considered corrins

System	μ_{01}	μ_{02}	μ_{03}	μ_{10}	μ_{12}	μ_{13}	μ_{20}	μ_{21}	μ_{23}	μ_{30}	μ_{31}	μ_{32}
Corrin	2.69	0.22	1.52	1.61	0.12	2.23	0.13	0.10	0.10	0.83	1.78	0.09
PFPh-Corrin	3.46	0.39	1.78	2.05	0.48	2.88	0.21	0.40	0.18	0.95	2.45	0.19
20-O-Corrin	2.20	0.72	1.30	1.33	0.40	2.10	0.42	0.37	0.95	0.70	1.90	0.93
20-O-PFPh-Corrin	2.07	1.37	0.56	1.21	1.08	0.56	0.78	1.06	0.58	0.32	0.51	0.58
21-O-Corrin	1.85	0.23	0.28	1.09	0.30	0.29	0.12	0.28	0.18	0.15	0.29	0.18
21-O-PFPh-Corrin	3.00	0.25	0.87	1.75	0.20	1.08	0.14	0.20	0.39	0.45	1.06	0.41
N1-Con-Corrin	1.87	2.18	1.38	1.11	2.17	1.40	1.27	2.04	0.43	0.79	1.08	0.42
N1-Con-PFPh-Corrin	2.88	2.43	2.86	1.70	3.23	2.62	1.40	3.09	0.81	1.69	2.37	0.68
N2-Con-Corrin	2.21	0.69	0.78	1.35	0.30	0.72	0.40	0.27	1.05	0.45	0.72	1.05
N2-Con-PFPh-Corrin	2.95	0.60	0.70	1.78	0.31	0.76	0.34	0.27	1.56	0.41	0.81	1.56
Neo-Con-Corrin	0.45	2.16	1.11	0.25	0.22	0.32	1.31	0.18	0.42	0.66	0.31	0.40
Neo-Con-PFPh-Corrin	0.51	2.97	0.78	0.29	0.24	0.23	1.79	0.24	0.51	0.45	0.22	0.48

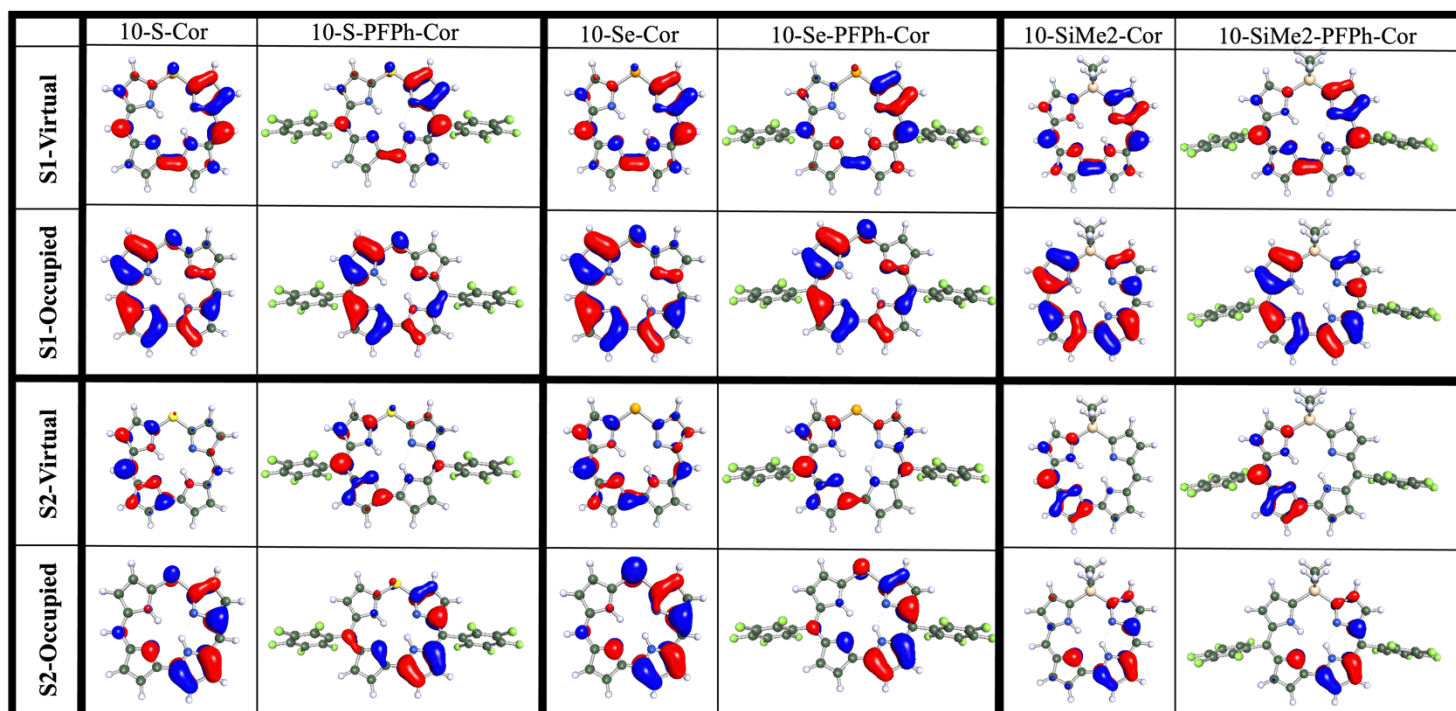
5. NTOs for $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions :

The following figures presents the NTOs for $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions of all considered heterocorrins and heterocorrins that were computed at RICC2/cc-pVDZ level of theory.

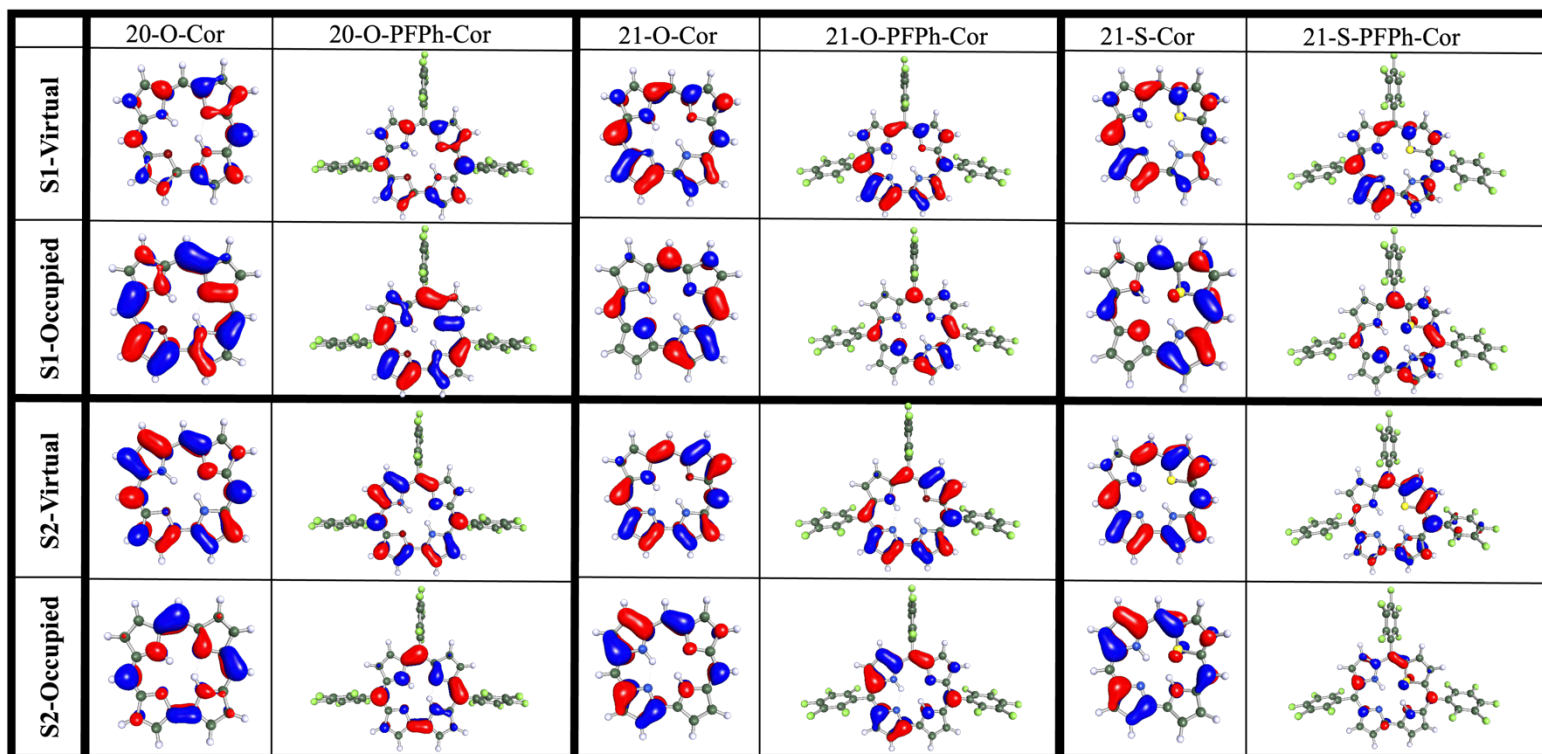
SF5a : NTOs of 10-NH-, 10-NMe-, 10-O- Corroles and their PFPh-substituted systems.



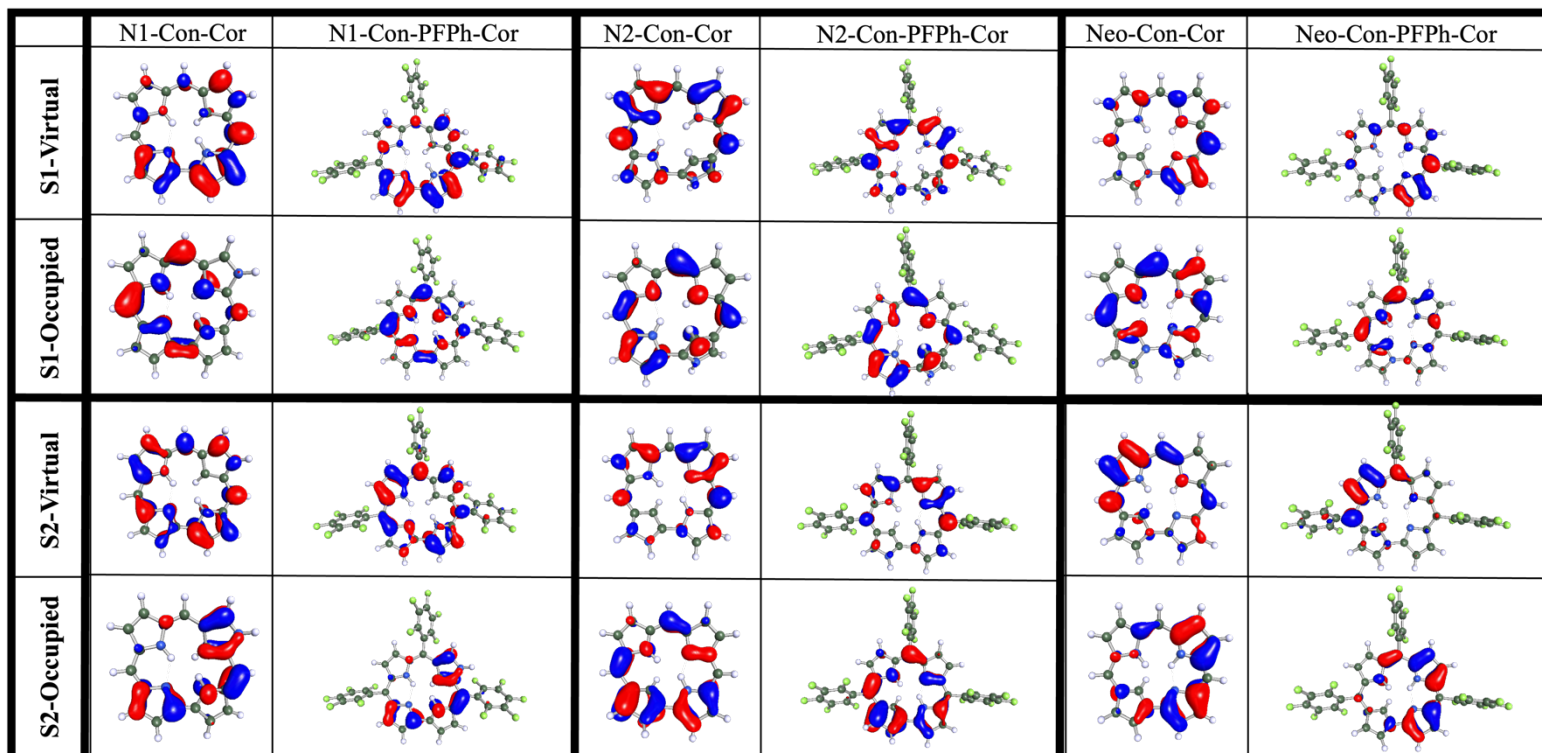
SF5b : NTOs of 10-S-, 10-Se-, 10-SiMe2- Corroles and their PFPh-substituted systems.



SF5c : NTOs of 20-O-, 21-O-, 21-S- Corroles and their PFPh-substituted systems



SF5d : NTOs of N1-Con-, N2-Con-, Neo-Con- Corroles and their PFPh-substituted systems



SF5e : NTOs of 10-NH-, 10-NMe-, 10-O- Corrins and their PFPh-substituted systems

	10-NH-Corrin	10-NH-PFPh-Corrin	10-NMe-Corrin	10-NMe-PFPh-Corrin	10-O-Corrin	10-O-PFPh-Corrin
S1-Virtual						
S1-Occupied						
S2-Virtual						
S2-Occupied						

SF5f : NTOs of 10-S-, 10-Se-, 10-SiMe2- Corrins and their PFPh-substituted systems

	10-S-Corrin	10-S-PFPh-Corrin	10-Se-Corrin	10-Se-PFPh-Corrin	10-SiMe2-Corrin	10-SiMe2-PFPh-Corrin
S1-Virtual						
S1-Occupied						
S2-Virtual						
S2-Occupied						

SF5g : NTOs of 20-O-, 21-O-, 21-S- Corrins and their PFPh-substituted systems

	20-O-Corrin	20-O-PFPh-Corrin	21-O-Corrin	21-OPFPh-Corrin	21-S-Corrin	21-S-PFPh-Corrin
S1-Virtual						
S1-Occupied						
S2-Virtual						
S2-Occupied						

SF5h : NTOs of N1-Con-, N2-Con-, Neo-Con- Corrins and their PFPh-substituted systems

	N1-Con-Corrin	N1-Con-PFPh-Corrin	N2-Con-Corrin	N2-Con-PFPh-Corrin	Neo-Con-Corrin	Neo-Con-PFPh-Corrin
S1-Virtual						
S1-Occupied						
S2-Virtual						
S2-Occupied						

6. Effect of basis set on magnitudes of different dipole moments and transition dipole moments :

ST6 : Dipole strengths of Pristine Corrole corresponding to $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions calculated using aug-cc-pVTZ, cc-pVTZ and cc-pVDZ basis sets at RI-CC2 level of theory.

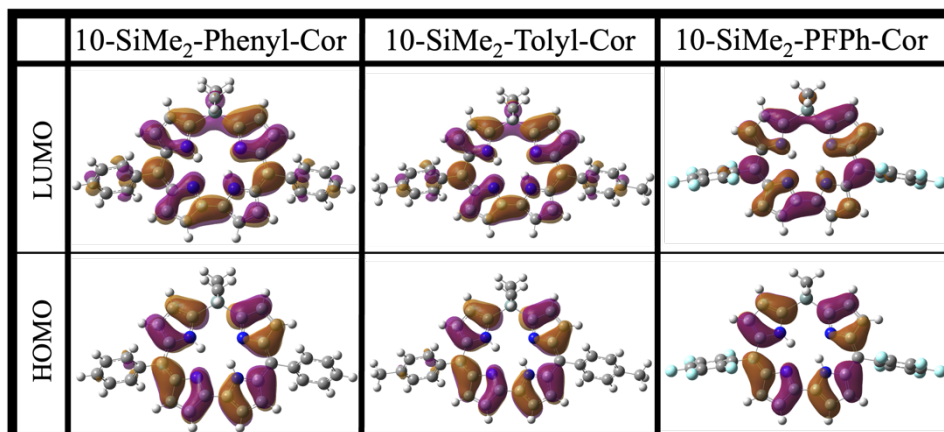
μ	aug-cc-pVTZ	cc-pVTZ	cc-pVDZ
μ_{00}	0.7492	0.7268	0.6976
μ_{11}	0.6557	0.6488	0.6546
μ_{22}	0.9119	0.8949	0.8758
μ_{01}	0.9986	1.0055	1.0482
μ_{02}	1.6567	1.6453	1.6761
μ_{10}	0.7943	0.7943	0.7983
μ_{20}	1.1928	1.1830	1.1861
μ_{12}	0.3651	0.3730	0.3940
μ_{21}	0.2583	0.2646	2843

7. Effect of different *meso*-substituents on OPA, TPA, excitation energies and MOs:

ST7 : Dipole strengths of Pristine Corrole calculated using aug-cc-pVTZ, cc-pVTZ and cc-pVDZ basis sets at RI-CC2 level of theory.

System	S1-OPA	S2-OPA	S1-TPA	S2-TPA	S1-Ex. Ene (eV)	S2-Ex. Ene (eV)
10-SiMe ₂ -Cor	0.1354	0.0124	2301	36155	2.21	3.17
10-SiMe ₂ -PFPh-Cor	0.2008	0.0231	3401	86031	2.07	2.92
10-SiMe ₂ -Tolyl-Cor	0.2226	0.0225	3509	106324	2.09	2.98
10-SiMe ₂ -OMe-Cor	0.1243	0.3631	1550	12309	2.50	3.48
10-SiMe ₂ -TFMe-Cor	0.1547	0.0301	3017	56337	2.01	2.90
10-SiMe ₂ -Phenyl-Cor	0.2105	0.0215	3250	97748	2.10	2.98
10-SiMe ₂ -Ethenyl-Cor	0.1777	0.0181	3406	72295	2.09	2.98
10-SiMe ₂ -Me-Cor	0.1499	0.0200	2954	43431	2.25	3.19

SF7 : HOMO and LUMOs of 10-SiMe₂-Phenyl-Cor, 10-SiMe₂-Tolyl-Cor and 10-SiMe₂-PFPh-Cor systems indicating the electron densities.



8. Optimized Coordinates of the ground-state geometry :

This section includes the ground-state optimized cartesian coordinates for all the systems considered in this work that are optimized at B3LYP/6-311+G(d,p) level of theory using Gaussian-16 program.

Coordinates of Heterocorroles (XYZ Format):

36

10-NH-Cor

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C      2.699241  0.978068  0.000057
N      1.947097 -0.137941  0.000099
C      4.062839  0.586817 -0.000068
C      4.085170 -0.803799 -0.000100
C      2.747062 -1.273522  0.000008
C      0.872823  2.674596  0.000026
N     -0.162903  1.852391  0.000133
C     -1.302450  2.658418 -0.000001
C     -0.893936  4.046004 -0.000198
C      0.474453  4.064885 -0.000172
C     -2.610813  2.172631 -0.000029
C     -2.943578  0.798624  0.000108
C     -4.141492  0.025748 -0.000097
C     -3.778641 -1.323940 -0.000150
C     -2.358488 -1.388104  0.000174
C     -1.292980 -2.358529  0.000119
N     -0.063948 -1.831692  0.000225
C      0.840168 -2.855075  0.000015
C      0.120785 -4.114686 -0.000204
C     -1.217795 -3.802591 -0.000149
C      2.210382 -2.574799 -0.000035
H      1.128207  4.925545 -0.000297

```

H	-1.558547	4.898131	-0.000354
H	-3.416430	2.897741	-0.000231
H	-5.146665	0.419766	-0.000266
H	-4.450072	-2.168543	-0.000367
H	-2.049519	-4.491921	-0.000295
H	0.559296	-5.102694	-0.000394
H	2.917081	-3.397207	-0.000140
H	4.963847	-1.430753	-0.000123
H	4.909894	1.255691	-0.000188
H	2.881788	2.985310	0.000064
N	-1.930991	-0.107122	0.000326
H	-0.960097	0.191054	0.000390
N	2.189812	2.251398	0.000117
H	0.931227	-0.235836	0.000088

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10-NH-PFPh-Cor

C	-1.227162	2.796895	-0.623917
N	-1.488168	1.506567	-0.342537
C	-2.465125	3.474136	-0.769143
C	-3.466891	2.534936	-0.565700
C	-2.856716	1.281781	-0.295363
C	1.264607	2.720111	-0.619677
N	1.434239	1.434160	-0.358675
C	2.811188	1.224241	-0.306765
C	3.486581	2.480557	-0.562112
C	2.519480	3.425115	-0.759315
C	3.404627	-0.020820	-0.048202
C	2.650764	-1.203978	0.169545
C	2.948614	-2.553017	0.526928
C	1.738951	-3.233766	0.661458
C	0.692830	-2.310113	0.388878
C	-0.742072	-2.250418	0.390373
N	-1.254349	-1.043241	0.123665
C	-2.613437	-1.136206	0.182514
C	-2.977688	-2.504700	0.506129
C	-1.803226	-3.201677	0.637149
C	-3.405423	0.005427	-0.029754
H	2.651828	4.476240	-0.972299
H	4.554739	2.633901	-0.592278
H	3.934662	-2.965719	0.674736
H	1.613247	-4.270436	0.932306
H	-1.688595	-4.248766	0.875623
H	-3.978263	-2.894035	0.624453
H	-4.529100	2.717792	-0.606903
H	-2.587549	4.522239	-0.995398
H	0.054117	4.314032	-0.946897
N	1.297715	-1.139086	0.088873
H	0.828536	-0.260324	-0.114243
N	0.030757	3.325975	-0.742491

H	-0.848606	0.723561	-0.188703
C	4.891632	-0.120638	0.020158
C	5.629269	-0.713002	-1.006701
C	5.610072	0.352493	1.119768
C	7.013397	-0.827523	-0.951784
C	6.994277	0.250080	1.197538
C	7.697911	-0.342940	0.156329
C	-4.891400	-0.114884	0.028558
C	-5.621257	0.350939	1.123715
C	-5.616875	-0.708028	-1.006301
C	-7.004522	0.234426	1.193637
C	-7.000323	-0.836421	-0.959176
C	-7.695984	-0.362962	0.146629
F	4.966813	0.916116	2.150209
F	7.651171	0.710518	2.266804
F	9.026173	-0.446439	0.220059
F	7.689839	-1.391932	-1.956925
F	5.005729	-1.178320	-2.096519
F	-4.988498	0.919640	2.158206
F	-7.672135	0.685207	2.260379
F	-9.023479	-0.480236	0.202520
F	-7.665417	-1.404096	-1.970017
F	-4.983860	-1.161500	-2.095226

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10-NMe-PFPh-Cor

C	2.410069	-1.172138	-0.015399
N	1.083326	-1.431879	-0.016592
C	3.086411	-2.423198	0.046226
C	2.115243	-3.415572	0.077621
C	0.842767	-2.799613	0.035318
C	2.282841	1.300805	-0.018734
N	0.958482	1.410576	-0.056717
C	0.673539	2.775695	0.016059
C	1.910183	3.511196	0.104129
C	2.926663	2.598489	0.083778
C	-0.602608	3.341893	0.020337
C	-1.803406	2.603522	-0.033613
C	-3.196733	2.888159	0.058245
C	-3.882041	1.670295	0.038492
C	-2.915024	0.634481	-0.067204
C	-2.824584	-0.803135	-0.051073
N	-1.573362	-1.272068	-0.065380
C	-1.629838	-2.633288	-0.003099
C	-3.019966	-3.046309	0.040915
C	-3.770428	-1.895359	0.013492
C	-0.444473	-3.368925	0.041400
H	3.980354	2.811462	0.160141
H	2.000701	4.585319	0.181508
H	-0.665150	4.421595	0.092773

H	-3.635833	3.870801	0.142907
H	-4.950247	1.533760	0.104984
H	-4.847569	-1.816338	0.036110
H	-3.385910	-4.062132	0.092286
H	-0.494793	-4.451000	0.092963
H	2.288719	-4.479695	0.130168
H	4.151359	-2.575436	0.085298
N	-1.715435	1.252035	-0.129794
H	-0.818522	0.779409	-0.164723
N	2.968475	0.087816	-0.064301
H	0.312432	-0.770485	-0.050549
C	4.437968	0.132603	-0.092326
H	4.763433	1.049841	-0.572131
H	4.857984	0.078009	0.915938
H	4.813146	-0.698080	-0.685577

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10-NMe-PFPh-Cor

C	-1.218301	2.731189	-0.371585
N	-1.462966	1.419459	-0.148755
C	-2.477244	3.373319	-0.543288
C	-3.457812	2.402520	-0.412917
C	-2.827324	1.160154	-0.160961
C	1.258206	2.659964	-0.366151
N	1.408275	1.355909	-0.149717
C	2.781310	1.108474	-0.163036
C	3.480418	2.346560	-0.414854
C	2.537872	3.323576	-0.543486
C	3.379902	-0.147044	0.029599
C	2.639840	-1.338191	0.228993
C	2.947658	-2.710967	0.466205
C	1.741415	-3.400762	0.585625
C	0.689627	-2.458137	0.424635
C	-0.744743	-2.400687	0.422350
N	-1.248629	-1.177400	0.227935
C	-2.606646	-1.275822	0.231894
C	-2.981350	-2.662298	0.452680
C	-1.810698	-3.367294	0.571624
C	-3.384188	-0.125175	0.037053
H	2.723030	4.362731	-0.759238
H	4.549638	2.469803	-0.496978
H	3.937377	-3.134566	0.539867
H	1.621784	-4.457191	0.768496
H	-1.701315	-4.428575	0.739469
H	-3.984848	-3.057843	0.510125
H	-4.521626	2.558915	-0.497020
H	-2.643443	4.414565	-0.758872
N	1.286488	-1.264049	0.215119
H	0.807796	-0.379453	0.075187
N	0.030483	3.311920	-0.418741

H	-0.801730	0.660577	0.001722
C	0.043465	4.772580	-0.611483
H	0.945376	5.187926	-0.174939
H	-0.004949	5.032031	-1.672183
H	-0.802782	5.212226	-0.090285
C	4.869113	-0.249883	0.026755
C	5.561244	-0.771842	-1.067381
C	5.633697	0.147712	1.124851
C	6.946219	-0.890042	-1.078091
C	7.019624	0.040032	1.138031
C	7.677547	-0.481500	0.030726
C	-4.872188	-0.243476	0.029694
C	-5.557306	-0.767947	-1.067543
C	-5.642949	0.152914	1.123914
C	-6.941561	-0.896333	-1.081289
C	-7.027858	0.035001	1.133868
C	-7.678781	-0.492878	0.025313
F	7.721959	0.428086	2.207247
F	9.007103	-0.589361	0.031979
F	7.578683	-1.386102	-2.146121
F	4.891246	-1.163490	-2.158665
F	5.034955	0.642852	2.215455
F	-4.882831	-1.153311	-2.157864
F	-7.567680	-1.397534	-2.150638
F	-9.007546	-0.610753	0.023243
F	-7.735923	0.418905	2.200820
F	-5.049869	0.654670	2.214910

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10-O-Cor

C	2.843196	0.029991	0.000007
N	1.762245	-0.765324	-0.000253
C	4.001191	-0.772695	0.000465
C	3.564214	-2.096425	0.000462
C	2.147165	-2.100506	0.000108
C	1.737244	2.177200	-0.000284
N	0.494641	1.760556	-0.000193
C	-0.292808	2.922020	0.000016
C	0.581069	4.075585	0.000088
C	1.868841	3.609832	-0.000209
C	-1.685354	2.922118	0.000226
C	-2.484310	1.752861	0.000254
C	-3.875059	1.447245	0.000251
C	-4.005959	0.053682	0.000124
C	-2.698091	-0.500312	0.000062
C	-2.023056	-1.779793	-0.000359
N	-0.691337	-1.694700	-0.000583
C	-0.178671	-2.962244	-0.000292
C	-1.278185	-3.908147	0.000024
C	-2.435373	-3.166145	0.000011

C	1.205362	-3.150124	0.000058
H	2.793556	4.165240	-0.000289
H	0.258745	5.107059	0.000273
H	-2.184507	3.884562	0.000331
H	-4.680360	2.166258	0.000285
H	-4.930280	-0.502752	0.000088
H	-3.449559	-3.537799	0.000297
H	-1.195913	-4.985874	0.000270
H	1.599356	-4.160541	0.000277
H	4.188124	-2.977270	0.000813
H	5.013922	-0.404107	0.000807
N	-1.853029	0.550870	0.000132
H	-0.841144	0.486681	-0.000024
H	0.770374	-0.526903	-0.000627
O	2.840193	1.375100	-0.000288

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10-O-PFPh-Cor

C	-1.186801	2.755207	-0.641640
N	-1.450658	1.473175	-0.344249
C	-2.402028	3.449894	-0.800672
C	-3.417261	2.522044	-0.589160
C	-2.823272	1.266137	-0.303111
C	1.227520	2.675680	-0.643438
N	1.393917	1.398419	-0.400070
C	2.781302	1.204390	-0.342498
C	3.439237	2.473921	-0.581325
C	2.459498	3.407823	-0.772214
C	3.383088	-0.032334	-0.084039
C	2.645279	-1.230609	0.122646
C	2.952888	-2.556127	0.545069
C	1.747713	-3.248427	0.683784
C	0.698289	-2.352881	0.347611
C	-0.741795	-2.287440	0.363370
N	-1.244531	-1.080484	0.093128
C	-2.605949	-1.157691	0.170282
C	-2.978249	-2.519917	0.509424
C	-1.808597	-3.226620	0.632882
C	-3.383456	-0.007413	-0.033841
H	2.556418	4.463441	-0.971242
H	4.505529	2.640665	-0.604475
H	3.939965	-2.945701	0.740683
H	1.629560	-4.271100	1.005959
H	-1.700855	-4.272825	0.877937
H	-3.980656	-2.898971	0.643803
H	-4.477252	2.715704	-0.638024
H	-2.494611	4.496569	-1.039800
N	1.294935	-1.193651	-0.005265
H	0.812012	-0.331626	-0.235518
H	-0.820847	0.684214	-0.184697

O	0.030399	3.308826	-0.769161
C	-4.870501	-0.109512	0.034535
C	-5.608555	-0.701897	-0.991639
C	-5.586902	0.375783	1.130039
C	-6.993273	-0.811161	-0.935709
C	-6.971018	0.277215	1.208837
C	-7.676080	-0.319372	0.170251
C	4.870393	-0.111502	0.010978
C	5.631447	-0.695116	-1.003464
C	5.562497	0.370862	1.123124
C	7.015702	-0.791587	-0.925244
C	6.946314	0.284804	1.224510
C	7.674734	-0.298780	0.194881
F	7.578664	0.751877	2.304829
F	9.002245	-0.385869	0.281330
F	7.715802	-1.347058	-1.918280
F	5.030651	-1.168204	-2.102353
F	4.893759	0.924676	2.142038
F	-7.671140	-1.378225	-1.937700
F	-4.986865	-1.172681	-2.079552
F	-9.004050	-0.419156	0.234787
F	-7.626127	0.744287	2.275583
F	-4.939728	0.943082	2.155814

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10-S-Cor

C	2.565240	-1.274178	0.000129
N	1.237427	-1.517306	-0.000147
C	3.240342	-2.516427	0.000108
C	2.266438	-3.508873	-0.000162
C	0.997012	-2.885794	-0.000313
C	2.289743	1.610331	0.000064
N	0.970212	1.596172	0.000326
C	0.580227	2.943365	-0.000011
C	1.757101	3.779937	-0.000474
C	2.841654	2.949101	-0.000394
C	-0.738911	3.389042	-0.000014
C	-1.870218	2.547104	0.000293
C	-3.279811	2.743521	-0.000194
C	-3.884440	1.484814	-0.000185
C	-2.849366	0.513788	0.000250
C	-2.701065	-0.917242	0.000375
N	-1.440824	-1.355848	0.000848
C	-1.477421	-2.723220	0.000278
C	-2.860814	-3.162803	-0.000543
C	-3.630033	-2.027569	-0.000448
C	-0.293704	-3.453445	-0.000070
H	3.888742	3.212175	-0.000726
H	1.760195	4.860560	-0.000833
H	-0.902145	4.460813	-0.000461

H	-3.781783	3.699250	-0.000690
H	-4.943466	1.279074	-0.000797
H	-4.708368	-1.965464	-0.001033
H	-3.205936	-4.187010	-0.001123
H	-0.344023	-4.536743	-0.000189
H	2.433911	-4.575229	-0.000507
H	4.311029	-2.645961	0.000189
N	-1.685508	1.199711	0.000621
H	-0.757202	0.787762	0.000852
H	0.462980	-0.856099	0.000432
S	3.406568	0.253691	0.000076

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10-Se-Cor

C	2.142184	-1.530540	0.000124
N	0.798689	-1.661031	-0.000190
C	2.710766	-2.822177	0.000532
C	1.657108	-3.732034	0.000382
C	0.445640	-3.005500	-0.000022
C	2.038308	1.561536	-0.000088
N	0.722296	1.598116	0.000056
C	0.386608	2.961615	0.000110
C	1.595325	3.750718	0.000108
C	2.645257	2.875508	-0.000072
C	-0.913182	3.456085	0.000174
C	-2.077142	2.660376	0.000136
C	-3.473807	2.926779	0.000144
C	-4.140383	1.699958	0.000012
C	-3.155352	0.679918	-0.000033
C	-3.095991	-0.757050	-0.000019
N	-1.870404	-1.282956	-0.000065
C	-2.008603	-2.645889	-0.000063
C	-3.419819	-2.983864	-0.000235
C	-4.103978	-1.796236	-0.000048
C	-0.887399	-3.466077	-0.000004
H	3.701997	3.097614	-0.000163
H	1.641509	4.830405	0.000183
H	-1.036538	4.533303	0.000211
H	-3.926426	3.906832	0.000154
H	-5.208156	1.546147	-0.000176
H	-5.174759	-1.654627	-0.000084
H	-3.837456	-3.980683	-0.000363
H	-1.024934	-4.541866	0.000026
H	1.734625	-4.808735	0.000462
H	3.766576	-3.043054	0.000915
N	-1.956620	1.304082	0.000013
H	-1.048817	0.847446	0.000108
H	0.079618	-0.939486	-0.000371
Se	3.188288	0.044132	-0.000189

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10-Se-PFPh-Cor

C	-1.534733	2.748921	-0.231829
N	-1.676518	1.411866	-0.115341
C	-2.821750	3.326383	-0.288413
C	-3.740140	2.286689	-0.203479
C	-3.023393	1.072370	-0.094084
C	1.560327	2.661103	-0.226591
N	1.618362	1.350172	-0.118866
C	2.985391	1.035677	-0.094623
C	3.756651	2.254345	-0.197599
C	2.865817	3.285002	-0.280757
C	3.488826	-0.264210	0.008080
C	2.670386	-1.417295	0.090368
C	2.928812	-2.810479	0.225885
C	1.700349	-3.466004	0.274841
C	0.686742	-2.479417	0.170770
C	-0.746008	-2.427681	0.169181
N	-1.289179	-1.213356	0.064120
C	-2.648590	-1.370749	0.090786
C	-2.966082	-2.782929	0.220493
C	-1.770360	-3.446147	0.269467
C	-3.492255	-0.261144	0.011938
H	3.073360	4.340922	-0.368933
H	4.833711	2.326052	-0.208637
H	3.904057	-3.268485	0.282317
H	1.540011	-4.527898	0.375779
H	-1.613442	-4.510389	0.363923
H	-3.953641	-3.217102	0.270188
H	-4.814605	2.379616	-0.219487
H	-3.034452	4.379726	-0.381275
N	1.316348	-1.287738	0.059140
H	0.871931	-0.375867	-0.019088
H	-0.967595	0.680149	-0.058122
Se	0.036804	3.790590	-0.315231
C	4.968662	-0.467568	0.038431
C	5.670611	-0.867314	-1.099223
C	5.707813	-0.284130	1.207504
C	7.045525	-1.071391	-1.083541
C	7.083225	-0.482189	1.248405
C	7.753369	-0.877493	0.096769
C	-4.971226	-0.468689	0.039351
C	-5.715009	-0.265151	1.202346
C	-5.670091	-0.881500	-1.095570
C	-7.090202	-0.463392	1.242354
C	-7.045114	-1.086170	-1.080600
C	-7.756598	-0.876307	0.094620
F	5.093195	0.087071	2.337306
F	7.762901	-0.300197	2.384252
F	9.072396	-1.070484	0.124187

F	7.690021	-1.447662	-2.191771
F	5.020554	-1.054769	-2.254524
F	-5.103450	0.123653	2.328159
F	-7.773297	-0.265770	2.373607
F	-9.075591	-1.069990	0.121019
F	-7.686217	-1.478354	-2.185332
F	-5.018236	-1.082636	-2.247332

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10-SiMe2-Cor

C	2.066653	-1.616727	-0.000191
N	0.714545	-1.736723	-0.000083
C	2.581097	-2.932124	-0.000582
C	1.505291	-3.824612	-0.000696
C	0.319967	-3.062349	-0.000414
C	2.023305	1.584365	-0.000317
N	0.697563	1.651895	-0.000019
C	0.357116	3.016759	-0.000314
C	1.566493	3.805557	-0.000763
C	2.606971	2.921245	-0.000722
C	-0.941446	3.497960	-0.000269
C	-2.108624	2.697782	0.000158
C	-3.497520	2.974757	-0.000487
C	-4.173913	1.748527	-0.000301
C	-3.196762	0.727934	0.000502
C	-3.163239	-0.718861	0.000355
N	-1.956862	-1.269431	0.000168
C	-2.129165	-2.636275	-0.000035
C	-3.548728	-2.936135	0.000022
C	-4.200743	-1.731426	0.000274
C	-1.034424	-3.481560	-0.000341
H	3.661944	3.157299	-0.000956
H	1.613704	4.885403	-0.001023
H	-1.077053	4.574401	-0.000709
H	-3.943192	3.957975	-0.000985
H	-5.242432	1.600591	-0.000601
H	-5.267218	-1.560617	0.000408
H	-3.992320	-3.921655	-0.000116
H	-1.205827	-4.552970	-0.000526
H	1.552249	-4.903393	-0.001079
H	3.628330	-3.194583	-0.000680
N	-1.992030	1.339158	0.000849
H	-1.078970	0.886148	0.000877
H	0.017969	-0.995601	0.000113
Si	3.061081	-0.002970	0.000295
C	4.147954	0.000414	1.544559
H	4.787167	0.887860	1.570390
H	4.795934	-0.880626	1.568716
H	3.540119	-0.003381	2.452939
C	4.149976	-0.000313	-1.542483

H	4.788464	0.887618	-1.568706
H	3.543229	-0.005835	-2.451593
H	4.798703	-0.880867	-1.564735

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10-SiMe2-PFPh-Cor

C	-1.593679	2.777114	0.035753
N	-1.741509	1.428988	0.004616
C	-2.897600	3.318929	0.068395
C	-3.812261	2.264436	0.057417
C	-3.075105	1.062595	0.017313
C	1.612799	2.702263	0.017827
N	1.682402	1.378659	0.012963
C	3.048523	1.037951	0.004131
C	3.836070	2.250918	0.003024
C	2.950588	3.287287	0.011384
C	3.519300	-0.269801	-0.009187
C	2.680545	-1.418746	-0.021747
C	2.929974	-2.813778	-0.028166
C	1.692181	-3.463552	-0.035141
C	0.692360	-2.465506	-0.031631
C	-0.750712	-2.419542	-0.028448
N	-1.301504	-1.213553	-0.007813
C	-2.667719	-1.388154	-0.011076
C	-2.965873	-2.809979	-0.036549
C	-1.762132	-3.458590	-0.046579
C	-3.520099	-0.291309	0.002087
H	3.186470	4.342079	0.012478
H	4.914142	2.309356	-0.005307
H	3.901829	-3.282230	-0.027537
H	1.522839	-4.528731	-0.040905
H	-1.590339	-4.524533	-0.065208
H	-3.947730	-3.259438	-0.046802
H	-4.888210	2.341334	0.077824
H	-3.138986	4.370655	0.097352
N	1.325676	-1.271560	-0.025111
H	0.897777	-0.345011	-0.013346
H	-1.019526	0.711524	-0.011034
Si	0.031672	3.752378	0.029162
C	0.041687	4.838111	-1.514461
H	0.026060	4.231464	-2.423422
H	0.935800	5.467586	-1.544104
H	-0.831989	5.495950	-1.533349
C	0.056708	4.831077	1.577213
H	0.950651	5.461056	1.599978
H	0.051288	4.220519	2.483639
H	-0.816815	5.488695	1.608362
C	-4.996695	-0.522828	0.003162
C	-5.750764	-0.415372	-1.165518
C	-5.680962	-0.854019	1.172558

C	-7.123910	-0.630291	-1.178197
C	-7.053919	-1.072607	1.185230
C	-7.776822	-0.960124	0.003720
C	4.995600	-0.508621	-0.010064
C	5.686425	-0.777347	-1.191311
C	5.737755	-0.486985	1.170400
C	7.057035	-1.008662	-1.205985
C	7.108933	-0.716030	1.181343
C	7.769744	-0.977269	-0.013128
F	-5.151401	-0.107935	-2.322412
F	-7.817880	-0.526943	-2.315292
F	-9.093856	-1.168749	0.003610
F	-7.681779	-1.385843	2.322288
F	-5.017208	-0.960685	2.330212
F	5.029810	-0.808416	-2.357642
F	7.692424	-1.257036	-2.354675
F	9.084724	-1.197968	-0.014685
F	7.793283	-0.689531	2.328453
F	5.130773	-0.245865	2.338803

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10-S-PFPh-Cor

C	-1.434119	2.883176	-0.415105
N	-1.607238	1.558696	-0.220343
C	-2.710318	3.485480	-0.510360
C	-3.649943	2.473716	-0.368053
C	-2.960753	1.250637	-0.185006
C	1.464021	2.798885	-0.407626
N	1.551391	1.494367	-0.227733
C	2.922877	1.210260	-0.188023
C	3.668288	2.437789	-0.359421
C	2.757820	3.444115	-0.497875
C	3.456955	-0.071778	-0.013941
C	2.662517	-1.235775	0.129892
C	2.936993	-2.615426	0.356108
C	1.716117	-3.281404	0.442484
C	0.689987	-2.315616	0.271000
C	-0.742922	-2.261861	0.269314
N	-1.274000	-1.049365	0.093569
C	-2.633146	-1.184963	0.133620
C	-2.968255	-2.583123	0.347888
C	-1.780528	-3.258333	0.433066
C	-3.457491	-0.064495	-0.005296
H	2.941911	4.497717	-0.644138
H	4.743520	2.531327	-0.376626
H	3.916970	-3.057513	0.447443
H	1.569013	-4.336388	0.612614
H	-1.638160	-4.317203	0.590264
H	-3.960825	-3.001353	0.426728
H	-4.721890	2.589810	-0.394123

H	-2.896324	4.536340	-0.665657
N	1.308790	-1.128464	0.082189
H	0.852761	-0.229296	-0.050289
H	-0.913955	0.816866	-0.120826
S	0.036728	3.806044	-0.541561
C	4.940320	-0.239474	0.032249
C	5.651508	-0.723231	-1.066675
C	5.675448	0.061195	1.179679
C	7.030288	-0.896824	-1.034877
C	7.054609	-0.104071	1.235975
C	7.733462	-0.585220	0.122777
C	-4.939594	-0.241238	0.035601
C	-5.682236	0.080211	1.172747
C	-5.644271	-0.743471	-1.059308
C	-7.060767	-0.089245	1.225964
C	-7.022720	-0.921744	-1.030282
C	-7.732513	-0.593183	0.118434
F	7.729652	0.190392	2.350812
F	9.056169	-0.747751	0.165364
F	7.683018	-1.355032	-2.106855
F	5.006743	-1.023502	-2.201015
F	5.053149	0.515912	2.274256
F	-5.066187	0.557328	2.261651
F	-7.742006	0.221910	2.332527
F	-9.054775	-0.760292	0.157913
F	-7.668824	-1.400759	-2.097201
F	-4.995056	-1.058604	-2.186771

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21-O-Cor

C	0.727106	-2.847438	0.000158
C	0.101151	-4.140807	0.000444
C	-1.259031	-3.962903	-0.000148
C	-1.535591	-2.551693	-0.000296
H	0.635867	-5.078653	0.000798
H	-2.017603	-4.731172	-0.000275
C	2.629272	-1.214149	0.000039
C	4.053812	-0.912191	-0.000303
C	4.166847	0.443966	-0.000234
C	2.814785	0.977353	0.000093
H	4.849858	-1.643304	-0.000534
H	5.072918	1.033282	-0.000397
C	2.078837	-2.512393	0.000166
N	-0.301674	-1.937283	-0.000163
N	1.912038	-0.062110	0.000253
H	2.777220	-3.341292	0.000276
H	-0.132933	-0.946198	-0.000208
C	1.134648	2.792936	0.000069
C	-1.104408	2.462964	0.000156
C	-0.876724	3.868008	0.000032

H	0.373285	0.886380	0.001016
H	-1.641386	4.629217	-0.000038
C	2.465193	2.335463	0.000064
H	3.262848	3.068290	-0.000013
C	0.498323	4.071163	-0.000297
N	0.123834	1.877786	0.000275
C	-2.968290	-0.521248	-0.000268
C	-4.081600	0.330378	0.000260
C	-3.611047	1.650318	0.000019
C	-2.219684	1.596457	0.000079
O	-1.849130	0.271660	0.000107
H	-5.112185	0.011531	0.000502
H	-4.206094	2.549927	-0.000026
C	-2.772872	-1.908370	-0.000501
H	-3.658167	-2.530877	-0.000792
H	1.005657	5.023938	-0.000905

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21-O-PFPh-Cor

C	-1.237983	1.571269	-0.049588
C	-2.532425	2.191236	-0.093208
C	-3.484382	1.206962	-0.063164
C	-2.822911	-0.065963	0.000911
H	-2.706445	3.254064	-0.146257
H	-4.553823	1.343302	-0.089566
C	1.273613	1.492966	-0.049376
C	2.575382	2.146045	-0.067945
C	3.508836	1.160245	-0.039999
C	2.787375	-0.100159	-0.003129
H	2.752720	3.210144	-0.097962
H	4.581832	1.277467	-0.048221
C	0.028198	2.169077	-0.069776
N	-1.473080	0.219228	0.007967
N	1.432528	0.144817	-0.011631
H	-0.726035	-0.451062	0.057586
C	2.599899	-2.567348	0.030645
C	0.645558	-3.695546	0.048174
C	1.694271	-4.655551	0.114881
H	0.823628	-1.542402	-0.045755
H	1.566292	-5.725271	0.169497
C	3.370437	-1.384520	0.024178
C	2.896110	-3.963207	0.104557
N	1.242528	-2.474793	-0.011108
C	-2.671824	-2.544402	0.056988
C	-3.003407	-3.905229	0.114509
C	-1.809002	-4.633788	0.116314
C	-0.763501	-3.716273	0.060841
O	-1.307000	-2.453454	0.022714
H	-4.002902	-4.307531	0.152846
H	-1.704772	-5.706489	0.154734

C	-3.402237	-1.342666	0.035504
H	3.883346	-4.395621	0.150586
C	0.053946	3.665370	-0.120929
C	0.123675	4.354132	-1.332469
C	0.012207	4.437143	1.040847
C	0.153777	5.742749	-1.393642
C	0.040544	5.826815	1.007509
C	0.111976	6.480869	-0.216720
C	4.854954	-1.518349	0.053845
C	5.595306	-1.242558	1.205523
C	5.571941	-1.942925	-1.066885
C	6.978692	-1.372588	1.244654
C	6.954727	-2.082787	-1.052392
C	7.660433	-1.794997	0.109680
C	-4.889403	-1.453477	0.049537
C	-5.630824	-1.216782	1.209316
C	-5.606540	-1.809716	-1.094825
C	-7.016809	-1.320630	1.234893
C	-6.991843	-1.923928	-1.093950
C	-7.698686	-1.676728	0.077141
F	-7.647376	-2.261989	-2.207770
F	-9.027255	-1.781643	0.090021
F	-7.695695	-1.088974	2.361748
F	-5.006571	-0.884413	2.345875
F	-4.959229	-2.044819	-2.243167
F	4.972875	-0.849893	2.324214
F	7.655617	-1.103885	2.365255
F	8.987469	-1.924971	0.135986
F	7.609491	-2.484204	-2.146255
F	4.927746	-2.217068	-2.209106
F	0.162422	3.674922	-2.486177
F	-0.055467	3.840189	2.237769
F	0.000028	6.536629	2.139316
F	0.139088	7.813628	-0.262133
F	0.219952	6.371794	-2.571187

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22-O-Cor

C	-3.031247	-0.332665	-0.000002
C	-3.944066	-1.414018	0.000119
C	-3.225168	-2.586567	0.000165
C	-1.845291	-2.261605	0.000020
O	-1.747158	-0.881658	0.000157
H	-5.017781	-1.304853	-0.000064
H	-3.614865	-3.592831	-0.000025
C	-0.739951	-3.096478	0.000015
H	-0.987496	-4.151760	-0.000028
C	0.639280	-2.806461	0.000120
C	2.586758	-1.634363	0.000217
H	0.788889	-0.638714	0.000601

C	2.909818	-3.024811	-0.000439
H	1.615306	-4.811619	-0.000594
H	3.911481	-3.427686	-0.000914
C	1.727790	-3.737849	-0.000273
N	1.210209	-1.567573	0.000540
C	3.400749	-0.486464	0.000209
C	2.889326	0.818801	0.000159
C	3.559550	2.107663	0.000226
N	1.543393	1.027004	-0.000208
C	2.575774	3.065985	0.000145
H	4.628031	2.271305	0.000404
C	1.318682	2.351207	-0.000195
H	2.707533	4.138146	0.000169
C	-2.227425	2.021083	-0.000216
C	-2.218123	3.447167	0.000254
C	-0.888664	3.871740	-0.000046
C	-0.063626	2.717297	-0.000385
N	-0.917350	1.656966	-0.000610
H	-3.094208	4.077832	0.000769
H	-0.542341	4.893639	0.000258
C	-3.238801	1.038514	-0.000027
H	-4.272151	1.361379	0.000310
H	-0.585220	0.710117	-0.000732
H	4.474138	-0.635527	0.000133

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22-O-PFPh-Cor

C	2.881763	-0.054300	0.065993
C	3.531500	1.197972	0.098033
C	2.570870	2.181245	0.115713
C	1.299447	1.560082	0.097441
O	1.507099	0.191571	0.072230
H	4.600366	1.338110	0.106902
H	2.738821	3.245422	0.136939
C	0.031732	2.143035	0.101907
C	-1.246991	1.534981	0.073632
C	-2.875987	-0.046563	0.020215
H	-0.898645	-0.611447	-0.011101
C	-3.506343	1.231528	0.075393
H	-2.666279	3.259043	0.154858
H	-4.571219	1.402019	0.094812
C	-2.520218	2.191989	0.107858
N	-1.519560	0.197257	0.017241
C	-3.429369	-1.347690	-0.012663
C	-2.628572	-2.505002	-0.012252
C	-2.985448	-3.912165	-0.114313
N	-1.275576	-2.396761	0.046696
C	-1.810059	-4.616214	-0.122644
H	-3.984091	-4.318220	-0.179752
C	-0.753685	-3.633142	-0.020520

H	-1.689970	-5.687359	-0.189045
C	2.621541	-2.526367	0.012923
C	2.922499	-3.909523	-0.173026
C	1.722424	-4.613926	-0.183378
C	0.669717	-3.678906	-0.004275
N	1.270146	-2.464089	0.134877
H	3.909885	-4.323733	-0.304473
H	1.603629	-5.676667	-0.325381
C	3.403648	-1.348795	0.021360
H	0.740697	-1.621418	0.264491
C	0.034862	3.641831	0.143979
C	0.056484	4.338048	1.353150
C	0.004582	4.404444	-1.024372
C	0.048094	5.727345	1.405944
C	-0.004651	5.794551	-0.998918
C	0.016923	6.456923	0.223083
C	-4.913195	-1.481874	-0.054170
C	-5.636329	-1.941725	1.048787
C	-5.647691	-1.165551	-1.199338
C	-7.018856	-2.083158	1.020345
C	-7.030302	-1.297004	-1.251827
C	-7.718024	-1.758696	-0.135927
C	4.886541	-1.489438	-0.043445
C	5.623151	-1.931123	1.058350
C	5.602847	-1.213416	-1.210515
C	7.002903	-2.091631	1.008937
C	6.982865	-1.362810	-1.283584
C	7.684446	-1.805147	-0.168169
F	-0.032808	6.496389	-2.135203
F	-0.014686	3.798224	-2.217539
F	0.009022	7.789325	0.260533
F	0.069098	6.364483	2.580042
F	0.086018	3.666043	2.510806
F	-5.018968	-0.733939	-2.300574
F	-5.000757	-2.247784	2.186984
F	-7.679989	-2.519541	2.096716
F	-9.044645	-1.889612	-0.174633
F	-7.700723	-0.991701	-2.367002
F	4.959376	-0.799008	-2.309253
F	5.002016	-2.202045	2.212568
F	7.677773	-2.509947	2.083012
F	9.007596	-1.953418	-0.226979
F	7.636816	-1.093249	-2.416814

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22-S-Cor

C	-1.382944	-2.674598	-0.110805
C	-0.818039	-3.838179	0.492117
C	0.561912	-3.851273	0.549541
C	1.189436	-2.697462	-0.006785

H	-1.437894	-4.581809	0.978114
H	1.127077	-4.604532	1.084265
C	2.475661	-2.195291	0.151471
H	3.235789	-2.883121	0.508873
C	2.887207	-0.842828	0.041951
C	2.758717	1.431163	-0.012251
H	1.050900	0.279381	-0.171313
C	4.125331	1.069452	0.176616
H	5.089130	-0.906861	0.363181
H	4.940216	1.768656	0.289176
C	4.201993	-0.309377	0.216375
N	2.066351	0.246967	-0.124888
C	2.131077	2.690025	0.010186
C	0.746827	2.903578	-0.036954
C	0.016020	4.142999	0.167911
N	-0.143317	1.878194	-0.180573
C	-1.315944	3.819593	0.177693
H	0.452359	5.121950	0.308450
C	-1.383909	2.393334	-0.044320
H	-2.153021	4.488223	0.315955
C	-2.996126	-0.765373	-0.078596
C	-4.142622	-0.022224	0.336777
C	-3.812698	1.334237	0.339350
C	-2.460841	1.447365	-0.078385
N	-2.066073	0.184665	-0.394735
H	-5.084463	-0.452710	0.642394
H	-4.449088	2.147119	0.653119
C	-2.662696	-2.140019	0.026833
H	-3.433568	-2.797665	0.415546
H	-1.082332	0.028175	-0.558016
H	2.776717	3.551522	0.138028
S	-0.046296	-1.793615	-0.873672

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22-S-PFPh-Cor

C	2.904101	-0.140367	-0.231401
C	3.352159	1.140498	0.181942
C	2.384498	2.128860	0.157651
C	1.105039	1.692075	-0.282199
H	4.344425	1.299529	0.584260
H	2.553798	3.127528	0.538386
C	-0.147776	2.315845	-0.183352
C	-1.407029	1.652159	-0.204137
C	-2.945682	-0.022395	-0.113863
H	-0.932163	-0.467980	-0.129373
C	-3.645861	1.220384	-0.122960
H	-2.918748	3.292958	-0.200557
H	-4.717887	1.334055	-0.087930
C	-2.713857	2.234475	-0.176854
N	-1.609207	0.293158	-0.179901

C	-3.417908	-1.353248	-0.046737
C	-2.571624	-2.478874	0.015618
C	-2.924567	-3.887374	-0.083008
N	-1.214481	-2.359289	0.087521
C	-1.749496	-4.587398	-0.095566
H	-3.922635	-4.293730	-0.153326
C	-0.696319	-3.603404	0.012975
H	-1.623783	-5.657623	-0.166571
C	2.713917	-2.598205	-0.083917
C	2.940665	-3.955235	-0.454741
C	1.722078	-4.630732	-0.408416
C	0.728648	-3.703082	0.001384
N	1.390821	-2.542071	0.252066
H	3.885247	-4.362624	-0.780527
H	1.547740	-5.656923	-0.691941
C	3.505466	-1.409227	-0.127173
H	0.883854	-1.723782	0.546675
S	1.269095	0.056377	-0.887841
C	-0.158985	3.789576	0.053506
C	0.215963	4.690144	-0.947366
C	-0.525886	4.337451	1.285751
C	0.221481	6.064802	-0.742228
C	-0.528772	5.708177	1.515002
C	-0.153944	6.574973	0.495007
C	4.978740	-1.518732	-0.026525
C	5.829694	-0.958720	-0.989178
C	5.599073	-2.195347	1.032616
C	7.212316	-1.064859	-0.909261
C	6.979317	-2.313989	1.131131
C	7.790299	-1.746411	0.155313
C	-4.894721	-1.563352	-0.061795
C	-5.584715	-1.977768	1.079693
C	-5.653915	-1.362710	-1.216780
C	-6.959202	-2.185064	1.078787
C	-7.029046	-1.562763	-1.242802
C	-7.683640	-1.976057	-0.088601
F	-0.152250	7.891477	0.703695
F	-0.878149	6.197458	2.708281
F	-0.871334	3.534000	2.300005
F	0.569344	4.237829	-2.156700
F	0.574930	6.897768	-1.725027
F	5.318981	-0.321532	-2.050187
F	7.989184	-0.530730	-1.855803
F	9.115802	-1.853950	0.240818
F	7.533156	-2.954093	2.164736
F	4.860872	-2.724224	2.016742
F	-4.924462	-2.173584	2.227833
F	-7.588807	-2.574778	2.191173
F	-9.002679	-2.171406	-0.101396
F	-7.723413	-1.368901	-2.368152

F -5.056548 -0.980962 -2.353410

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Corrole

C	0.384574	-2.841347	-0.082064
N	-0.508087	-1.816347	-0.054040
C	-0.321949	-4.112192	-0.128254
C	-1.652262	-3.824534	-0.123788
C	-1.770245	-2.378993	-0.068073
C	1.790912	-2.712912	-0.050084
C	2.526533	-1.533176	0.005618
N	1.964579	-0.273638	-0.014803
C	2.932988	0.724758	0.027856
C	4.184546	0.027320	0.116064
C	3.942137	-1.324595	0.104484
C	2.686954	2.096553	0.002665
C	1.399193	2.674044	0.022981
C	0.883984	3.937495	-0.353781
C	-0.513821	3.883173	-0.301846
C	-0.888420	2.592501	0.118123
C	-2.065213	1.793900	0.127420
N	-1.867312	0.442709	0.151379
C	-3.038426	-0.256368	0.083037
C	-4.071186	0.724761	0.059403
C	-3.471742	1.982689	0.082525
C	-2.972744	-1.659949	-0.014328
H	1.015060	-0.165025	-0.336252
H	-1.001948	-0.099706	0.056021
H	4.673595	-2.115832	0.172373
H	5.144579	0.514167	0.201707
H	3.543878	2.753509	-0.075779
H	1.476516	4.769258	-0.703519
H	-1.194331	4.660919	-0.612599
H	-3.976559	2.936369	0.081124
H	-5.130417	0.520457	0.019438
H	-3.899835	-2.218292	-0.060391
H	-2.480234	-4.518990	-0.144982
H	0.144972	-5.086483	-0.158823
H	2.362923	-3.633504	-0.054768
N	0.292894	1.905129	0.330093
H	0.352410	1.119396	0.960290

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N1-Con-Cor

C	-1.559785	-2.480029	-0.114205
C	0.098306	-3.959824	0.336627
C	0.728945	-2.784799	-0.105721
H	-1.919253	-4.428417	0.685175
H	0.526875	-4.883165	0.695016

C	2.141510	-2.514610	-0.115402
H	2.824185	-3.355387	-0.065920
C	2.711979	-1.256851	-0.118243
C	2.893189	1.025155	-0.019129
C	4.224407	0.464300	-0.052926
H	4.925670	-1.612096	-0.144615
H	5.134771	1.044737	-0.029870
C	4.117321	-0.896729	-0.109048
C	2.454002	2.343299	0.059170
C	1.082189	2.710509	0.111597
C	0.485268	4.034724	0.073269
C	-0.877045	3.858007	0.068482
H	1.020807	4.973163	0.038923
C	-1.097012	2.435267	0.117651
H	-1.636260	4.626162	0.038685
C	-3.043954	-0.539032	-0.011130
C	-4.134878	0.379728	-0.239584
C	-3.643606	1.670197	-0.174207
C	-2.237274	1.598830	0.105353
H	-5.147365	0.090402	-0.478302
H	-4.202558	2.577699	-0.343897
C	-2.877045	-1.917212	-0.102145
H	-3.747412	-2.558926	-0.172036
H	3.203802	3.124995	0.065538
N	2.037903	-0.050497	-0.080717
H	1.042806	0.138482	0.005326
C	-0.330636	-1.893669	-0.426604
H	-0.220450	-0.965598	-0.956919
N	0.102040	1.780684	0.150609
N	-1.973309	0.273020	0.253115
H	-1.050557	-0.041127	0.499412
N	-1.248112	-3.773847	0.314229

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N1-Con-PFPh-Cor

C	-2.728992	-0.270772	-0.117973
C	-2.415242	1.886300	-0.716904
C	-1.211515	1.456679	-0.136191
H	-4.214820	0.887082	-1.121852
H	-2.668893	2.831365	-1.170205
C	0.019639	2.218211	-0.075062
C	1.281342	1.648141	0.009076
C	2.920754	0.055525	0.035293
C	3.547393	1.352910	0.128180
H	2.711243	3.369939	0.190274
H	4.610286	1.523288	0.197671
C	2.569892	2.303090	0.118541
C	3.478369	-1.226114	0.014827
C	2.679041	-2.407333	-0.072469
C	3.086052	-3.793978	0.097534

C	1.942175	-4.547482	0.069508
H	4.094485	-4.152185	0.242628
C	0.858179	-3.620395	-0.132724
H	1.861350	-5.619227	0.175887
C	-2.569676	-2.707231	-0.129750
C	-2.758104	-4.091707	0.233840
C	-1.531292	-4.719576	0.211996
C	-0.543485	-3.749949	-0.166526
H	-3.696751	-4.532486	0.531609
H	-1.329144	-5.744209	0.483227
C	-3.374940	-1.565203	-0.080664
N	1.568513	0.296480	-0.021562
H	0.951952	-0.502597	-0.153419
C	-1.445076	0.113099	0.265657
H	-0.784593	-0.485876	0.867298
N	1.340896	-2.345003	-0.230271
N	-1.239213	-2.611037	-0.435981
H	-0.768435	-1.768570	-0.719290
N	-3.303145	0.862700	-0.691384
C	-0.086373	3.700284	-0.154641
C	0.407247	4.431358	-1.240695
C	-0.720814	4.437776	0.852115
C	0.289073	5.814257	-1.321775
C	-0.854004	5.819206	0.792119
C	-0.344406	6.511412	-0.300467
C	-4.841104	-1.666122	0.022186
C	-5.602028	-2.488514	-0.825286
C	-5.567755	-0.935527	0.977649
C	-6.983686	-2.587244	-0.726485
C	-6.949516	-1.014373	1.087779
C	-7.663508	-1.846916	0.233628
C	4.956751	-1.364254	0.126001
C	5.643383	-1.067944	1.306519
C	5.729856	-1.818187	-0.946497
C	7.021705	-1.207392	1.420029
C	7.108281	-1.970512	-0.857114
C	7.757084	-1.662129	0.332499
F	-0.464987	7.837932	-0.368822
F	0.765923	6.475515	-2.381413
F	-1.454786	6.488550	1.780894
F	-1.203467	3.812422	1.933609
F	0.996958	3.800105	-2.265686
F	-5.005168	-3.187405	-1.801104
F	-7.666936	-3.372309	-1.564472
F	-8.989977	-1.932902	0.333132
F	-7.595049	-0.312602	2.023534
F	-4.922527	-0.151822	1.852620
F	4.970532	-0.646427	2.386898
F	5.145903	-2.108068	-2.116595
F	7.815390	-2.399555	-1.907722

F	9.080606	-1.801369	0.429599
F	7.642672	-0.918161	2.568645

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N2-Con-Cor

C	-2.936601	0.880708	0.097024
C	-4.028048	-1.130676	-0.001789
C	-2.601888	-1.390477	0.003358
H	-5.171938	0.736208	0.063055
H	-4.784786	-1.899790	-0.045217
C	-1.926908	-2.595963	-0.070639
H	-2.539359	-3.487035	-0.140061
C	-0.515833	-2.790546	-0.077993
C	1.660381	-2.445840	-0.060805
C	1.465294	-3.880922	-0.178932
H	-0.394802	-5.043020	-0.263935
H	2.255936	-4.615152	-0.243863
C	0.123568	-4.097764	-0.186466
C	2.890566	-1.798675	-0.023890
C	3.051345	-0.390514	0.089452
C	4.125329	0.525742	0.010156
C	3.587392	1.825628	0.069436
H	5.169352	0.269479	-0.088061
C	2.189618	1.702559	0.191379
H	4.144911	2.749704	0.054496
C	-1.284810	2.713943	0.130567
C	-0.696568	3.746232	-0.607296
C	0.991569	2.515217	0.250435
H	-1.144891	4.515158	-1.216228
H	1.321444	4.150253	-1.074199
C	-2.647332	2.224086	0.095815
H	-3.476983	2.913361	-0.011870
H	3.782331	-2.408329	-0.111547
N	0.416360	-1.820564	-0.000917
H	-1.009825	-0.061123	-0.017996
N	1.925952	0.368213	0.217013
H	-0.285959	1.192302	1.420446
N	-2.006271	-0.157542	0.089604
C	-4.225484	0.216177	0.050785
C	-0.203282	2.011739	0.727170
N	0.664887	3.616243	-0.527597
H	1.018217	-0.100383	0.181658

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N2-Con-PFPh-Cor

C	-2.905440	-0.007131	-0.186500
C	-2.532919	2.243962	-0.305200
C	-1.250166	1.581060	-0.190839
H	-4.573556	1.474578	-0.395698

H	-2.665559	3.310540	-0.393922
C	0.019631	2.147968	-0.160393
C	1.267680	1.443513	-0.108278
C	2.790182	-0.145664	-0.053317
C	3.502865	1.117112	0.006195
H	2.742385	3.164429	-0.000373
H	4.574205	1.238110	0.057965
C	2.568113	2.099976	-0.030207
C	3.381555	-1.413751	-0.058579
C	2.637475	-2.624065	-0.168207
C	2.922138	-3.999205	0.003470
C	1.704333	-4.696809	-0.045244
H	3.898885	-4.430165	0.159225
C	0.681702	-3.750540	-0.252774
H	1.575474	-5.764986	0.037668
C	-2.688026	-2.459711	-0.156266
C	-2.818197	-3.608760	0.631060
C	-0.760802	-3.670423	-0.289369
H	-3.622236	-3.930901	1.273197
H	-1.443471	-5.134688	1.100738
C	-3.502996	-1.254348	-0.141467
N	1.420566	0.104730	-0.120651
H	-0.816865	-0.440988	0.056719
N	1.289947	-2.538480	-0.350923
H	-1.014362	-1.877164	-1.507278
N	-1.534457	0.239572	-0.134550
C	-3.513149	1.300845	-0.302065
C	-1.422371	-2.564342	-0.785810
N	-1.659831	-4.325896	0.539538
H	0.857488	-1.611818	-0.356314
C	0.081074	3.643084	-0.187614
C	-0.096814	4.406589	0.967444
C	0.326757	4.343907	-1.369857
C	-0.035253	5.795606	0.955732
C	0.395354	5.731770	-1.409275
C	0.212701	6.459811	-0.239471
C	4.860432	-1.534960	0.090181
C	5.668580	-1.919534	-0.981995
C	5.500882	-1.300198	1.308617
C	7.046117	-2.055496	-0.858529
C	6.876992	-1.430025	1.457028
C	7.652029	-1.809107	0.367777
C	-4.972545	-1.376595	-0.007133
C	-5.688776	-0.810948	1.055676
C	-5.721478	-2.120691	-0.929548
C	-7.063785	-0.962697	1.190766
C	-7.094756	-2.287474	-0.813298
C	-7.770869	-1.703849	0.252306
F	0.273960	7.792234	-0.264369
F	-0.209605	6.495358	2.081494

F	0.628653	6.370681	-2.560286
F	0.500770	3.676330	-2.518207
F	-0.331597	3.801625	2.139595
F	4.787187	-0.952241	2.386889
F	7.457640	-1.202034	2.639115
F	8.973110	-1.936476	0.498662
F	7.791246	-2.413664	-1.908557
F	5.121918	-2.151613	-2.182152
F	-5.048608	-0.122679	2.011940
F	-5.115639	-2.674456	-1.987597
F	-7.773534	-2.990075	-1.725267
F	-9.090137	-1.855722	0.373041
F	-7.707079	-0.416129	2.227261

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Neo-Con-Cor

C	3.033864	-0.379278	0.073617
C	3.715087	1.801898	0.054704
C	2.270647	1.793995	0.002036
H	5.194840	0.187124	0.144688
H	4.312763	2.701316	0.064236
C	1.415138	2.883510	-0.063887
H	1.892330	3.854319	-0.118420
C	-0.001933	2.898272	-0.077545
C	-2.154639	2.158563	-0.050653
C	-2.179673	3.572066	-0.207683
H	-0.538111	5.044292	-0.336962
H	-3.073546	4.169879	-0.304687
C	-0.871979	4.024181	-0.222469
C	-3.177428	1.194362	-0.010138
C	-2.950190	-0.180803	0.109314
C	-3.858532	-1.297265	0.028003
C	-3.091579	-2.444898	0.079534
H	-4.933075	-1.240132	-0.073771
C	-1.738864	-1.987038	0.199154
H	-3.431859	-3.469069	0.051416
C	1.723225	-2.468602	0.082638
C	1.288234	-3.638357	-0.658705
H	1.912257	-4.295356	-1.245256
H	-0.773904	-4.397455	-1.010341
C	2.976004	-1.756283	0.051269
H	3.908974	-2.293509	-0.077575
N	-0.818742	1.810071	0.029607
H	1.018741	0.095977	-0.234362
N	-1.662301	-0.664796	0.224882
H	0.460124	-1.148701	1.360140
N	1.915668	0.460335	0.045718
C	4.166994	0.513806	0.090700
C	0.582625	-1.973041	0.684791
H	-4.197351	1.547520	-0.112598

H	-0.625336	0.817043	0.181030
N	-0.517694	-2.680280	0.273841
C	-0.071230	-3.723514	-0.548991

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Neo-Con-PFPh-Cor

C	-2.884019	-0.052965	-0.218076
C	-2.545037	2.193896	-0.408318
C	-1.256804	1.573818	-0.206090
H	-4.565195	1.376201	-0.571074
H	-2.696015	3.251405	-0.556222
C	-0.011102	2.199495	-0.151034
C	1.271247	1.579297	-0.077307
C	2.880873	-0.025247	-0.042141
C	3.518129	1.234968	0.103696
H	2.695053	3.274197	0.188417
H	4.579512	1.389980	0.218092
C	2.541348	2.212248	0.084597
C	3.405439	-1.339502	-0.062689
C	2.601513	-2.479929	-0.190445
C	2.925782	-3.882911	-0.070562
C	1.735239	-4.573400	-0.122114
H	3.911286	-4.305692	0.057469
C	0.724315	-3.567168	-0.281396
H	1.588006	-5.641266	-0.067714
C	-2.593399	-2.498260	-0.159116
C	-2.701897	-3.726373	0.606622
H	-3.543077	-4.039840	1.205376
H	-1.171955	-5.301142	0.959001
C	-3.440076	-1.323415	-0.157527
N	1.527243	0.238592	-0.148736
H	-0.881858	-0.463428	0.266373
N	1.236372	-2.348467	-0.332790
H	-0.897442	-1.862490	-1.455820
N	-1.516596	0.220106	-0.115978
C	-3.508677	1.228811	-0.410829
C	-1.359016	-2.547935	-0.771881
H	0.922851	-0.568004	-0.325909
N	-0.673096	-3.656787	-0.351425
C	-1.518165	-4.394584	0.491290
C	-0.011718	3.694815	-0.176608
C	-0.311392	4.448151	0.960194
C	0.299319	4.406459	-1.337272
C	-0.307652	5.838487	0.950224
C	0.312132	5.795873	-1.373580
C	0.006743	6.513842	-0.223040
C	-4.905287	-1.484621	-0.015559
C	-5.633171	-2.286475	-0.905603
C	-5.635793	-0.898229	1.026199
C	-7.000944	-2.487989	-0.778901

C	-7.005134	-1.084858	1.171526
C	-7.691691	-1.882914	0.264911
C	4.879790	-1.505847	0.097164
C	5.695625	-1.833709	-0.987034
C	5.505932	-1.351052	1.335010
C	7.069280	-2.000040	-0.853167
C	6.877268	-1.512346	1.494146
C	7.661235	-1.838362	0.393776
F	0.014048	7.846976	-0.245661
F	0.608103	6.445215	-2.503492
F	-0.597660	6.528333	2.057337
F	-0.609588	3.832115	2.111501
F	0.588013	3.748111	-2.467238
F	-7.662476	-0.516292	2.187009
F	-5.014658	-0.154227	1.952690
F	-5.014323	-2.864235	-1.942660
F	-7.660570	-3.244616	-1.660863
F	-9.005655	-2.067476	0.394906
F	5.162375	-1.984561	-2.205584
F	7.823132	-2.307583	-1.912475
F	8.977736	-1.995606	0.534272
F	7.444704	-1.363306	2.694689
F	4.780148	-1.051316	2.420028

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PFPh-Corrole

C	-1.264590	1.470647	0.037112
N	-1.427194	0.119894	0.034001
C	-2.562798	2.124989	-0.023155
C	-3.499412	1.141804	-0.055036
C	-2.786335	-0.120505	-0.011546
C	-0.024249	2.156470	0.113066
C	1.248000	1.574334	0.163481
N	1.499973	0.222167	0.054561
C	2.862641	-0.050264	0.142529
C	3.489972	1.219335	0.349254
C	2.524026	2.193876	0.361515
C	3.448130	-1.324743	0.078438
C	2.686533	-2.519771	0.080472
C	2.951461	-3.841614	-0.352863
C	1.764001	-4.573569	-0.293135
C	0.747800	-3.720770	0.181371
C	-0.670210	-3.720075	0.195824
N	-1.273128	-2.496245	0.263417
C	-2.627837	-2.588262	0.132891
C	-2.919780	-3.980821	0.041662
C	-1.715215	-4.673719	0.076151
C	-3.382036	-1.399378	0.016116
H	0.799718	-0.390806	-0.334154
H	-0.867579	-1.554351	0.198902

H	4.547880	1.361220	0.504990
H	3.895361	-4.191378	-0.741035
H	1.620197	-5.586724	-0.635048
H	-1.585850	-5.743735	0.028802
H	-3.903530	-4.413173	-0.054448
H	-4.571304	1.263728	-0.090112
N	1.352291	-2.503246	0.426203
H	0.971582	-1.820819	1.064448
C	-0.064208	3.651861	0.167173
C	-0.315174	4.335511	1.357814
C	0.148388	4.430265	-0.971644
C	-0.357957	5.723661	1.419995
C	0.111860	5.819631	-0.936826
C	-0.143611	6.467732	0.265789
C	4.925695	-1.433767	-0.028793
C	5.627678	-0.945455	-1.135977
C	5.686039	-2.052936	0.969180
C	7.008436	-1.058129	-1.246693
C	7.066523	-2.179741	0.879304
C	7.730606	-1.678885	-0.234420
C	-4.862348	-1.523171	-0.100727
C	-5.529934	-1.277207	-1.302943
C	-5.649915	-1.911282	0.985765
C	-6.909238	-1.400642	-1.422477
C	-7.030203	-2.043441	0.891084
C	-7.661975	-1.785775	-0.319586
F	-0.180980	7.800169	0.312731
F	0.316439	6.534750	-2.047304
F	-0.598088	6.346803	2.577955
F	-0.518323	3.651565	2.491604
F	0.391271	3.839828	-2.149139
F	5.087469	-2.525177	2.070592
F	7.760417	-2.766371	1.858809
F	9.055069	-1.793414	-0.330969
F	7.643784	-0.587681	-2.323688
F	4.968251	-0.366574	-2.147673
F	-4.838489	-0.923582	-2.393895
F	-7.514577	-1.162149	-2.589945
F	-8.985900	-1.908701	-0.422945
F	-7.753259	-2.407763	1.954506
F	-5.079377	-2.153693	2.173519
H	2.679169	3.249016	0.521459
H	-2.737208	3.189767	-0.039494

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Coordinates of Heterocorrins (XYZ Format):

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10-NH-Corrin

C	-2.022601	1.933175	-0.199200
N	-0.791684	1.567894	-0.145386
C	-2.268506	3.432652	-0.198305
C	-0.819158	3.963058	-0.274405
C	0.018362	2.695715	-0.066942
C	-2.964469	-0.332999	-0.054040
N	-1.938438	-0.970157	-0.469918
C	-1.964093	-2.267638	0.064962
C	-3.361358	-2.566580	0.602484
C	-3.971550	-1.150068	0.740875
C	-0.835838	-2.986821	0.206657
C	0.489571	-2.498869	-0.209076
C	0.751944	-1.722771	-1.489081
C	2.287808	-1.681517	-1.510570
C	2.655813	-1.933255	-0.027798
C	2.880436	-0.632812	0.790770
N	1.763408	0.299174	0.622904
C	2.192356	1.484200	0.395589
C	3.715212	1.620816	0.410830
C	4.172937	0.149183	0.416249
C	1.349429	2.661701	0.172526
H	-4.987985	-1.068475	0.344834
H	-3.925015	-3.160270	-0.123997
H	-0.859623	-3.909738	0.776227
H	0.303067	-0.733691	-1.399932
H	2.678248	-0.737648	-1.896841
H	4.986804	-0.041355	1.118304
H	4.026940	2.159377	1.314434
H	1.867161	3.616788	0.192773
H	-0.613051	4.400365	-1.255436
H	-2.893788	3.743571	-1.039793
H	-3.997923	1.446220	-0.032157
N	1.514820	-2.676984	0.540984
H	2.690981	-2.486702	-2.131779
H	0.308455	-2.217074	-2.358435
H	3.562734	-2.537965	0.080541
H	-3.344575	-3.120079	1.541822
H	-3.995687	-0.807707	1.781907
H	2.896894	-0.936369	1.845158
H	-2.778918	3.741503	0.721086
H	-0.605575	4.725785	0.475944
H	4.089244	2.193490	-0.443062
H	4.524867	-0.144142	-0.576665
N	-3.086822	1.047371	-0.200598

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10-NH-PFPh-Corrin

C	-1.222988	3.048258	0.280016
N	-1.284599	1.764191	0.345067
C	-2.545053	3.767482	0.088352
C	-3.532092	2.585214	0.173914
C	-2.603217	1.365799	0.173393
C	1.237305	3.234750	0.338125
N	1.471267	2.027100	0.685691
C	2.806915	1.719157	0.423454
C	3.570514	2.984345	0.033228
C	2.438508	4.027693	-0.143620
C	3.210250	0.429877	0.471204
C	2.247188	-0.640504	0.864931
C	1.366041	-0.579519	2.100549
C	0.808043	-2.010927	2.144249
C	1.017303	-2.509712	0.692005
C	-0.234604	-2.382738	-0.211267
N	-0.816119	-1.036991	-0.160559
C	-2.089489	-1.103323	-0.062720
C	-2.650939	-2.528431	-0.046558
C	-1.377442	-3.370899	0.145503
C	-2.988895	0.072848	-0.002720
H	2.593309	4.936861	0.445071
H	4.258779	3.272274	0.832734
H	0.589883	0.168882	1.943300
H	-0.235987	-2.042924	2.461533
H	-1.361422	-4.265557	-0.479211
H	-3.144170	-2.746196	-1.000554
H	-4.111807	2.622950	1.099997
H	-2.709426	4.529187	0.855433
H	-0.120941	4.757717	0.144214
N	2.111337	-1.684856	0.141729
H	1.384792	-2.632061	2.834751
H	1.939249	-0.300999	2.989198
H	1.323598	-3.560566	0.656294
H	4.154924	2.859573	-0.876889
H	2.310435	4.331445	-1.187823
H	0.112311	-2.540289	-1.240384
H	-2.577950	4.268547	-0.885253
H	-4.240254	2.565937	-0.655633
H	-3.395599	-2.679653	0.739541
H	-1.290883	-3.696662	1.185719
N	-0.044297	3.768241	0.324544
C	4.562281	-0.009127	0.049506
C	5.064882	0.190892	-1.237903
C	5.381991	-0.729045	0.923990
C	6.311232	-0.280215	-1.633395
C	6.628478	-1.213452	0.555296
C	7.097368	-0.986614	-0.733384
C	-4.451495	-0.197317	-0.161891

C	-5.348808	-0.100633	0.903576
C	-4.996383	-0.573391	-1.391990
C	-6.707439	-0.359145	0.763757
C	-6.348887	-0.842167	-1.561462
C	-7.209856	-0.733853	-0.475928
F	7.385912	-1.885625	1.430327
F	8.297864	-1.442453	-1.101633
F	6.753655	-0.066898	-2.879003
F	4.334548	0.844348	-2.157503
F	4.967044	-0.960046	2.179842
F	-7.532141	-0.255063	1.812150
F	-4.907344	0.249145	2.123320
F	-4.200360	-0.678189	-2.467478
F	-6.829729	-1.194048	-2.758917
F	-8.512362	-0.984960	-0.624505

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10-NMe-Corrin

C	2.146016	1.515315	0.174240
N	0.889912	1.347042	-0.067552
C	2.575106	2.960581	0.396399
C	1.241171	3.706566	0.194401
C	0.241753	2.573324	-0.063097
C	2.655915	-0.856992	0.015838
N	1.556384	-1.312069	0.483531
C	1.305137	-2.569973	-0.090048
C	2.583644	-3.098911	-0.729257
C	3.421034	-1.811765	-0.894819
C	0.064388	-3.080718	-0.190553
C	-1.149660	-2.396721	0.270371
C	-1.242103	-1.551056	1.528296
C	-2.749882	-1.254901	1.585144
C	-3.200420	-1.498530	0.123940
C	-3.206153	-0.213909	-0.749297
N	-1.932138	0.498044	-0.630135
C	-2.129490	1.750851	-0.450318
C	-3.601316	2.167421	-0.466991
C	-4.323356	0.808366	-0.393520
C	-1.088016	2.756264	-0.247263
H	4.469482	-1.935956	-0.616994
H	3.084178	-3.797053	-0.050125
H	-0.087402	-3.974398	-0.786732
H	-0.637211	-0.654111	1.398809
H	-2.967772	-0.245445	1.940228
H	-5.175671	0.739932	-1.072124
H	-3.819678	2.706707	-1.397127
H	-1.441292	3.782922	-0.201461
H	0.961417	4.296067	1.070069
H	2.987519	3.096290	1.401366
N	-2.218981	-2.444110	-0.437794

H	-3.260334	-1.958135	2.249678
H	-0.862158	-2.088492	2.402224
H	-4.201515	-1.938332	0.060467
H	2.402765	-3.621248	-1.669032
H	3.399789	-1.431802	-1.923588
H	-3.300566	-0.552753	-1.788741
H	3.346350	3.272842	-0.312867
H	1.284889	4.390322	-0.656822
H	-3.852018	2.842703	0.356476
H	-4.697944	0.630453	0.618521
N	3.060902	0.473478	0.217498
C	4.498088	0.761511	0.210942
H	5.034369	-0.061633	0.680813
H	4.889135	0.906659	-0.802544
H	4.699972	1.657415	0.794224

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10-NMe-PFPh-Corrin

C	-1.207471	2.981485	0.232280
N	-1.222963	1.689653	0.197436
C	-2.574927	3.646720	0.157265
C	-3.504257	2.424033	0.078487
C	-2.528399	1.243707	0.070437
C	1.229355	3.167744	0.289629
N	1.460166	1.994548	0.746897
C	2.769203	1.621324	0.430836
C	3.541909	2.824105	-0.100668
C	2.424604	3.860049	-0.353271
C	3.159713	0.331203	0.528998
C	2.222923	-0.726793	0.989070
C	1.287162	-0.598991	2.177172
C	0.763633	-2.039722	2.302021
C	1.041713	-2.629297	0.897205
C	-0.161554	-2.539568	-0.074943
N	-0.730578	-1.187591	-0.098560
C	-2.007989	-1.240213	-0.060610
C	-2.581719	-2.661024	-0.034770
C	-1.329127	-3.504858	0.258163
C	-2.899287	-0.061376	-0.054999
H	2.643053	4.834552	0.087836
H	4.249026	3.180296	0.654445
H	0.501834	0.116082	1.936098
H	-0.290493	-2.079660	2.583308
H	-1.287487	-4.424161	-0.328439
H	-3.019924	-2.902461	-1.010189
H	-4.175724	2.374710	0.938265
H	-2.769242	4.263884	1.039012
N	2.153832	-1.831822	0.348550
H	1.330430	-2.595805	3.053698
H	1.815340	-0.241060	3.065489

H	1.344758	-3.680713	0.936887
H	4.107701	2.601038	-1.003390
H	2.240637	4.023141	-1.420890
H	0.237890	-2.739050	-1.077330
H	-2.659914	4.297088	-0.717935
H	-4.126369	2.436039	-0.818956
H	-3.372378	-2.786251	0.709421
H	-1.301754	-3.788448	1.314074
N	-0.047869	3.742045	0.293892
C	-0.134166	5.200965	0.143600
H	-0.063358	5.510047	-0.904374
H	-1.074254	5.561716	0.551184
H	0.667754	5.674486	0.706665
C	-4.363889	-0.344444	-0.192417
C	-4.928467	-0.686305	-1.422999
C	-5.239072	-0.299945	0.894145
C	-6.280608	-0.969793	-1.573818
C	-6.596309	-0.574428	0.774208
C	-7.119477	-0.912731	-0.467570
C	4.489968	-0.131585	0.055601
C	5.383445	-0.744472	0.937522
C	4.890870	-0.063124	-1.279234
C	6.608754	-1.251472	0.529131
C	6.113222	-0.559919	-1.715919
C	6.976407	-1.158035	-0.807897
F	-4.153393	-0.746216	-2.517045
F	-6.781555	-1.289162	-2.772378
F	-8.421265	-1.178697	-0.597610
F	-7.400443	-0.519308	1.842419
F	-4.775577	0.015864	2.115259
F	7.440833	-1.820011	1.410174
F	5.063492	-0.849583	2.237235
F	8.155237	-1.636992	-1.215526
F	6.459998	-0.473837	-3.006501
F	4.083495	0.486527	-2.201839

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10-O-Corrin

C	-2.131240	1.799538	-0.178546
N	-0.957751	1.534734	0.239347
C	-2.391990	3.197416	-0.674009
C	-1.055879	3.874179	-0.288137
C	-0.168845	2.680914	0.085852
C	-2.895572	-0.425840	0.012101
N	-1.907656	-1.019451	-0.514564
C	-1.845780	-2.317505	0.044109
C	-3.185631	-2.642495	0.697902
C	-3.782143	-1.231608	0.926304
C	-0.689846	-2.993796	0.145510
C	0.613902	-2.472492	-0.294292

C	0.850256	-1.691217	-1.574761
C	2.382701	-1.555418	-1.572506
C	2.749947	-1.810381	-0.089443
C	2.880482	-0.517910	0.758313
N	1.714077	0.348939	0.567157
C	2.078034	1.570446	0.449515
C	3.586151	1.793322	0.563565
C	4.128157	0.355263	0.451560
C	1.175915	2.700126	0.204811
H	-4.838961	-1.137179	0.668385
H	-3.815008	-3.212719	0.006740
H	-0.667233	-3.902087	0.738356
H	0.339397	-0.731339	-1.508419
H	2.718643	-0.582473	-1.936952
H	4.955100	0.152958	1.134621
H	3.817830	2.251179	1.533376
H	1.662371	3.659522	0.052588
H	-0.629260	4.474099	-1.092879
H	-2.567818	3.186355	-1.754773
N	1.641822	-2.615421	0.458569
H	2.841785	-2.322272	-2.202701
H	0.454386	-2.221373	-2.446134
H	3.686388	-2.367641	0.019827
H	-3.079419	-3.224959	1.613020
H	-3.661649	-0.885497	1.959226
H	2.880448	-0.840587	1.807535
H	-3.274834	3.637104	-0.205186
H	-1.189976	4.530265	0.577265
H	3.969040	2.469933	-0.206046
H	4.487249	0.164378	-0.564099
O	-3.164204	0.910683	-0.181798

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10-O-PFPh-Corrin

C	-1.191724	2.964622	0.655314
N	-1.260555	1.857093	0.029607
C	-2.473230	3.544094	1.187811
C	-3.490297	2.552212	0.582497
C	-2.590862	1.428441	0.056878
C	1.182005	3.074484	0.763223
N	1.389771	1.846129	1.004803
C	2.746519	1.575952	0.740576
C	3.509404	2.890148	0.581821
C	2.367977	3.915035	0.375690
C	3.165052	0.306893	0.565783
C	2.208753	-0.836871	0.652344
C	1.286471	-1.113249	1.824910
C	0.703908	-2.485856	1.435605
C	0.989655	-2.571250	-0.085394
C	-0.188862	-2.125934	-0.981237

N	-0.808325	-0.897712	-0.466825
C	-2.071827	-0.931965	-0.656507
C	-2.566815	-2.216319	-1.328559
C	-1.345940	-3.136529	-1.151616
C	-2.984650	0.173447	-0.279813
H	2.451353	4.812342	0.992473
H	4.066772	3.108017	1.498186
H	0.528304	-0.332481	1.876761
H	-0.357832	-2.571671	1.673513
H	-1.191814	-3.819162	-1.989080
H	-2.780075	-2.014247	-2.386171
H	-4.222063	2.194787	1.307748
H	-2.469358	3.534179	2.282613
N	2.116664	-1.648056	-0.329201
H	1.230183	-3.290014	1.956210
H	1.837044	-1.121696	2.769849
H	1.283515	-3.577556	-0.400535
H	4.217442	2.879253	-0.243901
H	2.275259	4.240112	-0.665783
H	0.245965	-1.881389	-1.959685
H	-2.609120	4.580506	0.871962
H	-4.041037	3.012802	-0.242631
H	-3.481294	-2.620511	-0.891712
H	-1.460567	-3.738486	-0.244450
O	-0.045432	3.676034	0.846236
C	4.546546	-0.025380	0.131799
C	5.358666	-0.844728	0.919761
C	5.078392	0.373820	-1.095386
C	6.630213	-1.237951	0.527805
C	6.349676	-0.002910	-1.512359
C	7.129602	-0.812740	-0.697630
C	-4.445789	-0.135619	-0.229649
C	-4.975842	-1.001544	0.730246
C	-5.357126	0.411903	-1.134800
C	-6.328037	-1.311917	0.793780
C	-6.716406	0.122227	-1.093923
C	-7.204025	-0.745551	-0.125162
F	4.357053	1.139465	-1.930090
F	6.823253	0.401738	-2.697003
F	8.353221	-1.179039	-1.087462
F	7.379749	-2.013258	1.319814
F	4.907312	-1.273910	2.109629
F	-7.554919	0.667696	-1.981323
F	-4.931175	1.249522	-2.093935
F	-8.506077	-1.031929	-0.074676
F	-6.794018	-2.141739	1.732870
F	-4.162236	-1.561548	1.639203

C	-2.034279	-1.900293	0.201499
N	-0.847245	-1.546003	-0.120966
C	-2.240147	-3.378679	0.495636
C	-0.877379	-3.945905	0.051621
C	-0.029915	-2.687567	-0.149300
C	-2.877864	0.795415	-0.013286
N	-1.778561	1.256701	0.437016
C	-1.565394	2.532252	-0.132501
C	-2.858594	3.026680	-0.769040
C	-3.671488	1.720974	-0.921075
C	-0.345784	3.092402	-0.207693
C	0.892014	2.477279	0.280950
C	1.006078	1.616665	1.526292
C	2.530050	1.432616	1.627442
C	3.007252	1.738613	0.186459
C	3.136618	0.478993	-0.709080
N	1.930457	-0.350988	-0.616192
C	2.247527	-1.582940	-0.479100
C	3.751092	-1.859320	-0.499366
C	4.338422	-0.442996	-0.362091
C	1.310496	-2.695278	-0.318011
H	-4.718084	1.807764	-0.619834
H	-3.368725	3.721043	-0.093472
H	-0.224315	3.998849	-0.791678
H	0.474386	0.679471	1.364058
H	2.812248	0.435651	1.972068
H	5.194622	-0.268251	-1.015946
H	4.023421	-2.334804	-1.449863
H	1.777718	-3.676486	-0.293899
H	-0.439507	-4.628281	0.781441
H	-2.429824	-3.521307	1.564528
N	1.975840	2.617448	-0.391381
H	2.964001	2.158799	2.320630
H	0.560144	2.107275	2.396228
H	3.973027	2.254368	0.163162
H	-2.691260	3.544212	-1.713950
H	-3.657947	1.332038	-1.945066
H	3.205840	0.842666	-1.741934
H	-3.092926	-3.794856	-0.045221
H	-0.971891	-4.489626	-0.893080
H	4.059986	-2.542983	0.296731
H	4.670563	-0.267345	0.665136
S	-3.462322	-0.856986	0.316531

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10-Se-Corrin

C	1.844014	1.740175	0.131517
N	0.630936	1.458452	-0.156135
C	2.160472	3.210334	0.361405
C	0.834321	3.856882	-0.084857

C	-0.104707	2.656579	-0.222180
C	2.478200	-1.198078	-0.084395
N	1.337329	-1.525893	0.374284
C	0.965623	-2.765228	-0.198950
C	2.180092	-3.401975	-0.862985
C	3.142745	-2.201387	-1.012831
C	-0.310354	-3.184075	-0.247504
C	-1.460945	-2.443389	0.276056
C	-1.444142	-1.560864	1.511133
C	-2.939179	-1.233850	1.668017
C	-3.498451	-1.507275	0.250256
C	-3.543497	-0.250196	-0.655822
N	-2.266612	0.472614	-0.611054
C	-2.472805	1.728812	-0.484069
C	-3.946988	2.133937	-0.464474
C	-4.648385	0.776330	-0.283040
C	-1.442549	2.761826	-0.373751
H	4.174868	-2.418193	-0.727325
H	2.612950	-4.162628	-0.205089
H	-0.545870	-4.068366	-0.830680
H	-0.834806	-0.679255	1.313429
H	-3.113734	-0.211697	2.010184
H	-5.539796	0.666715	-0.903129
H	-4.206832	2.615386	-1.415536
H	-1.828478	3.778228	-0.378522
H	0.459105	4.597335	0.622920
H	2.378963	3.381991	1.420599
N	-2.578170	-2.485617	-0.353979
H	-3.411439	-1.909905	2.386452
H	-1.010875	-2.079527	2.370981
H	-4.508776	-1.929400	0.269967
H	1.937209	-3.881835	-1.811419
H	3.163805	-1.801510	-2.032306
H	-3.676881	-0.615453	-1.681820
H	3.030507	3.542339	-0.209400
H	0.951046	4.354486	-1.052225
H	-4.170908	2.854736	0.327231
H	-4.956024	0.644154	0.758296
Se	3.307965	0.505122	0.283953

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10-Se-PFPh-Corrin

C	-1.478270	2.913218	0.114843
N	-1.388892	1.637910	0.166151
C	-2.872180	3.492509	-0.056678
C	-3.722815	2.210297	-0.048282
C	-2.677342	1.093838	0.025091
C	1.561862	3.174970	0.124452
N	1.665720	1.991621	0.581032
C	2.953713	1.502407	0.287668

C	3.824152	2.621817	-0.273533
C	2.804604	3.758160	-0.524635
C	3.246704	0.195693	0.454067
C	2.255984	-0.770654	0.990137
C	1.315855	-0.500592	2.150785
C	0.768241	-1.912239	2.422227
C	1.030985	-2.644354	1.083013
C	-0.173827	-2.637390	0.112667
N	-0.770215	-1.298564	-0.004627
C	-2.044712	-1.380024	0.042322
C	-2.588155	-2.806669	0.169194
C	-1.319255	-3.597115	0.523477
C	-2.972474	-0.230106	-0.039019
H	3.092243	4.712447	-0.075545
H	4.579225	2.916699	0.460931
H	0.542223	0.196434	1.830143
H	-0.284946	-1.906084	2.709446
H	-1.257437	-4.559206	0.012451
H	-3.017725	-3.125839	-0.787612
H	-4.386600	2.176786	0.818683
H	-3.119346	4.184384	0.752785
N	2.156912	-1.929191	0.457624
H	1.330167	-2.398497	3.224117
H	1.842282	-0.058273	3.000866
H	1.317340	-3.691230	1.227431
H	4.344701	2.331717	-1.184819
H	2.627486	3.940642	-1.588653
H	0.222278	-2.898347	-0.876594
H	-2.946699	4.049977	-0.994559
H	-4.346267	2.121211	-0.939789
H	-3.378309	-2.895870	0.918604
H	-1.283747	-3.793523	1.598843
Se	-0.058965	4.205529	0.176354
C	-4.422229	-0.584912	-0.195667
C	-4.945991	-0.971302	-1.430124
C	-5.314601	-0.564644	0.876540
C	-6.281014	-1.319097	-1.598746
C	-6.655019	-0.905012	0.738633
C	-7.140066	-1.285018	-0.506909
C	4.546377	-0.377148	0.014614
C	4.950872	-0.405638	-1.320229
C	5.398818	-0.992787	0.933824
C	6.139744	-1.001590	-1.723955
C	6.590583	-1.596192	0.558851
C	6.963420	-1.600443	-0.780169
F	-4.884175	-0.208613	2.098124
F	-7.478387	-0.872290	1.791835
F	-8.424643	-1.613922	-0.653968
F	-6.745010	-1.680591	-2.799229
F	-4.147234	-1.013880	-2.507240

F	5.071594	-1.004143	2.235613
F	7.385078	-2.164937	1.472980
F	8.109654	-2.173626	-1.155671
F	6.491723	-1.008974	-3.015256
F	4.179121	0.142781	-2.272834

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10-SiMe2-Corrin

C	-1.878481	1.705225	-0.015195
N	-0.601454	1.509621	-0.010819
C	-2.290915	3.122134	0.381240
C	-0.931956	3.840262	0.486715
C	0.070000	2.694912	0.350557
C	-2.446654	-1.311845	0.184939
N	-1.334900	-1.744066	-0.302935
C	-0.855748	-2.819976	0.478025
C	-1.984745	-3.333802	1.355388
C	-2.940312	-2.118389	1.385237
C	0.449247	-3.144486	0.536573
C	1.528095	-2.426333	-0.142988
C	1.384963	-1.609566	-1.414885
C	2.849599	-1.247717	-1.711392
C	3.529749	-1.427648	-0.333471
C	3.614151	-0.129302	0.505438
N	2.311665	0.549221	0.596168
C	2.464421	1.810868	0.453021
C	3.912844	2.261040	0.260089
C	4.623499	0.925550	-0.020033
C	1.401248	2.816540	0.534143
H	-3.998262	-2.381474	1.308402
H	-2.474233	-4.191464	0.880582
H	0.772956	-3.881264	1.264327
H	0.769026	-0.733881	-1.209232
H	2.959765	-0.240834	-2.119754
H	5.597488	0.845309	0.466099
H	4.271967	2.740419	1.179827
H	1.756165	3.820202	0.758563
H	-0.801151	4.562622	-0.324370
H	-2.966602	3.568867	-0.354464
N	2.694375	-2.397202	0.396177
H	3.286370	-1.946536	-2.430663
H	0.896026	-2.177543	-2.210409
H	4.548247	-1.822178	-0.417279
H	-1.642933	-3.648545	2.341610
H	-2.822368	-1.530128	2.304288
H	3.876469	-0.443233	1.524147
H	-2.835571	3.105330	1.332257
H	-0.805379	4.380471	1.426591
H	4.019090	2.995634	-0.543109
H	4.781394	0.799241	-1.094940

Si	-3.093082	0.318400	-0.534533
C	-3.118662	0.220783	-2.412684
C	-4.800642	0.721565	0.161493
H	-3.839852	-0.527224	-2.754938
H	-3.389162	1.181886	-2.859927
H	-2.130427	-0.066008	-2.778691
H	-5.526926	-0.044370	-0.127293
H	-4.794298	0.775653	1.254269
H	-5.170645	1.679545	-0.215840

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10-SiMe2-PFPh-Corrin

C	-1.496547	3.055361	0.238849
N	-1.860745	2.106170	-0.556362
C	-2.293846	3.100057	1.537597
C	-3.461215	2.139686	1.215291
C	-2.907605	1.368363	0.030924
C	1.570196	3.142218	0.045838
N	1.574541	1.872506	-0.178368
C	2.853322	1.337483	0.077567
C	3.770954	2.415840	0.639814
C	2.920050	3.696449	0.493427
C	3.136609	0.043748	-0.168026
C	2.130332	-0.898939	-0.745440
C	1.447686	-1.943701	0.122811
C	0.702926	-2.789496	-0.926808
C	0.743317	-1.902446	-2.203350
C	-0.577901	-1.188934	-2.538856
N	-1.143450	-0.522875	-1.359661
C	-2.416702	-0.571988	-1.410119
C	-2.981243	-1.352327	-2.593432
C	-1.717671	-2.071505	-3.104988
C	-3.248450	0.129589	-0.403571
H	2.835943	4.270593	1.420465
H	4.006149	2.215804	1.688100
H	0.767686	-1.434699	0.813125
H	-0.314027	-3.031321	-0.615032
H	-1.681114	-2.162956	-4.191924
H	-3.386101	-0.648736	-3.331986
H	-3.739179	1.489789	2.046058
H	-1.681022	2.729765	2.369025
N	1.784908	-0.881526	-1.968947
H	1.228784	-3.730420	-1.105861
H	2.158153	-2.518084	0.724889
H	1.034386	-2.478936	-3.087955
H	4.716092	2.468567	0.096198
H	3.319664	4.381867	-0.262933
H	-0.324787	-0.395127	-3.254047
H	-2.612133	4.111548	1.800797
H	-4.350903	2.705657	0.922327

H	-3.795467	-2.027626	-2.318852
H	-1.662095	-3.079351	-2.681769
Si	-0.024632	4.139069	-0.285968
C	0.011409	5.722534	0.739645
C	-0.139985	4.497173	-2.126031
H	0.870244	6.345566	0.472041
H	-0.889083	6.320114	0.568199
H	0.074034	5.515975	1.812289
H	0.737918	5.044206	-2.481967
H	-0.209641	3.556189	-2.675787
H	-1.027732	5.094108	-2.354269
C	-4.432195	-0.578238	0.145290
C	-4.333479	-1.872493	0.671309
C	-5.715626	-0.019740	0.141368
C	-5.427718	-2.565933	1.170576
C	-6.826690	-0.689906	0.639198
C	-6.683555	-1.970706	1.156318
C	4.458332	-0.538225	0.198055
C	5.330384	-1.047652	-0.770902
C	4.883052	-0.643398	1.525791
C	6.553083	-1.621282	-0.442296
C	6.100970	-1.210705	1.879837
C	6.940437	-1.704027	0.889463
F	-5.919636	1.201277	-0.378732
F	-8.034361	-0.115609	0.609675
F	-7.742833	-2.624661	1.636563
F	-5.280377	-3.795213	1.675858
F	-3.139064	-2.481473	0.723468
F	4.097496	-0.198544	2.521453
F	5.011091	-0.968698	-2.066424
F	7.365141	-2.083827	-1.399048
F	8.113358	-2.251767	1.215114
F	6.465461	-1.293771	3.164840

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10-S-PFPh-Corrin

C	-1.398770	3.096957	0.210417
N	-1.339682	1.817019	0.189999
C	-2.784437	3.715127	0.123940
C	-3.662749	2.452303	0.072946
C	-2.641133	1.311296	0.063894
C	1.457268	3.326358	0.226272
N	1.592359	2.134239	0.656376
C	2.896899	1.693703	0.367065
C	3.744639	2.859651	-0.130581
C	2.692424	3.963379	-0.387196
C	3.219107	0.387896	0.479781
C	2.237397	-0.623026	0.949770
C	1.296291	-0.438738	2.126095
C	0.750063	-1.866913	2.295194

C	1.021093	-2.504401	0.909795
C	-0.180732	-2.435042	-0.062899
N	-0.770050	-1.089677	-0.096819
C	-2.045112	-1.165150	-0.053306
C	-2.597486	-2.593403	-0.015022
C	-1.332245	-3.413911	0.282735
C	-2.961714	-0.003386	-0.055780
H	2.936178	4.921025	0.079724
H	4.457617	3.161417	0.642400
H	0.522751	0.279231	1.855511
H	-0.304703	-1.882369	2.576122
H	-1.277052	-4.338720	-0.293675
H	-3.033491	-2.847980	-0.988119
H	-4.315820	2.383137	0.945683
H	-2.988478	4.352040	0.988526
N	2.145507	-1.742281	0.338531
H	1.308167	-2.406784	3.064745
H	1.822605	-0.058913	3.006041
H	1.311794	-3.557414	0.983233
H	4.311742	2.617190	-1.027620
H	2.530413	4.153102	-1.452559
H	0.218822	-2.635468	-1.064785
H	-2.877237	4.339964	-0.768594
H	-4.299824	2.427732	-0.813274
H	-3.384961	-2.725127	0.730985
H	-1.297350	-3.684845	1.341768
S	-0.056976	4.250533	0.268284
C	-4.419529	-0.329707	-0.191882
C	-4.979948	-0.651100	-1.428940
C	-5.284682	-0.345979	0.902553
C	-6.323856	-0.971965	-1.579078
C	-6.633219	-0.660502	0.783520
C	-7.154880	-0.975942	-0.465237
C	4.538036	-0.137047	0.039057
C	5.384520	-0.780919	0.944447
C	4.968760	-0.093240	-1.287267
C	6.595302	-1.342391	0.565325
C	6.177072	-0.645975	-1.694797
C	6.994182	-1.274147	-0.764430
F	-4.818694	-0.052665	2.127769
F	-7.429597	-0.664343	1.857788
F	-8.447615	-1.279518	-0.594285
F	-6.823113	-1.270979	-2.782632
F	-4.209147	-0.654905	-2.527181
F	5.031745	-0.862276	2.237139
F	7.382968	-1.939797	1.466934
F	8.158767	-1.806273	-1.143720
F	6.554069	-0.584064	-2.977501
F	4.204856	0.485535	-2.228048

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C	-3.027938	0.157782	-0.018570
N	-2.017309	0.869660	-0.400036
C	-4.094826	0.958004	0.727129
C	-3.535428	2.396157	0.643393
C	-2.125740	2.162571	0.112084
C	-3.084255	-1.279678	-0.182615
C	-1.992541	-2.093969	-0.196964
N	-0.691171	-1.652393	-0.021598
C	0.131239	-2.661912	-0.046957
C	-0.546131	-4.006039	-0.295588
C	-2.035972	-3.616379	-0.337125
C	1.552114	-2.565770	0.149325
C	2.286903	-1.445117	0.392439
C	3.780019	-1.401548	0.635461
C	4.121938	0.069921	0.354143
C	2.815556	0.788736	0.708262
C	2.491151	2.064990	-0.080064
N	1.326790	2.726897	0.536330
C	0.296033	2.534656	-0.206735
C	0.573764	1.815345	-1.518048
C	2.109945	1.817939	-1.561041
C	-1.042505	2.960107	0.225406
H	-2.523365	-3.910934	-1.269334
H	-0.195821	-4.446554	-1.234729
H	2.112533	-3.493005	0.110735
H	4.322889	-2.113850	0.013407
H	4.361747	0.212480	-0.702928
H	2.484326	2.641913	-2.174166
H	0.108570	2.332367	-2.361493
H	-1.108002	3.885588	0.786781
H	-4.106546	3.003728	-0.065802
H	-5.081984	0.841754	0.270444
H	-4.066064	-1.743984	-0.198670
H	4.960581	0.437606	0.946538
H	3.979608	-1.656070	1.682980
H	2.765698	1.022244	1.776248
H	-0.305365	-4.719221	0.498344
H	-2.603142	-4.069207	0.480529
H	3.368700	2.714036	0.023649
H	-4.177460	0.603387	1.760353
H	-3.541159	2.918962	1.601093
H	0.145320	0.814695	-1.467071
H	2.521631	0.891630	-1.967079
O	1.776147	-0.213936	0.457961

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C	-1.037801	1.742054	0.024755
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N	-1.468251	0.704283	-0.611710
C	-1.903042	2.150820	1.211054
C	-3.107586	1.203206	1.059634
C	-2.608658	0.207582	0.020410
C	0.206647	2.443493	-0.324217
C	1.356255	1.787130	-0.649315
N	1.465419	0.402029	-0.599053
C	2.690672	0.050155	-0.817915
C	3.639413	1.204721	-1.089621
C	2.694159	2.419366	-1.024577
C	3.110382	-1.359774	-0.723915
C	2.382725	-2.357009	-1.299783
C	2.392738	-3.836076	-1.012460
C	0.923073	-4.197479	-1.313052
C	0.583718	-3.241655	-2.459023
C	-0.823447	-2.666237	-2.543384
N	-1.180081	-1.943803	-1.323692
C	-2.452896	-1.915893	-1.222949
C	-3.181844	-2.784154	-2.250576
C	-2.010525	-3.612652	-2.821984
C	-3.130163	-1.019330	-0.266042
H	3.020264	3.157906	-0.292008
H	4.437782	1.250800	-0.343434
H	2.704978	-4.066067	0.005729
H	0.292728	-3.977081	-0.448468
H	-2.129371	-3.863009	-3.877837
H	-3.640863	-2.145885	-3.016690
H	-3.395303	0.715782	1.992771
H	-1.356165	1.983995	2.145863
H	0.794103	-5.244207	-1.590524
H	3.068634	-4.350818	-1.703940
H	0.865229	-3.670878	-3.427543
H	4.124051	1.082705	-2.062822
H	2.615054	2.928495	-1.989109
H	-0.777456	-1.911703	-3.342882
H	-2.172975	3.208959	1.184674
H	-3.983899	1.737934	0.683865
H	-3.980892	-3.390208	-1.818047
H	-1.900746	-4.544502	-2.258139
O	1.466616	-2.093234	-2.238306
C	0.188177	3.931759	-0.224237
C	0.916810	4.640321	0.735070
C	-0.608459	4.698415	-1.080878
C	0.876154	6.026091	0.831926
C	-0.671366	6.084218	-1.004391
C	0.077843	6.752089	-0.043191
C	-4.393616	-1.485018	0.359216
C	-4.446100	-2.692086	1.067394
C	-5.602196	-0.787445	0.257786
C	-5.610946	-3.172589	1.649897

C	-6.781431	-1.241646	0.836876
C	-6.787301	-2.440966	1.536840
F	1.683789	3.981799	1.619311
F	1.589548	6.663846	1.766230
F	0.028852	8.082722	0.040471
F	-1.438340	6.779101	-1.850764
F	-1.341145	4.092409	-2.025717
F	-3.331148	-3.425621	1.213347
F	-5.607364	-4.325727	2.327873
F	-7.913775	-2.888987	2.095032
F	-7.913438	-0.540492	0.709715
F	-5.664836	0.356705	-0.442632
C	4.316801	-1.680502	0.072495
C	5.346887	-2.499908	-0.408645
C	4.515193	-1.154375	1.357266
C	6.482987	-2.795881	0.334428
C	5.646332	-1.423942	2.115413
C	6.636855	-2.253881	1.603615
F	3.578008	-0.365254	1.904855
F	5.781462	-0.905676	3.340580
F	7.725297	-2.527516	2.325677
F	7.438012	-3.583552	-0.172756
F	5.274371	-3.019475	-1.646482

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C	2.182354	-1.928708	-0.297526
C	2.307532	-3.407661	-0.571514
C	0.992394	-3.969234	-0.004002
C	0.097045	-2.749808	0.042367
C	3.158135	-1.001480	-0.242933
C	2.952451	0.418210	-0.009070
N	1.852365	1.014634	-0.320179
C	1.865279	2.328351	0.162821
C	3.261186	2.683916	0.667599
C	3.970355	1.310323	0.692819
C	0.733318	3.053506	0.246465
C	-0.575328	2.541216	-0.194364
C	-0.801332	1.832397	-1.520727
C	-2.332507	1.698846	-1.543899
C	-2.714156	1.875569	-0.053667
C	-2.865598	0.543048	0.719083
N	-1.714042	-0.345877	0.507953
C	-2.112409	-1.555606	0.382383
C	-3.625665	-1.742067	0.477831
C	-4.125174	-0.290361	0.364396
C	-1.234507	-2.714654	0.222355
H	4.936078	1.306611	0.178512
H	3.751856	3.371230	-0.028118
H	0.741138	4.004682	0.768196

H	-0.287934	0.871938	-1.501823
H	-2.666045	0.746436	-1.961715
H	-4.968133	-0.071410	1.022322
H	-3.880383	-2.195243	1.444389
H	-1.714902	-3.685969	0.281003
H	0.565192	-4.773580	-0.602689
H	2.364084	-3.566876	-1.653838
H	4.176464	-1.363045	-0.336977
N	-1.610570	2.643614	0.553889
H	-2.785048	2.497885	-2.137883
H	-0.396249	2.413124	-2.354891
H	-3.649998	2.430170	0.074644
H	3.237070	3.170482	1.643993
H	4.151153	0.949253	1.711217
H	-2.868120	0.809850	1.784129
H	3.202752	-3.839061	-0.124069
H	1.137726	-4.350003	1.012277
H	-4.015734	-2.406824	-0.298290
H	-4.443339	-0.079562	-0.660908
O	0.864733	-1.622689	-0.086702

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C	-1.292988	1.744966	0.141619
C	-2.702259	2.266013	0.275693
C	-3.555710	1.063291	-0.148492
C	-2.597320	-0.098167	-0.022490
C	-0.145400	2.464627	0.095166
C	1.198067	1.893615	0.009118
N	1.453813	0.672107	0.333214
C	2.793733	0.377184	0.073327
C	3.511721	1.599049	-0.487212
C	2.407349	2.678158	-0.483233
C	3.268302	-0.870813	0.291255
C	2.376174	-1.927968	0.843665
C	1.560708	-1.777875	2.115578
C	1.018256	-3.205878	2.300061
C	1.192746	-3.829359	0.892221
C	-0.073728	-3.776551	0.009893
N	-0.692394	-2.440082	0.004255
C	-1.964769	-2.554543	0.029405
C	-2.478084	-3.995062	0.071689
C	-1.192785	-4.767116	0.410819
C	-2.901033	-1.413334	-0.032531
H	2.636375	3.509224	0.190623
H	4.369513	1.874583	0.130623
H	0.774585	-1.042050	1.950617
H	-0.016640	-3.219895	2.647766
H	-1.113280	-5.721077	-0.112742
H	-2.880047	-4.274420	-0.909947

H	-4.448286	0.935194	0.461883
H	-2.886403	2.532645	1.322098
N	2.248340	-3.040640	0.230896
H	1.619882	-3.758369	3.026131
H	2.182464	-1.433300	2.946351
H	1.508538	-4.876783	0.936881
H	3.881715	1.411912	-1.495915
H	2.228513	3.110676	-1.471806
H	0.261179	-3.968077	-1.017729
H	-2.882974	3.153080	-0.327998
H	-3.877139	1.158029	-1.190895
H	-3.279587	-4.143440	0.798947
H	-1.150259	-4.973308	1.484343
O	-1.315723	0.381034	0.077499
C	-0.253104	3.956057	0.115772
C	0.102560	4.689787	1.249568
C	-0.666126	4.692413	-0.996248
C	0.048928	6.077923	1.286414
C	-0.733331	6.080561	-0.987481
C	-0.372495	6.776059	0.160629
C	4.641592	-1.284725	-0.081817
C	5.499353	-1.843604	0.871133
C	5.136306	-1.215235	-1.386308
C	6.774064	-2.293578	0.561078
C	6.410676	-1.655668	-1.724493
C	7.234117	-2.197786	-0.747243
C	-4.357338	-1.748955	-0.153058
C	-4.955575	-1.971970	-1.393622
C	-5.177465	-1.884111	0.967804
C	-6.297862	-2.310146	-1.522569
C	-6.522386	-2.220008	0.870063
C	-7.084105	-2.434739	-0.383340
F	-0.431725	8.107197	0.182299
F	0.393011	6.743676	2.391926
F	-1.136750	6.749119	-2.071517
F	-1.019600	4.057281	-2.124896
F	0.513148	4.048020	2.352652
F	7.566172	-2.807164	1.509454
F	8.460719	-2.622992	-1.060633
F	5.093079	-1.943912	2.147436
F	4.369966	-0.732666	-2.377851
F	6.843371	-1.573345	-2.988420
F	-4.668279	-1.685565	2.193594
F	-4.226704	-1.860585	-2.513767
F	-6.836603	-2.513263	-2.728154
F	-8.373251	-2.756606	-0.491925
F	-7.277157	-2.337823	1.966608

C	1.820536	-2.130767	-0.341310
C	1.489953	-3.585469	-0.572449
C	0.132767	-3.878731	0.104593
C	-0.681132	-2.603286	0.108984
C	3.051227	-1.554551	-0.301116
C	3.196577	-0.126458	-0.078785
N	2.201505	0.663398	-0.331034
C	2.407998	1.928540	0.222098
C	3.852091	2.032975	0.711138
C	4.363050	0.571273	0.607326
C	1.390547	2.801217	0.373421
C	0.010038	2.547463	-0.100813
C	-0.309055	2.101575	-1.519854
C	-1.849731	2.071192	-1.525713
C	-2.238650	2.304463	-0.037514
C	-2.842612	1.069939	0.675944
N	-1.982346	-0.103659	0.541002
C	-2.673507	-1.173868	0.389094
C	-4.178534	-0.935573	0.377206
C	-4.242108	0.599487	0.195391
C	-2.019784	-2.476874	0.268238
H	5.287538	0.477015	0.030134
H	4.424374	2.701779	0.062066
H	1.547862	3.705352	0.952433
H	0.146090	1.133824	-1.726093
H	-2.231540	1.121573	-1.905574
H	-5.057239	1.064738	0.752757
H	-4.613849	-1.254994	1.332386
H	-2.635662	-3.369313	0.327971
H	-0.401268	-4.698957	-0.381017
H	1.400979	-3.741097	-1.654611
H	3.938650	-2.177193	-0.362384
N	-1.004212	2.717343	0.661420
H	-2.258707	2.864348	-2.155623
H	0.108381	2.814384	-2.238431
H	-2.970856	3.113858	0.065283
H	3.916820	2.430756	1.725405
H	4.553169	0.122192	1.587696
H	-2.871758	1.325351	1.743732
H	2.283231	-4.246083	-0.214011
H	0.301595	-4.173813	1.147128
H	-4.689698	-1.494635	-0.411049
H	-4.380843	0.843465	-0.862247
S	0.351255	-1.179838	-0.078184

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C	-1.002262	1.726046	0.177833
C	-2.465508	2.088274	0.240689
C	-3.278738	0.920548	-0.351761

C	-2.496772	-0.354936	-0.147416
C	0.056420	2.591322	0.190079
C	1.426426	2.089949	0.168407
N	1.647754	0.843623	0.441166
C	2.973263	0.496948	0.203100
C	3.751312	1.730425	-0.246417
C	2.683458	2.855298	-0.211366
C	3.367674	-0.792381	0.344612
C	2.419393	-1.831767	0.863423
C	1.745207	-1.729730	2.220785
C	0.957319	-3.053043	2.302776
C	1.183369	-3.721839	0.914173
C	-0.091198	-3.885522	0.053532
N	-0.807452	-2.618786	-0.092968
C	-2.074003	-2.785081	-0.009764
C	-2.495073	-4.235139	0.197682
C	-1.148699	-4.888498	0.586959
C	-2.977606	-1.626666	-0.145916
H	2.909255	3.625379	0.533140
H	4.593030	1.931439	0.420251
H	1.112825	-0.843651	2.270400
H	-0.101285	-2.873120	2.497813
H	-1.024442	-5.889299	0.170555
H	-2.895403	-4.642644	-0.738505
H	-4.278346	0.861694	0.083664
H	-2.729927	2.226987	1.296188
N	2.168675	-2.889092	0.195398
H	1.334759	-3.690200	3.104521
H	2.503049	-1.635434	3.003920
H	1.616169	-4.723480	1.018602
H	4.153992	1.601903	-1.251796
H	2.572614	3.361069	-1.173121
H	0.250775	-4.176598	-0.947741
H	-2.676715	3.030551	-0.269202
H	-3.404597	1.068915	-1.430792
H	-3.267800	-4.354277	0.959121
H	-1.078214	-4.970873	1.675350
S	-0.771438	-0.025375	0.083955
C	-0.171722	4.067689	0.208712
C	-0.534657	4.736900	1.379027
C	-0.025651	4.852559	-0.936409
C	-0.743278	6.110588	1.416993
C	-0.221947	6.228250	-0.927200
C	-0.583627	6.859597	0.257185
C	4.717735	-1.260780	-0.047776
C	5.531428	-1.949112	0.858431
C	5.230819	-1.113318	-1.339602
C	6.779598	-2.449039	0.518607
C	6.479639	-1.601053	-1.706743
C	7.258665	-2.272657	-0.774393

C	-4.441419	-1.875516	-0.304337
C	-5.085476	-1.731341	-1.534708
C	-5.239618	-2.271350	0.770687
C	-6.446358	-1.965439	-1.695153
C	-6.600573	-2.517397	0.639149
C	-7.206755	-2.363072	-0.602195
F	-0.778852	8.178169	0.279855
F	-1.090832	6.715222	2.556727
F	-0.074278	6.944854	-2.045116
F	0.309285	4.275332	-2.101264
F	-0.693895	4.048250	2.519375
F	5.108573	-2.129481	2.121155
F	7.528623	-3.087051	1.425159
F	8.459921	-2.744783	-1.115834
F	6.929123	-1.440235	-2.956671
F	4.505956	-0.504304	-2.291647
F	-4.385553	-1.354021	-2.615415
F	-7.026435	-1.816039	-2.889882
F	-8.513038	-2.592010	-0.742435
F	-7.330596	-2.891484	1.694426
F	-4.691809	-2.416962	1.988130

45

Corrin

C	-1.691773	2.312280	-0.126810
N	-0.415124	1.827997	-0.020142
C	-1.684748	3.833071	-0.288028
C	-0.181611	4.169731	-0.347891
C	0.464126	2.812076	-0.112760
C	-2.826128	1.549823	-0.067728
C	-2.890296	0.122063	0.078360
N	-1.874540	-0.688736	-0.002822
C	-2.286393	-2.002644	0.225099
C	-3.775883	-2.055987	0.550299
C	-4.215342	-0.590655	0.345648
C	-1.400769	-3.014945	0.181839
C	0.013333	-2.733921	-0.158563
C	0.427801	-2.340043	-1.569024
C	1.956692	-2.205570	-1.445153
C	2.205639	-2.278404	0.088332
C	2.602775	-0.946590	0.753615
N	1.753459	0.192719	0.368620
C	2.410852	1.352483	0.254108
C	3.884885	1.099607	0.491976
C	4.009839	-0.431998	0.392160
C	1.852545	2.599074	0.005585
H	0.727697	0.192260	0.338030
H	-4.888660	-0.468311	-0.509694
H	-4.307671	-2.754774	-0.098772
H	-1.691824	-4.030360	0.427012

H	-0.073835	-1.408573	-1.842654
H	2.323952	-1.275271	-1.882722
H	4.775769	-0.843702	1.050435
H	4.143273	1.456261	1.495643
H	2.523855	3.444603	-0.075076
H	0.122071	4.573976	-1.318489
H	-2.223802	4.137535	-1.188125
H	-3.777217	2.071617	-0.106727
N	0.954326	-2.753278	0.704804
H	2.466495	-3.029581	-1.948776
H	0.116153	-3.100765	-2.290963
H	3.004350	-2.986362	0.337138
H	-3.934436	-2.384450	1.580891
H	-4.726268	-0.166244	1.214441
H	2.516813	-1.100544	1.836492
H	-2.179780	4.312191	0.561148
H	0.131334	4.892522	0.410429
H	4.514376	1.641359	-0.216138
H	4.257237	-0.721014	-0.633125

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N1-Con-Corrin

C	2.759803	-1.198149	-0.103392
C	3.509500	-2.520390	0.036691
C	2.396906	-3.501711	0.455741
C	1.135266	-2.678279	0.233611
C	3.344469	0.029520	-0.210756
C	2.636909	1.286667	-0.248172
C	0.970849	2.877204	-0.179334
C	3.264223	2.594109	0.196451
C	-0.294860	3.355416	0.045559
C	-1.473893	2.521321	-0.049766
C	-3.250291	1.272361	0.889638
C	-2.864545	0.800687	-0.529628
C	-2.621106	-0.702167	-0.764149
N	-1.340511	-1.166747	-0.223147
C	-1.318096	-2.466821	0.091626
C	-2.739820	-2.992391	0.027466
C	-3.597210	-1.714608	-0.134190
C	-0.174788	-3.206792	0.348132
H	4.122642	2.880099	-0.424114
H	-0.410971	4.326972	0.516537
H	-4.327072	1.256135	1.074063
H	-3.921881	-1.357595	0.846285
H	-3.001314	-3.586315	0.905528
H	-0.291578	-4.251097	0.608965
H	2.386283	-4.427841	-0.124081
H	3.944195	-2.805556	-0.926621
H	4.429201	0.067321	-0.163350
H	-2.764022	0.641701	1.641123

H	-3.342768	3.437491	0.548034
H	3.614166	2.525638	1.236094
H	4.327976	-2.459267	0.756529
H	2.470728	-3.784723	1.511369
H	-2.833740	-3.647458	-0.845805
H	-4.485345	-1.874710	-0.746904
N	1.394064	-1.416264	-0.061759
C	1.335138	1.524342	-0.540697
N	2.160346	3.552435	0.066577
H	0.624819	0.826151	-0.929760
N	-1.633388	1.532004	-0.866657
C	-2.639226	2.685044	0.927426
H	-2.320705	3.004424	1.921934
H	2.147822	4.355641	0.676474
H	-0.455494	-0.680024	-0.347790
H	-2.597473	-0.843139	-1.854189
H	-3.654407	1.093980	-1.238950

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N1-Con-PFPh-Corrin

C	1.320677	1.711206	-0.247191
C	2.656026	2.433038	-0.112943
C	3.636916	1.285386	0.184900
C	2.788277	0.052645	-0.084281
C	0.092054	2.319074	-0.295075
C	-1.175936	1.614183	-0.360083
C	-2.823713	-0.008878	-0.353699
C	-2.515775	2.310370	-0.512231
C	-3.390650	-1.264096	-0.199560
C	-2.515556	-2.443700	-0.270184
C	-1.184990	-4.201199	0.581107
C	-0.818190	-3.804954	-0.864740
C	0.661609	-3.601039	-1.233332
N	1.215113	-2.337392	-0.726852
C	2.515219	-2.380170	-0.432873
C	2.985570	-3.815415	-0.562110
C	1.675086	-4.622581	-0.685830
C	3.306210	-1.275056	-0.110431
H	-2.577995	2.907431	-1.430485
H	-1.144763	-5.277613	0.760591
H	1.359205	-4.969810	0.300448
H	3.610048	-4.125726	0.277144
H	4.533290	1.306129	-0.438652
H	2.910573	2.935551	-1.050935
H	-0.512976	-3.709047	1.291986
H	-3.361425	-4.331199	0.378633
H	-2.723394	2.974613	0.335877
H	2.638609	3.193586	0.669428
H	3.968116	1.293148	1.227797
H	3.593395	-3.901778	-1.469040

H	1.776635	-5.494083	-1.332998
N	1.516373	0.344674	-0.297341
C	-1.408791	0.281675	-0.280601
N	-3.450637	1.191825	-0.551559
H	-0.671753	-0.468669	-0.103708
N	-1.565248	-2.563314	-1.129088
C	-2.603084	-3.611887	0.709986
H	-2.865661	-3.296878	1.721804
H	-4.440373	1.328287	-0.440209
H	0.766203	-1.432464	-0.851773
H	0.711326	-3.569421	-2.329673
H	-1.195835	-4.573770	-1.555884
C	0.047106	3.813556	-0.266030
C	0.430995	4.589776	-1.362334
C	-0.391146	4.515097	0.860115
C	0.390710	5.979251	-1.346039
C	-0.447524	5.902838	0.903849
C	-0.053421	6.639143	-0.206947
C	-4.828418	-1.467747	0.037884
C	-5.555718	-2.461794	-0.640121
C	-5.574127	-0.727396	0.970730
C	-6.903969	-2.702429	-0.417117
C	-6.927966	-0.935425	1.199312
C	-7.601532	-1.931759	0.505052
C	4.748722	-1.492659	0.197531
C	5.677040	-1.843722	-0.786589
C	5.256122	-1.346991	1.492140
C	7.023841	-2.046900	-0.510378
C	6.598787	-1.533382	1.797495
C	7.487638	-1.888134	0.789732
F	0.858994	3.995598	-2.487449
F	0.767735	6.684082	-2.418253
F	-0.099509	7.972414	-0.178794
F	-0.868360	6.533910	2.005179
F	-0.767353	3.841614	1.959147
F	-4.944812	-3.217491	-1.569108
F	-7.544330	-3.657033	-1.102993
F	-8.902280	-2.147585	0.722075
F	-7.581381	-0.199044	2.107007
F	-4.969315	0.217901	1.716005
F	4.430189	-1.018229	2.498419
F	7.039614	-1.385667	3.051052
F	8.778377	-2.075758	1.069182
F	7.875989	-2.383245	-1.484375
F	5.276329	-1.992400	-2.060558

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N2-Con-Corrin

C	-2.871269	-0.439753	0.003748
C	-3.952392	-1.370201	-0.539836

C	-3.231285	-2.734531	-0.574568
C	-1.805648	-2.369827	-0.168348
C	-3.119467	0.977195	0.204374
C	-2.185392	1.963393	0.166637
C	-0.161372	2.829963	0.021417
C	-2.431710	3.453882	0.397906
C	1.276222	2.877476	-0.157859
C	2.037665	1.796804	-0.446906
C	2.847577	-0.467231	-0.736067
C	2.730486	-1.834348	-0.027631
N	1.602654	-2.549137	-0.659549
C	0.629831	-2.637634	0.164732
C	0.920311	-2.159507	1.579084
C	2.407649	-1.766974	1.495296
C	-0.704252	-3.142509	-0.231441
H	-2.992830	3.634507	1.316679
H	1.755963	3.840485	-0.003050
H	3.988168	0.289490	0.796685
H	3.034126	-2.475531	2.040931
H	0.726008	-2.962139	2.297323
H	-0.764770	-4.138609	-0.657117
H	-3.664198	-3.440278	0.139663
H	-4.839585	-1.363368	0.100908
H	-4.156451	1.268704	0.344997
H	4.050303	2.485635	0.113081
H	3.070426	-0.677240	-1.787380
H	-3.012252	3.879461	-0.425894
H	-4.276278	-1.036362	-1.531076
H	-3.266535	-3.205937	-1.558487
H	0.254415	-1.333117	1.836485
H	2.591352	-0.780153	1.928319
N	-1.738703	-1.027217	0.227674
C	3.552061	1.764457	-0.538493
C	1.560977	0.390731	-0.654559
H	0.890656	0.102609	0.156592
H	0.931511	0.307781	-1.544694
N	3.946202	0.381137	-0.214447
C	-0.999732	4.030645	0.438513
N	-0.849861	1.735627	-0.118929
H	3.859411	1.988444	-1.569843
H	-0.712126	4.368456	1.440071
H	-0.847702	4.877253	-0.236788
H	3.656789	-2.385135	-0.216658

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N2-Con-PFPh-Corrin

C	1.206974	1.805876	0.046654
C	2.452321	2.600870	0.426348
C	3.537805	1.509292	0.478229
C	2.803139	0.282427	-0.042905

C	-0.121127	2.419996	0.035102
C	-1.305454	1.741065	0.122826
C	-2.639976	-0.009280	0.191907
C	-2.696280	2.366622	0.084858
C	-3.040670	-1.411233	0.245580
C	-2.148881	-2.435554	0.289135
C	-0.141181	-3.776900	0.138898
C	1.109219	-3.878296	-0.758366
N	2.161146	-3.075958	-0.104776
C	2.396753	-2.031163	-0.797593
C	1.698868	-1.951890	-2.143406
C	0.949860	-3.299159	-2.195875
C	3.294646	-0.958033	-0.275863
H	-2.814329	3.041565	-0.765029
H	-1.337522	-4.489317	-1.373978
H	1.407680	-3.973559	-2.921687
H	2.434081	-1.837093	-2.944110
H	4.411563	1.746140	-0.132497
H	2.667098	3.361119	-0.330725
H	-3.375155	-4.142104	-0.371918
H	0.136694	-4.187854	1.114825
H	-2.880503	2.949053	0.991107
H	2.322356	3.125594	1.376429
H	3.886220	1.348548	1.499696
H	1.044926	-1.078449	-2.178898
H	-0.094350	-3.171898	-2.492786
N	1.448024	0.566163	-0.245371
C	-2.480443	-3.915928	0.210872
C	-0.656924	-2.327516	0.331012
H	-0.310102	-1.632407	-0.434881
H	-0.318543	-1.865962	1.262791
N	-1.290203	-4.562215	-0.361607
C	-3.620448	1.138171	0.009025
N	-1.395376	0.368204	0.261169
H	-2.647555	-4.300971	1.227009
H	-4.130017	1.060520	-0.956084
H	-4.394828	1.129576	0.780241
C	-0.164557	3.912460	-0.043604
C	-0.569226	4.711091	1.028171
C	0.216909	4.587944	-1.205764
C	-0.604746	6.098665	0.954471
C	0.195319	5.973119	-1.308017
C	-0.219661	6.732825	-0.220353
C	-4.508479	-1.711163	0.199510
C	-5.219838	-2.060465	1.347959
C	-5.233676	-1.664824	-0.991325
C	-6.579312	-2.350991	1.321085
C	-6.592675	-1.947431	-1.049394
C	-7.268246	-2.293339	0.115398
C	4.688075	-1.345889	0.044642

C	5.235130	-1.247077	1.327321
C	5.517486	-1.908829	-0.931407
C	6.530382	-1.658438	1.619793
C	6.811655	-2.331397	-0.667008
C	7.323488	-2.203550	0.619179
F	0.562643	6.578516	-2.441233
F	0.619365	3.887722	-2.277637
F	-0.935635	4.141686	2.187865
F	-0.998425	6.825382	2.004727
F	-0.248027	8.063145	-0.304147
F	5.061224	-2.040599	-2.189063
F	7.572108	-2.848553	-1.638414
F	8.568625	-2.601957	0.889192
F	7.011571	-1.547511	2.863197
F	4.500894	-0.765259	2.342739
F	-4.610424	-1.339386	-2.136692
F	-7.251265	-1.893904	-2.210694
F	-8.571739	-2.568808	0.075460
F	-7.226846	-2.680893	2.441667
F	-4.590565	-2.120804	2.530783
H	1.418213	-4.927336	-0.777708

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Neo-Con-Corrin

C	-2.827962	-0.580828	0.034643
C	-3.883673	-1.544784	-0.503849
C	-3.105318	-2.873438	-0.599780
C	-1.685399	-2.455228	-0.227033
C	-3.144531	0.817301	0.261718
C	-2.264530	1.853902	0.268917
C	-0.316378	2.858864	0.014346
C	-2.611683	3.331164	0.460198
C	1.105286	2.987966	-0.221315
C	1.934548	1.930675	-0.385898
C	2.790108	-1.648128	-0.126034
N	1.676302	-2.347842	-0.803345
C	0.763798	-2.620622	0.048491
C	1.098834	-2.317119	1.500876
C	2.567786	-1.878129	1.406315
C	-0.554510	-3.175329	-0.341661
H	-2.998943	3.507832	1.467186
H	1.513345	3.994079	-0.256884
H	4.822140	0.274357	-0.671061
H	3.234368	-2.669185	1.758080
H	0.949629	-3.206186	2.120998
H	-0.582013	-4.167243	-0.780644
H	-3.483754	-3.616838	0.107143
H	-4.749645	-1.595601	0.163394
H	-4.200077	1.056940	0.353123
H	3.916446	2.808909	-0.095979

H	-3.381266	3.658106	-0.242630
H	-4.252792	-1.198907	-1.474986
H	-3.150707	-3.318980	-1.595262
H	0.422024	-1.545517	1.878012
H	2.786549	-0.984499	1.995085
N	-1.662973	-1.122363	0.206477
C	3.425979	1.987284	-0.622303
C	1.544989	0.485667	-0.308302
H	1.110515	0.299421	0.687285
H	0.749619	0.219270	-1.005406
C	-1.256429	4.035863	0.231405
N	-0.908650	1.700916	0.048664
H	3.611964	2.112532	-1.695982
H	-0.937903	4.646540	1.081425
H	-1.258854	4.691528	-0.645391
N	2.779233	-0.258678	-0.575443
C	3.897846	0.590537	-0.179720
H	4.079254	0.591703	0.911940
H	3.740127	-2.076184	-0.460004

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Neo-Con-PFPh-Corrin

C	-1.193074	1.809808	0.018726
C	-2.408572	2.602697	-0.453024
C	-3.494337	1.514711	-0.549619
C	-2.803784	0.300459	0.054224
C	0.137366	2.415413	0.070027
C	1.320597	1.729650	0.044892
C	2.654168	-0.022322	-0.021469
C	2.713204	2.355181	0.064144
C	3.042652	-1.425963	-0.060667
C	2.143602	-2.439313	0.049230
C	-1.132229	-3.793876	1.042878
N	-2.123880	-3.023975	0.261374
C	-2.455560	-1.980402	0.916119
C	-1.914498	-1.872708	2.330856
C	-1.213602	-3.230809	2.499946
C	-3.315809	-0.930250	0.291573
H	2.856117	2.974775	0.952636
H	1.063348	-5.551784	0.578661
H	-1.814106	-3.901856	3.117937
H	-2.731365	-1.715917	3.039259
H	-4.407204	1.771324	-0.008085
H	-2.664152	3.378369	0.275694
H	3.417389	-4.147871	0.548446
H	2.869439	2.995837	-0.805947
H	-2.219511	3.108505	-1.403242
H	-3.771073	1.327489	-1.588410
H	-1.247047	-1.011132	2.409226
H	-0.230522	-3.150572	2.969025

N	-1.461532	0.581365	0.334566
C	2.457347	-3.915351	0.084817
C	0.667168	-2.288415	0.246330
H	0.500594	-1.658970	1.134494
H	0.185706	-1.743666	-0.567422
C	3.643727	1.128779	0.045518
N	1.406725	0.352216	-0.024380
H	2.476547	-4.294948	-0.944590
H	4.266546	1.057439	0.941444
H	4.319764	1.118375	-0.814013
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H	1.419638	-4.441438	1.919836
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C	0.185484	3.910603	0.090357
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C	0.622286	6.056687	-0.991756
C	-0.169060	6.017302	1.277095
C	0.242194	6.734900	0.159970
C	4.501041	-1.739245	-0.195481
C	5.057118	-2.121900	-1.416658
C	5.372465	-1.670857	0.891610
C	6.406993	-2.424622	-1.556095
C	6.726087	-1.964404	0.782343
C	7.244828	-2.344501	-0.450080
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C	-5.136533	-1.264760	-1.436262
C	-5.579790	-1.872580	0.811642
C	-6.406668	-1.687695	-1.810857
C	-6.850647	-2.306381	0.465053
C	-7.268908	-2.211446	-0.857154
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F	0.948467	4.053205	-2.150486
F	-5.216522	-1.972192	2.102362
F	-7.678067	-2.802667	1.391803
F	-8.490616	-2.620985	-1.206353
F	-6.797383	-1.608459	-3.087909
F	-4.332959	-0.805272	-2.407882
F	4.903202	-1.311538	2.098355
F	4.281043	-2.205857	-2.506620
F	6.903989	-2.787993	-2.741514
F	8.541269	-2.630760	-0.570252
F	7.528387	-1.888812	1.848302

C	-1.276522	1.661990	0.039474
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C	1.233543	1.774186	0.031228
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H	-0.079269	-3.370726	2.138043
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H	-4.209990	1.044716	0.994288
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H	1.447009	-4.197140	2.435636
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H	1.374908	-4.895383	0.189941
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H	2.402250	3.338590	-0.951642
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H	-2.802265	2.997276	-0.736226
H	-4.321655	1.186987	-0.754127
H	-3.423300	-4.208911	0.162020
H	-1.254390	-4.994049	0.806565
C	4.777648	-1.324112	-0.076774
C	5.448036	-1.045030	-1.273503
C	5.516807	-2.033010	0.878749
C	6.768240	-1.418401	-1.497122
C	6.832011	-2.424150	0.679378
C	7.465860	-2.111744	-0.517663
C	-0.159054	3.851556	0.162593
C	0.126189	4.530646	1.349281

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C	0.077673	5.915680	1.451004
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C	-0.269789	6.671272	0.337715
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C	-6.576969	-2.452943	0.997317
C	-6.741488	-1.708799	-1.282068
C	-7.344997	-2.211431	-0.135584
F	4.811513	-0.424035	-2.279320
F	7.364250	-1.132207	-2.660650
F	8.733805	-2.477190	-0.723182
F	7.498230	-3.085333	1.633217
F	4.947806	-2.342622	2.057771
F	-4.507936	-2.428422	2.085459
F	-7.154897	-2.934412	2.102625
F	-8.654917	-2.461296	-0.122459
F	-7.476870	-1.479173	-2.374457
F	-4.829343	-0.977697	-2.410680
F	0.461905	3.836573	2.448760
F	0.355954	6.525060	2.608374
F	-0.323568	8.001838	0.420465
F	-0.893465	6.757616	-1.936257
F	-0.782160	4.072906	-2.114193
