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1) Optimized 3D coordinates of EtIm-An/ACA for CD interactions

C	-0.08644	5.09362	-0.37710
C	-1.31497	5.97901	-0.44935
N	-2.46146	5.24709	-0.99016
C	-3.27107	4.37792	-0.27934
C	-4.21049	3.91369	-1.15246
N	-3.94444	4.50020	-2.38510
C	-2.88400	5.31203	-2.26197
C	-4.69614	4.30461	-3.63370
C	-4.80347	2.81798	-3.93009
C	-3.70669	2.14085	-4.56358
C	-3.76564	0.73391	-4.69732
C	-4.87323	0.03064	-4.22045
C	-5.96109	0.67994	-3.63339
C	-5.96027	2.08652	-3.49275
C	-2.55097	2.77817	-5.08441
C	-1.52297	2.06356	-5.70747
C	-1.60747	0.68555	-5.81961
C	-2.72075	0.02515	-5.31205
C	-7.05135	-0.08340	-3.18928
C	-8.16913	0.52021	-2.62284
C	-8.20872	1.89737	-2.49200
C	-7.12199	2.66650	-2.91477
H	-0.26513	4.22994	0.27167
H	0.17704	4.71419	-1.36945
H	-1.12346	6.84665	-1.08966
H	-1.58184	6.35080	0.54606
H	-3.07086	4.19891	0.76316
H	-5.03024	3.22510	-1.04353
H	-2.44509	5.91594	-3.04776
H	-4.20273	4.84048	-4.45063
H	-5.66165	4.80135	-3.52229
H	-4.89476	-1.05628	-4.31934
H	-2.42432	3.85487	-5.04454

H	-0.66029	2.58494	-6.11701
H	-0.81474	0.12377	-6.30908
H	-2.76700	-1.05891	-5.41400
H	-7.05200	-1.16882	-3.29193
H	-9.01152	-0.08944	-2.30152
H	-9.08667	2.37506	-2.06143
H	-7.22522	3.74009	-2.78132
H	0.76609	5.65167	0.02038
O	-3.93243	2.10929	-8.51332
O	-4.22094	-0.06878	-8.54041
N	-4.59059	1.08521	-8.28342
H	-5.48811	-1.20691	-8.07888
H	-5.67079	3.40330	-7.49753
C	-5.91249	1.24915	-7.66436
O	-6.35754	-1.15353	-7.62411
C	-6.32088	2.54817	-7.31147
C	-6.73749	0.14113	-7.40204
O	-6.98089	4.82773	-5.90765
C	-7.56066	2.73379	-6.68667
C	-7.99701	0.37502	-6.82653
N	-7.91782	4.06428	-6.19320
C	-8.42120	1.65925	-6.45586
O	-9.21419	-1.44324	-7.54575
N	-8.91042	-0.73170	-6.58192
O	-9.11609	4.32010	-6.04131
H	-9.38718	1.80247	-5.97182
O	-9.37330	-0.82898	-5.43736

2) Optimized 3D coordinates of EtIm-An/ACA for π - π interactions

C	-1.37595	0.92600	-1.28520
C	-2.10287	2.19776	-1.69597
N	-3.54890	1.97588	-1.85057
C	-4.47667	1.95802	-0.83313

C	-5.68251	1.66494	-1.39457
N	-5.46776	1.49999	-2.74297
C	-4.17504	1.69197	-2.99305
C	-6.50377	1.15548	-3.75021
C	-7.80739	1.84542	-3.46540
C	-8.83478	1.15676	-2.78811
C	-10.09639	1.81118	-2.58959
C	-10.27366	3.11659	-3.04580
C	-9.24616	3.81936	-3.67587
C	-7.98505	3.17674	-3.89512
C	-8.69510	-0.17612	-2.27020
C	-9.72778	-0.80144	-1.63321
C	-10.98867	-0.15510	-1.46797
C	-11.16199	1.11328	-1.93411
C	-9.44238	5.16570	-4.12384
C	-8.44086	5.85040	-4.74461
C	-7.18058	5.21983	-4.96172
C	-6.96139	3.93550	-4.55589
H	-1.75283	0.54368	-0.32844
H	-1.49061	0.14274	-2.04505
H	-1.73372	2.58335	-2.65303
H	-1.98217	2.99252	-0.95153
H	-4.20826	2.16707	0.19504
H	-6.67037	1.57781	-0.95898
H	-3.70668	1.63353	-3.96790
H	-6.61267	0.06823	-3.75558
H	-6.10407	1.44875	-4.72566
H	-11.24358	3.59718	-2.91777
H	-7.75612	-0.71671	-2.38089
H	-9.59238	-1.81324	-1.25078
H	-11.80303	-0.67750	-0.96733
H	-12.11796	1.62415	-1.81822
H	-10.41572	5.62795	-3.95853
H	-8.59681	6.87391	-5.08308

H	-6.38948	5.76680	-5.47404
H	-5.98778	3.49138	-4.75682
C	-10.72521	-0.77452	-5.22511
C	-9.48000	-1.43196	-5.45068
C	-8.47565	-0.77709	-6.09804
C	-8.64999	0.57291	-6.54755
C	-9.89482	1.24576	-6.30869
C	-10.92885	0.51131	-5.63475
C	-7.62341	1.23984	-7.21855
C	-7.76350	2.55293	-7.66813
C	-9.00521	3.23726	-7.45203
C	-10.05469	2.57398	-6.77230
C	-6.68612	3.22437	-8.33305
C	-6.82024	4.51157	-8.75836
C	-8.04845	5.20391	-8.53972
C	-9.09545	4.59645	-7.90987
C	-11.33728	3.30509	-6.58226
O	-12.08836	3.17925	-5.63684
H	-11.52717	-1.30816	-4.71570
H	-9.34470	-2.46087	-5.11778
H	-7.52775	-1.27640	-6.30650
H	-11.88017	0.99606	-5.44088
H	-6.68515	0.71268	-7.40859
H	-5.75660	2.67771	-8.49877
H	-5.99966	5.01463	-9.26962
H	-8.14818	6.23490	-8.87931
H	-10.00220	5.17173	-7.74010
H	-11.60677	4.01096	-7.39432
H	-0.30705	1.13901	-1.16947

3) Optimized 3D coordinates of EtIm-An/BAA for CD interactions

C	1.08021	2.73050	-1.31605
C	0.25541	3.47813	-2.34675
N	-1.18571	3.17897	-2.24159

C	-1.75702	1.98042	-1.88082
C	-3.10378	2.11439	-2.02821
N	-3.33211	3.39610	-2.47443
C	-2.15931	4.01480	-2.59827
C	-4.65335	4.00733	-2.73533
C	-5.53453	3.13956	-3.59712
C	-5.38367	3.18573	-4.99906
C	-6.25747	2.40453	-5.82475
C	-7.24044	1.61425	-5.22575
C	-7.37002	1.52933	-3.83969
C	-6.50117	2.30460	-2.99872
C	-4.37449	3.96482	-5.65746
C	-4.24620	3.95821	-7.01671
C	-5.11785	3.17729	-7.83103
C	-6.09687	2.42927	-7.24823
C	-8.34736	0.66497	-3.24527
C	-8.45859	0.55640	-1.89223
C	-7.59808	1.32102	-1.04886
C	-6.66235	2.16243	-1.57689
H	0.74707	2.95045	-0.29469
H	1.05557	1.64692	-1.48375
H	0.56791	3.21791	-3.36478
H	0.35519	4.56199	-2.22028
H	-1.16909	1.12268	-1.58218
H	-3.90390	1.39878	-1.88479
H	-2.01735	5.03438	-2.93370
H	-4.46105	4.97309	-3.21212
H	-5.11517	4.21735	-1.76730
H	-7.90785	1.02667	-5.85872
H	-3.67871	4.56835	-5.07790
H	-3.46544	4.55360	-7.49010
H	-4.99834	3.18687	-8.91362
H	-6.77252	1.82814	-7.85735
H	-8.99860	0.08945	-3.90392

H	-9.20132	-0.10562	-1.44851
H	-7.69585	1.23336	0.03321
H	-6.03341	2.72750	-0.89043
C	-4.29509	-0.37350	-4.59371
C	-4.20791	-1.38615	-3.59237
C	-2.99811	-1.70009	-3.04905
C	-1.80662	-1.01399	-3.45696
C	-1.89997	0.02479	-4.44538
C	-3.18818	0.30970	-5.00517
C	-0.57041	-1.32192	-2.88510
C	0.59303	-0.64133	-3.24805
C	0.52962	0.41134	-4.22505
C	-0.72528	0.72171	-4.77756
C	1.85776	-0.96651	-2.65268
C	2.99129	-0.29576	-3.00007
C	2.93183	0.74282	-3.97871
C	1.75079	1.08329	-4.57050
Br	-0.85221	2.19144	-5.98603
H	-5.26146	-0.14503	-5.03898
H	-5.10850	-1.91232	-3.27712
H	-2.91020	-2.48429	-2.29645
H	-3.27979	1.07652	-5.77156
H	-0.51083	-2.11581	-2.13906
H	1.89168	-1.77230	-1.91882
H	3.94707	-0.55554	-2.54611
H	3.84739	1.25929	-4.26679
H	1.73072	1.86020	-5.33181
H	2.12474	3.04627	-1.41248

4) Optimized 3D coordinates of EtIm-An/BAA for π - π interactions

C	-1.35484	0.96975	-1.33241
C	-2.09465	2.23621	-1.73612
N	-3.54115	2.00501	-1.87318
C	-4.45909	1.99667	-0.84670

C	-5.66899	1.69149	-1.39281
N	-5.46623	1.50978	-2.74091
C	-4.17690	1.70376	-3.00576
C	-6.50868	1.14509	-3.73276
C	-7.80904	1.84747	-3.46015
C	-8.84699	1.17277	-2.78640
C	-10.10497	1.83987	-2.60351
C	-10.26630	3.14273	-3.07321
C	-9.22870	3.83181	-3.70313
C	-7.97095	3.17663	-3.90326
C	-8.72175	-0.15629	-2.25454
C	-9.76237	-0.76669	-1.61699
C	-11.01854	-0.10745	-1.46446
C	-11.17900	1.15726	-1.94437
C	-9.40809	5.17517	-4.16532
C	-8.39369	5.84526	-4.78023
C	-7.13627	5.20320	-4.97605
C	-6.93306	3.92020	-4.55778
H	-1.71964	0.58514	-0.37189
H	-1.47141	0.18551	-2.09101
H	-1.73930	2.62309	-2.69787
H	-1.97070	3.03260	-0.99401
H	-4.18128	2.21894	0.17622
H	-6.65219	1.60548	-0.94653
H	-3.71792	1.63423	-3.98440
H	-6.62075	0.05862	-3.71064
H	-6.11585	1.41293	-4.71842
H	-11.22923	3.63862	-2.94353
H	-7.78639	-0.70498	-2.35403
H	-9.63757	-1.77536	-1.22301
H	-11.83914	-0.61731	-0.96100
H	-12.13050	1.67782	-1.83297
H	-10.37969	5.64720	-4.01984
H	-8.53882	6.86479	-5.13459

H	-6.33537	5.73902	-5.48479
H	-5.96206	3.46495	-4.74504
C	-10.65567	-0.83431	-5.23331
C	-9.38520	-1.44972	-5.44332
C	-8.39176	-0.76309	-6.07440
C	-8.59616	0.58049	-6.53325
C	-9.87565	1.19960	-6.32679
C	-10.89279	0.43866	-5.65958
C	-7.57848	1.28683	-7.17500
C	-7.76687	2.59419	-7.62474
C	-9.03774	3.23713	-7.43837
C	-10.05577	2.51395	-6.79189
C	-6.71252	3.31148	-8.27920
C	-6.89925	4.58586	-8.72323
C	-8.16341	5.22440	-8.54426
C	-9.19266	4.57672	-7.92707
Br	-11.74881	3.34496	-6.54302
H	-11.44465	-1.38921	-4.72676
H	-9.22044	-2.47323	-5.10686
H	-7.42386	-1.23180	-6.26109
H	-11.86725	0.89181	-5.49536
H	-6.61805	0.79705	-7.35040
H	-5.75648	2.80656	-8.42536
H	-6.09263	5.11727	-9.22841
H	-8.30754	6.24016	-8.91236
H	-10.14991	5.07688	-7.80166
H	-0.28641	1.19023	-1.22751

5) Optimized 3D coordinates of EtIm-An/NAA for CD interactions

C	-0.74932	1.63695	0.56520
C	-1.74088	2.77655	0.40697
N	-3.05451	2.31851	-0.07718

C	-4.27272	2.87576	0.25064
C	-5.21756	2.25105	-0.50309
N	-4.55679	1.32156	-1.27548
C	-3.25553	1.38307	-1.00395
C	-5.16957	0.44144	-2.29358
C	-6.08978	1.21834	-3.20050
C	-7.48752	1.15010	-3.02398
C	-8.33634	1.91725	-3.89454
C	-7.76652	2.71220	-4.88842
C	-6.38324	2.79835	-5.05771
C	-5.52297	2.04064	-4.19772
C	-8.12947	0.36825	-2.00147
C	-9.48742	0.35111	-1.86777
C	-10.32271	1.10851	-2.74265
C	-9.75938	1.86474	-3.72488
C	-5.81160	3.63830	-6.06833
C	-4.45997	3.73859	-6.21633
C	-3.59750	2.99562	-5.35841
C	-4.10757	2.17808	-4.39134
H	-1.12337	0.87518	1.25956
H	-0.51790	1.16305	-0.39663
H	-1.37294	3.52478	-0.30494
H	-1.92647	3.27173	1.36644
H	-4.36603	3.66441	0.98668
H	-6.28970	2.39201	-0.56296
H	-2.48685	0.79794	-1.49898
H	-5.68567	-0.36619	-1.77108
H	-4.34018	-0.01225	-2.84567
H	-8.41897	3.29288	-5.54271
H	-7.53943	-0.23207	-1.31158
H	-9.94458	-0.25213	-1.08312
H	-11.40454	1.07537	-2.61907
H	-10.38239	2.45259	-4.39949
H	-6.48393	4.20309	-6.71493

H	-4.03424	4.38405	-6.98344
H	-2.51768	3.08376	-5.48053
H	-3.41455	1.63052	-3.75653
C	-1.55800	-0.16656	-7.23574
C	-0.63656	-0.01210	-8.31281
C	0.54573	0.63060	-8.10240
C	0.87546	1.15916	-6.81196
C	-0.04986	0.99923	-5.72799
C	-1.28020	0.31259	-5.98823
C	2.08146	1.82857	-6.59886
C	2.42703	2.37088	-5.35996
C	1.51308	2.26815	-4.26085
C	0.30627	1.58227	-4.49664
C	3.68593	3.02810	-5.16973
C	4.02931	3.54211	-3.95635
C	3.12772	3.42208	-2.85764
C	1.91372	2.81363	-2.99727
N	-0.63809	1.47958	-3.38964
O	-1.07684	0.37423	-3.08779
H	-2.50280	-0.68100	-7.41117
H	-0.88349	-0.40984	-9.29633
H	1.26354	0.76079	-8.91267
H	-1.99808	0.15907	-5.18853
H	2.78076	1.93090	-7.43060
H	4.36524	3.10069	-6.01946
H	4.98898	4.03850	-3.81668
H	3.41807	3.82377	-1.88644
H	1.24935	2.74852	-2.14002
O	-0.96218	2.50173	-2.80106
H	0.18672	2.03728	0.97040

6) Optimized 3D coordinates of EtIm-An/NAA for π - π interactions

C	-1.21595	1.76509	-1.19389
C	-2.14951	2.83846	-1.73204

N	-3.51892	2.33349	-1.91799
C	-4.41362	2.04465	-0.91110
C	-5.54949	1.58430	-1.50405
N	-5.32584	1.59321	-2.86121
C	-4.09613	2.04928	-3.08550
C	-6.30387	1.18084	-3.89866
C	-7.68651	1.66566	-3.56166
C	-8.63519	0.78517	-3.00200
C	-9.95132	1.27888	-2.70949
C	-10.25614	2.61727	-2.95913
C	-9.30945	3.50348	-3.47524
C	-7.99867	3.02194	-3.79383
C	-8.36620	-0.59289	-2.69454
C	-9.32436	-1.40008	-2.15109
C	-10.63297	-0.90532	-1.87750
C	-10.93237	0.39472	-2.15418
C	-9.63164	4.87987	-3.70085
C	-8.70669	5.74231	-4.20866
C	-7.40362	5.26767	-4.53557
C	-7.06117	3.96060	-4.33906
H	-1.55214	1.39518	-0.21735
H	-1.14693	0.91660	-1.88581
H	-1.81452	3.21078	-2.70659
H	-2.21472	3.69709	-1.05392
H	-4.17654	2.20230	0.13373
H	-6.49731	1.27002	-1.08446
H	-3.64127	2.17777	-4.06021
H	-6.25362	0.09295	-3.97998
H	-5.95096	1.59870	-4.84757
H	-11.25984	2.98328	-2.73928
H	-7.38323	-1.02144	-2.88416
H	-9.08812	-2.43991	-1.92486
H	-11.38362	-1.56958	-1.45107
H	-11.92801	0.79133	-1.95398

H	-10.64059	5.21912	-3.47033
H	-8.96161	6.78670	-4.38305
H	-6.67646	5.95698	-4.96458
H	-6.06434	3.63995	-4.63597
C	-12.31690	0.33825	-5.54381
C	-11.45369	-0.79397	-5.44106
C	-10.15189	-0.69681	-5.82855
C	-9.62752	0.53611	-6.33527
C	-10.49318	1.67546	-6.42948
C	-11.86087	1.53226	-6.01952
C	-8.29368	0.64810	-6.72986
C	-7.76215	1.84575	-7.21136
C	-8.60808	2.99551	-7.34268
C	-9.94589	2.85675	-6.94869
C	-6.38053	1.95492	-7.57996
C	-5.86876	3.13353	-8.03716
C	-6.71260	4.27894	-8.16031
C	-8.03485	4.21627	-7.83221
N	-10.83880	4.01739	-7.11020
O	-11.41073	4.43733	-6.11892
H	-13.35950	0.24443	-5.24076
H	-11.84445	-1.73455	-5.05448
H	-9.48539	-1.55685	-5.76168
H	-12.53487	2.38257	-6.08469
H	-7.64932	-0.23098	-6.66245
H	-5.75478	1.06272	-7.51493
H	-4.82219	3.20195	-8.33458
H	-6.29526	5.21276	-8.53647
H	-8.66280	5.09640	-7.94869
O	-10.95524	4.48155	-8.22786
H	-0.21327	2.18928	-1.06746

7) Optimized 3D coordinates of EtIm-An/PA for CD interactions

C	-0.44770	4.69473	0.15225
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C	-1.61445	5.65341	-0.02981
N	-2.77351	5.00105	-0.65975
C	-3.77183	4.32541	0.00079
C	-4.61043	3.82138	-0.94487
N	-4.10214	4.19032	-2.17046
C	-2.99185	4.89830	-1.97060
C	-4.70176	3.87968	-3.48721
C	-4.78921	2.40036	-3.77780
C	-3.71880	1.75727	-4.43904
C	-3.86114	0.38690	-4.83802
C	-5.01940	-0.31038	-4.49109
C	-6.05314	0.29464	-3.77761
C	-5.96326	1.68945	-3.44701
C	-2.47335	2.40103	-4.75020
C	-1.48398	1.75258	-5.43517
C	-1.65546	0.40561	-5.86992
C	-2.81142	-0.25441	-5.57299
C	-7.20927	-0.45802	-3.38856
C	-8.23810	0.13539	-2.72273
C	-8.17880	1.53042	-2.43054
C	-7.09233	2.27775	-2.78105
H	-0.74403	3.81880	0.74169
H	-0.05622	4.35940	-0.81708
H	-1.34351	6.50992	-0.65746
H	-1.96637	6.04579	0.93022
H	-3.79977	4.24197	1.07956
H	-5.50437	3.21840	-0.84403
H	-2.37602	5.33946	-2.74437
H	-4.09431	4.39767	-4.23416
H	-5.68893	4.34863	-3.50785
H	-5.12044	-1.35740	-4.78362
H	-2.29504	3.43185	-4.45003
H	-0.55082	2.27036	-5.65648
H	-0.86015	-0.08781	-6.42655

H	-2.95774	-1.28803	-5.88967
H	-7.24309	-1.51893	-3.63818
H	-9.11274	-0.44199	-2.42616
H	-9.01933	2.00542	-1.92496
H	-7.10544	3.34116	-2.54641
H	0.36361	5.20913	0.67954
O	0.64925	-0.24186	-3.56517
O	0.33652	1.57248	-2.45422
N	-0.00730	0.43911	-2.82006
H	-0.86762	2.10475	-1.48794
H	-1.05101	-1.89986	-3.45640
C	-1.27547	-0.07975	-2.32406
O	-1.74267	1.92158	-1.06677
C	-1.67954	-1.33064	-2.77643
C	-2.06881	0.69958	-1.45154
O	-2.67432	-3.66527	-3.70547
C	-2.90581	-1.81463	-2.36640
C	-3.28276	0.11989	-1.03173
N	-3.39710	-3.08370	-2.92114
C	-3.72424	-1.10037	-1.49989
O	-3.58439	1.38529	0.86006
N	-4.13208	0.82293	-0.06737
O	-4.50545	-3.44626	-2.57611
H	-4.69176	-1.49370	-1.19526
O	-5.33474	0.78603	-0.25780

8) Optimized 3D coordinates of EtIm-An/PA for π - π interactions

C	-0.08644	5.09362	-0.37710
C	-1.31497	5.97901	-0.44935
N	-2.46146	5.24709	-0.99016
C	-3.27107	4.37792	-0.27934
C	-4.21049	3.91369	-1.15246
N	-3.94444	4.50020	-2.38510
C	-2.88400	5.31203	-2.26197

C	-4.69614	4.30461	-3.63370
C	-4.80347	2.81798	-3.93009
C	-3.70669	2.14085	-4.56358
C	-3.76564	0.73391	-4.69732
C	-4.87323	0.03064	-4.22045
C	-5.96109	0.67994	-3.63339
C	-5.96027	2.08652	-3.49275
C	-2.55097	2.77817	-5.08441
C	-1.52297	2.06356	-5.70747
C	-1.60747	0.68555	-5.81961
C	-2.72075	0.02515	-5.31205
C	-7.05135	-0.08340	-3.18928
C	-8.16913	0.52021	-2.62284
C	-8.20872	1.89737	-2.49200
C	-7.12199	2.66650	-2.91477
H	-0.26513	4.22994	0.27167
H	0.17704	4.71419	-1.36945
H	-1.12346	6.84665	-1.08966
H	-1.58184	6.35080	0.54606
H	-3.07086	4.19891	0.76316
H	-5.03024	3.22510	-1.04353
H	-2.44509	5.91594	-3.04776
H	-4.20273	4.84048	-4.45063
H	-5.66165	4.80135	-3.52229
H	-4.89476	-1.05628	-4.31934
H	-2.42432	3.85487	-5.04454
H	-0.66029	2.58494	-6.11701
H	-0.81474	0.12377	-6.30908
H	-2.76700	-1.05891	-5.41400
H	-7.05200	-1.16882	-3.29193
H	-9.01152	-0.08944	-2.30152
H	-9.08667	2.37506	-2.06143
H	-7.22522	3.74009	-2.78132
H	0.76609	5.65167	0.02038

O	-3.93243	2.10929	-8.51332
O	-4.22094	-0.06878	-8.54041
N	-4.59059	1.08521	-8.28342
H	-5.48811	-1.20691	-8.07888
H	-5.67079	3.40330	-7.49753
C	-5.91249	1.24915	-7.66436
O	-6.35754	-1.15353	-7.62411
C	-6.32088	2.54817	-7.31147
C	-6.73749	0.14113	-7.40204
O	-6.98089	4.82773	-5.90765
C	-7.56066	2.73379	-6.68667
C	-7.99701	0.37502	-6.82653
N	-7.91782	4.06428	-6.19320
C	-8.42120	1.65925	-6.45586
O	-9.21419	-1.44324	-7.54575
N	-8.91042	-0.73170	-6.58192
O	-9.11609	4.32010	-6.04131
H	-9.38718	1.80247	-5.97182
O	-9.37330	-0.82898	-5.43736

9) Optimized 3D coordinates of DNP

C	-0.75754	1.19086	-0.04620
C	-1.38482	-0.03651	-0.04793
C	-0.61335	-1.20461	-0.07296
C	0.76406	-1.16278	-0.09611
C	1.38969	0.08256	-0.09439
C	0.64661	1.28454	-0.06937
O	1.18308	2.49827	-0.06615
N	2.84491	0.10506	-0.11940
O	3.40410	1.20665	-0.11809
O	3.44611	-0.94413	-0.14018
N	-1.28516	-2.50964	-0.07471
O	-0.58664	-3.50569	-0.09410
O	-2.50285	-2.51138	-0.05659

H	-1.32673	2.11833	-0.02725
H	-2.46982	-0.11510	-0.02986
H	1.35520	-2.07484	-0.11481
H	2.15621	2.38592	-0.08392

10) Optimized 3D coordinates of MNP

C	-0.76699	1.17573	-0.04722
C	-1.40666	-0.05359	-0.06002
C	-0.64172	-1.21791	-0.06859
C	0.74793	-1.17946	-0.06466
C	1.38778	0.05276	-0.05191
C	0.63102	1.22945	-0.04318
O	1.20008	2.46001	-0.03055
N	-1.31828	-2.51784	-0.08214
O	-0.62391	-3.52000	-0.08783
O	-2.53704	-2.52393	-0.08699
H	-1.33328	2.10560	-0.04040
H	-2.49205	-0.12483	-0.06352
H	1.31203	-2.10954	-0.07141
H	2.47806	0.10067	-0.04875
H	2.15839	2.38045	-0.02901

11) Optimized 3D coordinates of ONP

C	-0.72193	1.19445	-0.02515
C	-1.33348	-0.04436	0.02757
C	-0.57769	-1.22711	0.02515
C	0.79951	-1.14732	-0.03033
C	1.42492	0.10507	-0.08362
C	0.67718	1.30083	-0.08269
O	1.20556	2.52541	-0.13258
N	2.87493	0.13642	-0.13952
O	3.43343	1.23880	-0.18889
O	3.48805	-0.90955	-0.13576
H	-1.29919	2.11786	-0.02380
H	-2.42186	-0.09824	0.07184

H	-1.06812	-2.19815	0.06688
H	1.42347	-2.03833	-0.03392
H	2.17672	2.41604	-0.16889

12) Optimized 3D coordinates of PA

C	-0.67297	1.21718	0.00464
C	-1.38019	0.03406	0.00843
C	-0.67695	-1.16697	0.03142
C	0.70310	-1.19764	0.02183
C	1.39633	0.00669	-0.01119
C	0.73874	1.26203	-0.01896
O	1.35469	2.42292	-0.08231
N	-1.44842	2.46828	0.02424
O	-1.05335	3.35728	0.74751
O	-2.44918	2.49811	-0.66747
N	2.85436	-0.06142	-0.04495
O	3.47872	1.00141	-0.10789
O	3.38502	-1.14564	-0.01117
N	-1.42235	-2.43333	0.05868
O	-0.77473	-3.46220	0.06566
O	-2.63606	-2.36345	0.07277
H	-2.46818	0.04273	-0.00315
H	1.24349	-2.14122	0.03236
H	2.31864	2.23761	-0.11799

13) Optimized 3D coordinates of PBB

C	-0.78204	1.16085	-0.03059
C	-1.40247	-0.08096	-0.00960
C	-0.61291	-1.23302	-0.00530
C	0.77752	-1.16563	-0.02177
C	1.38516	0.08708	-0.04285
C	0.61419	1.25046	-0.04721
C	1.28327	2.57543	-0.06991
Br	-1.45586	-2.92868	0.02467
H	2.39759	2.54149	-0.08227

O	0.69896	3.63501	-0.07526
H	-1.37022	2.07864	-0.03425
H	-2.48819	-0.16179	0.00357
H	1.37319	-2.07682	-0.01826
H	2.47463	0.15781	-0.05604

14) Optimized 3D coordinates of PBH

C	-0.73164	1.17788	-0.02624
C	-1.36310	-0.06056	-0.01090
C	-0.59953	-1.22600	-0.01245
C	0.78908	-1.16370	-0.02926
C	1.42105	0.07809	-0.04448
C	0.66204	1.24881	-0.04297
O	1.22439	2.49091	-0.05711
Br	-1.46464	-2.91585	0.00946
H	-1.31087	2.10040	-0.02533
H	-2.45065	-0.11798	0.00236
H	1.38111	-2.07785	-0.03037
H	2.51172	0.12886	-0.05754
H	2.18218	2.41294	-0.06915

15) Optimized 3D coordinates of PHB

C	-0.78809	1.15784	-0.06532
C	-1.40697	-0.08245	-0.05623
C	-0.62657	-1.24659	-0.04681
C	0.76808	-1.16793	-0.04640
C	1.37384	0.08100	-0.05544
C	0.60874	1.25189	-0.06505
C	1.27598	2.56983	-0.07528
O	-1.17761	-2.48786	-0.03765
H	2.39094	2.53208	-0.07359
O	0.69928	3.63621	-0.08507
H	-1.37648	2.07573	-0.07263
H	-2.49656	-0.15596	-0.05644
H	1.35145	-2.08748	-0.03918

H	2.46374	0.15060	-0.05519
H	-2.13666	-2.41897	-0.03923

16) Optimized 3D coordinates of PIP

C	-0.77012	1.17347	-0.03071
C	-1.39331	-0.06800	-0.00967
C	-0.61164	-1.22809	-0.00530
C	0.78190	-1.15404	-0.02181
C	1.39468	0.09645	-0.04286
C	0.62587	1.26186	-0.04736
C	1.28412	2.59539	-0.07040
I	-1.54850	-3.10643	0.02707
H	2.40323	2.56539	-0.08294
O	0.69090	3.64258	-0.07543
H	-1.35355	2.09750	-0.03460
H	-2.48286	-0.13685	0.00341
H	1.38519	-2.06386	-0.01841
H	2.48691	0.16451	-0.05607

17) Optimized 3D coordinates of PNB

C	-0.79378	1.17036	-0.06588
C	-1.42535	-0.06563	-0.05956
C	-0.63520	-1.21246	-0.05261
C	0.75282	-1.17242	-0.05170
C	1.37089	0.07446	-0.05820
C	0.60357	1.24088	-0.06525
C	1.28606	2.56610	-0.07244
H	2.39939	2.52676	-0.07095
O	0.70291	3.62427	-0.07946
N	-1.30311	-2.53156	-0.04585
O	-0.59484	-3.52090	-0.03587
O	-2.51936	-2.54616	-0.05068
H	-1.36966	2.09527	-0.07124
H	-2.50877	-0.15932	-0.06000
H	1.32064	-2.09976	-0.04610

H	2.46012	0.14018	-0.05779
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18) Optimized 3D coordinates of PNP

C	-1.37417	-0.09343	-0.00352
C	-0.74404	1.14542	-0.00848
C	0.64690	1.24348	-0.04349
C	1.37336	0.06260	-0.07264
C	0.78002	-1.19490	-0.06865
C	-0.61057	-1.26437	-0.03380
O	-1.28416	-2.44622	-0.02744
N	2.84771	0.13089	-0.10967
O	3.36296	1.23279	-0.11920
O	3.46214	-0.92093	-0.12850
H	-2.46009	-0.17546	0.02397
H	-1.34566	2.05383	0.01471
H	1.16022	2.20122	-0.04825
H	1.40519	-2.08637	-0.09166
H	-0.66260	-3.17926	-0.05012

19) Optimized 3D coordinates of ACA

C	-1.20773	0.68695	-0.00063
C	-1.20885	-0.74764	0.00196
C	1.23184	0.71528	-0.00258
C	1.26066	-0.72058	-0.00056
C	0.00504	1.37567	-0.00333
C	0.03329	-1.44277	-0.00008
C	-2.44414	1.40982	-0.00092
C	-2.48937	-1.39813	0.00297
C	2.45208	1.46762	-0.00238
C	2.56563	-1.33034	0.00630
C	-3.63666	0.75134	0.00077
C	-3.64846	-0.67292	0.00224
C	3.66117	0.84309	0.00182
C	3.70732	-0.58140	0.00698
H	-0.00738	2.46782	-0.00526

C	0.09780	-2.92553	-0.00950
H	-2.40591	2.50010	-0.00269
H	-2.52521	-2.48157	0.00627
H	2.38524	2.55650	-0.00474
H	2.67457	-2.41031	0.01295
H	-4.57609	1.30444	0.00069
H	-4.60413	-1.19843	0.00314
H	4.58671	1.41850	0.00240
H	4.67450	-1.08482	0.01268
O	-0.83774	-3.70138	0.02938
H	1.11687	-3.35269	-0.06046

20) Optimized 3D coordinates of ANT

C	-1.21995	0.71713	0.00004
C	-1.21994	-0.71719	0.00009
C	1.21992	0.71711	0.00005
C	1.21995	-0.71722	0.00002
C	-0.00000	1.40024	0.00007
C	-0.00001	-1.40030	0.00010
C	-2.47817	1.40583	-0.00008
C	-2.47823	-1.40578	0.00003
C	2.47816	1.40577	0.00000
C	2.47822	-1.40585	-0.00012
C	-3.65404	0.71523	-0.00016
C	-3.65406	-0.71510	-0.00010
C	3.65402	0.71515	-0.00014
C	3.65405	-0.71517	-0.00023
H	0.00001	2.49224	0.00007
H	-0.00003	-2.49231	0.00010
H	-2.47603	2.49699	-0.00014
H	-2.47616	-2.49694	0.00004
H	2.47603	2.49693	0.00005
H	2.47612	-2.49700	-0.00017
H	-4.60384	1.25094	-0.00029

H	-4.60390	-1.25074	-0.00018
H	4.60382	1.25086	-0.00019
H	4.60388	-1.25083	-0.00035

21) Optimized 3D coordinates of BAA

C	-1.21701	0.72197	-0.00014
C	-1.23388	-0.71448	-0.00019
C	1.21700	0.72191	-0.00015
C	1.23386	-0.71452	-0.00011
C	0.00001	1.40328	-0.00011
C	-0.00001	-1.38817	-0.00022
C	-2.46192	1.43392	-0.00009
C	-2.50925	-1.37227	-0.00009
C	2.46191	1.43387	-0.00008
C	2.50923	-1.37232	-0.00005
C	-3.65178	0.77111	0.00005
C	-3.67020	-0.65639	0.00005
C	3.65176	0.77104	-0.00005
C	3.67018	-0.65645	0.00003
H	0.00003	2.49464	-0.00011
Br	-0.00002	-3.29382	-0.00022
H	-2.43183	2.52443	-0.00009
H	-2.54274	-2.45940	-0.00010
H	2.43182	2.52437	-0.00014
H	2.54270	-2.45945	-0.00001
H	-4.59129	1.32409	0.00014
H	-4.62623	-1.18065	0.00013
H	4.59127	1.32401	-0.00004
H	4.62620	-1.18073	0.00011

22) Optimized 3D coordinates of BNP

C	0.00638	-0.73995	-0.00000
C	0.00674	0.68528	-0.00000
C	1.25125	-1.42813	-0.00001
C	1.25309	1.36989	-0.00003

C	-1.22593	-1.44860	-0.00002
C	-1.26220	1.34027	0.00001
C	2.43807	-0.74218	-0.00003
C	2.43566	0.67420	-0.00003
C	-2.41864	-0.77547	-0.00003
C	-2.44079	0.64059	-0.00001
H	1.24314	-2.51920	-0.00001
H	1.26042	2.45833	-0.00002
H	-1.20527	-2.53911	-0.00004
Br	-1.35481	3.24011	0.00005
H	3.38436	-1.28372	-0.00003
H	3.38141	1.21672	-0.00005
H	-3.36211	-1.32143	-0.00004
H	-3.39088	1.17243	-0.00000

23) Optimized 3D coordinates of BPN

C	-0.71931	-0.39323	0.00017
C	0.74095	-0.40764	0.00019
C	-1.42155	0.84065	0.00024
C	1.43653	0.82189	0.00020
C	-0.64699	2.06350	0.00026
C	0.70507	2.05980	0.00032
C	-1.47532	-1.58741	0.00018
C	1.49940	-1.60054	0.00008
C	-2.83394	0.83666	0.00022
C	2.84978	0.83381	0.00019
C	-2.85386	-1.57037	0.00015
C	2.87879	-1.57151	0.00005
C	-3.54129	-0.34578	0.00016
C	3.56488	-0.34342	0.00008
Br	-1.53331	3.74613	0.00031
H	1.26021	2.99706	0.00038
H	-0.96599	-2.54868	0.00020
H	0.99945	-2.56684	0.00006

H	-3.36593	1.78589	0.00025
H	3.36795	1.79393	0.00023
H	-3.40846	-2.50891	0.00013
H	3.43917	-2.50668	-0.00003
H	-4.63120	-0.32766	0.00014
H	4.65487	-0.32485	0.00004

24) Optimized 3D coordinates of BPY

C	-0.70389	0.01554	0.00017
C	0.72782	0.02848	0.00006
C	-1.41306	1.24758	0.00000
C	1.43729	1.25840	0.00008
C	-1.42645	-1.21255	-0.00002
C	1.44339	-1.19615	-0.00001
C	-0.66682	2.48412	0.00005
C	0.68688	2.49116	0.00011
C	-0.64702	-2.43629	0.00017
C	0.70566	-2.43476	0.00013
C	-2.81258	1.23577	-0.00004
C	2.83743	1.23906	0.00001
C	-2.82491	-1.18036	-0.00005
C	2.84324	-1.17655	-0.00009
C	-3.50779	0.03262	-0.00008
C	3.53196	0.03299	-0.00014
H	-1.22419	3.42184	-0.00003
H	1.23606	3.43365	0.00010
Br	-1.54197	-4.11332	0.00012
H	1.25792	-3.37377	0.00009
H	-3.35356	2.18307	-0.00006
H	3.38254	2.18403	0.00001
H	-3.38341	-2.11439	-0.00012
H	3.39106	-2.11982	-0.00017
H	-4.59793	0.03459	-0.00015
H	4.62223	0.03520	-0.00022

25) Optimized 3D coordinates of DPY

C	-0.71591	-0.01155	-0.00005
C	0.71594	0.01159	0.00011
C	-1.42988	1.21506	-0.00000
C	1.43616	1.24063	0.00014
C	-1.43616	-1.24059	-0.00009
C	1.42986	-1.21504	0.00007
C	-0.69482	2.45482	-0.00007
C	0.65718	2.46320	0.00005
C	-0.65717	-2.46321	0.00003
C	0.69481	-2.45487	-0.00000
C	-2.82922	1.20430	0.00001
C	2.83486	1.21068	0.00007
C	-2.83488	-1.21069	-0.00013
C	2.82920	-1.20431	-0.00002
C	-3.52140	-0.00022	-0.00003
C	3.52139	0.00023	-0.00003
H	-1.25161	3.39106	-0.00014
Br	1.54718	4.14123	0.00007
Br	-1.54724	-4.14120	0.00025
H	1.25164	-3.39110	-0.00001
H	-3.37091	2.15089	0.00006
H	3.39070	2.14622	0.00001
H	-3.39073	-2.14621	-0.00008
H	3.37089	-2.15090	-0.00016
H	-4.61139	-0.00086	0.00001
H	4.61138	0.00092	-0.00017

26) Optimized 3D coordinates of NAA

C	-1.22048	0.75176	0.01088
C	-1.23569	-0.68172	0.00933
C	1.22134	0.75048	-0.02054
C	1.23546	-0.68304	-0.00591
C	0.00072	1.42968	-0.00804
C	-0.00046	-1.33465	0.00445

C	-2.47103	1.45268	0.03248
C	-2.49697	-1.36363	0.03259
C	2.47238	1.45022	-0.04806
C	2.49618	-1.36597	-0.02204
C	-3.65229	0.77392	0.05404
C	-3.66145	-0.65511	0.05523
C	3.65319	0.77044	-0.06256
C	3.66119	-0.65847	-0.05033
H	0.00124	2.52105	-0.01311
N	-0.00146	-2.80809	0.01091
H	-2.45533	2.54327	0.03275
H	-2.52116	-2.45243	0.02534
H	2.45751	2.54077	-0.05855
H	2.51975	-2.45466	-0.00456
H	-4.59749	1.31659	0.07069
H	-4.61472	-1.18363	0.07296
H	4.59881	1.31225	-0.08379
H	4.61407	-1.18789	-0.06218
O	-0.34270	-3.37202	-1.01245
O	0.33923	-3.36407	1.03869

27) Optimized 3D coordinates of NAP

C	-0.00000	-0.71083	-0.00001
C	-0.00001	0.71083	-0.00001
C	1.24475	-1.40002	-0.00002
C	1.24473	1.40004	-0.00001
C	-1.24474	-1.40004	-0.00001
C	-1.24476	1.40002	-0.00001
C	2.43003	-0.70931	-0.00003
C	2.43002	0.70934	-0.00002
C	-2.43003	-0.70934	-0.00001
C	-2.43004	0.70931	-0.00002
H	1.24175	-2.49138	-0.00003
H	1.24172	2.49139	-0.00001

H	-1.24173	-2.49139	-0.00001
H	-1.24177	2.49138	-0.00001
H	3.37747	-1.24930	-0.00004
H	3.37745	1.24935	-0.00003
H	-3.37746	-1.24935	-0.00001
H	-3.37748	1.24931	-0.00002

28) Optimized 3D coordinates of NNP

C	0.02000	-0.73755	0.02100
C	0.03216	0.68861	0.01857
C	1.25430	-1.44415	-0.00053
C	1.28738	1.35960	-0.02802
C	-1.21483	-1.44130	0.03710
C	-1.24452	1.32916	0.01559
C	2.44750	-0.77263	-0.03793
C	2.45706	0.64304	-0.05836
C	-2.41262	-0.77517	0.02548
C	-2.42689	0.63593	0.00178
H	1.23042	-2.53467	0.00749
H	1.31773	2.44500	-0.02964
H	-1.19140	-2.53180	0.05260
N	-1.36293	2.79707	0.03912
H	3.38863	-1.32246	-0.05597
H	3.40867	1.17381	-0.09597
H	-3.35473	-1.32184	0.03366
H	-3.36484	1.18713	-0.01861
O	-2.28138	3.29522	-0.58679
O	-0.55789	3.42846	0.70190

29) Optimized 3D coordinates of NPA

C	0.00945	-0.76353	0.00238
C	-0.02757	0.66117	-0.00639
C	1.26318	-1.43544	0.01078
C	1.21460	1.36091	-0.00651
C	-1.20826	-1.49587	0.00249

C	-1.31027	1.30622	-0.01485
C	2.43879	-0.73171	0.01043
C	2.40860	0.68397	0.00163
C	-2.42184	-0.85483	-0.00581
C	-2.46697	0.55446	-0.01453
H	1.27155	-2.52652	0.01741
H	1.23356	2.44844	-0.01318
H	-1.16115	-2.58620	0.00936
C	-1.45375	2.78725	-0.02373
H	3.39460	-1.25583	0.01678
H	3.34465	1.24315	0.00126
H	-3.34885	-1.42799	-0.00562
H	-3.42164	1.08062	-0.02107
O	-2.52363	3.35819	-0.03254
H	-0.51928	3.38540	-0.02200

30) Optimized 3D coordinates of NPY

C	-0.71880	-0.01938	-0.03120
C	0.71425	-0.00760	-0.01500
C	-1.41914	1.21829	-0.00926
C	1.42654	1.22001	0.04231
C	-1.44804	-1.24409	-0.07670
C	1.43627	-1.22838	-0.06568
C	-0.67047	2.45183	0.05066
C	0.68221	2.45562	0.07891
C	-0.65330	-2.45710	-0.11757
C	0.69965	-2.45903	-0.12906
C	-2.81721	1.21588	-0.05039
C	2.82649	1.19689	0.05513
C	-2.84749	-1.20172	-0.12503
C	2.83655	-1.21332	-0.05264
C	-3.51728	0.01782	-0.11535
C	3.52484	-0.00651	0.00867
H	-1.22768	3.38922	0.07199

H	1.23537	3.39447	0.12387
N	-1.29246	-3.78493	-0.12452
H	1.23324	-3.40674	-0.17663
H	-3.35294	2.16594	-0.03478
H	3.37070	2.14139	0.09934
H	-3.41881	-2.12444	-0.15726
H	3.38136	-2.15724	-0.09191
H	-4.60659	0.02698	-0.15382
H	4.61477	-0.00261	0.01822
O	-0.75343	-4.66585	-0.77025
O	-2.30443	-3.93676	0.53767

31) Optimized 3D coordinates of PCA

C	-0.70340	0.03789	-0.01997
C	0.72930	0.04990	-0.02970
C	-1.40666	1.27205	0.04469
C	1.44071	1.27835	0.02431
C	-1.41860	-1.19357	-0.07451
C	1.44997	-1.17201	-0.09395
C	-0.65905	2.50666	0.09791
C	0.69426	2.51184	0.08828
C	-0.64957	-2.42996	-0.14067
C	0.71142	-2.40053	-0.14893
C	-2.80574	1.26393	0.05457
C	2.84055	1.25765	0.01325
C	-2.82028	-1.15055	-0.06193
C	2.85110	-1.15259	-0.10269
C	-3.50099	0.06221	0.00185
C	3.53926	0.05455	-0.04944
H	-1.21558	3.44360	0.14531
H	1.24583	3.45206	0.12790
C	-1.30430	-3.76573	-0.20296
H	1.24933	-3.34846	-0.19892
H	-3.34560	2.21046	0.10362

H	3.38466	2.20248	0.05404
H	-3.40285	-2.06833	-0.10080
H	3.39590	-2.09616	-0.15151
H	-4.59109	0.06513	0.01036
H	4.62933	0.06014	-0.05696
O	-0.69293	-4.81116	-0.26631
H	-2.41327	-3.78695	-0.18944

32) Optimized 3D coordinates of PHN

C	-0.73034	-0.38126	0.00017
C	0.73036	-0.38122	0.00015
C	-1.42004	0.85492	0.00022
C	1.42001	0.85497	0.00020
C	-0.67683	2.08899	0.00025
C	0.67673	2.08901	0.00023
C	-1.49481	-1.57073	0.00011
C	1.49484	-1.57068	0.00007
C	-2.83321	0.86855	0.00025
C	2.83319	0.86863	0.00021
C	-2.87409	-1.53677	0.00016
C	2.87411	-1.53670	0.00006
C	-3.55440	-0.30535	0.00024
C	3.55441	-0.30527	0.00016
H	-1.23158	3.02840	0.00028
H	1.23144	3.02844	0.00027
H	-0.99665	-2.53844	0.00003
H	0.99674	-2.53843	0.00001
H	-3.34818	1.83072	0.00030
H	3.34813	1.83081	0.00028
H	-3.43860	-2.46962	0.00013
H	3.43866	-2.46954	-0.00000
H	-4.64444	-0.28186	0.00027
H	4.64445	-0.28176	0.00017

33) Optimized 3D coordinates of PYR

C	-0.71585	-0.00002	0.00015
C	0.71588	0.00003	0.00009
C	-1.42697	1.22962	0.00007
C	1.42694	1.22970	0.00006
C	-1.42695	-1.22967	0.00007
C	1.42697	-1.22962	0.00008
C	-0.67728	2.46438	0.00009
C	0.67719	2.46442	0.00008
C	-0.67721	-2.46441	0.00007
C	0.67727	-2.46438	0.00009
C	-2.82696	1.20830	-0.00004
C	2.82692	1.20841	-0.00008
C	-2.82693	-1.20843	-0.00006
C	2.82694	-1.20830	-0.00003
C	-3.51833	-0.00007	-0.00011
C	3.51832	0.00006	-0.00013
H	-1.22963	3.40525	0.00008
H	1.22947	3.40533	0.00009
H	-1.22950	-3.40530	0.00007
H	1.22961	-3.40526	0.00010
H	-3.37451	2.15204	-0.00008
H	3.37442	2.15219	-0.00014
H	-3.37445	-2.15218	-0.00012
H	3.37451	-2.15204	-0.00007
H	-4.60875	-0.00009	-0.00021
H	4.60875	0.00011	-0.00024