

## Revisiting the electron transfer between amicyanin and cytochrome c from a theoretical perspective

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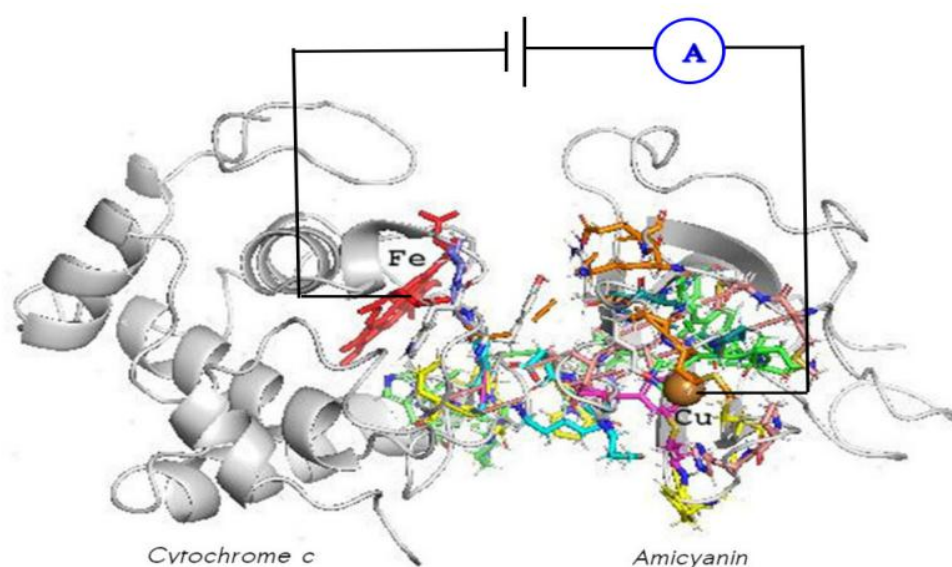
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### Supplementary Documents



**Figure S1.** Collection of all the ET(ET1-ET10) pathways between the Cytochrome c and amicyanin and were given in the picture.

Geometric coordinates which are considered for each pathways from ET1-ET10 are given below.

#### Geometry of Pathway ET1

N	-13.10723	0.13269	-0.92119
C	-13.71837	-0.63248	0.09194
C	-12.73598	-1.20504	1.11291
O	-13.01587	-2.26990	1.58812
C	-14.63205	-1.82502	-0.37233
C	-15.68127	-1.38775	-1.34718
S	-17.29888	-0.60459	-0.68914
C	-18.06955	-0.32454	-2.31559
H	-13.43361	1.06872	-0.97255
H	-14.23710	0.09586	0.69629
H	-13.98384	-2.63350	-0.78351
H	-15.13821	-2.25479	0.50408
H	-15.27389	-0.74147	-2.14571
H	-16.17616	-2.23563	-1.86736
H	-19.00872	0.25246	-2.21802

H	-17.44970	0.29182	-3.00027
H	-18.28308	-1.30179	-2.80107
N	-11.68899	-0.48758	1.41961
C	-10.64315	-1.10906	2.26542
C	-9.70465	0.01096	2.70471
O	-9.65537	1.12693	2.21219
C	-9.80833	-2.19000	1.56175
C	-8.89269	-1.77433	0.45680
C	-8.29494	-3.09276	-0.18134
C	-6.81164	-2.93687	-0.48862
N	-6.50304	-2.02370	-1.60356
H	-11.43029	0.35681	0.96291
H	-11.18268	-1.38400	3.15958
H	-9.20227	-2.70062	2.34919
H	-10.48006	-3.01100	1.22406
H	-9.43159	-1.23731	-0.34452
H	-8.08127	-1.10545	0.80650
H	-8.49133	-3.88124	0.57518
H	-8.87101	-3.27129	-1.10398
H	-6.32237	-2.47426	0.39575
H	-6.51123	-3.91972	-0.91142
H	-6.36590	-1.03812	-1.30622
H	-5.59403	-2.16998	-2.07270
H	-7.25579	-2.02903	-2.32401
N	-5.62272	0.48575	2.90529
C	-4.45166	0.03531	2.24664
C	-3.53117	-0.78678	3.14190
O	-3.04876	-1.87430	2.72348
C	-3.65474	1.25042	1.64098
C	-4.37114	1.92003	0.47060
C	-4.75721	0.85016	-0.62982
O	-3.89314	0.51062	-1.47516
O	-5.83499	0.27894	-0.59118
H	-5.68536	1.47914	2.87747
H	-4.79441	-0.72353	1.55117
H	-3.38113	1.97044	2.43244
H	-2.71762	0.77089	1.28652
H	-5.31654	2.45768	0.70821
H	-3.72536	2.58212	-0.15295
N	1.03096	-1.62217	1.27903
C	-0.33255	-1.65724	0.77443
C	-0.75241	-2.95870	0.06442
O	0.10840	-3.67707	-0.42909
C	-0.36869	-0.46286	-0.16256
C	0.59240	0.59641	0.44346
C	1.69369	-0.39017	0.89923
H	-1.00306	-1.47694	1.59790
H	-0.01986	-0.71127	-1.18798
H	-1.39280	-0.03431	-0.17475
H	0.85465	1.42016	-0.26595
H	0.28981	1.07958	1.38982
H	2.34728	-0.71254	0.05507
H	2.38346	0.07678	1.63806
N	-2.03718	-3.25995	0.01836
C	-2.77702	-4.26801	-0.68054
C	-3.09312	-3.90158	-2.05401
O	-4.23802	-3.54278	-2.34395
H	-2.47551	-2.57463	0.59134
H	-2.26400	-5.21110	-0.79138
H	-3.74874	-4.27349	-0.20543
Cu	-16.80855	5.20568	0.82407
C	5.43517	1.97071	-4.08777
C	9.99440	-5.61982	-0.09156
C	11.05470	0.39573	5.01784

C	6.85233	5.10693	0.28403
N	7.71677	0.14529	-1.74166
C	4.05273	1.55230	-3.58272
C	10.01559	-6.69093	-0.81577
C	11.64894	-0.06131	6.13828
C	7.11159	5.70504	-1.15014
N	8.81348	-2.11618	-0.51188
C	2.79200	2.36887	-3.98767
C	7.83263	7.07911	-0.99188
N	8.24995	1.62549	0.56312
C	6.93119	2.42801	-1.25933
C	7.87938	-1.98171	-2.73061
C	9.92109	-2.94802	1.53002
C	9.59825	1.70373	2.64011
C	6.71550	-0.56110	-5.23650
C	8.68290	-4.82435	-2.88679
C	10.89753	-2.65757	4.35846
C	8.54179	4.58366	2.89692
C	6.99765	1.27771	-2.08090
C	8.51750	-2.66347	-1.70279
C	9.98125	-1.70891	2.20366
C	8.76654	2.25416	1.70102
O	2.42163	2.43264	-5.13298
O	8.94855	7.09767	-1.52974
C	6.49220	1.13818	-3.43074
C	8.86194	-4.01418	-1.71860
C	10.58060	-1.54356	3.48781
C	8.32461	3.57340	1.81933
O	2.21776	2.95782	-3.03794
O	7.22830	8.03925	-0.46900
C	6.96714	-0.01417	-3.90056
C	9.47119	-4.40109	-0.55065
C	10.63519	-0.27215	3.88609
C	7.49642	3.81262	0.69441
C	7.62300	-0.62533	-2.76785
C	9.41608	-3.15305	0.19464
C	9.97604	0.36065	2.69933
C	7.51792	2.58115	-0.01631
N	9.54948	-0.51421	1.70904
Fe	8.56917	-0.21183	-0.01042
H	-12.10239	0.15244	-0.74688
H	-9.05745	-0.19139	3.48278
H	-6.44026	0.08693	2.44369
H	-3.30263	-0.45274	4.09151
H	-3.06645	0.95043	-1.50320
H	1.01258	-1.69093	2.29671
H	-2.36286	-3.94189	-2.78179
H	5.60038	3.00256	-3.85559
H	5.48128	1.82649	-5.14650
H	10.37873	-5.66252	0.86522
H	10.88530	1.41368	5.00432
H	5.79523	4.96497	0.37167
H	7.31272	5.82243	0.93242
H	3.89219	0.54997	-3.91995
H	4.11914	1.71378	-2.52671
H	9.63724	-6.67245	-1.77595
H	10.41136	-7.56419	-0.43378
H	11.85623	-1.06745	6.23877
H	11.89578	0.59478	6.89616
H	7.72896	5.03634	-1.71350
H	6.18285	5.83632	-1.66551
H	6.39335	3.22983	-1.62315
H	7.56853	-2.54009	-3.54114
H	10.26812	-3.77788	2.03615

H	9.97717	2.33425	3.36454
H	6.20351	0.16742	-5.83013
H	6.11275	-1.44148	-5.15366
H	7.64674	-0.80929	-5.70115
H	8.17567	-4.25719	-3.63967
H	8.10059	-5.68683	-2.63706
H	9.63842	-5.13372	-3.25659
H	11.33768	-2.29007	5.26234
H	11.58760	-3.31054	3.86489
H	10.00202	-3.19464	4.59118
H	8.04465	5.49474	2.63745
H	9.58985	4.76845	3.00700
H	8.14726	4.21177	3.81912
H	2.88808	1.97247	-5.80239
H	9.30663	6.31156	-1.89154

### Geometry of Pathway ET2

N	-9.11219	-0.87918	-0.21757
C	-8.06118	-0.78144	0.74629
C	-6.70672	-0.90789	-0.01024
O	-6.59178	-1.76729	-0.91535
C	-8.26468	-1.77711	1.84271
C	-9.53274	-1.58801	2.62940
C	-9.63382	-0.49146	3.54267
C	-10.75565	-2.34385	2.48080
C	-10.81388	-0.17728	4.17216
C	-11.87382	-2.05468	3.14411
C	-11.88463	-0.98867	3.95830
O	-13.14317	-0.74891	4.62904
H	-9.28180	-1.84065	-0.39370
H	-8.09582	0.13643	1.32302
H	-8.35075	-2.82635	1.49019
H	-7.41781	-1.71369	2.55747
H	-8.87334	0.26091	3.70699
H	-10.78009	-3.19094	1.81026
H	-10.98930	0.55973	4.93776
H	-12.80859	-2.54906	2.91003
H	-13.10459	0.09986	5.07982
N	-5.74177	-0.00732	0.29168
C	-4.44401	-0.10515	-0.26898
C	-3.70619	-1.37847	0.12962
O	-3.11081	-2.06413	-0.74553
C	-3.57793	1.15166	0.11665
C	-4.05335	2.44078	-0.54935
C	-4.16337	2.24853	-2.11637
O	-3.12986	2.37842	-2.81743
O	-5.20564	1.86854	-2.62497
H	-5.82990	0.81936	0.83970
H	-4.60730	-0.28399	-1.32651
H	-3.50114	1.25027	1.21395
H	-2.57185	0.87709	-0.26573
H	-5.04481	2.83082	-0.22658
H	-3.31291	3.27480	-0.53040
N	2.44505	-4.50824	0.68583
C	2.21718	-3.05742	0.54981
C	1.10996	-2.63695	-0.31816
O	0.19090	-3.39947	-0.53099
H	2.34482	-5.03457	-0.15869
H	2.07490	-2.62846	1.53543
H	3.15467	-2.71786	0.15586
N	1.17106	-1.42168	-0.96204
C	-0.05360	-1.02538	-1.63891

C	-0.27124	-1.62774	-3.04033
O	0.69746	-2.00785	-3.68665
C	0.06908	0.48746	-1.68456
C	0.84540	0.90113	-0.40425
C	1.85790	-0.26876	-0.41400
H	-0.88814	-1.29043	-1.01162
H	0.63414	0.84551	-2.57192
H	-0.94305	0.94132	-1.63747
H	1.22390	1.95309	-0.43104
H	0.33444	0.77443	0.56707
H	2.68495	-0.10516	-1.14401
H	2.36072	-0.38520	0.57257
N	-1.50680	-1.71993	-3.49683
C	-2.04909	-2.05994	-4.77836
C	-2.08063	-0.93787	-5.70602
O	-3.14994	-0.36806	-5.94157
H	-2.07839	-1.45370	-2.72709
H	-1.49339	-2.80955	-5.32074
H	-3.09838	-2.24460	-4.59155
N	-15.81697	-4.02977	-0.56873
C	-14.48765	-3.59873	-0.19280
C	-14.04830	-4.29427	1.11426
O	-14.80278	-4.11714	2.07586
C	-14.50994	-2.11277	0.24936
C	-14.86882	-1.14062	-0.88797
S	-15.02402	0.56328	-0.24248
C	-13.41705	0.86350	0.49841
H	-16.63842	-3.48140	-0.36896
H	-13.81158	-3.78915	-1.01486
H	-15.23321	-2.01775	1.09313
H	-13.46919	-1.87352	0.57387
H	-14.08351	-1.18194	-1.66955
H	-15.83167	-1.31448	-1.41901
H	-12.61473	0.55493	-0.20448
H	-13.22197	1.92200	0.76474
H	-13.24687	0.20016	1.37569
Cu	-16.38757	6.10851	-0.70615
C	6.48612	4.16375	-2.25114
C	10.34903	-4.73928	-2.68288
C	10.10983	-2.92659	5.06786
C	6.84601	4.03655	3.29965
N	8.28117	1.10600	-1.03866
C	5.04288	3.66737	-2.36051
C	10.55769	-5.18983	-3.87689
C	10.46941	-4.00276	5.79583
C	7.38174	5.32534	2.56901
N	9.16818	-1.54369	-1.18605
C	3.86952	4.68571	-2.44054
C	8.00749	6.27634	3.63533
N	8.26761	0.91952	1.74565
C	7.33668	2.75216	0.52938
C	8.71862	-0.06029	-3.03289
C	9.84755	-3.50645	0.14591
C	9.14469	-0.34995	3.68396
C	8.06260	2.65318	-4.39631
C	9.63040	-2.35031	-4.66845
C	10.19600	-5.00256	2.73012
C	7.96335	1.93670	5.37268
C	7.61268	2.28938	-0.77916
C	9.14800	-1.26915	-2.50120
C	9.72349	-2.89851	1.41391
C	8.51180	0.72007	3.10854
O	3.74687	5.43599	-3.37598
O	9.21044	6.49384	3.43408

C	7.40787	3.00648	-2.02046
C	9.53244	-2.38742	-3.23942
C	10.03303	-3.56584	2.63639
C	8.01157	1.76306	3.89061
O	3.08894	4.66919	-1.45615
O	7.27519	6.81030	4.49505
C	8.00891	2.29878	-2.97550
C	9.89437	-3.43575	-2.43010
C	9.96048	-2.77190	3.70526
C	7.43154	2.68822	2.98714
C	8.43120	1.08469	-2.31644
C	9.64229	-2.85080	-1.12228
C	9.54565	-1.50870	3.01566
C	7.64295	2.09995	1.70990
N	9.36643	-1.60279	1.64197
Fe	8.76097	-0.26774	0.27813
H	-8.83281	-0.41389	-1.08117
H	-3.69401	-1.67955	1.11694
H	-2.33080	2.67031	-2.42507
H	1.77637	-4.87054	1.36523
H	-1.21250	-0.62062	-6.16457
H	-15.79853	-4.15545	-1.58122
H	-13.98903	-5.34653	0.92759
H	-13.10852	-3.85917	1.38521
H	-15.67362	-4.49704	1.87807
H	6.56454	4.84898	-1.43247
H	6.75899	4.65492	-3.16115
H	10.52435	-5.36478	-1.88102
H	9.91357	-2.07788	5.62129
H	5.79946	3.97383	3.08500
H	7.13558	4.19607	4.31700
H	4.99017	3.06634	-3.24377
H	4.87993	3.18078	-1.42119
H	10.38974	-4.58256	-4.69448
H	10.89270	-6.15657	-4.01227
H	10.68397	-4.89591	5.32505
H	10.52923	-3.93389	6.82415
H	8.12568	5.04955	1.85056
H	6.57862	5.82023	2.06358
H	6.86139	3.66437	0.61027
H	8.60412	-0.01334	-4.05762
H	10.10736	-4.50510	0.12453
H	9.34144	-0.29531	4.69601
H	7.66341	3.63646	-4.53454
H	7.48532	1.95099	-4.96104
H	9.07851	2.63029	-4.73114
H	9.27474	-1.40607	-5.02578
H	9.03734	-3.13655	-5.08731
H	10.65207	-2.47999	-4.95977
H	10.42345	-5.27069	3.74114
H	10.99575	-5.31304	2.08966
H	9.28978	-5.48491	2.42903
H	7.50224	2.87306	5.60751
H	8.95801	1.92059	5.76649
H	7.39587	1.14046	5.80671
H	4.35883	5.40514	-4.08450
H	9.66247	6.03164	2.75649

### Geometry of Pathway ET3

N	-7.00389	-1.29352	-0.06627
C	-5.95226	-1.27440	-1.03422
C	-4.60065	-1.17653	-0.26841
O	-4.50904	-0.39822	0.70977

C	-6.18659	-0.19135	-2.03770
C	-7.45008	-0.34639	-2.83906
C	-7.52098	-1.35969	-3.84649
C	-8.69414	0.35733	-2.62462
C	-8.69258	-1.65071	-4.50235
C	-9.80466	0.09603	-3.31190
C	-9.78603	-0.89307	-4.21785
O	-11.03831	-1.10860	-4.90823
H	-7.20101	-0.35691	0.19471
H	-5.96131	-2.13785	-1.69047
H	-6.30243	0.81937	-1.59314
H	-5.33955	-0.16618	-2.75463
H	-6.73928	-2.07199	-4.07662
H	-8.74192	1.14024	-1.88128
H	-8.84794	-2.32136	-5.33071
H	-10.75296	0.54020	-3.03539
H	-10.97594	-1.91235	-5.43283
N	-1.62976	-0.06176	-1.56809
C	-1.00011	1.27940	-1.88279
C	-2.08629	2.31043	-2.21683
O	-2.73475	2.16635	-3.23827
C	-0.07175	1.30934	-3.08651
C	0.94154	2.46725	-3.13430
O	0.60572	0.09278	-3.12413
H	-2.02521	-0.66668	-2.25350
H	-0.47253	1.55924	-0.97430
H	-0.64726	1.45277	-4.03788
H	0.87919	-0.03078	-4.03366
H	0.53873	3.48017	-2.92091
H	1.78481	2.33320	-2.41749
H	1.36478	2.50050	-4.15820
N	-2.39842	3.45581	-1.48534
C	-3.70827	4.07088	-1.60363
C	-3.69555	5.07853	-2.69477
O	-4.81674	5.35692	-3.18503
C	-3.76822	4.91781	-0.32676
C	-2.29015	5.01448	0.15531
C	-1.76365	3.66169	-0.18373
H	-4.45324	3.30739	-1.67970
H	-4.36241	5.85941	-0.25368
H	-4.19253	4.39962	0.55456
H	-1.86120	5.75511	-0.55749
H	-2.16930	5.32735	1.21474
H	-0.65020	3.59263	-0.24902
H	-2.16502	2.93409	0.55680
N	-0.14372	3.16983	4.47412
C	0.10705	3.06270	3.07122
C	0.37639	4.43776	2.54012
O	-0.27934	5.39357	2.92722
H	0.62801	3.25600	5.10103
H	0.95046	2.40087	2.95788
H	-0.72903	2.61481	2.56272
N	1.39484	4.55715	1.66622
C	1.70459	5.76072	1.01324
C	2.48768	5.44956	-0.26082
O	1.85499	5.21697	-1.27803
C	2.39604	6.78810	1.91617
C	2.43128	8.18808	1.36101
C	3.10963	9.26075	2.33861
C	2.97079	10.71631	1.82229
N	3.86073	11.08921	0.63277
H	1.93100	3.75637	1.42254
H	0.76729	6.22096	0.73421
H	1.80484	6.90363	2.84979

H	3.37394	6.34007	2.22840
H	3.00477	8.18052	0.41235
H	1.45869	8.58435	1.01013
H	2.62904	9.26024	3.33928
H	4.16575	8.97658	2.52500
H	1.95294	10.97211	1.46699
H	3.26424	11.46968	2.58989
H	3.52761	10.60261	-0.22061
H	3.93689	12.08541	0.34178
H	4.83585	10.76354	0.74975
N	3.83773	5.30718	-0.26018
C	4.55709	5.00951	-1.58174
C	4.48659	3.47623	-1.76879
O	4.44562	2.95533	-2.93977
C	6.04816	5.25904	-1.56643
C	6.24727	6.70751	-1.22232
C	6.59009	4.95504	-2.99699
C	7.72257	7.15214	-1.25046
H	4.38332	5.52408	0.54100
H	3.98172	5.46549	-2.37718
H	6.59183	4.56093	-0.89616
H	5.79983	7.29335	-2.04730
H	5.62865	7.02840	-0.35783
H	7.67236	5.15772	-3.07591
H	6.39370	3.97409	-3.49834
H	6.04534	5.58216	-3.73017
H	8.20139	6.49069	-0.49329
H	8.24477	7.07960	-2.23298
H	7.91469	8.21858	-1.00124
N	4.44147	2.73606	-0.63401
C	4.25605	1.27289	-0.62798
C	3.16311	0.74474	0.19824
O	2.22270	1.45823	0.47747
H	4.32756	3.18193	0.25398
H	4.12447	0.92949	-1.64801
H	5.20373	0.92697	-0.26516
N	3.26064	-0.52077	0.73130
C	2.04925	-1.01124	1.36924
C	1.81680	-0.54271	2.81860
O	2.77525	-0.19369	3.49695
C	2.21587	-2.51791	1.28000
C	3.00151	-2.79312	-0.03150
C	3.97965	-1.59981	0.08322
H	1.20621	-0.71572	0.76744
H	2.79272	-2.93702	2.13234
H	1.21726	-2.99501	1.19189
H	3.41043	-3.83184	-0.09827
H	2.48529	-2.59530	-0.98805
H	4.81244	-1.80369	0.79637
H	4.47705	-1.38138	-0.88867
N	0.57993	-0.52752	3.28058
C	0.03036	-0.31895	4.58690
C	0.03311	-1.51965	5.41085
O	-1.01878	-2.13903	5.59389
H	0.01489	-0.74062	2.48975
H	0.56507	0.39519	5.19434
H	-1.02419	-0.14897	4.41650
N	1.16926	-1.92492	5.95660
C	1.26722	-3.05844	6.83820
C	0.69070	-2.84213	8.26499
O	1.42139	-2.43913	9.22012
C	2.68827	-3.53338	7.13340
C	3.53373	-3.86747	5.92704
C	2.79237	-4.73721	4.89160



C	4.32166	-2.76607	5.25393
H	2.05356	-1.58257	5.63767
H	0.71380	-3.93377	6.54488
H	3.28001	-2.75576	7.65074
H	2.62467	-4.48645	7.71245
H	4.29144	-4.52311	6.40423
H	3.51028	-5.04692	4.10338
H	2.31651	-5.55379	5.46680
H	1.99122	-4.06819	4.50178
H	4.88139	-3.17545	4.38860
H	3.69834	-1.91165	4.88866
H	5.11465	-2.31666	5.88385
N	-14.23937	0.39274	-4.39499
C	-14.76071	-0.98605	-4.49109
C	-16.28778	-0.99070	-4.56753
O	-16.98657	-0.49441	-3.70567
C	-14.27754	-1.89648	-3.28616
S	-14.35713	-3.69091	-3.65519
H	-14.23001	0.62702	-3.42931
H	-14.30751	-1.33538	-5.40485
H	-13.21419	-1.62475	-3.12639
H	-14.88411	-1.61996	-2.40201
H	-13.67299	-4.01527	-2.56829
N	-16.39139	2.64308	0.78289
C	-15.44181	3.18735	1.74968
C	-14.07479	2.68803	1.38194
O	-13.13525	3.36638	1.78755
C	-15.87082	2.82342	3.25171
C	-16.03005	1.35140	3.54223
C	-17.29017	0.93848	4.06967
C	-15.01960	0.36839	3.53254
C	-17.51514	-0.38416	4.53925
C	-15.24234	-0.92868	3.89059
C	-16.46197	-1.35682	4.37410
H	-17.03253	1.94450	1.11018
H	-15.51194	4.23510	1.52227
H	-15.26056	3.30583	4.04781
H	-16.88680	3.27034	3.34191
H	-18.11607	1.61598	4.16184
H	-14.01264	0.65691	3.26110
H	-18.47928	-0.64731	4.96888
H	-14.38870	-1.58796	3.86321
H	-16.53427	-2.29780	4.88403
N	-13.79663	1.61698	0.55922
C	-12.45605	1.25998	0.14737
C	-12.03949	2.08168	-1.09218
O	-12.79028	1.96907	-2.06631
C	-12.43602	-0.18070	-0.42546
C	-12.76444	-1.26033	0.62044
S	-12.87130	-2.90373	-0.17443
C	-11.25767	-3.08990	-0.93793
H	-14.60218	1.06494	0.31076
H	-11.78428	1.39598	0.98363
H	-13.15778	-0.22115	-1.27489
H	-11.38936	-0.35972	-0.76922
H	-11.97921	-1.26599	1.40319
H	-13.73094	-1.16254	1.16414
H	-10.46334	-2.82199	-0.20973
H	-11.03243	-4.11434	-1.29737
H	-11.10843	-2.34637	-1.75248
Cu	-14.07247	-8.50550	-0.20777
C	8.73794	-6.04193	1.52154
C	12.34161	2.89575	2.74782
C	12.14083	1.77463	-5.13379

C	9.08376	-5.41029	-3.99555
N	10.44125	-2.83744	0.58771
C	7.28111	-5.59944	1.67363
C	12.53930	3.24400	3.97739
C	12.46769	2.92139	-5.76269
C	9.65801	-6.74292	-3.38227
N	11.25125	-0.18675	0.97130
C	6.13795	-6.65455	1.66171
C	10.30914	-7.57655	-4.52862
N	10.41715	-2.40410	-2.16891
C	9.54204	-4.36410	-1.12149
C	10.84834	-1.84123	2.67827
C	11.87091	1.90580	-0.17995
C	11.25344	-0.94202	-3.98573
C	10.27387	-4.68331	3.79397
C	11.69628	0.31950	4.51207
C	12.17102	3.63569	-2.62030
C	10.13585	-3.10249	-5.87239
C	9.80691	-4.01192	0.22329
C	11.24147	-0.57784	2.25674
C	11.76220	1.40990	-1.49717
C	10.65294	-2.07700	-3.50843
O	6.03886	-7.48843	2.52648
O	11.51826	-7.77604	-4.34665
C	9.62529	-4.84241	1.39559
C	11.59465	0.48092	3.09196
C	12.04999	2.19221	-2.65509
C	10.18174	-3.06027	-4.38070
O	5.35540	-6.57309	0.68212
O	9.59106	-8.05285	-5.43306
C	10.20730	-4.20544	2.41035
C	11.92450	1.60726	2.37954
C	11.99855	1.49489	-3.79051
C	9.63049	-4.07871	-3.56370
C	10.59295	-2.92570	1.86242
C	11.68710	1.13408	1.02461
C	11.62182	0.16375	-3.21653
C	9.82708	-3.60068	-2.23896
N	11.44249	0.12982	-1.84005
Fe	10.87855	-1.33847	-0.60106
H	-6.70953	-1.82558	0.75265
H	-3.79022	-1.74474	-0.56230
H	-0.90213	-0.60617	-1.10527
H	-2.82397	5.51930	-3.02743
H	-0.65945	2.33417	4.74937
H	-0.30907	-3.03066	8.43873
H	-14.84476	1.03391	-4.90616
H	-16.74277	-1.43173	-5.38170
H	-16.94393	3.42266	0.42455
H	-12.01044	3.11441	-0.81244
H	-11.08798	1.69997	-1.40012
H	-13.67141	2.30437	-1.83610
H	8.83471	-6.64893	0.64513
H	9.02663	-6.60409	2.38436
H	12.49722	3.59504	2.00502
H	11.96827	0.97326	-5.76080
H	8.03622	-5.39739	-3.77696
H	9.37596	-5.47004	-5.02286
H	7.21261	-5.08129	2.60690
H	7.10238	-5.03605	0.78128
H	12.39056	2.56168	4.73748
H	12.84636	4.20417	4.19862
H	12.65710	3.77489	-5.21404
H	12.52758	2.94618	-6.79302

H	10.39496	-6.51073	-2.64154
H	8.87053	-7.30402	-2.92355
H	9.09329	-5.27890	-1.28370
H	10.73714	-1.98261	3.69465
H	12.10166	2.90570	-0.06947
H	11.44983	-0.90053	-4.99847
H	9.90364	-5.68618	3.84373
H	9.67749	-4.05130	4.41859
H	11.28930	-4.66081	4.13027
H	11.36883	-0.66277	4.78357
H	11.08142	1.04772	4.99888
H	12.71429	0.45236	4.81455
H	12.38873	3.99933	-3.60323
H	12.96260	3.91100	-1.95412
H	11.25174	4.06275	-2.27810
H	9.70169	-4.02722	-6.19006
H	11.12890	-3.02246	-6.26245
H	9.54470	-2.28759	-6.23415
H	6.65096	-7.50305	3.23538
H	11.95793	-7.36310	-3.63023

#### Geometry of Pathway ET4

N	-3.26110	2.18990	-0.44252
C	-4.24263	1.17011	-0.38053
C	-4.45550	0.54697	-1.78427
O	-4.91032	1.27412	-2.62765
C	-5.67312	1.58149	0.21735
C	-5.57200	2.67850	1.36214
C	-6.34516	0.31111	0.94419
C	-6.83329	3.24308	1.95840
H	-3.52383	2.99276	-0.97692
H	-3.87999	0.35414	0.21343
H	-6.27588	1.92930	-0.65277
H	-4.88202	2.28026	2.12858
H	-4.94528	3.51422	0.97163
H	-7.28774	0.51203	1.49162
H	-6.42565	-0.43259	0.11459
H	-5.65890	-0.03368	1.74709
H	-6.59536	3.78592	2.89275
H	-7.40808	3.88629	1.26422
H	-7.51656	2.41888	2.28512
N	-4.16459	-0.76352	-2.04693
C	-4.58422	-1.41843	-3.35933
C	-4.55056	-2.89555	-3.09954
O	-3.88373	-3.39933	-2.19996
C	-3.54560	-1.18536	-4.50295
H	-3.97353	-1.37052	-1.28035
H	-5.61187	-1.13396	-3.54912
H	-3.85019	-1.74562	-5.40485
H	-3.57409	-0.09136	-4.70801
H	-2.50177	-1.43373	-4.20812
N	-5.58993	-4.81099	0.29607
C	-4.63680	-4.72704	1.42740
C	-4.12777	-3.28932	1.47259
O	-4.24960	-2.46703	0.57850
C	-3.42491	-5.66474	1.31543
C	-2.41996	-5.40288	0.24137
C	-1.38707	-6.60104	0.25985
C	0.04087	-6.10501	0.07587
N	0.35196	-5.60059	-1.27357
H	-5.45471	-4.14882	-0.43313
H	-5.27538	-4.82134	2.29316
H	-2.90107	-5.64278	2.30195

H	-3.77928	-6.71908	1.26980
H	-2.88396	-5.38534	-0.76128
H	-1.89872	-4.43401	0.37444
H	-1.54391	-7.08777	1.24528
H	-1.68131	-7.26789	-0.56703
H	0.19112	-5.22923	0.74364
H	0.66223	-7.02521	0.12220
H	0.17030	-4.58449	-1.38826
H	1.34944	-5.60918	-1.54334
H	-0.19676	-6.09893	-2.00586
N	-15.59714	7.62668	1.03873
C	-15.04988	6.76361	0.04489
C	-14.22129	7.54903	-0.92873
O	-14.67123	8.50036	-1.54625
C	-16.16350	5.91671	-0.67284
C	-16.98419	4.95426	0.18812
S	-16.06271	3.67791	0.86657
C	-17.40865	2.99510	1.88942
H	-16.51901	8.01625	0.97168
H	-14.44749	6.03705	0.55689
H	-16.91538	6.54785	-1.19183
H	-15.75173	5.42349	-1.58633
H	-17.33973	5.56167	1.04417
H	-17.83064	4.59988	-0.43450
H	-17.87789	3.81657	2.46951
H	-18.22121	2.51233	1.30762
H	-17.06599	2.15072	2.52574
N	4.51059	-4.70230	1.17630
C	4.21858	-6.07111	0.87120
C	4.13390	-6.33674	-0.55809
O	3.02946	-6.48546	-1.08883
H	3.79988	-4.03400	1.37217
H	4.96136	-6.77834	1.20736
H	3.19839	-6.21370	1.20119
N	-12.90563	7.16524	-1.03574
C	-11.90233	7.64238	-1.92366
C	-11.94559	7.10391	-3.34647
O	-11.82561	5.89307	-3.45997
C	-10.46630	7.54322	-1.49496
C	-10.30003	8.13981	-0.06253
S	-8.52403	8.02717	0.40409
C	-8.70715	6.29824	1.18369
H	-12.52697	6.47192	-0.44167
H	-12.11429	8.70073	-2.01013
H	-10.21088	6.45718	-1.40186
H	-9.64020	7.97559	-2.10218
H	-10.57883	9.20848	-0.10512
H	-10.96627	7.66033	0.68761
H	-8.56409	5.44286	0.48845
H	-7.88180	6.16853	1.91312
H	-9.66526	6.27044	1.75216
N	5.24964	-6.41990	-1.26598
C	5.27853	-6.74280	-2.66834
C	4.98058	-8.22820	-3.01432
O	5.91202	-9.08196	-3.12429
C	6.61927	-6.51293	-3.36238
C	7.19167	-5.12025	-3.24198
C	6.15330	-4.01408	-3.51835
C	8.04993	-4.77937	-2.04440
H	6.12022	-6.07740	-0.91147
H	4.53767	-6.25733	-3.27985
H	7.41478	-7.15212	-2.93683
H	6.47645	-6.67099	-4.45888
H	7.88410	-5.12594	-4.10927

H	6.67157	-3.03246	-3.53866
H	5.63408	-4.31145	-4.44898
H	5.43474	-4.10117	-2.67130
H	8.38459	-3.72398	-2.10652
H	7.54129	-4.92255	-1.05811
H	8.99941	-5.34703	-1.98228
N	-15.71689	-1.30721	3.36840
C	-16.36253	-2.32273	2.49847
C	-15.76883	-3.77023	2.69510
O	-16.33248	-4.78305	2.30950
C	-16.07380	-1.93021	1.00912
C	-16.00214	-0.40852	1.14998
C	-15.27363	-0.20004	2.50921
H	-17.40965	-2.37367	2.75447
H	-15.05115	-2.28207	0.72400
H	-16.83630	-2.37459	0.33501
H	-15.46249	0.09899	0.32117
H	-17.03418	0.00440	1.10331
H	-14.16996	-0.26681	2.52200
H	-15.50340	0.80062	2.94701
N	-14.60356	-3.85299	3.36838
C	-13.99386	-5.18928	3.59285
C	-13.33370	-5.28738	4.93377
O	-12.16900	-4.91941	4.96004
C	-12.77035	-5.34335	2.62141
C	-13.23493	-5.65233	1.23892
C	-13.99526	-6.69087	0.90389
N	-12.74516	-5.01002	0.10871
C	-13.24889	-5.67787	-0.90259
N	-13.95445	-6.75770	-0.47218
H	-14.03139	-3.04322	3.46833
H	-14.67573	-5.99848	3.38491
H	-12.13192	-4.44764	2.70636
H	-12.16665	-6.21828	2.94241
H	-14.37007	-7.42282	1.61499
H	-12.99662	-5.55576	-1.95542
H	-14.23879	-7.59169	-0.94611
Cu	-11.70064	-1.62947	-3.09730
C	11.16589	0.79805	-3.87439
C	16.46611	-3.02061	3.31574
C	14.83746	4.42278	5.63101
C	10.75314	5.55864	-1.02425
N	13.25094	0.74611	-0.76120
C	9.85447	0.17319	-3.39371
C	16.91296	-4.21372	3.09437
C	15.26302	4.60652	6.89693
C	11.16682	5.65683	-2.54116
N	14.57468	-0.46023	1.38865
C	8.55249	0.34980	-4.22669
C	11.46995	7.14953	-2.87725
N	12.87470	3.03597	0.78873
C	11.83573	2.67798	-1.33186
C	14.15236	-1.42545	-0.78008
C	15.37319	-0.11666	3.69786
C	13.66609	4.26866	2.78675
C	13.25726	-1.43374	-3.75513
C	15.65140	-3.72832	0.31549
C	15.59462	1.45252	6.25257
C	11.89697	6.56030	1.74047
C	12.36653	1.39486	-1.60472
C	14.69569	-1.45850	0.49746
C	14.97249	1.23196	3.81392
C	12.95321	4.15661	1.62234
O	8.44131	-0.11814	-5.33199

O	12.63675	7.32682	-3.25415
C	12.22388	0.63274	-2.82776
C	15.35980	-2.54376	1.06708
C	15.21181	2.02308	4.97687
C	12.18228	5.21987	1.14815
O	7.65407	1.02434	-3.66418
O	10.54549	7.98942	-2.85593
C	13.06237	-0.39822	-2.73684
C	15.77154	-2.27670	2.34932
C	14.85887	3.30048	4.82922
C	11.59129	4.76906	-0.05854
C	13.58162	-0.32626	-1.39077
C	15.24404	-0.93113	2.51453
C	14.34312	3.22730	3.42496
C	12.07531	3.43975	-0.20265
N	14.37798	1.97096	2.83472
Fe	13.75966	1.31636	1.04638
H	-3.05965	2.49428	0.50993
H	-5.11266	-3.51530	-3.70379
H	-5.51326	-5.74391	-0.10991
H	-3.63970	-2.98651	2.33009
H	-15.57680	7.10010	1.91193
H	5.11776	-4.71880	1.99592
H	-12.06856	7.72147	-4.16382
H	4.00284	-8.52616	-3.15762
H	-16.38592	-0.96524	4.05890
H	-13.36655	-6.30988	5.24689
H	-13.87227	-4.62895	5.58288
H	-11.63676	-5.48895	4.38293
H	11.01363	1.84053	-4.06399
H	11.47992	0.30934	-4.77237
H	16.62701	-2.59675	4.24280
H	14.42764	5.26011	5.18825
H	9.77229	5.13129	-0.99989
H	10.86560	6.56392	-0.67628
H	10.02708	-0.87919	-3.31094
H	9.64284	0.71162	-2.49319
H	16.76448	-4.65820	2.17468
H	17.41857	-4.72132	3.83723
H	15.68636	3.82248	7.41792
H	15.16462	5.53107	7.34560
H	12.04009	5.06307	-2.71592
H	10.37274	5.29602	-3.16135
H	11.20989	3.08435	-2.04443
H	14.17778	-2.30295	-1.32297
H	15.79454	-0.55732	4.53066
H	13.70600	5.20049	3.22950
H	12.72496	-1.16540	-4.64392
H	12.88946	-2.36906	-3.38751
H	14.30002	-1.52339	-3.97717
H	15.19902	-3.65706	-0.65200
H	15.26144	-4.58212	0.82958
H	16.71125	-3.83042	0.20696
H	15.71788	2.23606	6.97135
H	16.51705	0.92035	6.14254
H	14.83220	0.78012	6.58597
H	11.25922	7.11272	1.08272
H	12.81483	7.09274	1.87732
H	11.41300	6.43643	2.68643
H	9.14394	-0.61376	-5.70364
H	13.25005	6.61959	-3.22599

Geometry of Pathway ET5

N	10.64460	-3.82043	0.29063
C	10.20688	-2.89117	-0.80586
C	11.21051	-1.80869	-0.86113
O	11.05702	-0.78844	-1.55856
C	8.76000	-2.26348	-0.65143
C	7.64233	-3.33271	-0.46609
C	7.36047	-4.09930	-1.79059
N	6.20869	-5.04651	-1.56992
C	5.55228	-5.61460	-2.58570
N	6.09992	-5.55995	-3.80016
N	4.28931	-5.95730	-2.44875
H	10.66775	-3.48446	1.21922
H	10.25097	-3.41188	-1.75049
H	8.80735	-1.61736	0.24834
H	8.64148	-1.73775	-1.61686
H	7.79733	-4.01919	0.39625
H	6.77021	-2.66829	-0.30816
H	7.20503	-3.46448	-2.69571
H	8.23681	-4.74432	-1.98601
H	5.52434	-4.73900	-0.90351
H	6.94728	-5.11836	-4.06861
H	5.50787	-5.65010	-4.60138
H	3.88446	-5.53624	-1.64419
H	3.78537	-5.94426	-3.31470
N	12.37842	-1.90378	-0.25115
C	13.33867	-0.85553	-0.28100
C	14.65269	-1.41848	-0.69687
O	14.87459	-2.59966	-0.82716
C	13.42039	-0.14013	1.01855
C	14.06705	-0.79334	2.24933
C	14.05028	-0.05005	3.54426
O	13.27935	0.91946	3.71141
O	14.80782	-0.49457	4.40741
H	12.51315	-2.68849	0.34204
H	13.09914	-0.09948	-1.02080
H	13.84877	0.88221	0.91559
H	12.36097	0.08940	1.26645
H	13.75156	-1.85638	2.38391
H	15.12712	-0.91270	1.93850
N	4.93650	4.80478	0.56892
C	4.72583	3.55446	-0.08578
C	3.28683	3.30079	-0.29057
O	2.50973	3.54019	0.57823
C	5.36573	2.42335	0.78492
C	5.17664	1.10781	0.09890
C	6.03384	0.78630	-1.00343
C	4.15432	0.27340	0.44847
C	5.81697	-0.47093	-1.65439
C	3.92635	-0.93468	-0.21030
C	4.73053	-1.26306	-1.30614
O	4.47523	-2.46732	-2.03002
H	4.36979	4.92876	1.38559
H	5.18278	3.48612	-1.06201
H	6.45318	2.65573	0.71519
H	5.01144	2.33992	1.83816
H	6.86407	1.35690	-1.38307
H	3.39685	0.60334	1.14230
H	6.41656	-0.80815	-2.48972
H	3.09945	-1.58920	0.04627
H	4.31119	-3.09855	-1.32693
N	2.88070	2.87144	-1.51850
C	1.54097	2.80095	-1.88939
C	1.61935	1.79581	-2.89684
O	2.60938	1.52981	-3.59547

C	1.15365	4.11522	-2.64495
C	1.28153	5.37823	-1.72894
C	0.45680	5.85577	-0.76626
C	2.34507	6.29288	-1.88835
C	2.07006	7.34169	-0.99238
C	3.52883	6.34155	-2.67443
N	0.87691	7.08712	-0.36191
C	2.90045	8.42365	-0.90735
C	4.27815	7.51004	-2.69773
C	3.96204	8.52828	-1.84621
H	3.58152	2.49626	-2.12207
H	0.87014	2.66342	-1.05971
H	1.80842	4.38622	-3.49538
H	0.09108	4.07674	-2.95216
H	-0.44434	5.35363	-0.43116
H	0.26342	7.68332	0.12580
H	3.54462	5.54095	-3.40702
H	2.71125	9.20232	-0.18156
H	4.97094	7.66228	-3.51734
H	4.63501	9.37695	-1.89157
Cu	16.19898	-1.70582	5.92106
C	-5.10443	1.94126	-1.96806
C	-12.39708	2.35487	4.43652
C	-11.92474	-5.29703	2.28192
C	-5.85996	-3.54963	-2.45404
N	-8.12261	0.77507	-0.07790
C	-4.01383	1.88998	-0.89602
C	-12.69838	3.54271	4.84938
C	-12.76271	-6.03315	3.03911
C	-5.73496	-2.71571	-3.78474
N	-10.05557	0.89176	1.94186
C	-2.51313	1.90116	-1.30587
C	-5.95894	-3.67476	-4.99430
N	-8.38010	-2.00315	-0.12832
C	-6.66824	-0.80343	-1.28362
C	-8.88469	2.74957	0.94639
C	-11.60534	-0.45280	3.31245
C	-9.84913	-3.90161	0.48460
C	-7.02928	4.16023	-1.10780
C	-10.58339	4.36413	2.75144
C	-12.74086	-3.05413	4.30317
C	-7.91312	-5.59506	-1.20662
C	-7.02760	0.50422	-0.87928
C	-9.82944	2.20957	1.80909
C	-11.31709	-1.69926	2.71575
C	-8.77844	-3.34368	-0.16266
O	-2.01501	2.85219	-1.85397
O	-6.93294	-3.34975	-5.68756
C	-6.44917	1.75009	-1.33779
C	-10.60838	2.93204	2.71163
C	-11.96690	-2.91420	3.08624
C	-7.93089	-4.12414	-0.95149
O	-1.88524	0.84662	-1.03700
O	-5.12804	-4.57681	-5.23183
C	-7.23068	2.72678	-0.88007
C	-11.44194	2.11644	3.43619
C	-11.63106	-3.94963	2.31606
C	-6.94808	-3.24120	-1.46441
C	-8.17996	2.05922	-0.01988
C	-11.05124	0.81710	2.91164
C	-10.66518	-3.24885	1.41092
C	-7.30572	-1.97630	-0.92198
N	-10.45142	-1.90408	1.68277
Fe	-9.23728	-0.54798	0.84857



H	10.01130	-4.61957	0.27646
H	15.42291	-0.75793	-0.88628
H	4.72247	5.55425	-0.08982
H	0.76916	1.23452	-3.06111
H	-4.93433	1.16441	-2.68464
H	-5.07568	2.89372	-2.45368
H	-12.87955	1.54715	4.86050
H	-11.41898	-5.82938	1.55671
H	-4.93145	-3.43933	-1.93348
H	-6.12046	-4.52662	-2.80325
H	-4.16626	2.73718	-0.26106
H	-4.14144	0.91912	-0.46381
H	-12.22934	4.36599	4.43994
H	-13.40831	3.66752	5.58801
H	-13.30975	-5.58317	3.78986
H	-12.85656	-7.04703	2.86875
H	-6.47432	-1.94183	-3.79609
H	-4.76455	-2.26868	-3.84693
H	-5.85204	-0.88989	-1.90885
H	-8.69185	3.75964	1.03548
H	-12.26918	-0.44995	4.10274
H	-10.07115	-4.88677	0.26990
H	-6.23590	4.30206	-1.81189
H	-6.77538	4.63593	-0.18342
H	-7.92992	4.58969	-1.49393
H	-9.83115	4.72632	2.08156
H	-10.36154	4.68962	3.74651
H	-11.53833	4.74624	2.45553
H	-13.12993	-4.04934	4.36618
H	-13.55070	-2.35396	4.29297
H	-12.11406	-2.86261	5.14875
H	-7.10969	-5.83218	-1.87205
H	-8.84121	-5.89192	-1.64846
H	-7.77651	-6.11568	-0.28212
H	-2.53049	3.61416	-2.03039
H	-7.49317	-2.65261	-5.40968

### Geometry of Pathway ET6

N	10.66926	-3.80496	0.65697
C	10.23118	-2.89136	-0.45245
C	11.23569	-1.81069	-0.52452
O	11.08233	-0.80055	-1.23656
C	8.78501	-2.26021	-0.30564
C	7.66661	-3.32564	-0.10357
C	7.38267	-4.11117	-1.41648
N	6.23030	-5.05405	-1.18084
C	5.57231	-5.63628	-2.18755
N	6.11869	-5.59979	-3.40325
N	4.30918	-5.97584	-2.04429
H	10.69370	-3.45553	1.58055
H	10.27379	-3.42579	-1.38945
H	8.83389	-1.60111	0.58459
H	8.66591	-1.74848	-1.27849
H	7.82194	-3.99964	0.76849
H	6.79523	-2.65822	0.04560
H	7.22681	-3.48945	-2.33058
H	8.25823	-4.75974	-1.60343
H	5.54693	-4.73628	-0.51825
H	6.96615	-5.16290	-3.67900
H	5.52571	-5.70106	-4.20245
H	3.90557	-5.54276	-1.24551
H	3.80433	-5.97495	-2.90980
N	12.40416	-1.89793	0.08553

C	13.36529	-0.85108	0.03942
C	14.67838	-1.42118	-0.36961
O	14.89911	-2.60432	-0.48293
C	13.44903	-0.11692	1.32834
C	14.09644	-0.75272	2.56781
C	14.08170	0.00935	3.85180
O	13.31180	0.98186	4.00564
O	14.83978	-0.42324	4.72053
H	12.53885	-2.67405	0.68993
H	13.12563	-0.10565	-0.71105
H	13.87819	0.90344	1.21006
H	12.39008	0.11714	1.57400
H	13.78017	-1.81341	2.71817
H	15.15607	-0.87752	2.25763
N	4.96896	4.82843	0.81579
C	4.75650	3.56890	0.17958
C	3.31706	3.31355	-0.01997
O	2.54110	3.56625	0.84607
C	5.39635	2.45001	1.06596
C	5.20538	1.12481	0.39936
C	6.06112	0.78653	-0.69909
C	4.18271	0.29647	0.76212
C	5.84246	-0.47984	-1.33146
C	3.95299	-0.92086	0.12123
C	4.75571	-1.26586	-0.97056
O	4.49859	-2.48029	-1.67657
H	4.40323	4.96478	1.63118
H	5.21235	3.48597	-0.79603
H	6.48392	2.68039	0.99171
H	5.04311	2.38223	2.12068
H	6.89144	1.35082	-1.08787
H	3.42628	0.63714	1.45187
H	6.44086	-0.82971	-2.16243
H	3.12580	-1.57085	0.38817
H	4.33475	-3.10109	-0.96420
N	2.90924	2.86675	-1.24110
C	1.56906	2.79205	-1.60950
C	1.64549	1.77230	-2.60230
O	2.63453	1.49529	-3.29804
C	1.18207	4.09554	-2.38369
C	1.31203	5.37162	-1.48630
C	0.48875	5.86385	-0.52979
C	2.37619	6.28291	-1.66012
C	2.10305	7.34490	-0.77922
C	3.55915	6.31909	-2.44808
N	0.91036	7.10058	-0.14385
C	2.93447	8.42724	-0.71081
C	4.30946	7.48647	-2.48917
C	3.99515	8.51726	-1.65222
H	3.60909	2.48221	-1.83988
H	0.89900	2.66720	-0.77720
H	1.83616	4.35355	-3.23867
H	0.11914	4.05353	-2.68919
H	-0.41247	5.36743	-0.18646
H	0.29791	7.70435	0.33579
H	3.57346	5.50791	-3.16896
H	2.74673	9.21656	0.00377
H	5.00150	7.62615	-3.31164
H	4.66881	9.36459	-1.71063
N	0.49103	1.14405	-2.87696
C	0.34307	0.02725	-3.83187
C	0.47749	0.58921	-5.24393
O	0.83695	-0.03818	-6.20016
C	-1.10294	-0.46232	-3.70432

C	-1.45531	-1.63524	-4.64634
O	-1.39540	-1.01937	-2.43437
H	-0.23134	1.27750	-2.21538
H	1.11998	-0.67023	-3.56179
H	-1.84859	0.34938	-3.85040
H	-1.61929	-0.27427	-1.85704
H	-1.40816	-1.26950	-5.68952
H	-0.65389	-2.39942	-4.53390
H	-2.47546	-2.04120	-4.43783
Cu	16.23151	-1.61358	6.25016
C	-5.07716	1.93719	-1.66862
C	-12.36259	2.45038	4.73698
C	-11.89921	-5.23247	2.69343
C	-5.83799	-3.55952	-2.07386
N	-8.09433	0.80128	0.24150
C	-3.98547	1.90054	-0.59710
C	-12.66241	3.64436	5.13284
C	-12.73700	-5.95676	3.46214
C	-5.71369	-2.74516	-3.41668
N	-10.02502	0.94905	2.26139
C	-2.48520	1.90443	-1.00866
C	-5.93980	-3.72151	-4.61193
N	-8.35429	-1.97714	0.23178
C	-6.64263	-0.79587	-0.94267
C	-8.85360	2.79115	1.23775
C	-11.57449	-0.37405	3.65304
C	-9.82432	-3.86519	0.87381
C	-6.99916	4.17014	-0.83870
C	-10.54896	4.43330	3.02092
C	-12.71121	-2.95969	4.68271
C	-7.89159	-5.58477	-0.79464
C	-7.00042	0.51784	-0.55701
C	-9.79789	2.26460	2.10922
C	-11.28796	-1.62931	3.07424
C	-8.75383	-3.31768	0.21737
O	-1.98684	2.84695	-1.57107
O	-6.91425	-3.40576	-5.30881
C	-6.42139	1.75639	-1.03422
C	-10.57524	3.00081	3.00198
C	-11.93844	-2.83816	3.46305
C	-7.90781	-4.11028	-0.56092
O	-1.85793	0.85336	-0.72515
O	-5.10994	-4.62765	-4.83718
C	-7.20157	2.74033	-0.58992
C	-11.40873	2.19658	3.73921
C	-11.60431	-3.88498	2.70766
C	-6.92478	-3.23576	-1.08768
C	-8.15051	2.08619	0.28089
C	-11.01972	0.88939	3.23321
C	-10.63880	-3.19829	1.79139
C	-7.28074	-1.96280	-0.56332
N	-10.42358	-1.84990	2.04342
Fe	-9.20916	-0.50716	1.18830
H	10.03525	-4.60366	0.65510
H	15.44897	-0.76413	-0.56942
H	4.75488	5.56842	0.14645
H	0.24130	1.58315	-5.38637
H	-4.90851	1.14985	-2.37400
H	-5.04811	2.88245	-2.16808
H	-12.84531	1.64933	5.17318
H	-11.39469	-5.77576	1.97552
H	-4.90882	-3.44249	-1.55594
H	-6.09971	-4.54126	-2.40854
H	-4.13648	2.75703	0.02562

H	-4.11345	0.93619	-0.15068
H	-12.19309	4.46119	4.71097
H	-13.37144	3.78053	5.87032
H	-13.28284	-5.49542	4.20685
H	-12.83191	-6.97292	3.30665
H	-6.45239	-1.97087	-3.43852
H	-4.74296	-2.29994	-3.48640
H	-5.82718	-0.89214	-1.56744
H	-8.65979	3.80225	1.31194
H	-12.23749	-0.35912	4.44391
H	-10.04742	-4.85317	0.67370
H	-6.20642	4.30101	-1.54561
H	-6.74387	4.65902	0.07840
H	-7.89985	4.59474	-1.23008
H	-9.79712	4.78505	2.34505
H	-10.32576	4.77304	4.01092
H	-11.50388	4.81192	2.72050
H	-13.10108	-3.95352	4.76060
H	-13.52045	-2.25902	4.66317
H	-12.08334	-2.75644	5.52475
H	-7.08908	-5.83226	-1.45740
H	-8.82040	-5.88721	-1.23113
H	-7.75444	-6.09201	0.13719
H	-2.50185	3.60672	-1.75801
H	-7.47359	-2.70415	-5.04051

#### Geometry of Pathway ET7

N	-7.49953	1.72807	2.15858
C	-7.03865	1.35529	0.77799
C	-7.95365	0.29688	0.30402
O	-7.75044	-0.34357	-0.74452
C	-5.54057	0.85334	0.65504
C	-4.50508	1.85842	1.24186
C	-4.34578	3.11044	0.33166
N	-3.26494	3.99320	0.90176
C	-2.70281	4.97563	0.19166
N	-3.29861	5.35806	-0.93819
N	-1.46652	5.34985	0.44234
H	-7.45366	1.05024	2.87561
H	-7.16702	2.20200	0.12073
H	-5.49521	-0.09845	1.22191
H	-5.42399	0.76772	-0.44113
H	-4.67554	2.12845	2.30813
H	-3.57620	1.26889	1.11284
H	-4.18096	2.90463	-0.75318
H	-5.27899	3.69677	0.41860
H	-2.52871	3.51035	1.38323
H	-4.11907	4.98386	-1.35283
H	-2.75252	5.81295	-1.64209
H	-0.99324	4.68283	1.00766
H	-1.00280	5.72816	-0.36131
N	-12.19420	-1.32618	-0.19124
C	-13.54529	-0.95004	-0.53719
C	-14.46923	-0.84991	0.65516
O	-15.30310	0.06653	0.74950
C	-14.04423	-1.92988	-1.58746
H	-11.94253	-2.21206	-0.56309
H	-13.65640	0.03279	-0.97135
H	-13.23743	-2.27788	-2.27125
H	-14.32632	-2.84893	-1.01792
H	-14.91060	-1.44677	-2.07696
N	-14.39630	-1.83843	1.57130
C	-15.13560	-1.89559	2.84219

C	-14.53474	-1.16777	4.05089
O	-13.52076	-1.56647	4.60432
C	-15.28955	-3.40723	3.20846
C	-16.40331	-3.88461	4.15780
S	-18.04037	-3.20514	4.01062
C	-18.83148	-4.06287	5.44764
H	-13.79591	-2.63142	1.44166
H	-16.10898	-1.51952	2.56434
H	-15.42362	-4.01320	2.28465
H	-14.28934	-3.78589	3.51227
H	-16.46350	-4.99521	4.21297
H	-16.08311	-3.55926	5.16939
H	-18.37937	-3.72078	6.40162
H	-19.89856	-3.76942	5.47800
H	-18.75575	-5.16722	5.46697
N	-12.93959	4.10861	0.29824
C	-11.73962	3.69459	-0.42096
C	-10.89579	4.87285	-0.93257
O	-11.47465	5.69054	-1.61258
C	-12.16389	2.95709	-1.68985
C	-11.08330	2.13871	-2.43011
C	-11.61907	1.34912	-3.66218
C	-10.57526	0.33770	-4.14870
N	-11.23604	-0.47808	-5.22335
H	-13.80973	3.85352	-0.14175
H	-11.19824	3.03529	0.23658
H	-12.89810	2.19162	-1.33502
H	-12.70638	3.63012	-2.39108
H	-10.33684	2.82129	-2.88681
H	-10.60447	1.52741	-1.64149
H	-12.62842	0.93302	-3.46964
H	-11.82804	2.13513	-4.43484
H	-9.69391	0.79034	-4.64453
H	-10.30237	-0.37418	-3.33836
H	-11.51027	-0.01496	-6.10727
H	-10.55033	-1.18453	-5.57509
H	-12.05611	-1.03457	-4.88987
N	-9.55368	4.91720	-0.58922
C	-8.64717	5.98820	-1.04921
C	-9.16605	7.32131	-0.54138
O	-9.40197	8.35538	-1.18047
C	-8.40199	5.96611	-2.58404
C	-7.60744	4.81758	-3.26973
C	-6.13072	5.06447	-3.13388
O	-5.55240	5.76064	-3.96640
O	-5.46340	4.34244	-2.32768
H	-9.09197	4.23939	-0.03615
H	-7.64260	5.93004	-0.65621
H	-9.37917	5.85950	-3.10275
H	-7.91879	6.89365	-2.97530
H	-8.02378	3.84414	-2.91749
H	-7.80981	4.82814	-4.36181
N	-1.11095	-5.73525	-1.08781
C	-1.03110	-4.31417	-1.19005
C	0.37217	-3.86935	-1.28985
O	1.20444	-4.36191	-0.59652
C	-1.71971	-3.68590	0.06617
C	-1.66799	-2.19481	-0.03850
C	-2.59716	-1.54181	-0.91231
C	-0.70117	-1.47812	0.60587
C	-2.51152	-0.11533	-1.00843
C	-0.60089	-0.09240	0.48285
C	-1.47753	0.56914	-0.38276
O	-1.35266	1.97974	-0.56724

H	-0.49980	-6.12101	-0.39414
H	-1.53571	-3.90579	-2.05324
H	-2.78703	-3.97002	-0.08043
H	-1.32602	-3.99572	1.06157
H	-3.39522	-1.98806	-1.48059
H	0.11090	-1.98565	1.10281
H	-3.17337	0.46953	-1.63364
H	0.18156	0.47907	0.97190
H	-1.20820	2.29182	0.32799
N	0.68664	-2.95224	-2.24752
C	1.99825	-2.61778	-2.57186
C	1.79402	-1.30691	-3.09272
O	0.75528	-0.87716	-3.61745
C	2.45526	-3.48218	-3.79340
C	2.47066	-5.01108	-3.45749
C	3.37371	-5.75404	-2.77375
C	1.47784	-5.88036	-3.95925
C	1.87634	-7.16881	-3.55988
C	0.26749	-5.72094	-4.68811
N	3.07247	-7.07753	-2.89143
C	1.14014	-8.26661	-3.90666
C	-0.38592	-6.84730	-5.16955
C	0.04903	-8.08640	-4.79907
H	-0.06858	-2.43408	-2.64418
H	2.69269	-2.76037	-1.76270
H	1.78659	-3.45174	-4.67507
H	3.49633	-3.22764	-4.06956
H	4.24588	-5.34611	-2.27433
H	3.75324	-7.75948	-2.68849
H	0.15442	-4.70030	-5.03941
H	1.42382	-9.24864	-3.55447
H	-1.10059	-6.72415	-5.97514
H	-0.55502	-8.90496	-5.17359
Cu	-12.60618	-2.94863	6.52608
C	8.54287	-1.19270	-2.36263
C	16.12713	-3.44676	3.27391
C	14.94538	4.35297	4.36233
C	8.83259	4.08336	-0.62017
N	11.54005	-0.60228	-0.19228
C	7.50123	-1.67172	-1.34929
C	16.54113	-4.66781	3.17467
C	15.75493	4.80107	5.34276
C	8.71491	3.83913	-2.17204
N	13.56543	-1.33418	1.59421
C	5.98929	-1.65657	-1.71535
C	8.80632	5.21593	-2.89942
N	11.57122	1.97814	0.86968
C	9.91070	1.18484	-0.65277
C	12.50363	-2.74233	-0.04990
C	15.06264	-0.50901	3.37341
C	12.90936	3.60272	2.17660
C	10.67648	-3.38428	-2.47922
C	14.40624	-4.77811	0.94322
C	16.02936	1.57670	5.31072
C	10.76925	5.64355	1.32159
C	10.39175	-0.13691	-0.80826
C	13.44001	-2.50545	0.94784
C	14.64863	0.83980	3.32747
C	11.85874	3.25233	1.37035
O	5.54484	-2.35285	-2.59322
O	9.77093	5.28383	-3.67391
C	9.89503	-1.14534	-1.72114
C	14.31441	-3.45235	1.47898
C	15.21493	1.86150	4.14663

C	10.91652	4.20072	0.96727
O	5.29159	-0.85802	-1.04147
O	7.89583	6.05783	-2.74875
C	10.77228	-2.14742	-1.69936
C	15.11172	-2.91913	2.46130
C	14.76262	3.08218	3.85776
C	9.98556	3.50824	0.15340
C	11.70283	-1.79264	-0.65298
C	14.59470	-1.56008	2.50359
C	13.81618	2.71341	2.75705
C	10.46770	2.17052	0.14158
N	13.72353	1.35791	2.47065
Fe	12.58568	0.33984	1.17534
H	-6.93369	2.52141	2.45910
H	-8.79363	0.08032	0.86315
H	-12.11421	-1.36216	0.82482
H	-14.99911	-0.31751	4.40669
H	-12.91649	3.68115	1.22452
H	-9.34622	7.37282	0.47339
H	-0.86746	-6.13828	-1.99320
H	2.58814	-0.65123	-3.02689
H	8.27877	-0.21425	-2.70729
H	8.56873	-1.87209	-3.18822
H	16.56190	-2.83347	3.98089
H	14.36629	5.08085	3.91518
H	7.94040	3.69076	-0.17842
H	8.99780	5.13806	-0.55214
H	7.74970	-2.68360	-1.10740
H	7.56992	-0.94525	-0.56624
H	16.12165	-5.29985	2.47468
H	17.29144	-5.01019	3.79513
H	16.36968	4.14203	5.84587
H	15.75932	5.80313	5.59103
H	9.51272	3.20475	-2.49875
H	7.78170	3.36675	-2.39865
H	9.06279	1.43741	-1.18362
H	12.39669	-3.71770	-0.37021
H	15.75961	-0.76477	4.09041
H	13.04168	4.60791	2.37155
H	9.86604	-3.30674	-3.17383
H	10.50361	-4.20917	-1.81974
H	11.59031	-3.54050	-3.01327
H	13.65599	-4.91161	0.19150
H	14.25642	-5.49099	1.72725
H	15.37442	-4.92197	0.51029
H	16.33976	2.49604	5.76265
H	16.89148	1.01562	5.01387
H	15.45881	1.00845	6.01507
H	9.92014	6.05084	0.81399
H	11.64961	6.17519	1.02658
H	10.63322	5.73912	2.37836
H	6.11130	-2.93128	-3.06436
H	10.39729	4.58819	-3.70314

#### Geometry of Pathway ET8

N	11.27590	-0.70891	-2.37985
C	11.94810	0.16229	-1.49976
C	11.03942	0.80930	-0.45527
O	11.32749	1.92037	-0.10793
C	12.78421	1.32374	-2.15128
C	13.75944	0.81718	-3.16850
S	15.44897	0.13453	-2.58329
C	16.08706	-0.28374	-4.23725

H	11.62379	-1.63854	-2.37161
H	12.53704	-0.49388	-0.87735
H	12.08034	2.07545	-2.57835
H	13.35003	1.84588	-1.36629
H	13.30488	0.08908	-3.86458
H	14.18371	1.62153	-3.80679
H	17.04748	-0.82903	-4.16820
H	15.42966	-0.97560	-4.80474
H	16.23029	0.64680	-4.82876
N	10.04340	0.10279	0.00711
C	9.05529	0.78040	0.87882
C	8.19023	-0.31178	1.50093
O	8.13188	-1.47056	1.12114
C	8.13289	1.77136	0.15241
C	7.13950	1.23283	-0.82496
C	6.45187	2.47137	-1.52921
C	4.95304	2.25585	-1.69036
N	4.57785	1.23393	-2.68390
H	9.77161	-0.78665	-0.34435
H	9.66033	1.15086	1.69300
H	7.58107	2.34224	0.93834
H	8.74953	2.57012	-0.31775
H	7.62402	0.63296	-1.61634
H	6.38033	0.58369	-0.34496
H	6.68860	3.33256	-0.86974
H	6.94238	2.57276	-2.51111
H	4.55399	1.86990	-0.72740
H	4.58953	3.18724	-2.17552
H	4.49503	0.27868	-2.28485
H	3.62853	1.31563	-3.08380
H	5.26647	1.18599	-3.46442
N	4.15542	-0.85032	2.09936
C	2.92025	-0.48952	1.50584
C	2.05534	0.39508	2.39691
O	1.50789	1.42726	1.92214
C	2.11056	-1.77339	1.08814
C	2.74449	-2.53683	-0.07233
C	3.00484	-1.56936	-1.29741
O	2.06285	-1.33040	-2.09242
O	4.06499	-0.97469	-1.40627
H	4.24429	-1.84028	2.15926
H	3.18076	0.20627	0.71525
H	1.92591	-2.41991	1.96427
H	1.13328	-1.34965	0.77324
H	3.72180	-3.02942	0.13139
H	2.06776	-3.26890	-0.57265
N	-4.83152	6.68884	0.39323
C	-3.60735	6.64573	-0.36582
C	-2.70250	7.75505	-0.10264
O	-1.54891	7.68058	-0.59404
C	-3.88901	6.53583	-1.88094
C	-4.79651	5.31958	-2.20292
C	-6.09197	5.23374	-2.81310
N	-4.42545	4.00407	-1.98720
C	-5.43857	3.25293	-2.41555
N	-6.44669	3.92436	-2.87845
H	-5.50406	7.29523	-0.03288
H	-2.98525	5.79942	-0.13205
H	-4.27109	7.44797	-2.38296
H	-2.87397	6.37478	-2.31067
H	-3.66011	3.69519	-1.42778
H	-6.77686	5.98036	-3.17225
H	-5.41919	2.16585	-2.39357
N	0.65898	6.24235	0.47273



C	0.28553	5.32560	1.50355
C	-0.18333	6.11927	2.68494
O	0.39851	7.14083	3.01855
H	-0.05254	6.65501	-0.09247
H	-0.48738	4.69656	1.09231
H	1.11187	4.69148	1.77419
N	18.36803	-1.07252	4.58113
C	18.11607	0.29627	4.06081
C	17.44916	1.17002	5.07830
O	16.22887	1.11131	5.08368
C	17.01513	0.20570	2.94542
C	17.60031	-0.30268	1.67195
C	18.61654	0.25764	1.02217
N	17.00799	-1.29768	0.90454
C	17.70851	-1.32869	-0.20488
N	18.65107	-0.34860	-0.21516
H	17.60225	-1.59237	4.95049
H	18.99204	0.74028	3.61523
H	16.16378	-0.38066	3.33075
H	16.64564	1.22905	2.72352
H	19.13835	1.14794	1.36419
H	17.47679	-1.89380	-1.10707
H	19.16074	0.06878	-0.96818
Cu	15.25733	-5.51321	-0.49626
C	-7.40675	-3.22824	-3.73560
C	-11.82990	4.61306	-0.08566
C	-12.27899	-0.90670	5.63689
C	-8.35725	-5.96057	1.01707
N	-9.53367	-1.23470	-1.38101
C	-5.99925	-2.73465	-3.39408
C	-11.94338	5.60926	-0.90230
C	-12.78931	-0.35703	6.75708
C	-8.71946	-6.69847	-0.32684
N	-10.58757	1.11070	-0.27748
C	-4.75414	-3.55973	-3.82898
C	-9.38434	-8.06583	0.02140
N	-9.82673	-2.49833	1.08975
C	-8.64416	-3.44388	-0.75741
C	-9.84106	0.78403	-2.54671
C	-11.54212	2.11083	1.76622
C	-10.99160	-2.40557	3.27432
C	-8.85264	-0.84527	-5.00040
C	-10.73709	3.58127	-2.89765
C	-12.26688	2.07209	4.68360
C	-9.83404	-5.22502	3.70656
C	-8.81326	-2.37913	-1.67409
C	-10.40944	1.54756	-1.53558
C	-11.50906	0.94090	2.55550
C	-10.22671	-3.02586	2.32207
O	-4.48031	-3.72507	-4.99116
O	-10.54075	-8.15907	-0.41325
C	-8.42811	-2.35890	-3.06988
C	-10.79304	2.88307	-1.64766
C	-11.99255	0.88673	3.89673
C	-9.73825	-4.31821	2.52439
O	-4.08474	-4.04296	-2.88188
O	-8.71031	-8.95870	0.57724
C	-8.97435	-1.26698	-3.60235
C	-11.31226	3.36718	-0.47248
C	-11.97632	-0.34159	4.41544
C	-9.00161	-4.64665	1.35902
C	-9.54948	-0.56404	-2.47904
C	-11.15808	2.19762	0.37867
C	-11.40185	-1.07116	3.24027

C	-9.11891	-3.48957	0.54079
N	-11.08620	-0.28639	2.13914
Fe	-10.24653	-0.73140	0.37678
H	10.29041	-0.73286	-2.11771
H	7.60559	-0.04945	2.30999
H	4.91905	-0.48052	1.53312
H	1.91777	0.14876	3.38988
H	1.24987	-1.78804	-2.00717
H	-4.62733	7.02792	1.33357
H	-2.99558	8.56682	0.46313
H	1.28751	5.74334	-0.15656
H	-1.00527	5.80064	3.22199
H	18.75942	-1.61855	3.81304
H	17.73250	2.18320	4.88388
H	17.77189	0.81703	6.03547
H	15.88630	1.42272	4.23140
H	-7.52169	-4.23636	-3.39440
H	-7.54643	-3.18700	-4.79513
H	-12.13298	4.73910	0.89272
H	-12.08186	-1.91752	5.70399
H	-7.30110	-5.78883	0.99876
H	-8.74016	-6.62018	1.76714
H	-5.89699	-1.76606	-3.83628
H	-5.97136	-2.79567	-2.32584
H	-11.64726	5.50688	-1.88579
H	-12.33060	6.50663	-0.57071
H	-13.01647	0.64955	6.78066
H	-12.95198	-0.94259	7.59161
H	-9.40144	-6.09978	-0.89444
H	-7.83425	-6.85905	-0.90649
H	-8.11598	-4.26544	-1.09002
H	-9.61624	1.26865	-3.42987
H	-11.86902	2.97790	2.22075
H	-11.28940	-2.97163	4.08476
H	-8.37178	-1.61641	-5.56555
H	-8.27085	0.05139	-5.05303
H	-9.82667	-0.66219	-5.40346
H	-10.27913	2.95538	-3.63542
H	-10.16103	4.47567	-2.78131
H	-11.72906	3.83382	-3.21025
H	-12.61812	1.78367	5.65273
H	-13.01491	2.66027	4.19300
H	-11.37086	2.64755	4.78626
H	-9.33440	-6.14617	3.49120
H	-10.86322	-5.42026	3.92419
H	-9.37385	-4.75842	4.55209
H	-5.01490	-3.34092	-5.65757
H	-10.95083	-7.41885	-0.81449

### Geometry of Pathway ET9

N	10.24320	-5.33118	-0.20753
C	10.85906	-4.06644	0.16146
C	10.43785	-3.01534	-0.89185
O	10.57501	-3.16522	-2.08676
C	12.42777	-4.26468	0.32682
C	13.08733	-2.89451	0.65253
N	14.14466	-2.62230	-0.13293
O	12.59920	-2.07850	1.41756
H	10.79116	-6.05044	-0.61864
H	10.43434	-3.82326	1.12462
H	12.55606	-4.93535	1.20246
H	12.86257	-4.65335	-0.61552
H	14.55984	-3.34021	-0.68641

H	14.34861	-1.65501	-0.21144
N	10.00521	-1.79864	-0.37006
C	9.40120	-0.75737	-1.26913
C	10.25282	0.44354	-1.14802
O	9.93687	1.54112	-1.64440
C	7.89391	-0.36900	-0.97158
C	6.93358	-1.59555	-0.95994
C	6.69283	-2.14564	-2.39550
N	5.68455	-3.26415	-2.32617
C	5.06127	-3.72635	-3.41396
N	5.54100	-3.38313	-4.60973
N	3.86083	-4.25583	-3.31437
H	10.02724	-1.63299	0.60348
H	9.46892	-1.09112	-2.29354
H	7.89848	0.10735	0.02961
H	7.66427	0.29890	-1.82227
H	7.21541	-2.39688	-0.24067
H	5.99101	-1.09414	-0.66472
H	6.41528	-1.38713	-3.16623
H	7.63534	-2.62091	-2.72413
H	4.99744	-3.17553	-1.60020
H	6.31094	-2.79021	-4.81155
H	4.92950	-3.40887	-5.40093
H	3.44223	-4.04320	-2.43798
H	3.32029	-4.15755	-4.15232
N	17.73121	-1.09654	1.97037
C	17.11912	-2.43595	2.15347
C	16.32761	-2.82414	3.36847
O	16.43830	-2.22953	4.45303
C	18.33820	-3.42209	2.09800
C	19.21452	-2.73040	1.01259
C	19.03068	-1.25228	1.34345
H	16.53769	-2.63160	1.26518
H	18.82918	-3.33235	3.09213
H	18.05864	-4.46965	1.84448
H	20.22902	-3.16734	1.10887
H	18.88936	-3.06151	-0.00009
H	19.78805	-1.08471	2.13762
H	19.25247	-0.50282	0.55577
N	3.24838	5.78576	1.59874
C	3.17139	4.65482	0.73194
C	1.76943	4.24899	0.51563
O	1.00853	4.22271	1.43015
C	3.99143	3.48431	1.36790
C	3.94282	2.29829	0.45796
C	4.78298	2.29688	-0.70284
C	3.05410	1.28436	0.67175
C	4.70092	1.15770	-1.56709
C	2.95434	0.19298	-0.19099
C	3.74316	0.17653	-1.34550
O	3.61285	-0.90327	-2.27095
H	2.70842	5.68475	2.43644
H	3.58813	4.82356	-0.25008
H	5.03534	3.87053	1.31811
H	3.69954	3.16788	2.39575
H	5.51416	3.03298	-0.99008
H	2.29292	1.38008	1.43034
H	5.30017	1.05864	-2.46269
H	2.23166	-0.60262	-0.04009
H	3.56421	-1.66568	-1.69124
N	1.36639	3.99363	-0.76087
C	0.03145	3.80931	-1.10925
C	0.19291	3.01918	-2.28442
O	1.17596	3.01815	-3.04113

C	-0.55680	5.17212	-1.60413
C	-0.55149	6.25778	-0.47635
C	-1.38606	6.44049	0.57489
C	0.37639	7.32172	-0.48948
C	0.00941	8.14759	0.58832
C	1.50665	7.66919	-1.27903
N	-1.11064	7.62579	1.18759
C	0.69591	9.29959	0.85102
C	2.09669	8.91381	-1.10530
C	1.69091	9.71219	-0.07588
H	2.08144	3.83011	-1.43775
H	-0.57722	3.43697	-0.30415
H	0.01776	5.67605	-2.40496
H	-1.61842	5.04523	-1.89009
H	-2.19839	5.76942	0.83237
H	-1.77309	8.03716	1.78896
H	1.59225	7.02112	-2.14539
H	0.44106	9.90400	1.71046
H	2.72568	9.30166	-1.89829
H	2.24568	10.63865	0.01956
N	-0.88200	2.30414	-2.65346
C	-0.92844	1.38187	-3.80596
C	-0.93397	2.21742	-5.08253
O	-0.54129	1.84015	-6.15054
C	-2.29133	0.68471	-3.74750
C	-2.53237	-0.32239	-4.89421
O	-2.44960	-0.14029	-2.60604
H	-1.58390	2.20850	-1.96390
H	-0.05600	0.75790	-3.69416
H	-3.14182	1.40015	-3.71594
H	-2.74093	0.44257	-1.88911
H	-2.58171	0.23975	-5.84592
H	-1.63436	-0.97760	-4.95055
H	-3.48051	-0.89586	-4.74867
Cu	15.49161	0.01473	5.42957
C	-6.44352	2.08501	-1.19904
C	-13.42719	0.36232	5.33036
C	-12.06847	-6.64937	1.80801
C	-6.50406	-3.28310	-2.66076
N	-9.19572	0.20358	0.51203
C	-5.30748	1.99232	-0.17820
C	-13.86034	1.40597	5.95916
C	-12.76861	-7.61494	2.43641
C	-6.54908	-2.21692	-3.81965
N	-11.03293	-0.30338	2.56069
C	-3.84120	2.27934	-0.61162
C	-6.70234	-2.96718	-5.17855
N	-9.09379	-2.53033	-0.03810
C	-7.60622	-0.92377	-0.99235
C	-10.15901	1.84295	1.89519
C	-12.33134	-2.06740	3.69667
C	-10.27532	-4.68872	0.25040
C	-8.59772	3.83427	0.09263
C	-11.96772	2.86588	4.00060
C	-13.07430	-4.93284	4.22128
C	-8.21612	-5.77660	-1.76263
C	-8.11276	0.23031	-0.34884
C	-10.98545	1.03534	2.66536
C	-11.91197	-3.13730	2.87676
C	-9.31657	-3.88485	-0.30745
O	-3.49590	3.37119	-0.98795
O	-7.74093	-2.65918	-5.77970
C	-7.72194	1.60451	-0.58514
C	-11.80910	1.47367	3.70110

C	-12.38153	-4.47539	3.03372
C	-8.41226	-4.39060	-1.24346
O	-3.07054	1.28876	-0.55306
O	-5.77353	-3.69166	-5.59441
C	-8.60139	2.36931	0.05971
C	-12.49610	0.43704	4.28285
C	-11.95025	-5.30231	2.08068
C	-7.57643	-3.30571	-1.60814
C	-9.41595	1.43720	0.80426
C	-11.96508	-0.68334	3.52201
C	-11.12562	-4.32758	1.29762
C	-8.06942	-2.21761	-0.83671
N	-11.07533	-3.03614	1.80522
Fe	-10.08629	-1.40163	1.20591
H	9.83798	-5.72104	0.64365
H	11.14390	0.36984	-0.63263
H	17.13106	-0.52463	1.37562
H	15.66767	-3.61444	3.29984
H	2.90926	6.60433	1.09238
H	-1.30329	3.17862	-5.02202
H	-6.20741	1.47815	-2.04868
H	-6.56048	3.10356	-1.50353
H	-13.78121	-0.56568	5.61045
H	-11.53188	-6.97091	0.98716
H	-5.57474	-3.14228	-2.14908
H	-6.65176	-4.20865	-3.17639
H	-5.53894	2.68465	0.60363
H	-5.28852	0.95193	0.07255
H	-13.52097	2.34472	5.69649
H	-14.54585	1.30022	6.72339
H	-13.33427	-7.38382	3.26827
H	-12.73826	-8.58563	2.08626
H	-7.38205	-1.56075	-3.67379
H	-5.64851	-1.63867	-3.82040
H	-6.81521	-0.78638	-1.64043
H	-10.09454	2.83779	2.16261
H	-12.95306	-2.29497	4.48847
H	-10.37767	-5.64091	-0.13532
H	-7.86246	4.20509	-0.59087
H	-8.36538	4.16812	1.08248
H	-9.56308	4.19946	-0.18916
H	-11.30014	3.43984	3.39177
H	-11.74447	3.03641	5.03327
H	-12.97662	3.16153	3.80005
H	-13.32811	-5.96679	4.11034
H	-13.96750	-4.35827	4.35638
H	-12.43946	-4.81147	5.07380
H	-7.42011	-5.78067	-2.47740
H	-9.11728	-6.11321	-2.23092
H	-7.97110	-6.42981	-0.95164
H	-4.11314	4.07541	-1.01138
H	-8.37329	-2.10493	-5.36737

#### Geometry of Pathway ET10

N	-0.57411	6.55764	1.42944
C	-0.05101	6.46206	0.04173
C	0.25350	7.80752	-0.39316
O	-0.44644	8.74609	-0.18515
C	-1.18532	5.87778	-0.96526
C	-1.44602	4.37994	-1.01643
C	-0.19542	3.53703	-1.25643
C	-2.11271	3.90044	0.19361
H	-1.55360	6.75566	1.48500

H	0.87088	5.90627	-0.07453
H	-2.09188	6.45649	-0.70709
H	-0.82622	6.12777	-1.98871
H	-2.12746	4.19789	-1.87170
H	0.36301	3.83835	-2.16526
H	0.47397	3.83027	-0.41077
H	-0.35527	2.44391	-1.37190
H	-2.99964	4.51635	0.47254
H	-2.50321	2.86342	0.14262
H	-1.34865	3.97211	1.00000
N	1.45237	8.02047	-1.02645
C	1.97382	9.34368	-1.42906
C	1.99308	9.30760	-2.89030
O	2.69705	8.50963	-3.47449
C	3.32900	9.85275	-0.79950
C	3.32636	9.90129	0.75377
C	2.36878	9.74273	1.69254
N	4.47946	10.26232	1.32902
C	4.30293	10.22857	2.60644
N	3.03708	9.84023	2.86590
H	2.09636	7.34048	-1.34629
H	1.24542	10.10713	-1.20307
H	4.05087	9.03623	-0.99648
H	3.53274	10.83955	-1.27196
H	1.35416	9.37146	1.62613
H	4.92708	10.59979	3.42254
H	2.66445	9.52659	3.73197
N	-6.23729	5.15334	-8.07105
C	-5.90343	4.20318	-7.06929
C	-6.85149	2.98399	-7.26875
O	-8.06171	3.03124	-7.60642
C	-5.99633	4.76103	-5.58714
C	-5.78018	3.76899	-4.49542
C	-4.99606	5.93335	-5.51681
H	-6.92504	5.78281	-7.73973
H	-4.86104	3.93350	-7.20040
H	-6.96056	5.29360	-5.44705
H	-5.84702	4.21025	-3.47924
H	-6.46468	2.90222	-4.62176
H	-4.76634	3.36631	-4.69357
H	-5.20026	6.41752	-4.53922
H	-3.94500	5.59575	-5.53924
H	-5.28864	6.67717	-6.29381
N	-7.98876	-0.59315	-5.18821
C	-7.95561	-1.36245	-4.05774
C	-8.34947	-2.76099	-4.35366
O	-9.09547	-2.89435	-5.29297
C	-8.92434	-0.90143	-2.90850
C	-8.52332	0.42346	-2.25617
C	-7.79049	0.59427	-1.10657
C	-8.75896	1.76650	-2.69642
C	-8.12862	2.64202	-1.79756
C	-9.33217	2.18795	-3.85396
N	-7.51070	1.83568	-0.83071
C	-8.15206	3.97050	-1.95468
C	-9.47998	3.61942	-4.00582
C	-8.85279	4.46623	-3.01884
H	-8.87478	-0.57345	-5.64808
H	-6.90772	-1.39159	-3.80621
H	-9.96623	-0.82280	-3.30256
H	-8.80598	-1.60018	-2.05725
H	-7.51089	-0.27726	-0.53162
H	-7.14289	2.18460	0.00755
H	-9.89704	1.50264	-4.47634

H	-7.55054	4.60364	-1.32642
H	-9.86257	3.99205	-4.94777
H	-8.94214	5.53830	-3.13586
N	-14.22633	-6.68001	1.75006
C	-13.89024	-5.30605	2.18797
C	-14.42229	-4.38781	1.11766
O	-14.59872	-4.77906	-0.01349
C	-12.31202	-5.12845	2.26140
C	-11.57559	-5.77998	3.45538
C	-10.45724	-6.57474	3.48051
N	-11.97823	-5.54581	4.69282
C	-11.06974	-6.03326	5.48796
N	-10.13037	-6.71366	4.80296
H	-14.29323	-6.85644	0.77109
H	-14.40361	-5.02829	3.09069
H	-11.92135	-5.61741	1.33771
H	-11.89444	-4.09943	2.31075
H	-9.89639	-6.92551	2.62040
H	-11.11756	-5.84013	6.56472
H	-9.43383	-7.29235	5.22493
N	-14.41571	-3.07536	1.41369
C	-14.77916	-1.98256	0.56965
C	-14.06483	-0.74427	1.08584
O	-13.63181	-0.63839	2.23536
C	-16.20853	-1.56865	0.19150
C	-16.95544	-0.79644	1.29115
N	-18.01301	-0.01999	0.89457
O	-16.68492	-0.87828	2.50194
H	-14.16953	-2.72862	2.32745
H	-14.25146	-2.13085	-0.36187
H	-16.23464	-0.94459	-0.72390
H	-16.71549	-2.48167	-0.19318
H	-18.13916	0.02950	-0.09124
H	-18.47136	0.42132	1.66416
N	-13.81807	0.25999	0.26203
C	-13.48963	1.59532	0.76198
C	-14.74184	2.52896	0.89870
O	-15.88484	2.36302	0.39302
C	-12.40125	2.31891	-0.16172
C	-11.12902	1.63725	0.14631
C	-12.77333	2.19867	-1.69954
H	-14.11855	0.16098	-0.68307
H	-13.02147	1.63001	1.74092
H	-12.35023	3.38609	0.11275
H	-10.41539	2.12108	-0.55228
H	-10.74985	1.96891	1.13481
H	-11.09548	0.52439	0.02792
H	-13.68830	2.76003	-1.98518
H	-11.96046	2.58457	-2.35499
H	-13.05287	1.15478	-1.95872
N	10.48976	1.70957	5.57946
C	9.43385	1.02616	4.88793
C	8.37859	0.49157	5.80288
O	7.21168	0.57749	5.50432
C	9.96256	-0.07103	3.96514
S	11.16862	0.54692	2.81608
H	11.28288	1.15036	5.79336
H	9.03431	1.78320	4.23170
H	10.38041	-0.92793	4.55661
H	9.10334	-0.40439	3.35154
H	12.00419	-0.42269	3.17131
N	4.39484	1.73931	6.49910
C	4.74328	3.08489	6.30184
C	4.98264	3.32478	4.81239

O	4.02110	3.61192	4.11806
C	5.90282	3.55437	7.18725
C	6.07505	5.04942	7.25477
C	7.25686	5.52688	8.22527
C	7.29422	7.06548	8.41449
N	7.81452	7.87135	7.22040
H	4.62721	1.09848	5.77560
H	3.89667	3.68090	6.61204
H	5.68588	3.27931	8.24165
H	6.80020	2.95182	6.89375
H	6.29542	5.42873	6.23670
H	5.15835	5.62268	7.49378
H	7.13677	5.11114	9.24754
H	8.22294	5.12165	7.86006
H	6.30255	7.51825	8.61272
H	7.98210	7.37653	9.23484
H	7.12326	7.83927	6.44766
H	8.01750	8.88547	7.33552
H	8.67439	7.46530	6.81254
Cu	-13.39545	-8.08298	5.85837
C	8.68767	-8.13289	-0.59977
C	14.42686	-0.93528	2.50323
C	11.45297	1.59300	-4.43801
C	7.37512	-5.13026	-5.09624
N	10.68174	-4.96619	-0.79417
C	7.49811	-7.71139	0.26544
C	15.08315	-1.18574	3.58893
C	11.81195	2.87601	-4.64392
C	7.79712	-6.63060	-5.32580
N	12.15241	-2.82368	0.24325
C	6.20358	-8.57385	0.28890
C	7.83743	-6.90551	-6.86066
N	9.87172	-3.34808	-2.91852
C	8.95845	-5.50822	-2.46660
C	11.95471	-5.03592	1.18151
C	12.82764	-0.48237	-0.14456
C	10.38869	-1.28665	-4.19177
C	11.13914	-8.03336	1.23034
C	13.81515	-3.98017	3.22473
C	12.71216	2.13101	-1.62606
C	8.26347	-2.30113	-6.17429
C	9.71441	-5.81092	-1.30924
C	12.46782	-3.74559	1.16845
C	12.19139	-0.33036	-1.39551
C	9.73211	-2.47381	-4.00160
O	6.20094	-9.69756	0.72510
O	8.96198	-7.24308	-7.25604
C	9.73558	-7.06345	-0.58280
C	13.30179	-3.19598	2.14093
C	12.26147	0.86586	-2.16993
C	8.79491	-2.93186	-4.92980
O	5.18781	-8.01345	-0.19356
O	6.77825	-6.88068	-7.52249
C	10.74170	-6.98525	0.28657
C	13.63204	-1.89412	1.85617
C	11.69051	0.75326	-3.36969
C	8.31932	-4.16971	-4.42967
C	11.21102	-5.62346	0.17721
C	12.87053	-1.69668	0.63255
C	11.22610	-0.66661	-3.26205
C	9.03471	-4.34672	-3.21353
N	11.49616	-1.29934	-2.05592
Fe	11.04231	-3.12617	-1.37350