

Supporting Information

Electrostatic repulsion as an additional selectivity factor in asymmetric proline catalysis

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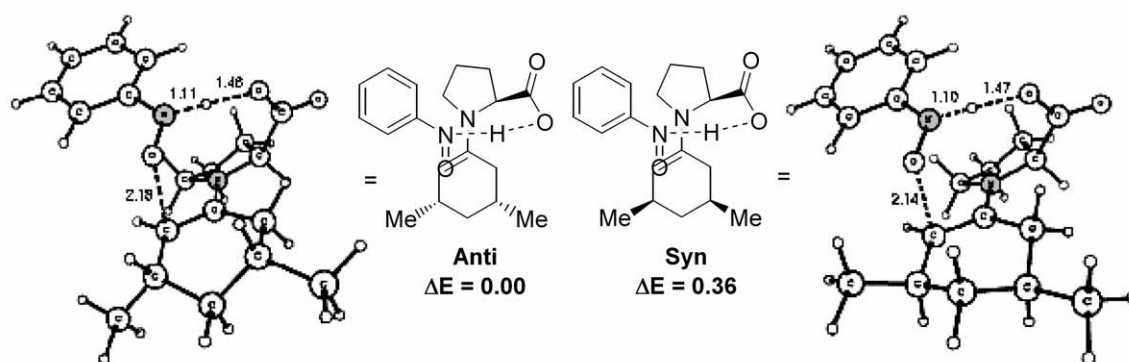


Figure S1: Lowest energy transition state structures for α -aminoxylation for substrate **1a**.

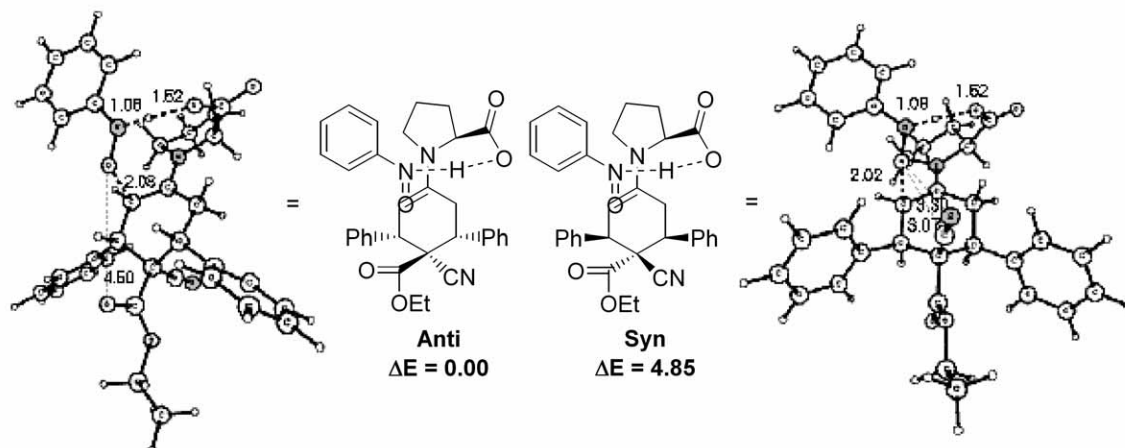


Figure S2: Lowest energy transition state structures for α -aminoxylation for substrate **1h**.

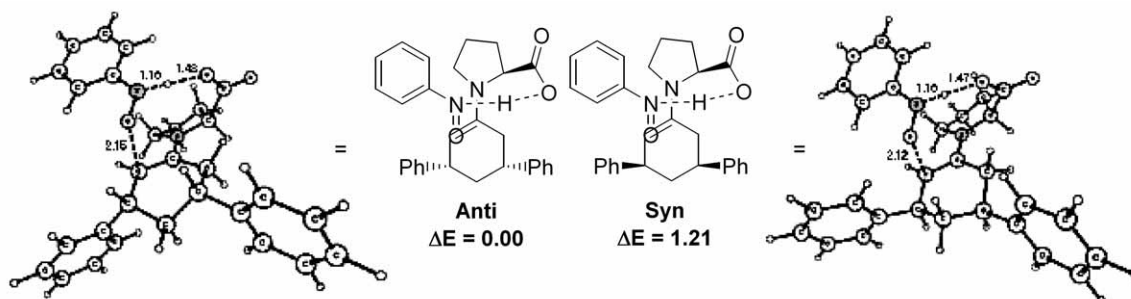


Figure S3: Lowest energy transition state structures for α -aminoxylation for substrate **26**.

Molecular Energies (in Hartree) and Geometries (in Å⁰):

Anti-10

B3LYP/6-31G*

E+ZPE = -1590.006654

O	2.254942	.637863	-1.665654
O	3.199815	.903646	.526447
O	2.126522	.262791	2.343836
O	.284750	-.287449	-2.002095
H	1.182002	6.196886	-.293638
C	1.681307	-3.096212	-.682040
H	1.154219	-2.747912	-1.565496
C	2.626174	-4.115663	-.814583
H	2.812198	-4.549945	-1.793373
C	3.324970	-4.578548	.301907
H	4.056070	-5.375640	.197799
C	3.075589	-4.010996	1.551855
H	3.613717	-4.361194	2.428483
C	2.131863	-2.991254	1.683382
H	1.951799	-2.545446	2.657477
C	1.418490	-2.519440	.571733
C	.390757	-1.405554	.759337
H	.252142	-1.284241	1.837404
C	-.975367	-1.795932	.157419
H	-.841458	-2.272032	-.819500
H	-1.416437	-2.561815	.807879
C	-1.950044	-.666667	-.051957
C	-1.623492	.700060	.223185
H	-2.620024	.939884	1.047577
H	-1.979222	1.372183	-.562245
C	-.231190	1.057611	.734272
H	-.222995	.958204	1.824823
C	.897020	.006020	.300192
C	1.119168	.074333	-1.200003
C	3.444730	.845784	-.884778
C	2.123553	.364107	1.139527
C	4.403079	-.308627	-1.158356
H	3.954061	-1.259322	-.857155
H	5.328211	-.160785	-.594328
H	4.636561	-.351306	-2.225982
C	3.988066	2.207942	-1.285864
H	3.246963	2.980027	-1.064819
H	4.208865	2.217120	-2.356742

H	4.904753	2.418552	-.728392
C	.152537	2.500088	.423195
C	.651475	3.318568	1.446098
H	.751296	2.915109	2.450225
C	1.022286	4.639719	1.191728
H	1.401059	5.257158	2.001682
C	.899923	5.166513	-.094510
C	.404087	4.362152	-1.122980
H	.300925	4.762920	-2.127937
C	.033596	3.041506	-.866351
H	-.345771	2.429485	-1.680035
C	-4.763599	.551642	.808824
C	-4.278134	.030719	-.599588
C	-5.353021	-.739252	-1.364865
C	-5.184606	-2.177852	-.857519
C	-3.664528	-2.340920	-.732665
H	-3.894896	.882387	-1.172387
H	-5.172944	-.683410	-2.445205
H	-6.336135	-.326228	-1.136236
H	-5.619369	-2.930537	-1.520940
H	-5.655708	-2.271242	.126107
H	-3.212537	-2.690638	-1.669965
H	-3.373592	-3.031890	.063450
N	-3.178765	-.973319	-.439175
O	-3.829462	.993518	1.588756
O	-5.961634	.510611	1.056977

Syn-11

B3LYP/6-31G*

E+ZPE = -1590.007020

O	-2.057736	.551118	-1.695829
O	-3.298581	.676631	.357739
O	-2.371587	.266248	2.313605
O	.039423	-.105045	-1.771888
H	-4.369433	-5.062540	-.528578
C	.494196	3.034654	-.403270
H	1.079563	2.450277	-1.105395
C	.272905	4.388245	-.665038
H	.679330	4.827845	-1.571848
C	-.451238	5.175595	.232283

H	-.614478	6.230255	.026718
C	-.953133	4.601274	1.401251
H	-1.509990	5.205043	2.113074
C	-.732985	3.248291	1.664879
H	-1.125314	2.807280	2.577911
C	-.012133	2.445472	.766779
C	.195284	.966088	1.092340
H	-.011805	.855602	2.163018
C	1.632011	.515363	.827803
H	2.267072	.920664	-.233908
H	2.315406	1.017675	1.521216
C	1.934369	-.867224	.623227
C	.853608	-1.886245	.375035
H	1.103682	-2.821826	.890860
H	.855280	-2.113636	-.696010
C	-.549195	-1.454263	.838416
H	-.542597	-1.422685	1.932421
C	-.895478	.033761	.434466
C	-.916226	.169209	-1.082853
C	-3.249013	1.008901	-1.038943
C	-2.232535	.351925	1.115448
C	-3.326236	2.523990	-1.178301
H	-2.474786	3.000815	-.687635
H	-4.250097	2.887660	-.719582
H	-3.321539	2.795037	-2.237810
C	-4.407625	.270239	-1.693351
H	-4.279585	-.807203	-1.559395
H	-4.434650	.498138	-2.762345
H	-5.350833	.579865	-1.235288
C	-1.613049	-2.467441	.427183
C	-2.483797	-2.983448	1.397968
H	-2.394706	-2.644385	2.426544
C	-3.469628	-3.911157	1.059087
H	-4.132203	-4.297013	1.829053
C	-3.603816	-4.339014	-.261980
C	-2.745399	-3.832002	-1.239519
H	-2.839378	-4.159730	-2.271424
C	-1.757417	-2.906405	-.899228
H	-1.102509	-2.525844	-1.677633
C	4.387198	.605876	-.796723
C	4.363932	-.319628	.483237
C	5.560060	-1.267132	.556161
C	5.100050	-2.466780	-.283395
C	3.617194	-2.619622	.082202
H	4.286474	.319405	1.370234
H	5.755223	-1.567132	1.593005

H	6.443477	-.778006	.144315
H	5.662206	-3.383414	-.084567
H	5.202829	-2.223838	-1.345652
H	3.477543	-3.289796	.940551
H	3.010322	-2.994990	-.746247
N	3.193163	-1.249465	.456756
O	3.261746	1.167655	-1.098675
O	5.450726	.734842	-1.389187

Anti-20

B3LYP/6-31G*

E+ZPE = -1489.512413

O	-4.720730	.497666	1.185603
O	-5.161523	-.958735	-.632686
O	-3.551827	-1.821583	-1.889348
O	-2.678506	1.081420	1.807787
C	-1.706979	-1.386024	.351763
H	-1.534081	-2.026755	-.524573
C	-.393896	-.738188	.691244
H	.238584	-1.302525	1.366512
C	-.060983	.576151	.387226
C	-.935984	1.396063	-.522978
H	-.327402	1.778306	-1.348962
H	-1.296403	2.266274	.040243
C	-2.115546	.630699	-1.141752
H	-1.719295	-.024825	-1.924202
C	-2.793984	-.367164	-.123043
C	-3.361708	.437699	1.051292
C	-5.487286	-.582421	.690110
C	-3.843496	-1.139463	-.941909
N	1.111752	1.103635	.789963
C	1.877936	.581130	1.946062
C	2.525430	1.833641	2.544933
C	2.810773	2.693002	1.309735
C	1.607432	2.443131	.377482
H	2.634063	-.139425	1.609839
H	1.201846	.075538	2.639217
H	1.814369	2.335926	3.211496
H	3.422013	1.593071	3.124426
H	2.925558	3.756772	1.522486
H	3.732289	2.356442	.820470
H	.818355	3.177799	.568729
C	2.044335	2.653084	-1.126500

O	2.339020	3.821298	-1.369040	H	-2.188292	-.559394	2.195202
O	2.077775	1.643511	-1.910450	C	-2.805879	-.013092	.242927
H	1.959261	.243687	-1.543230	C	-2.769835	-.465259	-1.229433
H	-6.523035	-.247997	.673504	C	-4.211047	-.136886	.876517
H	-5.373660	-1.446680	1.355420	N	1.289307	1.265011	.922900
C	-3.105218	1.613626	-1.781632	C	1.884609	2.477432	.309919
H	-2.576853	2.260529	-2.489830	C	3.284505	2.563558	.950023
H	-3.894986	1.096759	-2.336353	C	3.141877	1.822759	2.283624
H	-3.577358	2.261143	-1.032821	C	2.201847	.666911	1.927894
C	-2.195725	-2.292102	1.497269	H	1.281044	3.345571	.593309
H	-3.103821	-2.837753	1.213189	H	4.013289	2.051707	.310944
H	-1.433974	-3.042046	1.736268	H	3.607724	3.600912	1.048279
H	-2.397809	-1.720356	2.409873	H	4.093201	1.462858	2.687104
C	5.396090	-1.434680	-.344634	H	2.674124	2.466648	3.038144
C	4.249345	-.809449	-.822021	H	2.754899	-.174948	1.495773
C	3.008412	-1.461259	-.694646	H	1.622904	.299716	2.779055
C	2.918198	-2.726555	-.092375	C	1.997150	2.521825	-1.273637
C	4.076717	-3.333155	.383987	O	2.368311	3.626116	-1.670610
C	5.315214	-2.694327	.260070	O	1.745866	1.464413	-1.931592
H	6.357613	-.939567	-.445266	H	1.521734	.029337	-1.443351
H	4.287170	.165603	-1.299607	C	-3.316500	2.408079	-.525566
H	1.951947	-3.213894	-.029332	H	-3.060556	3.459311	-.355209
H	4.016686	-4.314185	.847106	H	-3.192155	2.207330	-1.594415
H	6.214913	-3.178396	.628776	H	-4.372345	2.283817	-.262183
N	1.883903	-.808906	-1.209981	C	-1.980309	-2.359217	1.069833
O	.725786	-1.308225	-1.098284	H	-2.989323	-2.684047	1.346725

Syn-21

B3LYP/6-31G*

E+ZPE

=-1489.502539

O	-3.815799	-1.218202	-1.694769
O	-5.162331	-.852835	.218404
O	-4.499993	.398120	1.916909
O	-1.925103	-.136242	-2.017187
C	-2.411790	1.505999	.326153
H	-2.574865	1.766567	1.377715
C	-.932448	1.769014	-.007890
H	-.741920	1.645628	-1.079197
H	-.723398	2.818271	.229022
C	.014236	.882295	.754352
C	-.392682	-.405569	1.128706
H	.255361	-.989396	1.772983
C	-1.840066	-.830231	1.186766

H	-2.188292	-.559394	2.195202
C	-2.805879	-.013092	.242927
C	-2.769835	-.465259	-1.229433
C	-4.211047	-.136886	.876517
N	1.289307	1.265011	.922900
C	1.884609	2.477432	.309919
C	3.284505	2.563558	.950023
C	3.141877	1.822759	2.283624
C	2.201847	.666911	1.927894
H	1.281044	3.345571	.593309
H	4.013289	2.051707	.310944
H	3.607724	3.600912	1.048279
H	4.093201	1.462858	2.687104
H	2.674124	2.466648	3.038144
H	2.754899	-.174948	1.495773
H	1.622904	.299716	2.779055
C	1.997150	2.521825	-1.273637
O	2.368311	3.626116	-1.670610
O	1.745866	1.464413	-1.931592
H	1.521734	.029337	-1.443351
C	-3.316500	2.408079	-.525566
H	-3.060556	3.459311	-.355209
H	-3.192155	2.207330	-1.594415
H	-4.372345	2.283817	-.262183
C	-1.980309	-2.359217	1.069833
H	-2.989323	-2.684047	1.346725
H	-1.746376	-2.718059	.064120
H	-1.288963	-2.850389	1.763110
C	3.747661	-3.440261	.493089
C	2.558027	-2.792138	.171113
C	2.602638	-1.623888	-.607170
C	3.833101	-1.112945	-1.063460
C	5.009002	-1.779731	-.737420
C	4.973744	-2.941958	.041853
H	3.717802	-4.346166	1.092472
H	1.596967	-3.179102	.490112
H	3.837168	-.211244	-1.669350
H	5.959143	-1.391741	-1.093455
H	5.896090	-3.458321	.291392
N	1.442243	-.944104	-.982581
O	.290399	-1.314186	-.575427
C	-4.763117	-1.753363	-.800584
H	-5.657048	-1.967506	-1.384891
H	-4.376183	-2.671193	-.347124

Anti (for 1a)

B3LYP/6-31G*

E+ZPE =-1074.343124

C	-2.395571	-2.218993	.359881
H	-2.103347	-2.780967	-.542838
C	-1.243277	-1.306653	.689969
H	-.424370	-1.752484	1.244464
C	-1.284775	.078149	.541288
C	-2.409872	.741526	-.220231
H	-1.986232	1.416243	-.970037
H	-2.975339	1.373369	.484148
C	-3.364451	-.249583	-.909614
H	-2.841339	-.648107	-1.789415
C	-3.669320	-1.425817	.024941
N	-.252440	.846059	.952706
C	.704265	.416469	2.000459
C	1.049843	1.718166	2.729647
C	1.019444	2.755174	1.603746
C	-.142264	2.305547	.692694
H	1.594376	-.035905	1.546006
H	.234048	-.326905	2.648279
H	.282438	1.938496	3.481653
H	2.015837	1.656939	3.240335
H	.874733	3.781560	1.944039
H	1.959714	2.726979	1.040774
H	-1.076969	2.785005	1.001132
C	.128599	2.791419	-.786983
O	.081171	4.015582	-.891499
O	.392535	1.923583	-1.686363
H	.622800	.498220	-1.495399
C	4.433962	-.367435	-.622428
C	3.140135	-.006810	-.982894
C	2.111720	-.964129	-.898378
C	2.378391	-2.269591	-.455001
C	3.679010	-2.609089	-.093951
C	4.708375	-1.665321	-.176210
H	5.232820	.365431	-.690424
H	2.902257	.992888	-1.335563
H	1.569778	-2.990815	-.420267
H	3.894699	-3.618158	.246419
H	5.721415	-1.941194	.102072
N	.829275	-.568047	-1.291698
O	-.157754	-1.356949	-1.203524
H	-4.407089	-2.097500	-.432385

H	-4.123608	-1.046501	.953767
C	-4.633837	.465318	-1.383942
H	-4.393545	1.310195	-2.039677
H	-5.284026	-.218120	-1.942081
H	-5.209335	.854820	-.533879
C	-2.634977	-3.243087	1.483086
H	-1.735068	-3.837735	1.680888
H	-2.923397	-2.745950	2.417260
H	-3.439111	-3.935190	1.208285

Syn (for 1a)

B3LYP/6-31G*

E+ZPE =-1074.342549

C	-3.713542	-.282651	-.013918
H	-4.127754	-.218651	1.004727
C	-2.480278	.636802	-.082353
H	-2.162418	.766699	-1.126165
H	-2.748877	1.638034	.274070
C	-1.294386	.117071	.697404
C	-1.162552	-1.251969	.953683
H	-.317719	-1.596800	1.540762
C	-2.300725	-2.229129	.792580
H	-2.828910	-2.261013	1.763037
C	-3.306326	-1.741074	-.261556
N	-.279516	.959840	.971585
C	-.234266	2.382831	.544366
C	1.030369	2.927081	1.236395
C	1.185204	2.053005	2.484803
C	.763632	.667157	1.985478
H	-1.122927	2.892649	.930598
H	1.896533	2.797353	.576580
H	.932368	3.993426	1.446066
H	2.201517	2.047594	2.890404
H	.505741	2.388618	3.277523
H	1.605964	.134098	1.529312
H	.344556	.034964	2.772617
C	-.184202	2.698531	-1.002505
O	-.403945	3.883344	-1.247423
O	.117733	1.756955	-1.810504
H	.486992	.379190	-1.461685
C	3.787091	-2.385778	.091472
C	2.450179	-2.153637	-.220877
C	2.086356	-.926608	-.798918

C	3.056688	.058634	-1.064353	N	1.321367	1.099168	.674233
C	4.387482	-.195718	-.751939	C	2.039420	.667288	1.897219
C	4.758319	-1.414658	-.172142	C	2.697903	1.952965	2.408549
H	4.075846	-3.334558	.535524	C	3.017136	2.709910	1.116346
H	1.686981	-2.903474	-.046548	C	1.815457	2.415944	.195247
H	2.745509	.995190	-1.518844	H	2.788109	-.096367	1.653062
H	5.140239	.558813	-.961890	H	1.329864	.238950	2.609174
H	5.799709	-1.607852	.068510	H	1.984936	2.517829	3.020971
N	.766558	-.639497	-1.155305	H	3.580860	1.746013	3.021053
O	-.175037	-1.465112	-.930078	H	3.154904	3.784387	1.246838
H	-4.193142	-2.387855	-.246104	H	3.933789	2.312531	.664146
H	-2.857660	-1.830938	-1.259428	H	1.030388	3.164060	.349956
C	-1.798093	-3.654788	.513287	C	2.257201	2.555117	-1.307522
H	-1.111632	-3.993905	1.298994	O	2.477276	3.716502	-1.639098
H	-2.640192	-4.355288	.482846	O	2.388755	1.495596	-2.021893
H	-1.272182	-3.706243	-.443826	H	2.251385	.207386	-1.566656
C	-4.790598	.192363	-.995518	C	-2.773054	1.380782	-2.136513
H	-5.694932	-.421528	-.913214	H	-2.172555	1.836911	-2.931661
H	-5.072805	1.234608	-.805865	H	-3.572719	.807333	-2.610961
H	-4.432222	.128177	-2.030247	H	-3.223189	2.186166	-1.549513

Anti-22

B3LYP/6-31G*

E+ZPE =-1529.991527

O	-4.159394	1.281188	.558833	C	5.653145	-1.440591	-.169659
O	-4.716590	-1.437162	.089516	C	4.521253	-.846622	-.717404
O	-3.687410	-1.651198	-1.904201	C	3.275629	-1.487239	-.582547
O	-2.574848	.693952	2.044303	C	3.165746	-2.712000	.095477
C	-1.520624	-1.388523	.365909	C	4.308822	-3.287982	.641767
H	-1.334439	-2.053029	-.492527	C	5.551779	-2.658812	.511843
C	-.209951	-.725307	.693697	H	6.618655	-.954328	-.275378
H	.412900	-1.250818	1.408196	H	4.574579	.095290	-1.256022
C	.143139	.549972	.293191	H	2.196063	-3.191766	.163799
C	-.714307	1.302236	-.692486	H	4.233790	-4.236940	1.165595
H	-.090366	1.648869	-1.521983	H	6.439611	-3.118763	.936212
H	-1.103190	2.207586	-.201215	N	2.166052	-.862324	-1.167646
C	-1.871269	.477316	-1.284458	O	1.018670	-1.378300	-1.081587
H	-1.436974	-.274247	-1.952018	C	-5.786494	-2.260095	-.410737
C	-2.583834	-.361443	-.164299	H	-6.264648	-1.780388	-1.268336
C	-3.089707	.561081	.953607	H	-5.407314	-3.238930	-.714801
C	-3.717474	-1.192865	-.783169	H	-6.488753	-2.357737	.417209
				C	-4.696349	2.184583	1.540952
				H	-5.033566	1.631002	2.420965
				H	-3.942456	2.914755	1.845712
				H	-5.535919	2.678898	1.052097

Syn-23

B3LYP/6-31G*

E+ZPE =-1529.987365

O	2.599693	-1.878064	1.038651
O	4.859177	-.240348	.255879
O	4.413656	-.036419	-1.943497
O	2.049766	.063105	2.029329
C	2.240261	1.595013	-.372669
H	2.397414	1.900441	-1.416224
C	.762968	1.863125	-.026291
H	.580700	1.681612	1.039011
H	.561997	2.927262	-.198491
C	-.195431	1.033483	-.841497
C	.228016	-.174369	-1.394916
H	-.451438	-.731783	-2.029836
C	1.674546	-.583803	-1.495495
H	2.078194	-.125236	-2.410683
C	2.558838	.055788	-.367915
C	2.357463	-.553336	1.033829
C	4.030987	-.098239	-.794331
N	-1.495337	1.387754	-.888399
C	-2.071354	2.537795	-.147598
C	-3.512585	2.629635	-.685746
C	-3.429562	2.037964	-2.096186
C	-2.432804	.887036	-1.923526
H	-1.510727	3.441021	-.410133
H	-4.177235	2.020487	-.061695
H	-3.878198	3.657071	-.651755
H	-4.392689	1.688196	-2.480245
H	-3.030470	2.776164	-2.802229
H	-2.933753	-.026611	-1.583272
H	-1.880901	.654483	-2.837845
C	-2.089029	2.476785	1.431445
O	-2.373940	3.560268	1.937717
O	-1.876315	1.356062	2.004302
H	-1.644163	.065643	1.369423
C	3.158561	2.464740	.499103
H	2.866834	3.516494	.398728
H	3.086450	2.187053	1.552026
H	4.204944	2.386336	.187119
C	1.802056	-2.102485	-1.713655
H	2.850533	-2.395839	-1.811848
H	1.353790	-2.675045	-.902252

H	1.296666	-2.367970	-2.650410
C	-3.792528	-3.391918	-.723858
C	-2.619521	-2.714594	-.401753
C	-2.684213	-1.604466	.456243
C	-3.915667	-1.178986	.990410
C	-5.074520	-1.873739	.662170
C	-5.019733	-2.978750	-.195423
H	-3.749074	-4.253087	-1.385075
H	-1.656070	-3.032357	-.783720
H	-3.932563	-.320739	1.656190
H	-6.025957	-1.553468	1.077139
H	-5.928772	-3.517520	-.446707
N	-1.540064	-.895270	.833128
O	-.394475	-1.212969	.383343
C	2.424763	-2.524210	2.311536
H	3.104788	-2.096981	3.052719
H	1.394980	-2.403865	2.655928
H	2.655019	-3.575740	2.137380
C	6.260800	-.324021	-.061184
H	6.454691	-1.191306	-.697095
H	6.589730	.580564	-.578775
H	6.768721	-.426418	.897575

Anti (with 1h)

B3LYP/6-31G*

E+ZPE =-1817.057541

O	4.192827	.690746	-.065145
O	2.971376	.930832	-1.950995
C	.679030	1.319822	-.209727
H	.639912	1.359850	-1.306464
C	-.655268	.804087	.267517
H	-1.382807	1.567522	.511540
C	-.876626	-.510322	.701539
C	.130528	-1.595716	.408379
H	-.367740	-2.398510	-.144425
H	.466698	-2.024937	1.361139
C	1.332958	-1.119064	-.425413
H	.975310	-.920911	-1.440122
C	1.833468	.290522	.079364
C	3.059594	.687107	-.766153
N	-2.048617	-.865678	1.248872
C	-2.992732	.087352	1.876848
C	-3.562696	-.712751	3.050678

C -3.663424 -2.132212 2.480151
C -2.455926 -2.265483 1.525091
H -3.777787 .366125 1.162811
H -2.464460 .991440 2.184382
H -2.863775 -.677129 3.894812
H -4.523231 -.312545 3.389280
H -3.650234 -2.911860 3.243340
H -4.592797 -2.255396 1.914842
H -1.623113 -2.773944 2.020764
C -2.833399 -3.178431 .276241
O -3.251630 -4.280246 .627223
O -2.661947 -2.712918 -.895342
H -2.645922 -1.260345 -1.350944
C -6.205928 .562386 -1.410048
C -5.012135 -.151173 -1.429731
C -3.795500 .547768 -1.544806
C -3.777700 1.949271 -1.636424
C -4.983147 2.644379 -1.608151
C -6.197526 1.959013 -1.497009
H -7.147478 .027222 -1.326567
H -4.995714 -1.235733 -1.366824
H -2.828570 2.461743 -1.744756
H -4.976923 3.728390 -1.681330
H -7.133271 2.510200 -1.482423
N -2.620552 -.204765 -1.579745
O -1.473367 .352174 -1.588793
C 5.408524 .981335 -.807297
H 5.500182 .245543 -1.611496
H 5.304382 1.970796 -1.262422
C 2.139868 .235192 1.515521
N 2.295774 .154566 2.663471
C .979311 2.733345 .278661
C 1.477225 3.683373 -.624513
C 1.759050 4.985126 -.208055
C 1.545319 5.357436 1.119774
C 1.050001 4.419931 2.027667
C .767955 3.118911 1.610506
H 1.647150 3.396528 -1.658822
H 2.140795 5.708404 -.923770
H 1.761810 6.371369 1.445324
H .883559 4.699493 3.064497
H .391635 2.396722 2.329328
C 2.426749 -2.173483 -.522443
C 2.995499 -2.776332 .609900
C 3.995543 -3.739601 .475223
C 4.443271 -4.119395 -.791387

C 3.886960 -3.525505 -1.924482
C 2.888585 -2.559933 -1.788539
H 2.670258 -2.490018 1.605366
H 4.422816 -4.195661 1.364201
H 5.217573 -4.874996 -.893548
H 4.224113 -3.815263 -2.916070
H 2.460072 -2.099370 -2.674954
C 6.561498 .913186 .174079
H 6.436464 1.646891 .976315
H 6.632290 -.082223 .622879
H 7.500940 1.126194 -.347431

Syn (with 1h)

B3LYP/6-31G*

E+ZPE =-1817.049811

C 1.625976 -1.227754 .615564
H 1.737328 -1.179893 1.704700
C .213099 -1.755285 .305643
H .040147 -1.847460 -.773183
H .135395 -2.767887 .710943
C -.869964 -.870456 .871061
C -.676629 .525438 .881794
H -1.438345 1.154833 1.327372
C .710271 1.134975 .915740
H 1.032599 1.042938 1.962736
C 1.791399 .275874 .160601
N -2.065531 -1.392758 1.165601
C -2.450045 -2.808051 .919666
C -3.839539 -2.929622 1.575652
C -3.849623 -1.842381 2.654982
C -3.089324 -.694780 1.984400
H -1.732083 -3.455485 1.432633
H -4.617949 -2.728250 .830385
H -4.004823 -3.938376 1.956842
H -4.855664 -1.538364 2.959402
H -3.310445 -2.177063 3.549369
H -3.751059 -.101845 1.342821
H -2.599429 -.022736 2.692896
C -2.500244 -3.302685 -.585496
O -2.660408 -4.520286 -.661847
O -2.411364 -2.435266 -1.510488
H -2.485236 -.915877 -1.409848
C -4.914921 2.844741 -.507791

C	-3.690614	2.201020	-.669893
C	-3.674635	.851269	-1.059239
C	-4.878419	.156181	-1.285223
C	-6.089769	.820270	-1.125180
C	-6.115009	2.163833	-.734506
H	-4.932276	3.889664	-.210215
H	-2.752853	2.724767	-.521450
H	-4.837268	-.885210	-1.592825
H	-7.019220	.287912	-1.306475
H	-7.064163	2.677347	-.611888
N	-2.483876	.153376	-1.257382
O	-1.345448	.690594	-1.015280
C	.762469	2.630376	.611139
C	.337187	3.184837	-.607627
C	.418224	4.561669	-.822750
C	.923465	5.407395	.166281
C	1.353467	4.866897	1.378031
C	1.273774	3.490687	1.594880
H	-.051751	2.543581	-1.388014
H	.087781	4.971892	-1.773299
H	.983975	6.478402	-.007999
H	1.752006	5.512639	2.156036
H	1.622068	3.075964	2.537562
C	2.719342	-2.151739	.095620
C	2.703698	-2.673182	-1.206394
C	3.721876	-3.521736	-1.642104
C	4.770314	-3.864527	-.786921
C	4.796237	-3.352172	.510648
C	3.777487	-2.504359	.946727
H	1.901816	-2.417406	-1.891020
H	3.690650	-3.917259	-2.653457
H	5.558622	-4.530012	-1.128381
H	5.603953	-3.616658	1.188051
H	3.803024	-2.107634	1.958681
C	1.698331	.391729	-1.300557
N	1.618010	.449847	-2.456687
C	3.173967	.748108	.674922
O	3.430029	.795241	1.861053
O	4.019661	1.059679	-.302196
C	5.354951	1.468151	.102314
H	5.801413	.650476	.675793
H	5.262442	2.335751	.762251
C	6.130775	1.780018	-1.161747
H	6.191995	.899666	-1.808553
H	5.653749	2.589105	-1.723073
H	7.148193	2.091080	-.900871

Anti-24 (with 17a)

B3LYP/6-31G*

E+ZPE

=-1394.404440

O	-5.241093	-.393770	.077117
O	-4.018497	-1.732373	-1.269080
C	-1.801212	-1.265316	.535570
H	-1.754505	-1.913529	-.350460
C	-.431730	-.677446	.750255
H	.222078	-1.251666	1.396048
C	-.093953	.647054	.451743
C	-.995560	1.486263	-.419083
H	-.415116	1.851664	-1.272212
H	-1.313990	2.368253	.155689
C	-2.226379	.740899	-.958021
H	-1.894764	.041760	-1.733306
C	-2.850629	-.168301	.159302
C	-4.092997	-.868308	-.423790
N	1.099991	1.150021	.804147
C	1.933787	.599098	1.897783
C	2.593840	1.843925	2.497472
C	2.833164	2.729188	1.269506
C	1.624236	2.461751	.347073
H	2.680808	-.095129	1.492767
H	1.305535	.058995	2.608717
H	1.902975	2.326205	3.199143
H	3.511317	1.597775	3.040607
H	2.921694	3.791139	1.502981
H	3.756797	2.435070	.759519
H	.845406	3.215277	.502944
C	2.053817	2.596305	-1.177177
O	2.517000	3.708158	-1.424969
O	1.881664	1.602240	-1.954501
H	1.758712	.135540	-1.591931
C	5.175851	-1.646854	-.519492
C	4.037473	-.981879	-.962601
C	2.775634	-1.574420	-.767149
C	2.658127	-2.821048	-.131211
C	3.809207	-3.467226	.310165
C	5.067875	-2.887538	.118799
H	6.152189	-1.196124	-.672648
H	4.098987	-.020009	-1.463947
H	1.675979	-3.264920	-.014538

H	3.726141	-4.433850	.799289
H	5.960930	-3.402225	.461046
N	1.658563	-.885483	-1.243929
O	.475937	-1.309014	-1.035008
C	-6.445580	-.977578	-.459430
H	-6.504947	-.801179	-1.536138
H	-6.461813	-2.053407	-.269670
H	-7.262609	-.479331	.061147
C	-3.184930	.651320	1.336102
N	-3.369957	1.317522	2.268982
C	-3.222406	1.731247	-1.571450
H	-3.655705	2.387988	-.808475
H	-2.714087	2.360151	-2.310012
H	-4.039636	1.215466	-2.085823
C	-2.236632	-2.130236	1.730372
H	-2.340529	-1.536196	2.644385
H	-3.193173	-2.624249	1.529308
H	-1.494963	-2.915218	1.914266

Syn-25 (with 17a)

B3LYP/6-31G*

E + ZPE = -1394.398352

C	-2.476100	1.343003	.203048
H	-2.678956	1.547589	1.261883
C	-.998869	1.656631	-.084214
H	-.770076	1.536664	-1.151686
H	-.823593	2.712911	.142527
C	-.050453	.791181	.705226
C	-.413018	-.538249	.987888
H	.243545	-1.132412	1.614176
C	-1.844470	-1.017310	.977612
H	-2.248642	-.816272	1.980452
C	-2.778136	-.188255	.030366
N	1.190941	1.223993	.955736
C	1.756524	2.499363	.444086
C	3.137866	2.583993	1.121879
C	2.985917	1.758560	2.403614
C	2.094682	.597642	1.953045
H	1.117649	3.322164	.780713
H	3.894935	2.131819	.470624
H	3.428201	3.621973	1.290667
H	3.937865	1.404362	2.810431
H	2.478575	2.340220	3.182683

H	2.685634	-.198631	1.486126
H	1.504745	.162171	2.763305
C	1.897092	2.661618	-1.127527
O	2.207943	3.810568	-1.440719
O	1.719905	1.638517	-1.859794
H	1.584956	.156838	-1.464625
C	3.678244	-3.477265	.318394
C	2.512902	-2.797152	-.026388
C	2.610634	-1.568589	-.699958
C	3.869903	-1.030825	-1.029116
C	5.021102	-1.729841	-.683141
C	4.932559	-2.952026	-.006849
H	3.607058	-4.430024	.836044
H	1.532894	-3.204949	.193787
H	3.916742	-.082422	-1.557244
H	5.993153	-1.319965	-.942417
H	5.835458	-3.493540	.259778
N	1.482165	-.846423	-1.087389
O	.300355	-1.224210	-.767456
C	-2.625142	-.578333	-1.380728
N	-2.503697	-.857611	-2.500390
C	-4.229647	-.419668	.515760
O	-4.554700	-.271694	1.674458
O	-5.068459	-.764300	-.465963
C	-6.442604	-.963540	-.076146
H	-6.857348	-.039659	.334229
H	-6.960990	-1.249038	-.990664
H	-6.511999	-1.754423	.674382
C	-1.946465	-2.534024	.743162
H	-2.980238	-2.874758	.865381
H	-1.602473	-2.810522	-.255444
H	-1.335823	-3.068971	1.479182
C	-3.387287	2.233592	-.650876
H	-3.249698	2.033558	-1.718664
H	-4.444288	2.082709	-.408019
H	-3.154905	3.288806	-.472336

Anti (for 26)

B3LYP/6-31G*

E+ZPE = -1457.706260

C	1.128176	1.781794	-0.467686
H	0.931437	1.834567	-1.550158
C	-0.041226	1.046574	0.140395

O	.335761	-4.683470	-.453037
O	-.368150	-2.758452	-1.406993
H	-1.033717	-1.452739	-1.339617
C	-4.902807	.942799	-.799281
C	-3.512945	.882131	-.854742
C	-2.895900	-.341713	-1.163076
C	-3.666027	-1.492885	-1.416246
C	-5.053118	-1.408464	-1.363308
C	-5.676598	-.194387	-1.053108
H	-5.387192	1.886570	-.564085
H	-2.898371	1.758964	-.683789
H	-3.160293	-2.423477	-1.658862
H	-5.651468	-2.292489	-1.564677
H	-6.760411	-.134633	-1.013395
N	-1.507860	-.465015	-1.249820
O	-.743123	.522447	-.999800
C	.151754	3.222288	.580739
C	-.192856	3.521708	-.746707
C	-.780880	4.745225	-1.071059
C	-1.036460	5.693663	-.078436
C	-.697836	5.409184	1.244240
C	-.108001	4.185249	1.565308
H	-.009225	2.794203	-1.529021
H	-1.037511	4.958026	-2.105662
H	-1.491631	6.646489	-.335245
H	-.885974	6.139583	2.026918
H	.159848	3.976354	2.599267
C	3.958902	-.141699	-.021207
C	4.009636	-.437208	-1.391647
C	5.221989	-.730454	-2.015246
C	6.408994	-.733423	-1.279576
C	6.372826	-.441619	.083866
C	5.156728	-.148929	.704094
H	3.095810	-.443655	-1.980560
H	5.238062	-.960829	-3.077154
H	7.353080	-.964516	-1.765520
H	7.289668	-.443389	.667726
H	5.137322	.076915	1.768423
H	2.789131	2.325058	.227607
H	1.777665	1.424738	-.903023
