

Understanding and Quantifying the Impact of Solute-Solvent Van-der-Waals Interactions on the Selectivity of Asymmetric Catalytic Transformations in Organic Solvents – Supporting Information

Riya Kayal ^[a], Lorenzo Baldinelli^[b], Ingolf Harden ^{*[a]}, Frank Neese ^[a], Giovanni Bistoni ^{*[b]}

^[a]*Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm Platz 1, 45470 Mülheim an der Ruhr (Germany)*

^[b]*Department of Chemistry, Biology and Biotechnology, University of Perugia Via Elce di Sotto, 8, 06123 Perugia (Italy).*

E-mail: ingolf.harden@mpg.kofo.de

E-mail: giovanni.bistoni@unipg.it

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S1 Effect of implicit solvation models on the relative stability of TS conformers

Table S1. Relative electronic energies (in kcal mol⁻¹) between transition state conformers using different implicit solvation models and solvents at the B3LYP-D3(BJ)/def2-TZVP level of theory. **Major₀** was used as reference in all cases. CyH: cyclohexane, Ac: acetone, GP: Gas phase. $E(\text{SMD}') = E(\text{SMD}) - E(\text{CDS})$.

	GP	CPCM/CyH	CPCM/Ac	SMD/CyH	SMD/Ac	SMD'/CyH	SMD'/Ac
Major₀	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Major₁	0.51	0.54	0.49	0.37	0.30	0.41	0.25
Major₂	2.19	2.24	2.20	2.17	1.99	2.17	2.07
Major₃	5.87	5.14	4.36	4.03	3.33	4.86	3.82
Major₄	6.46	5.81	5.08	5.60	4.99	5.70	4.89
Minor₀	3.72	3.79	3.74	4.36	3.48	3.58	3.41
Minor₁	4.50	4.69	5.04	4.18	3.99	4.36	4.48
Minor₂	5.98	5.38	4.76	5.73	4.76	5.34	4.59
Minor₃	6.33	5.16	4.00	4.60	2.75	4.62	2.89
Minor₄	9.69	9.44	9.30	8.43	7.99	9.00	8.51

Table S2. Cavity-dispersion solvent structure (CDS) term contribution to the relative energy between TS conformers at the B3LYP-D3(BJ)/def2-TZVP +SMD level (SMD – SMD'). All energies are in kcal mol⁻¹.

	SMD – SMD' (CyH)	SMD – SMD' (Ac)
Major₀	0.00	0.00
Major₁	-0.04	0.05
Major₂	-0.01	-0.08
Major₃	-0.83	-0.49
Major₄	-0.10	0.10
Minor₀	0.77	0.07
Minor₁	-0.18	-0.48
Minor₂	0.39	0.17
Minor₃	-0.02	-0.14
Minor₄	-0.57	-0.52

S2 Decomposition of relative electronic energies in geometric preparation and catalyst-substrate interaction contributions

The relative electronic energies between the conformers were decomposed into additive contributions corresponding to the catalyst/substrate distortion and catalyst-substrate interaction (Table S3). The results confirm that the lowest in energy TS conformer, **Major₀**, features the smallest energetic contribution from the geometric distortion over the entire set of conformers considered in this work. Hence, the design of highly selective catalysts should consider the structural features of the substrate and of the chiral pocket of the catalyst.

Table S3. Relative electronic energies ΔE_{el} , relative geometric preparation energies $\Delta E_{\text{Geo_prep}}$ and relative catalyst-substrate interaction energies ΔE_{int} for five major and minor transition state conformers at the B3LYP-D4/def2-TZVP level of theory. All energies are in kcal mol⁻¹.

	ΔE_{el}	$\Delta E_{\text{Geo_prep}}$	ΔE_{int}
Major₀	0.00	0.00	0.00
Major₁	0.37	0.56	-0.20
Major₂	2.58	1.95	0.63
Major₃	5.54	2.64	2.90
Major₄	7.03	5.59	1.44
Minor₀	3.70	6.13	-2.44
Minor₁	4.46	8.28	-3.82
Minor₂	6.17	1.78	4.39
Minor₃	6.65	7.85	-1.20
Minor₄	9.57	13.38	-3.81

S3 3D Structures of selected conformers

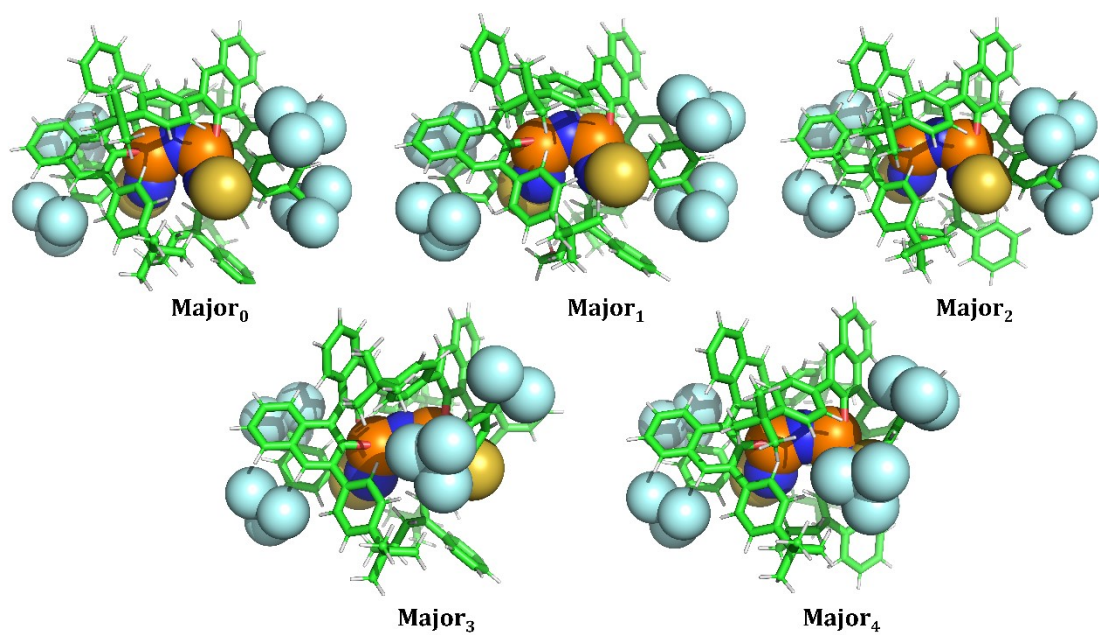


Figure S1. 3D structures of **Major₀** to **Major₄** highlighting the core catalyst and the Ph-(CF₃)₂ groups.

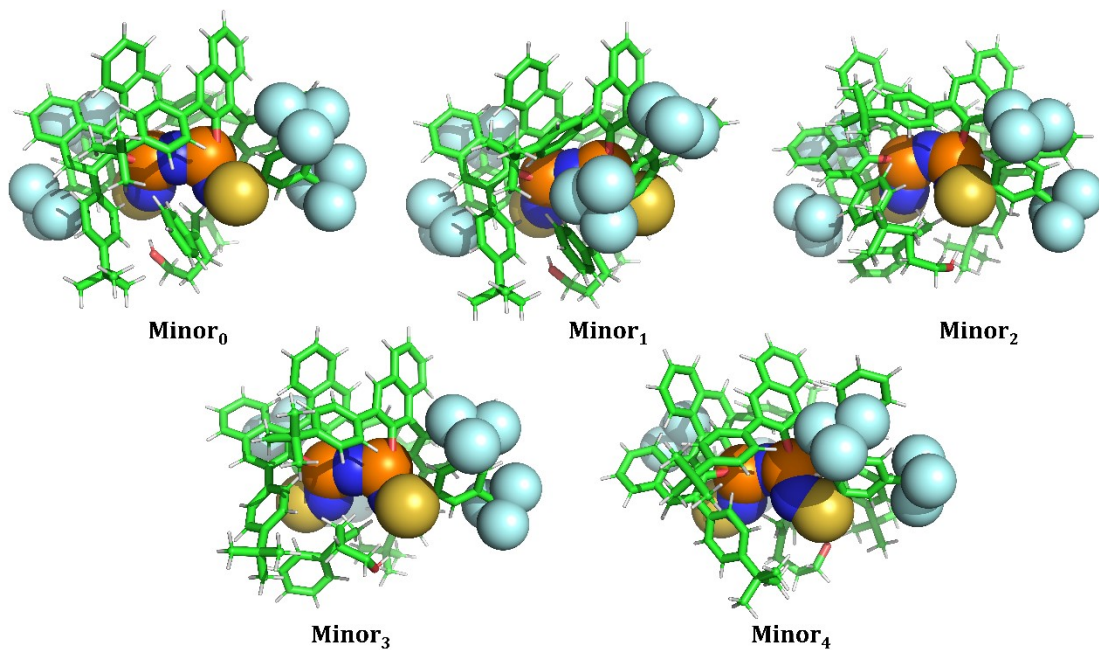


Figure S2. 3D structures of **Minor₀** to **Minor₄** highlighting the core catalyst and the Ph-(CF₃)₂ groups.

S4 Hybrid implicit/explicit solvation model: Computational details and number of optimized conformers at each step

The hybrid explicit/implicit solvation was carried out in an iterative manner, adding one solvent (cyclohexane) molecule at each step to the most stable conformer of both the major and minor stereoisomers of the TS complex (**Major**₀ and **Minor**₀, respectively). The starting geometries of the conformers without solvent molecules were obtained from a previous work by our group¹. Conformational sampling in the presence of a single solvent molecule was performed using the Conformer–Rotamer Ensemble Sampling Tool^{2,3} (CREST) from the Extended Tight-Binding Program Package⁴⁻⁶ (xTB), at the xTB-GFN-FF⁷ levels of theory. For the metadynamics simulations, a simulation time of 50 ps was chosen. In addition, the solute was kept frozen at its DFT-optimized TS structure. In order to avoid dissociation of the solute-solvent aggregate, an ellipsoid wall potential³ was used. Afterwards, the whole conformer ensemble was optimized at the GFN2-xTB level, again with fixed solute. For the next iteration, another solvent molecule was added to the most stable optimized structure and the above conformational sampling was reapplied. This scheme was repeated up to the addition of four solvent molecules. The most stable conformers with significantly different structural features were subjected to constrained geometry optimizations PBE-D3⁸/def2-SVP level of theory. Afterwards, fully relaxed transition state geometries were obtained using Grimme’s r2SCAN-3c composite method⁹. From this protocol we obtained the lowest-in energy transition states for the major and minor enantiomeric pathways with 0 to 4 added solvent molecules. The number of TS conformers optimized at the xTB and DFT level at each step are reported in Table S4.

Table S4. Numbers of xTB/DFT geometry optimizations performed for **Major**₀ and **Minor**₀ with one to four cyclohexane (CyH) molecules.

	xTB	DFT
1 CyH	1382	78
2 CyH	469	59
3 CyH	809	43
4 CyH	884	35

For the solvated system with four solvent molecules the xTB optimized structures together with their relative electronic energies are given in **Figure S3** and **Figure S4**.

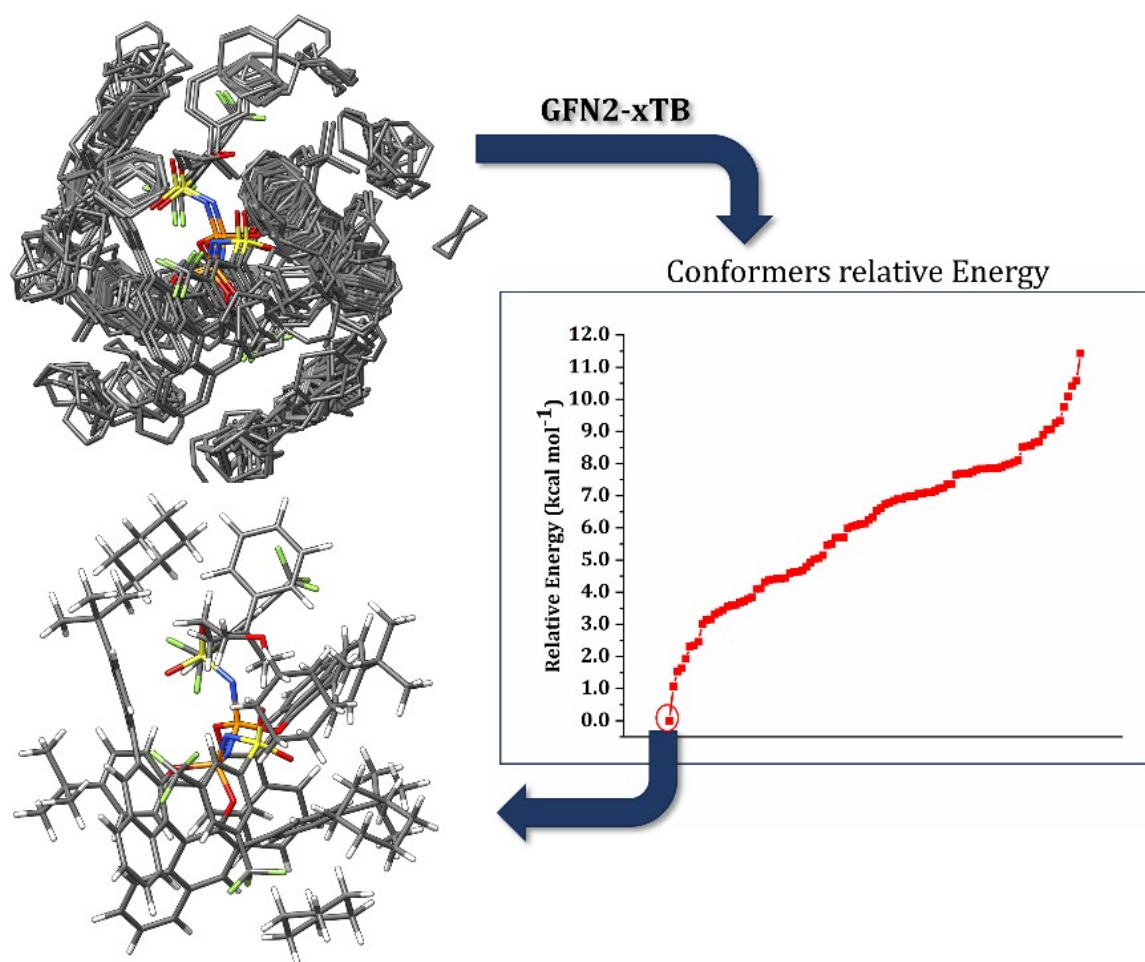


Figure S3. Low energy conformers for **Major₀** with 4 CyH molecules optimized at the GFN2-xTB level. Only the solvent network was optimized while the transition state was kept frozen in its DFT optimized structure. For clarity, the hydrogen atoms are omitted in the overlay of the individual conformers. The lowest-in energy conformer is shown at the bottom.

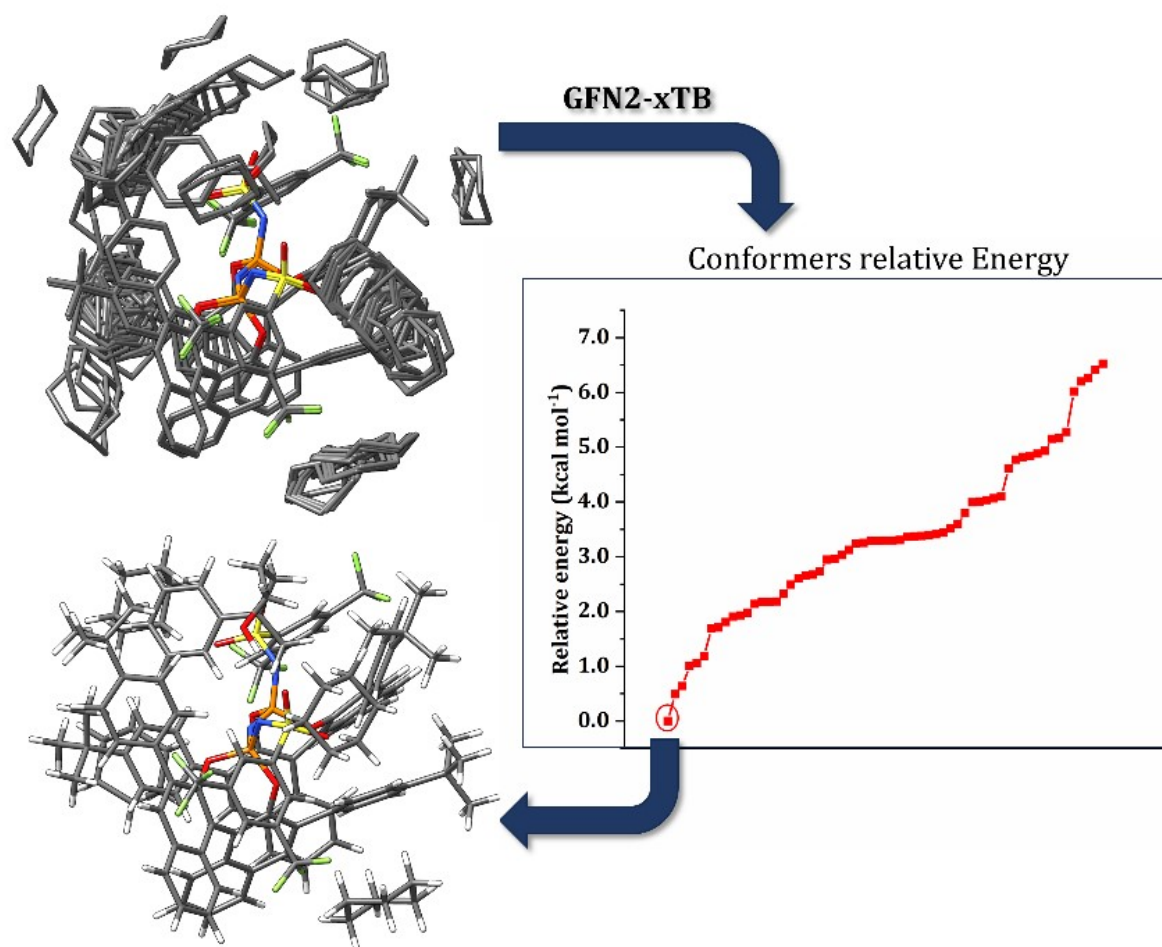


Figure S4. Low energy conformers for **Minor₀** with 4 CyH molecules optimized at the GFN2-xTB level. Only the solvent network was optimized while the transition state was kept frozen in its DFT optimized structure. For clarity, the hydrogen atoms are omitted in the overlay of the individual conformers. The lowest-in energy conformer is shown at the bottom.

S5 Effect of hybrid explicit/implicit solvation models on the relative stability of TS conformers

Table S5. Relative electronic energies (in kcal/mol) between **Minor₀** and **Major₀** with 0 – 4 solvent molecules at different levels of theory.

	B3LYP-D3	M06-2X	ω B97M-V
	ΔE_{adduct}	ΔE_{adduct}	ΔE_{adduct}
0 CyH	3.38	7.47	5.98
1 CyH	3.88	8.1	6.65
2 CyH	4.79	8.86	8.25
3 CyH	4.24	8.75	7.04
4 CyH	2.76	8.02	5.94

S6 Influence of explicit solvation on transition state structures

To test the influence of explicit solvation on the transition state geometry, the geometries of the fully relaxed transition states optimized *in vacuo* are compared with the fully relaxed transition states explicitly solvated by four cyclohexane molecules (**Figure S5**).

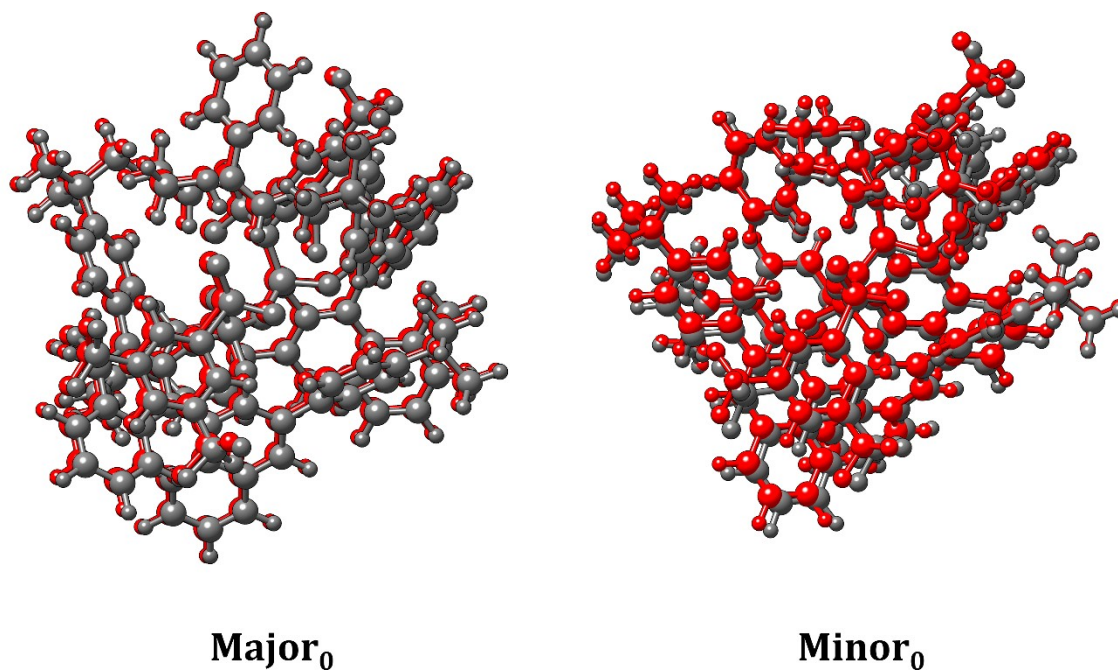


Figure S5. Optimally aligned transition state structures of the transition states optimized at the r2SCAN-3c level of theory in gas phase (dim grey) and with four explicit cyclohexane molecules (red) for **Major₀** and **Minor₀**. RSMD: 0.09 Å (**Major₀**), 0.32 Å (**Minor₀**).

As can be seen from the small RMSD values, implicit solvation has rather small impact on the transition state structure. As expected, the largest deviations in structure occur for the groups that are in direct interaction with the solvent molecules.

S7 References

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S8 XYZ Coordinates

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Major0

C	0.95233617156085	-4.15906190571433	-0.19026716977022
C	-0.24753804718309	-4.26749649187697	0.69994190794283
C	-0.94871694601085	-5.63413049101322	0.68786552371341
C	-1.73537055920114	-5.87034627138391	-0.59855393129617
O	-0.91758569956540	-5.69570473954126	-1.75830891151776
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C	2.03262218463091	-5.15233466427240	-0.08522917323837
C	2.76703020805937	-5.50205306429230	-1.23250990662907
C	2.36531795646483	-5.76273203148524	1.13788446120265
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C	-1.62486159035388	-2.31144690358167	3.94773646914565
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H	-3.59032329531320	-5.00140468321707	3.31662736708111
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C	-1.35601196618926	-4.62669956006515	4.97185397535700
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Major1

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C	3.26730118668847	4.49120269207650	-0.78168113348962
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P	-1.60869831816929	0.22922109209463	-0.34577962167887
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S	2.13309733035949	-1.04341592815220	2.46590807818259
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Major4

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Major2

C	-1.18107351519381	4.33134819791149	0.28843096117256
C	-0.19448269347373	4.68839680712555	1.35885999758153
C	1.28873335152467	4.67304300855516	0.98107208799469
C	1.64732128727465	5.84108971586546	0.06972433343125
O	0.83456868189270	5.89828914360175	-1.10170829059460
H	-0.46584994645980	5.66123001647718	1.79435427269587
H	1.56086596994021	3.71844480124675	0.50882430777701
H	2.71940080481480	5.79139857968981	-0.19819996203422
C	-2.40208199503392	5.14275799084936	0.18210355740370
C	-3.64712067372956	4.52813844403955	-0.03267875198559
C	-2.34827943125385	6.54555058922028	0.27030569393935
C	-4.81043370305300	5.28597825591644	-0.12558239784987
H	-3.69066054916876	3.44296933577120	-0.11461543540801
C	-3.50786665114441	7.30586164764793	0.13581958518286
H	-1.38293962069674	7.03830258319649	0.38557937594876
C	-4.74378674738047	6.67963020750741	-0.04615759018416

H	-5.77245511750960	4.78844695510845	-0.26109984621887
H	-3.44753569369201	8.39427637860924	0.17817571432283
H	-5.65323890657165	7.27680931126602	-0.12776281878326
C	-1.03542255870780	3.19731716355198	-0.49238640180342
H	-1.68229557934329	3.08324367101513	-1.36468193469476
H	-0.03679719346017	2.76005517966268	-0.57681536851167
H	-4.72677332600623	-2.38675156375687	-5.31389241881675
C	-3.86178187304042	-2.45178345858245	-4.63666566232877
C	-2.55561978754467	-2.52884671327476	-5.45207054715957
H	-3.99554279720008	-3.33765555063877	-4.00137792878510
H	-3.87081737742661	-1.56657046439482	-3.98730690262839
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C	-2.59556996205424	1.09687832795350	-3.19180428236266
C	-0.25293492369955	-1.81227015862689	-4.53433639528130
C	-1.32685970706210	-3.72128398258901	-3.57255760606097
H	-1.57477196668299	-1.29479728061404	-6.98135705513407
H	-3.34705907981789	-1.21848617933137	-6.98277538173481
H	-2.43336831449543	-0.35510026577215	-5.73046758623135
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C	0.83815662775820	-1.99122697443036	-3.68314372896419
H	-0.22291961310798	-0.97713474915570	-5.23374582085913
C	-0.24487553728990	-3.90586468738785	-2.72056207103171
H	-2.17075992073694	-4.40747723075994	-3.49375563430961
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C	-4.52226147692221	2.35265175649841	-2.50005761731572
C	-2.81875500337872	3.43605194475462	-3.86631293009596
H	-1.15894409659685	2.13711671044371	-4.37759034991894
C	0.86873610906557	-3.04859962982179	-2.76171893267912
H	1.66572281687523	-1.28817860120119	-3.74241676284758
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C	-3.52286097435629	-0.96192262539175	-1.07513842993131
C	-5.72182507182935	-0.23999628681843	-1.67413951620787
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H	-5.45586471460976	2.43469429434383	-1.94106401320480
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C	2.01868218134635	-3.30734592904367	-1.86638111050643
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C	-3.99259616799448	-2.12067522019370	-0.46950298900692
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C	-6.27771855538026	-1.31893929819023	-0.95056167886119
H	-4.61809013598969	4.39056412648218	-3.13908298652878
C	-3.14133077191913	5.88815226388083	-4.45644994879550
C	-1.99992071836572	4.33919923291096	-6.05383322381485

C	-0.87579375230787	5.00726103340793	-3.89915056781027
C	2.74712691401963	-2.26631834021711	-1.22512570868697
C	2.42694338011691	-4.60341815933765	-1.59387215943975
P	-1.33069425611623	-0.43468887638760	0.25021658501502
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C	-3.04107317917205	-3.16500859681345	-0.00424426662721
C	-7.68345767169362	-1.46686810465105	-0.81469241727275
H	-3.30432939720026	6.18312089044133	-3.40883336322907
H	-2.67368144097926	6.73941135790078	-4.97145434610611
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H	-1.56797026742648	5.21125984940558	-6.56709137586999
H	-0.41021449474417	5.86296079445104	-4.41072398017774
H	-1.01869001313417	5.28477928778457	-2.84554848060398
H	-0.16938683891203	4.16654020984324	-3.93634194478258
O	2.37399214434575	-0.94936993574858	-1.50151229187227
C	3.81332019128662	-2.47000268115878	-0.36067771985161
H	1.91743622507500	-5.43413050688742	-2.08583375997396
C	3.48182242323572	-4.89298207128399	-0.69783077542559
O	-1.91566868136448	-1.51007832191740	1.29682663509647
N	0.14513580866831	-0.67090560344572	-0.14742067712596
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C	-5.99330073430792	-3.33149010022440	0.42015303789665
C	-3.11127031518034	-4.50997702905187	-0.50024123334212
C	-2.00916607313465	-2.84438153928338	0.86339333421648
H	-8.33263555794017	-0.72782881779171	-1.28820941936239
C	-8.21821392893677	-2.50225308709079	-0.07912332331934
P	1.59135255871646	-0.09491798758186	-0.37114850748856
C	4.48963933837769	-1.31312327528680	0.28744240661385
C	4.18637731279644	-3.82104827036638	-0.05338084691494
C	3.83687126739129	-6.23587285175495	-0.39870953430955
S	-2.29841049469482	1.23831635940969	2.46182500218405
H	-1.48405508875922	2.13856918080323	0.29324393295333
C	-7.36289116473953	-3.43602997924864	0.54898471546087
H	-5.34373898148904	-4.04909018999136	0.91924315837155
C	-4.04676452029881	-4.92648664407308	-1.48295289783922
C	-2.15513993566667	-5.46835014715002	-0.02344232143214
C	-1.04408667963513	-3.76719152605410	1.35179994262046
H	-9.29965049010451	-2.59750448234767	0.02812647842019
O	2.35403547453503	-0.51363968700410	0.99269631058516
N	1.79133545957756	1.44834236950886	-0.70983536478393
C	3.74587836370489	-0.38962660816750	1.01218466479705
C	5.90673572446352	-1.12316124837953	0.20365383829791
C	5.18492774261300	-4.15359287281966	0.89964768907164
H	3.29929890844388	-7.03958382039945	-0.90654670864943
C	4.82290059624647	-6.52263867770251	0.51939827669367
O	-2.38444622212854	2.68443638613515	2.60918200189187
O	-1.52371244939040	0.46002573948867	3.41467009971034
H	-7.78779793309168	-4.23938489952648	1.15202576388170

H	-4.75692205857074	-4.20361598809009	-1.88018591645936
C	-4.05779268354464	-6.22427149224826	-1.95130036688810
C	-2.20554118920163	-6.80084124481914	-0.51373915803627
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S	2.20383621273437	2.03222583879418	-2.15080569016941
C	4.31179222273529	0.64522374499234	1.81310677467823
C	6.50689090683652	-0.07766292632243	0.97995956557086
C	6.73564035371105	-1.89745119919499	-0.64790635247890
C	5.49426207046164	-5.46871548178103	1.17999393710504
H	5.70717807440465	-3.35381337859354	1.42156908907085
H	5.08117130204775	-7.55839452328602	0.74412113638380
H	-4.78157194094171	-6.51587519855157	-2.71388548922457
C	-3.13629916514655	-7.17552113890368	-1.45751291249542
H	-1.47793264042282	-7.52114891386959	-0.13381234725539
H	-0.45814648375994	-5.82296255504626	1.26661958037470
C	-0.16541397046202	-2.51814215459405	3.36656479871838
C	1.32190722017738	-3.93404058510215	2.12335063849433
O	1.59683461443824	1.32574519169393	-3.27602365706459
O	2.03428408686848	3.48645440393337	-2.08842709818675
C	5.69531192582975	0.74715197619101	1.79099103823311
C	3.50002013405250	1.53944542238772	2.67287640869855
C	7.91225454758961	0.11443978824283	0.90991249420544
C	8.09507695328634	-1.67063437726835	-0.70969979739235
H	6.28166303571248	-2.66531663864668	-1.27255047551121
H	6.26154577806739	-5.69569471035106	1.92178838963654
H	-3.15889517866736	-8.20008775806714	-1.83122701846596
C	0.86758522536333	-2.22428091436014	4.25626049661184
H	-1.13795362985510	-2.05854044939149	3.52554345318320
C	2.34326178898603	-3.64484094233952	3.02022105168414
H	1.52787379386388	-4.57956376460533	1.26841625387076
H	6.18606740988947	1.49065277230178	2.41990599115319
C	2.28429471931436	1.14111208215016	3.25534395717816
C	3.97049751632954	2.82667729708875	2.99590182294438
H	8.35927007667902	0.91130611901888	1.50729245624170
C	8.69259902762621	-0.66456848585184	0.08333281027988
H	8.71079337779262	-2.26384910267102	-1.38694427765220
F	-7.65775600480476	2.81341884673632	2.14111793005212
C	2.14368999372171	-2.78428125815265	4.11238069549814
H	0.65565427880127	-1.54221915049257	5.07896848004495
H	3.32053587996952	-4.09790166128291	2.85136817040043
C	1.57971707816745	1.98515002063866	4.11307491984963
H	1.87565502240612	0.15343734388199	3.05913031052027
C	3.27453615515791	3.65234897408047	3.87250033754042
H	4.88938316682291	3.19656224489580	2.53826052611069
H	9.76916073328787	-0.49690497714798	0.02824620932146
C	-7.40683039501934	1.71700110758374	1.37188161031770
C	3.28269453749607	-2.52896993747966	5.10508975576332
C	2.05679529539724	3.25646751162522	4.45363578149352
H	0.63488306981402	1.62128512365023	4.51488006008221

H	3.68834213739730	4.63685652083860	4.09798736186896
F	-7.07708562525969	2.18642838209911	0.13041658847190
C	-6.30442042487693	0.87375480856073	1.96190175684196
F	-8.57397276885515	1.03926087288654	1.24749572994597
C	3.57444816288380	-3.84812159355395	5.85160942234940
C	2.93055487533048	-1.44656156117115	6.13550798432569
C	4.55273362628657	-2.08375491497403	4.35428403240956
C	1.33188564871036	4.16782830104256	5.44910922652004
C	-6.59612853854447	-0.33368613704197	2.60137225782948
C	-4.99599532739070	1.35478912073122	1.91135572228486
H	2.68832205298342	-4.18765210610614	6.40732223231379
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H	2.07099643794366	-1.73536305168109	6.75787666145913
H	3.78680659537362	-1.29097331370912	6.80779778647458
H	2.70455786490461	-0.48425256232090	5.65339268353727
H	4.88027227876055	-2.83850054991851	3.62703072319692
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H	5.37509158958358	-1.92504134441855	5.06793038700470
C	-0.06789016121258	3.64127228968162	5.79920209365230
C	1.18102663133573	5.59068765806511	4.87572582135346
C	2.17598010166401	4.23469257455774	6.74012298321453
C	-5.56457661634521	-1.05555732204146	3.20092454637963
H	-7.61709605498129	-0.70836998261560	2.62982456161779
C	-3.97717301611538	0.60648480651054	2.49900540197902
H	-4.76893660650711	2.31075963976851	1.44042985935988
H	-0.56464421005528	4.34700162103367	6.48062417265797
H	-0.70043934247801	3.53028449699260	4.90638289447892
H	-0.02346120743836	2.66741657065502	6.30731110188276
H	0.56977656594961	5.58687425094115	3.96289653746993
H	0.68543405177648	6.23936702543608	5.61324507668349
H	2.15219394685398	6.04423884905553	4.63464708497566
H	3.17593254252964	4.64563514145030	6.54090720347346
H	1.68342245972308	4.87724446025505	7.48590653939543
H	2.30191091808506	3.23286716860281	7.17527377260477
C	-4.24792558209915	-0.59170554113684	3.15227534531539
C	-5.84772064834731	-2.32458788316135	3.96682669051847
H	-3.43703207610990	-1.14455985235825	3.62387108499199
F	-7.12247721611695	-2.75934295848517	3.80483751404225
F	-5.65320668437059	-2.13975348049972	5.30380311357588
F	-5.01826831918272	-3.33774596403742	3.59060476384035
C	4.48897442359654	0.77327299823738	-3.07719277108630
C	3.97973550748993	1.77307324179937	-2.25498389769896
H	3.80626116608802	0.15564448625909	-3.65894589849333
C	5.87235646604262	0.58842262644232	-3.14693026219326
C	4.82693130788717	2.59596786860648	-1.51388770643049
C	6.73706488131774	1.40004253164205	-2.41369272509512
C	6.40684388502599	-0.47713602754796	-4.06972471718985
C	6.20634668798028	2.40649456087145	-1.60293945098556
H	4.40758393442307	3.38323755348961	-0.88740853041484

H	7.81267573383692	1.24701159129492	-2.46686531132344
F	6.19655208444699	-0.14965081918840	-5.37714921936069
F	5.78932115709901	-1.67621831931594	-3.86810584446008
F	7.74123270727545	-0.67873201142122	-3.91954202066206
C	7.11596861421761	3.35361057417706	-0.86305946109047
F	8.39662086999115	2.90857459208318	-0.79816141198096
F	7.14952666886840	4.57755919856071	-1.46386795450666
F	6.69671424050186	3.56689052420614	0.41936980576990
H	1.05723825734420	5.09535409482379	-1.61944984535021
H	1.48424039689653	6.79587350821046	0.59683990516612
H	1.88751100752600	4.73821041582766	1.90167439833743
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Minor0

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C	-1.67246186559458	-5.74604738511730	-2.68837943162214
O	-2.38879748842436	-4.79469636232902	-1.89991693900367
H	1.15573172553289	-5.45693931505936	-2.28919145987365
H	-1.22286918164959	-6.85451571875080	-0.91350166006187
H	-2.38214427309999	-6.46342286141596	-3.14109471079965
C	-0.34897568686094	-4.40581978229382	0.63166549818400
C	-0.19660396667881	-5.53395421454186	1.46465645875869
C	-0.92216952570991	-3.25053818896625	1.19135691084291
C	-0.57318335052161	-5.48752526777269	2.80282041464058
H	0.25800665553199	-6.44423610884316	1.07641602668745
C	-1.29771421746290	-3.20086059070024	2.52585879700572
H	-1.08959265826628	-2.38064036327388	0.56561269399438
C	-1.11556940583684	-4.31684195325291	3.34205249887312
H	-0.43113434886021	-6.36596696965055	3.43388322588249
H	-1.73365738671932	-2.28302384492874	2.91834454236440
H	-1.40102019637445	-4.27823841165605	4.39480731839982
C	0.37216531501778	-3.20541837943153	-1.42738208888423
H	0.75591540772508	-3.25934598080108	-2.44774624292144
H	-0.28541488469848	-2.35163078094618	-1.22881662145718
H	5.29780992652240	2.34786086187297	-5.49572637910433
C	4.58789796813458	2.38401699019772	-4.65568182746869
C	3.32163927078007	3.15767916143612	-5.07587377496400
H	5.09911698142765	2.85689517622928	-3.80570704036106
H	4.34011538061421	1.35284713819137	-4.37089448021938
C	2.34873881024822	3.25802114523027	-3.89686955695662
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Minor3

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Minor2

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Major0 0 CyH

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H	-2.44180069361146	3.83528515135101	6.67143752229946
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C	-2.05060357335187	-5.94430171810755	5.05192742828316
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Major0 1 CyH

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F	6.63465646415346	2.39731468380907	2.18855316284482
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H	-0.30030086159616	-6.28507781309174	0.84020765428650
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C	-4.35924406818328	-4.08161921962303	-3.90439607240981
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Major0 2 CyH

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H	3.21273762480385	-4.55954800458707	-2.22745197457732
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H	-3.30238005855165	-6.09860932150857	-4.54501523024082
H	-3.95463623980612	-7.89306964098195	-2.96136986444909
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C	-1.17091528763560	0.12743068420404	7.98587605817273
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C	-1.26085392351978	-3.03001947859903	3.25055410271310
C	-0.66261184319810	1.27478889535165	5.19145042175422
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H	-3.04907701983868	0.14299442153406	5.95214029319341
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H	-1.59886881596129	1.72160559430190	5.50940121367405
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C	1.36791253698516	1.47870999214108	3.87979261679592
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H	-1.98934646932249	2.60280335187657	-1.68257808677237
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Major0 3 CyH

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300 Major0 4 CyH

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Minor0 1 CyH

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Minor0 2 CyH

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Minor0 3 CyH

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Minor0 4 CyH

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