

Dimerization of Confined Brønsted Acids in Enantioselective Organocatalytic Reactions– Supporting Information

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: giovanni.bistoni@unipg.it*

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S1 Most stable dimer structures

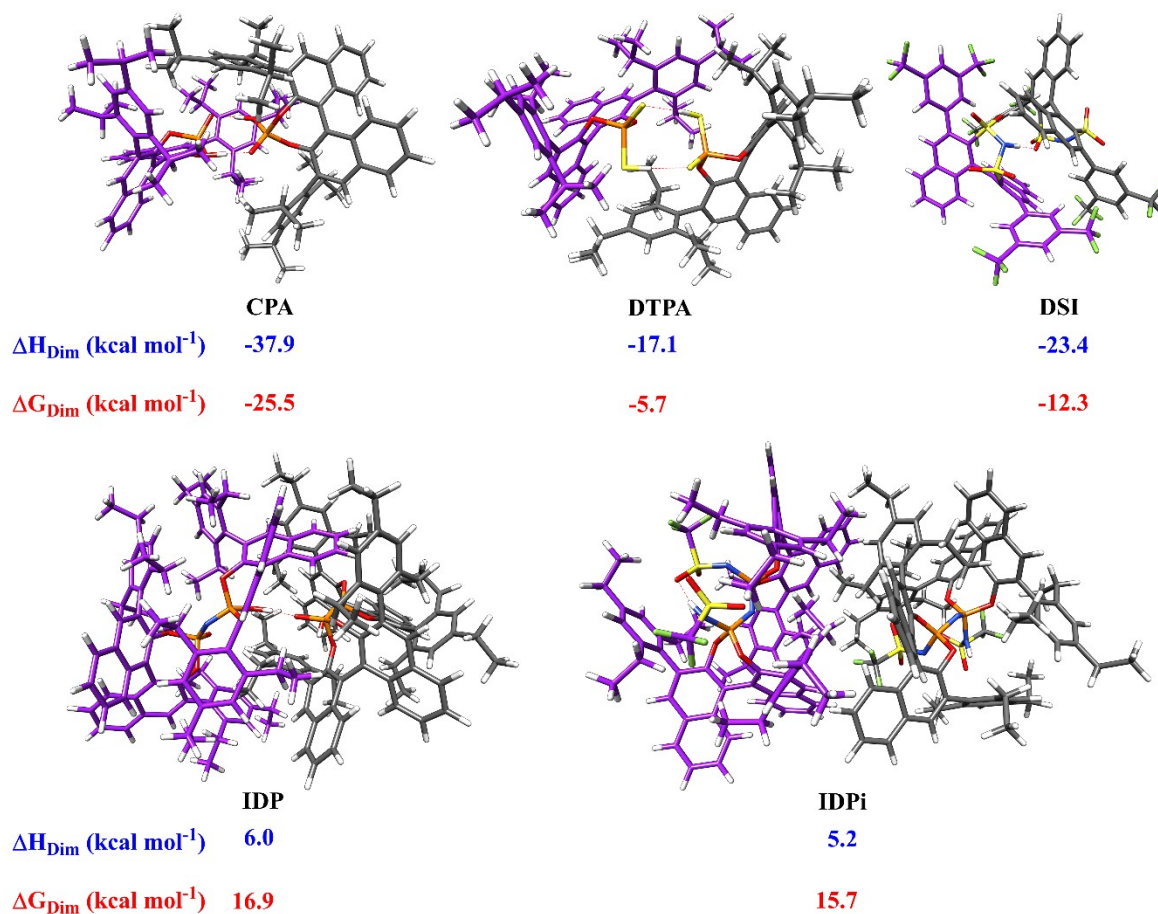


Figure S1. Most stable dimer conformers for **CPA**, **DTPA**, **DSI**, **IDP** and **IDPi** together with the corresponding dimerization enthalpies (ΔH_{dim}) and free dimerization energies (ΔG_{dim}) at the ω B97M-V/def2-TZVP level at 173 K. All energies are in kcal mol⁻¹. For a discussion of the structural features, see main text.

S2 Effect of the electronic structure method on the dimerization electronic energy

Table S1. Dimerization energies ΔE_{dim} for different acids (**CPA**, **DTPA**, **DSI**, **IDP**, **IDPi**) at various levels of theory *in vacuo*. All energies are in kcal mol⁻¹. All DFT calculations were carried out with the def2-TZVP basis set. HFLD calculations were carried out with the def2-TZVP(-f) basis set and NormalPNO settings with a TCutPairs cutoff of 1e-05. †: Geometric preparation energy was calculated at the ω B97M-V level of theory. *: Basis set extrapolation with the def2-TZVP and def2-QZVP basis sets was carried out, TightPNO settings were used.

	CPA	DTPA	DSI	IDP	IDPi
B3LYP-D3BJ	-46.7	-26.7	-33.0	-4.1	-5.1
B3LYP-ABC	-43.7	-23.6	-30.0	-0.4	-2.0
M06-2x-D3	-48.7	-22.6	-31.2	-3.9	-2.4
ω B97M-V	-48.1	-25.5	-36.0	-5.0	-5.2
HFLD†	-40.7	-32.9*	-31.0	-6.4	0.4

As can be seen from **Table S1**, fairly similar dimerization energies are obtained for the different density functionals. Interestingly, the three-body dispersion correction used in the B3LYP-ABC calculations increase the dimerization energy by a relatively constant amount between 3.0 kcal mol⁻¹ and 3.7 kcal mol⁻¹. In addition, interaction energies obtained by HFLD are systematically smaller than their DFT counterparts. For **DTPA**, we noticed a more pronounced basis set incompleteness error. Hence, HFLD calculations were carried out with a larger basis set and TightPNO settings. **DTPA** features two S-H hydrogen bonds and it is suspected that the smaller def2-TZVP(-f) basis set is not appropriate for describing the extended charge distribution of sulfur sufficiently well.

S3 Effect of the dispersion correction scheme on the dimerization energy

For the **DTPA** dimer, the electronic dimerization energy was computed using different approximations for the London dispersion correction within the density functional theory framework. ω B97M/def2-TZVP calculations were carried out with D3, D4^[1] and NL dispersion corrections, respectively. For the NL calculations, the VV10 kernel was used in a post-SCF fashion, as detailed in the main text.

Table S2. Electronic dimerization energy of **DTPA** at the ω B97M/def2-TZVP level of theory. Dispersion corrections were included at the D3BJ/D4/VV10 level, respectively. All energies are in kcal mol⁻¹.

	ΔE_{dim}
ω B97M-D3BJ	-22.6
ω B97M-D4	-18.2
ω B97M-V	-25.5

Interestingly, deviations between the different dispersion schemes are relatively large. This is especially true for D4 which differs much larger from D3 and VV10 than those two differ from each other.

S4 Dispersion vs non-dispersion contributions to the dimerization energy

Table S3. Decomposition of the interaction energies between the monomers in their dimer geometries for different acids (**CPA**, **DTPA**, **DSI**, **IDP**, **IDPi**) at various levels of theory. All energies are in kcal mol⁻¹. *: Basis set extrapolation with def2-TZVP and def2-QZVP was carried out, TightPNO settings were used.

		CPA	DTPA	DSI	IDP	IDPi
B3LYP-D3BJ	E_{dim}^{disp}	-47.0	-51.9	-45.6	-86.3	-53.3
	$E_{dim}^{non-disp}$	-19.2	11.2	3.0	12.2	14.9
B3LYP-ABC	E_{dim}^{disp}	-43.9	-48.8	-42.7	-80.3	-49.5
	$E_{dim}^{non-disp}$	-19.2	11.2	3.0	12.2	14.9
ω B97M-V	E_{dim}^{disp}	-38.6	-39.7	-39.4	-69.6	-44.3
	$E_{dim}^{non-disp}$	-28.1	1.1	-6.0	-6.6	2.8
HFLD	E_{dim}^{disp}	-46.3	-71.9*	-49.3	-87.0	-53.3
	$E_{dim}^{non-disp}$	-12.1	25.7*	8.9	24.2	21.1

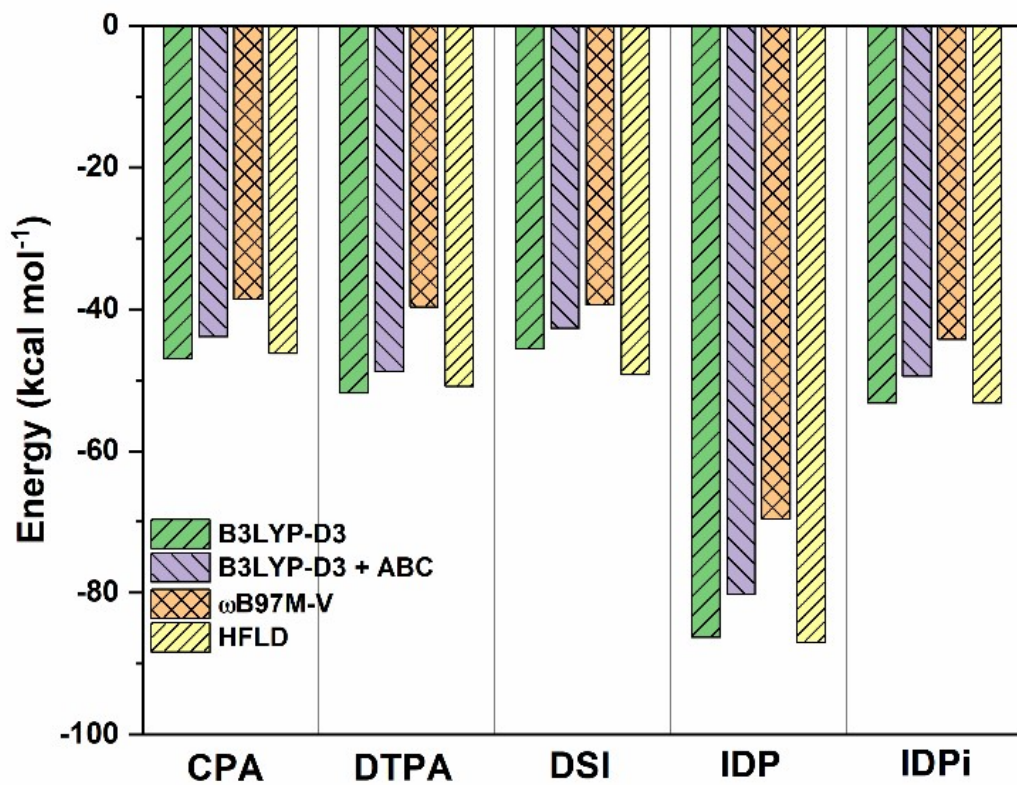


Figure S2. London dispersion contribution to ΔG_{Dim} at various levels of theory. All energies are in kcal mol⁻¹.

S5 Effect of the solvent on the dimerization energy.

In this section the influence of different solvation schemes (C-PCM vs. SMD) and the influence of the solvent on dimerization energies are discussed. The C-PCM calculations were performed using the gaussian charge scheme [2] as implemented in ORCA.

Table S4. Dimerization energies for various acids (**CPA**, **DTPA**, **DSI**, **IDP**, **IDPi**) with the C-PCM and SMD solvation schemes. All calculations were carried out at the B3LYP-D3BJ/def2-TZVP level of theory. All energies are in kcal mol⁻¹.

	$\Delta E_{\text{dim}}(\text{C-PCM})$	$\Delta E_{\text{dim}}(\text{SMD})$	$\Delta \Delta E_{\text{dim}}(\text{SMD} - \text{C-PCM})$
CPA	-42.2	-37.7	4.5
DTPA	-24.3	-18.7	5.6
DSI	-26.5	-22.2	4.3
IDP	-0.8	6.2	7.0
IDPi	-3.0	4.6	7.6

As can be seen from **Table S4**, the solvation scheme has significant influence on the dimerization energies. For all acid dimers, SMD predicts larger (closer to zero) dimerization energies. This effect increases with the size of the acid and is therefore largest for **IDPi**. Comparing the dimerization energies in solution (**Table S4**) with the dimerization energies *in vacuo* (**Table S1**), it becomes evident that implicit solvation favors dissociation for all acid dimers. The association process decreases the solvent accessible surface and therefore consequently reduces the interactions between solute and solvent. SMD takes into account short-range interactions like London dispersion between solute and solvent. These interactions are important for an accurate description of the dimerization energy as well.

The influence of the solvation scheme and solvent was also studied for the aggregation of **I-1** and **X-TBS** to form **I-2** (see **Figure 4**, main text). In **Figure S3**, the reaction energy for the Reaction **I-1** + **X-TBS** → **I-2** is shown as a function of the dielectric constant. In practice, calculations for five different solvents (toluene, acetone, water, dichloromethane, methanol) were carried out.

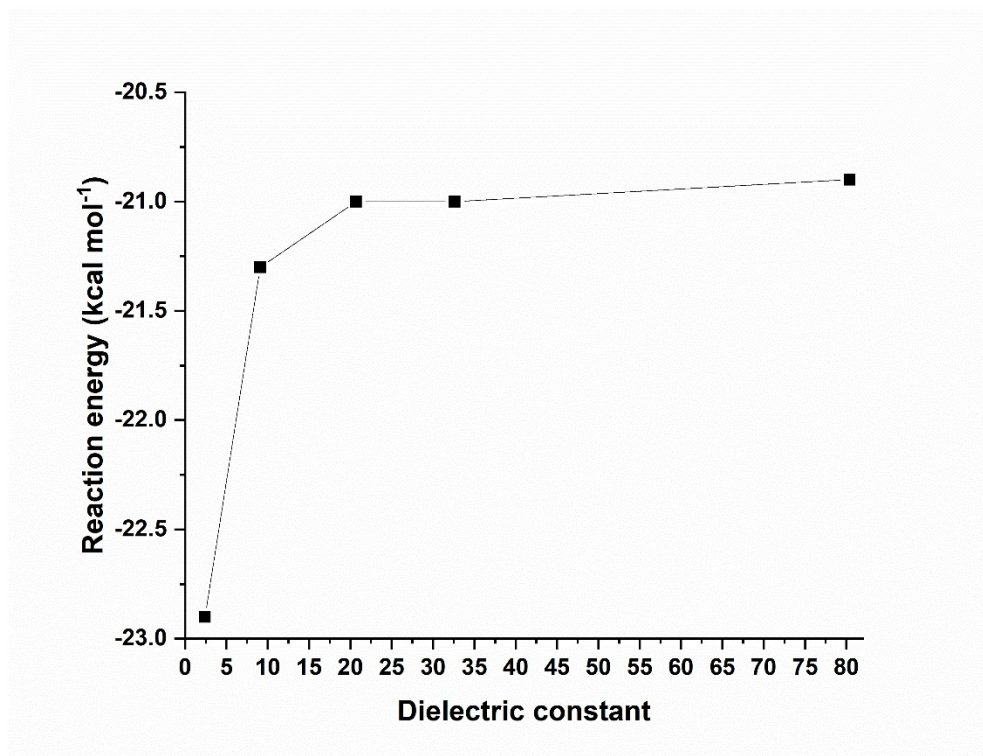


Figure S3. Electronic reaction energy for the association of **I-1** with **X-TBS** for five different solvents (toluene, acetone, water, dichloromethane, methanol) at the ω B97M-V/def2-TZVP level of theory. All energies are in kcal mol⁻¹. Free solvation enthalpies were calculated using the C-PCM model.

Increasing solvent polarity decreases the reaction energy in absolute value. Interestingly, the reaction energy changes most for the change from toluene ($\epsilon = 2.4$) to dichloromethane ($\epsilon = 9.1$). Increasing the polarity of the solvent further only has minor effects on the reaction energy.

It should be kept in mind, however, that the description of the solute-solvent interaction with the C-PCM scheme misses the dispersive interactions between solute and solvent. For toluene and dichloromethane additional calculations with the SMD model were carried out.

Table S5. Electronic reaction energy for the association of **I-1** with **X-TBS** at the ω B97M-V/def2-TZVP level of theory with C-PCM and SMD (toluene and dichloromethane, respectively). All energies are in kcal mol⁻¹.

	Reaction energy
C-PCM(Toluene)	-22.9
SMD(Toluene)	-18.8
C-PCM(CH ₂ Cl ₂)	-21.3
SMD(CH ₂ Cl ₂)	-18.0

Like for the acid dimers, the SMD model favors dissociation much stronger than the C-PCM model, as can be seen from **Table S5**. However, the change in free energies when replacing toluene by dichloromethane is smaller for SMD (1.6 kcal mol⁻¹ for C-PCM, 0.8 kcal mol⁻¹ for SMD).

S6 Effect of the DFT functional on the solvation energy

For CPA, the free solvation energies were calculated using the C-PCM model and toluene as solvent at the B3LYP-D3/def2-TZVP and ω B97M-V/def2-TZVP levels of theory. The solvation contribution to the free dimerization energy amounts to 4.5 kcal mol⁻¹ at the B3LYP-D3 level and 4.2 kcal mol⁻¹ at the ω B97M-V level. The difference in contributions is only 0.3 kcal mol⁻¹, thus showing that the implicit solvation correction is fairly independent of the underlying density functional used and that the choice of the implicit solvation model (C-PCM vs. SMD) is much more important in this regard.

S7 Decomposition of ΔG_{corr} into thermochemical and solvation corrections

In Table S6, we show the decomposition of the correction term ΔG_{corr} that was introduced in Figure 3 into its contributions from implicit solvation and thermochemistry.

Table S6. Decomposition of the correction term ΔG_{corr} to the free dimerization energy at 173 K. Thermochemical corrections were computed at the PBE-D3/def2-SVP level of theory, solvation corrections were computed at the B3LYP-D3/def2-TZVP/SMD(Toluene) level of theory. All energies are in kcal mol⁻¹.

	ΔG_{corr}	ΔG_{solv}	ΔG_{thermo}
CPA	22.6	9.0	13.6
DTPA	19.7	8.0	11.7
DSI	23.7	10.7	13.0
IDP	21.9	10.3	11.6
IDPi	21.0	9.7	11.3

Interestingly, implicit solvation and thermochemistry both contribute significantly to ΔG_{corr} , with thermochemical corrections slightly being more important. It is noted here that thermochemical

corrections in **Table S6** were computed at 173 K. The contribution from implicit solvation is roughly temperature independent so that at lower temperatures ΔG_{corr} should be dominated by solvation effects. As has been discussed before (**Table S4**, **Table S5**), solute-solvent dispersive interactions play an important role for the magnitude of ΔG_{solv} .

S8 Basis set extrapolation for DTPA

For the electronic dimerization energy of **DTPA**, basis set extrapolation was carried out. For achieving this, single point energy calculations of the monomer and the dimer were carried out at the ω B97M-V with the def2-SVP, def2-TZVP and def2-QZVP basis sets, respectively. The def2-TZVP and def2-QZVP were used further to compute the (3/4) extrapolated dimerization energy. The results are shown in **Table S7**.

Table S7. Electronic dimerization energy of **DTPA** at the ω B97M-V level of theory for different basis set sizes. All energies are in kcal mol⁻¹.

Basis set	ΔE_{dim}
def2-SVP	-32.2
def2-TZVP	-25.5
def2-QZVP	-24.0
(3/4)-extrapolation	-23.6

As can be seen from **Table S7**, basis sets of at least triple-zeta quality are required to get a reasonable accurate description of the dimerization energy.

S9 Noncovalent interaction analysis in I-2

I-2 consists of three individual molecules. The catalyst anion **X**, the nitronate cation **N** and the activated catalyst molecule **X-TBS**. **X** and **N** already form a dimer in **I-1**. In the first step, the geometric preparation energies of the fragments in **I-2** were computed. For **X** and **N**, the corresponding geometries in **I-1** were taken as reference. For **X-TBS** the equilibrium structure was taken as reference. The geometric preparation energies were calculated at the ω B97M-V/def2-TZVP level of theory using the r²SCAN-3c/xTB optimized geometries (see main text for details) and account for -1.2 kcal mol⁻¹ for **X**, 8.7 kcal mol⁻¹ for **N** and 1.2 kcal mol⁻¹ for **X-TBS**. Interestingly, the overall geometric preparation is very small, especially compared to the **IDPi** dimer (see **Figure 3**, main text). This indicates that all three fragments do not have to distort much to optimize their interaction. The low geometric preparation is therefore one of the driving forces that possibly might lead to dimerization. Dispersive interactions between the fragments were calculated at the HFLD level of theory. For the computation of the non-dispersive interactions, Hartree-Fock single point calculations of each fragment and each pair of fragments were carried out.

Table S8. Fragment-pairwise dispersive and non-dispersive interactions in **I-2** at the HFLD/def2-TZVP(-f) level of theory. All energies are in kcal mol⁻¹.

Fragment pair	E_{disp}	$\Delta E_{\text{non-disp}}$
X, N	-47.5	-50.6
X, X-TBS	-5.7	7.3
N, X-TBS	-18.4	-2.4

As expected, very strong dispersive and non-dispersive interactions arise between the catalyst anion **X** and the nitronate **N** in **I-2**, which are the driving force for the formation of **I-1** in the first place. Interestingly, **X** and **X-TBS** feature very weak dispersive interactions, while non-dispersive

interactions are repulsive and slightly larger in magnitude leading to a weak overall repulsion between **X** and **X-TBS**. The nitronate **N** and **X-TBS** are held together by strong dispersive interactions and weak attractive non-dispersive interactions. In contrast to the **IDP** and **IDPi** acid dimers case (**Figure 3**), in **I-2** the nitronate seems to act as “glue” between **X** and **X-TBS**, allowing for strong intermolecular interactions without the need of significant distortions. These much more favorable interactions lead to free dimerization energies of approximately 0 kcal mol⁻¹ at 153 K (see **Figure 4**).

S10 Comparison of r²SCAN-3c and r²SCAN-3c/GFN2-xTB optimized structures

Geometry optimizations of the conformers of the species in **Figure 4** were performed at the r²SCAN-3c/GFN2-xTB level of theory using the multiscale approach in ORCA, as discussed in the main text. Final single point energies were obtained at various levels of theory. The aggregation energy of **I-2** was recomputed using r²SCAN-3c optimized structures. Computation of the formation energies of **I-2** *in vacuo* gives -22.9 kcal mol⁻¹ for the r²SCAN-3c/ GFN2-xTB optimized structures and -22.2 kcal mol⁻¹ for the r²SCAN-3c optimized structures at the ωB97M-V/def2-TZVP level of theory, thus justifying the use of the computationally less demanding ONIOM approach.

S11 Reaction energies at various levels of theory

In Table S9 the relative free energies of the species **I-1**, **RC-1**, **TS-1**, **P-1**, **I-2**, **RC-2**, **TS-2** and **P-2** are given at various levels at theory.

Table S9. Computed free energies for the reaction of the monomeric (**I-1**) and dimeric (**I-2**) ion pair with the nucleophile **2** at different levels of theory. Geometries and thermal corrections at 153 K were obtained at the r²SCAN-3c/xTB level of theory. Final single point energy calculations with the i) B3LYP-D3, ii) B3LYP-D3 + ABC, iii) ω B97M-V and iv) ω B97M-D4 functionals were carried out with the def2-TZVP basis set and the SMD solvation model (CH₂Cl₂). The gCP correction was included in all cases. All free energies are relative to that of **I-1**. All energies are in kcal mol⁻¹.

	B3LYP-D3	B3LYP-D3 + ABC	ω B97M-V	ω B97M-D4
I-1	0.0	0.0	0.0	0.0
RC-1	8.3	9.6	9.1	11.1
TS-1	14.2	15.7	16.7	19.5
P-1	-2.1	-0.8	-8.0	-3.8
I-2	-0.8	2.2	-0.8	4.1
RC-2	4.6	8.5	5.0	11.2
TS-2	7.8	11.8	9.4	16.4
P-2	-8.2	-4.2	-14.6	-6.1

Remarkably enough, the aggregation of **I-1** with **X-TBS** to give **I-2** features a free reaction energy (ΔG_R) close to zero. While B3LYP-D3 and ω B97M-V predict slightly negative ΔG_R values, B3LYP-D3 + ABC and ω B97M-D4 predict a slightly endergonic association process. The direct comparison of B3LYP-D3 and B3LYP-D3 + ABC results reveals that many-body dispersion corrections favor dissociation. The small value of ΔG_R suggests that the spontaneity of this process might change for

different substituents and/or for different reaction conditions. The difference in the activation barrier between the pathways ranges from 7.3 kcal/mol (ω B97M-V) to 3.1 kcal mol⁻¹ (ω B97M-D4). While the significant variations observed with different functionals as well as the complex nature of the system and of its interaction with the environment effectively limit the confidence of quantitative computational estimates of reaction barriers in this case, the relatively small energy difference between the two pathways suggest that experimental variables like temperature and solvent nature are likely crucial to determine the actual mechanistic details of the transformation, *e.g.*, the reaction order with respect to the catalyst.

S12 Reaction barriers at different temperatures

In **Table S10**, the activation barriers for the monomeric and dimeric pathways are shown for different temperatures.

Table S10. Computed reaction barriers for the reaction of the monomeric (TS-1) and dimeric (TS-2) pathway at the ω B97M-V/def2-TZVP level of theory at different temperatures. All energies are in kcal mol⁻¹.

Temperature (K)	ΔG^\ddagger (TS-1)	ΔG^\ddagger (TS-2)	$\Delta\Delta G^\ddagger$ (TS-2 – TS-1)
153.15	16.7	9.4	-7.3
173.15	17.9	11.9	-6.0
193.15	19.1	14.5	-4.7

The temperature has large impact on the reaction barriers with higher temperatures favoring the monomeric pathway. The large deviations in activation barriers found for different exchange-correlation functionals have no influence on their temperature dependence as the temperature dependence is governed by entropy.

S13 References

- [1] E. Caldeweyher, S. Ehlert, A. Hansen, H. Neugebauer, S. Spicher, C. Bannwarth, S. Grimme, *The Journal of Chemical Physics* **2019**, *150*, 154122.
- [2] M. Garcia-Ratés, F. Neese, *Journal of Computational Chemistry* **2020**, *41*, 922-939.

S14 XYZ Coordinates

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CPA Monomer

C	3.77206190407251	-0.76791343120771	-1.31986945817998
C	3.57215151681695	-0.36983400716490	0.02888725472592
C	4.48643144913036	-1.95138747751393	-1.57844273097015
C	3.26428241126354	0.06137615752097	-2.49604742878370
C	2.82273563664126	0.88770202084147	0.33003820507075
C	4.07168139381630	-1.17182343990755	1.09307084959380
C	5.00308238527750	-2.75248726493136	-0.54878439152298
H	4.64865905087704	-2.26516544771246	-2.62277413164037
C	1.42176548393041	0.97043738100766	0.06715931018331
C	3.43738439492038	2.01096475770045	0.87045213924009
C	4.78327741215445	-2.34152533759199	0.77665578988166
C	3.86581871486868	-0.80277776937886	2.56032716078570
O	0.80627938473644	-0.15279321823500	-0.48426045400421
C	0.65545592193924	2.12074952738620	0.29742623315667
H	4.52126472946647	1.98822425148254	1.05831291454771
C	2.70158863784362	3.17532677726885	1.22979147503887
H	5.16864263426800	-2.96086627862879	1.60151057653383
P	-0.12617071188605	-1.03102980432856	0.56226509760586
C	1.28465210728079	3.23157916180568	0.96569187771354
C	-0.75329554439614	2.16083628205807	-0.17872169329135
C	3.33380693226152	4.28240343945534	1.86972747055896
O	-1.21946660789673	0.12092180034618	1.01908932386301
C	0.55684043315626	4.37397072480891	1.41264957214706
C	-1.23724036148562	3.19913643829828	-1.05918920449995
C	-1.62373943399955	1.11449726406293	0.13655344838315
H	4.41787733756708	4.23089292556622	2.05557098439809
C	2.60165453904865	5.38999581306897	2.26755984129424
C	1.19914694510203	5.42638254654848	2.04884857698478
H	-0.53027662445944	4.40767885509376	1.25679223577180
C	-0.39979721073673	4.23439739284282	-1.57191550850517
C	-2.61981662477761	3.17716333538283	-1.47560163962237
C	-2.94751404558790	1.00181127855290	-0.38959511356822
H	3.10124115702538	6.23384804697141	2.76673043794408
H	0.61491536226271	6.29337236220078	2.39239600606250
H	0.66746755859822	4.23498278103835	-1.31524202572489
C	-0.91081627737541	5.23016519933087	-2.39209310182958
C	-3.11790788811056	4.22712735166270	-2.30258529380387
C	-3.44130699646630	2.06644939638327	-1.13012271943989

H	-0.24097183395737	6.01460066339285	-2.77541329257547
C	-2.28511931706120	5.24190014328851	-2.74652344825240
H	-4.17810940020602	4.20201452772625	-2.59904441153552
H	-4.47106720925836	2.02710286047187	-1.51569937520632
H	-2.68049763734937	6.04269780910975	-3.38930517921965
C	5.77137189680737	-4.02908062900901	-0.86006753914608
C	5.06723900777689	-5.27017185563708	-0.28637425976049
C	7.23007758440006	-3.94150550643640	-0.38019645120984
C	3.32895932982029	-1.97645816158457	3.39457358114700
C	5.16271972716898	-0.23690006256139	3.16742358177603
C	4.43304968515079	0.63466054820768	-3.31647127003289
C	2.28744547945512	-0.73212308116463	-3.37994567751399
O	0.54282734927302	-1.65772326239544	1.72848910526806
O	-0.88885978016511	-2.01398628561292	-0.46001191441578
H	2.70583825871528	0.92640125911032	-2.08498635634613
H	3.09537795355363	-0.00671659683441	2.59702441611154
C	-3.65715470204687	-0.30735277276205	-0.25050872093694
H	5.78702886936174	-4.13245686431817	-1.96742828308729
H	5.02784459129868	-5.23237449922945	0.82204836455633
H	5.60571956660607	-6.19790260018773	-0.57032330609383
H	4.02463738047061	-5.34778288988776	-0.65392984933165
H	7.74600305960005	-3.06347496568900	-0.81765180489523
H	7.79685621396003	-4.85270918249294	-0.66272145470848
H	7.28237407279643	-3.84431680310434	0.72428669033332
H	3.11989061596138	-1.64047173707356	4.43114164201410
H	4.06147312153231	-2.80765829414651	3.46361271900936
H	2.38727166148810	-2.35960579312914	2.95900116499834
H	5.96996753207175	-0.99895254139128	3.15418939004387
H	5.00429581808242	0.07121784880032	4.22157056189530
H	5.53228740270038	0.64333765020952	2.60414661742767
H	4.05860738564227	1.28176553043375	-4.13655607387394
H	5.03816250939807	-0.17391258864137	-3.77664308155276
H	5.11134751286369	1.23994524302725	-2.68194035024651
H	1.88357364903075	-0.08813704062627	-4.18854069989673
H	1.43660745718628	-1.11328084392396	-2.78279666639012
H	2.78655539276057	-1.59764802213373	-3.86333953315574
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C	6.46246778414266	-3.64372337406489	-3.13124952405542
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H	7.90312220788034	-4.61516963401987	2.72431640310870
H	6.99503274974766	-3.20553064783718	-3.98959735798424
C	5.73006229600460	-5.56722921472443	-1.84174118608197
C	6.43852737985748	-5.01656656648745	-2.94215742733129
H	5.69186426816048	-6.65875803376720	-1.70749659842617
H	6.95682896544053	-5.68176497522559	-3.64908825139990

DTPA Monomer

C	4.16532168423123	0.49376485588485	0.95148470375306
C	3.75524143008467	0.24803751380287	-0.38540452327482
C	4.92072710790202	1.64668445464548	1.22906886223834
C	3.86735326450897	-0.48820001556233	2.08001734239147
C	2.91411340242230	-0.94364619673000	-0.70883079006360
C	4.12116197188437	1.15358547731744	-1.42316417844026
C	5.28321006435924	2.56099835440660	0.22867278558226
H	5.24205651717781	1.84329934993069	2.26480496010044
C	1.56593496238742	-1.03189977033763	-0.23958448432324
C	3.37803930413707	-1.98404976162907	-1.50482415810583
C	4.87996882139560	2.28759377605882	-1.08907422442963
C	3.73671741150987	0.92788813815902	-2.88481409897075
O	1.13633002858601	-0.05075939850987	0.64951040997818
C	0.69493050738217	-2.07423431160429	-0.57196834064021
H	4.42313020545351	-1.96924902007445	-1.84799002337424
C	2.53024499831785	-3.04085019810499	-1.93963232030800
H	5.15543498730799	2.99136969643958	-1.88978506441569
P	0.04370740370768	1.10320996646793	0.15302850754853
C	1.15470378699210	-3.07270783366721	-1.50781001246369
C	-0.67537715869115	-2.12521476099559	0.00447694049360
C	3.00531931968226	-4.04622691125181	-2.83300318811562
O	-1.03634428722115	0.14888288279260	-0.68048028184970
C	0.29992937876991	-4.07556736357867	-2.05472569699912
C	-1.17803202990811	-3.30614349694389	0.66238307063573
C	-1.52172479228774	-1.01586251657822	-0.09772358501028
H	4.06137203746114	-4.01453848795656	-3.14312069518679
C	2.15560459705238	-5.02716521558909	-3.31914276967098
C	0.78807380934758	-5.02769005765764	-2.93816388283045
H	-0.76261350369905	-4.08268190762494	-1.77760562938449
C	-0.35044950192787	-4.42083341775941	0.98940960615739
C	-2.57015138970881	-3.35574895544238	1.03242430718692
C	-2.89912079842372	-1.02548799396783	0.30050402680244
H	2.53273450027730	-5.79321987057418	-4.01325926320044
H	0.10607377682756	-5.78599426767724	-3.35152057257488
H	0.72153564736099	-4.37701518822018	0.75369651392721
C	-0.87821576717339	-5.54485136165962	1.60853499734928
C	-3.08581452709645	-4.53455055480515	1.64822845952936
C	-3.39804842364569	-2.22038309062913	0.80673965657062
H	-0.21788963167510	-6.38880099530574	1.85878145692678
C	-2.26011395576692	-5.61230534645191	1.92726533791386
H	-4.15400527940131	-4.56281669365024	1.91415594506979
H	-4.46202202539724	-2.28744106960652	1.07442823366517
H	-2.66887630484794	-6.51286692516476	2.40971619185169
C	6.07279592950195	3.81774405640546	0.56430766640824
C	5.24887527605577	5.08550738425485	0.28033980455632
C	7.42749288098943	3.85461895260571	-0.16205091491928
C	3.14941287461565	2.17872261311555	-3.55694091537279
C	4.94047662249640	0.40133357169073	-3.68794431414445

C	5.14987160510533	-1.22811724706706	2.50169354977003
C	3.17973770868862	0.18168329598821	3.27950358031310
S	0.57958904135190	2.62257036716243	-0.89378597946267
S	-0.72060971849949	1.42209088330986	2.09621893215449
H	3.17065948619131	-1.25533491934812	1.68683259005311
H	2.94806167405690	0.14896153805982	-2.90643199849597
C	-3.72778171491163	0.21348831323595	0.18712483214996
H	6.27714853905180	3.78663657569270	1.65714053307638
H	5.02742708089493	5.18374485994949	-0.80277093760963
H	5.80011691904090	5.99614009929542	0.59370705217490
H	4.27935498439914	5.06310069784183	0.81671513082708
H	8.03233978179495	2.95433708811577	0.06641778100033
H	8.01279399152936	4.74925488458623	0.13494997700770
H	7.29172946460240	3.89633982717628	-1.26286546536332
H	2.28802031756632	2.56853706928741	-2.98158671391990
H	2.79957927914967	1.93363166987144	-4.58060855656373
H	3.89918440782198	2.99095568887792	-3.65431838964449
H	4.65279992941176	0.18817843800090	-4.73830887863059
H	5.35783227716437	-0.52802057168130	-3.25150805784755
H	5.75857024962713	1.15148758046289	-3.70587919685753
H	4.92991464572188	-1.98433763841472	3.28355905186210
H	5.90287339665566	-0.52451578572404	2.91390271322293
H	5.61414540447296	-1.74824277393684	1.63967093070221
H	2.91288585163262	-0.57499423828692	4.04566346721431
H	2.25241261518829	0.70000471465619	2.96783861437393
H	3.84224277542872	0.92552971763303	3.76841105921060
H	-1.37080932747181	2.54698561382312	1.68471482611857
C	-4.28376837617131	0.82186338292094	1.35229197624888
C	-4.97895115435899	2.03774861119925	1.21191748990203
C	-5.15600817232387	2.66839684256972	-0.02874041383284
C	-4.63612799900336	2.02887024702870	-1.16591217520740
C	-3.93254239799949	0.81629155787090	-1.08771524183792
C	-4.20474989996113	0.18607624557142	2.73996023886174
C	-3.49746359120357	0.14470939560264	-2.38771674210493
C	-5.88118508196123	4.00171230268341	-0.13461314367664
C	-7.11304882828502	3.91717625386344	-1.05073843947908
C	-4.92376928551541	5.11856630596883	-0.58597297467545
C	-4.72577115338908	-0.43573975803795	-3.11372079048382
C	-2.68835656167637	1.07746055611346	-3.30187697090122
C	-3.86955590967851	1.17759165309389	3.86483047223604
C	-5.52507996368655	-0.53927988323807	3.06902629081418
H	-5.40306265690147	2.51824072937089	2.10781177676741
H	-4.78706703139305	2.48649274337789	-2.15604176831453
H	-3.39296971517497	-0.56845728455062	2.71762452907996
H	-2.84459233315864	-0.71228033885073	-2.13158598215950
H	-6.23812596027362	4.25561629295552	0.88776296347196
H	-7.81250469131815	3.12582426895550	-0.71478028712153
H	-6.82162969373423	3.68589308678597	-2.09626552940348
H	-7.66151084558552	4.88135804071894	-1.06471021552264
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H	-4.05379093374756	5.20334674045094	0.09557289460393
H	-5.44068244130826	6.10002057738253	-0.61092986631537
H	-4.42051496079664	-0.96854609398499	-4.03795375142708
H	-5.43576590165920	0.36661404404756	-3.40366167415704
H	-5.27459781098113	-1.15078434030491	-2.46812914061151
H	-1.81010090805723	1.49317848928395	-2.77131229637150
H	-3.30260224006688	1.92397974257892	-3.67347704648722
H	-2.32530117023948	0.52294223968733	-4.19123850271363
H	-2.93031381405834	1.72782008452019	3.66221862062645
H	-3.73943028493855	0.63580343511573	4.82360310636931
H	-4.67499093721527	1.92427511213092	4.02139099507508
H	-5.45098548020668	-1.07866571536668	4.03590553719867
H	-5.80467313812388	-1.27118734081425	2.28616845808810
H	-6.36050935355381	0.18724396726713	3.14684850853130

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C	-0.34173635123434	2.50042340084594	-3.13841534587626
C	0.78007741113608	1.76837708076572	-3.60175682778894
C	-1.62082628346258	2.14064720494118	-3.59127449911468
C	-0.20040095831606	3.64426204797265	-2.14253479937604
C	2.16184132424726	2.15706796197759	-3.17665501949765
C	0.60238244866292	0.66604322982127	-4.48048289289902
C	-1.82668022600115	1.07276639047942	-4.48158355198699
H	-2.49655206772965	2.69548993479091	-3.21733731435572
C	2.72539259707614	1.65467153268766	-1.96316700375774
C	2.94577651017037	3.00356957336617	-3.94833168556810
C	-0.70188806434518	0.34231107825284	-4.90171225089416
C	1.79777024690717	-0.13224359507672	-4.99900803093635
O	1.86102624585420	0.95768425936171	-1.13505825890834
C	4.03666972061082	1.92263092490600	-1.55170217662489
H	2.51691751382648	3.44877795513337	-4.85898466946130
C	4.30324143580138	3.27838936288920	-3.62210855103301
H	-0.83676497106224	-0.51284150140354	-5.57725586678430
P	2.08054566767138	-0.62148766232627	-0.65128790953687
C	4.88148552507647	2.69176229246477	-2.43782335484238
C	4.59536497653483	1.35149756325574	-0.29500615674395
C	5.11681092475185	4.07888268152453	-4.47715424974135
O	3.71713443329476	-0.79996000606066	-0.90207601752076
C	6.27988233430709	2.87463965433734	-2.21653871683782
C	5.29027508654684	2.14590528957488	0.68651639524968
C	4.53630715366619	-0.02869517061931	-0.08238316167569
H	4.65328829420438	4.52919943336224	-5.36874047215765
C	6.46348164278438	4.26760020450067	-4.21026661381695
C	7.04954534176694	3.64184164009676	-3.07943810957285
H	6.75553231763326	2.38970960893546	-1.35428382168533
C	5.25192928817941	3.57096265179313	0.68325405306198
C	6.02106741803158	1.47766146828685	1.73577736448648
C	5.31059286264013	-0.72470973757185	0.89861377398433
H	7.08201714194562	4.88145754257142	-4.88211634340544
H	8.12658874524265	3.75918123143683	-2.88639771257586

H	4.67312868179904	4.08402484116696	-0.09711174615614
C	5.90920630127351	4.30458602441965	1.66059167506077
C	6.70210215011325	2.26267725562527	2.71236325366614
C	6.05658003494321	0.05265889130862	1.77626622002991
H	5.85163724982870	5.40336868559438	1.64856591717301
C	6.64844213200154	3.64782091560018	2.67946204726507
H	7.26025923403818	1.74303193246770	3.50635193347316
H	6.68706357778374	-0.44304045486577	2.52974011721360
H	7.17072890686000	4.23958780458777	3.44617780988127
C	-3.24311264495035	0.76603413428913	-4.95237434477332
C	-3.39791901983784	-0.60121540589015	-5.62162597149187
C	-3.75999597401950	1.88556812495533	-5.87493241965871
C	1.49389352385523	-1.61762447100280	-5.23932515914890
C	2.36593500930940	0.49975860232155	-6.28430520346990
C	-0.67006227223324	4.97863515778994	-2.74565569482869
C	-0.94647366465956	3.32296107695645	-0.83994858908715
S	1.13060791855799	-2.02171181522138	-1.60614002967590
S	1.76813684813697	-0.35900436335002	1.39804944588499
H	0.87679074239758	3.75014336622305	-1.89778720203766
H	2.58750017523713	-0.07920636595718	-4.21868142960177
C	5.37125934405426	-2.21916712914869	0.87113601121194
H	-3.88125651029088	0.77116842537526	-4.04011062935907
H	-2.84072229574505	-0.65178335303881	-6.58017882770176
H	-4.46393896408441	-0.80003746516367	-5.85070473141352
H	-3.03153885158008	-1.41991504304230	-4.97118191361262
H	-3.70896849731887	2.87564783050358	-5.38085671565511
H	-4.81654669083714	1.70453857068189	-6.16222524442678
H	-3.15374366149953	1.93653368836198	-6.80337315545333
H	1.03210650736036	-2.08573859856177	-4.34915583511725
H	2.43182135864472	-2.16501073555463	-5.46332302549808
H	0.81702444869320	-1.76552409037320	-6.10629607995965
H	3.24517036873357	-0.07212237832449	-6.64620065455157
H	2.68432149333470	1.54715940908168	-6.12460586427890
H	1.59977105208672	0.49631924267097	-7.08737914957806
H	-0.52186164141206	5.81005448698280	-2.02573897050557
H	-1.75013409620533	4.94394855554197	-3.00043033107365
H	-0.11460265715145	5.22282221391226	-3.67378552745996
H	-0.84676792974429	4.15339350896882	-0.11241426259166
H	-0.56442155911548	2.39694874157304	-0.37194009254024
H	-2.02651155696559	3.17448192071600	-1.03106070752684
H	0.68467686111826	-1.23591425072291	1.39573320966035
C	4.88382992955753	-3.00400191038994	1.95084295931046
C	4.99268261475218	-4.40563747791237	1.87371516813066
C	5.55343635413987	-5.05788090811449	0.76703340350687
C	6.02132542313091	-4.26134792517645	-0.29154769444995
C	5.94372572729055	-2.85999657100349	-0.26729226601412
C	4.24272317264395	-2.39136047559804	3.19146377514762
C	6.51593545128183	-2.08636777803197	-1.45366346194182
C	5.62687314121197	-6.57645246289722	0.70455343522601
C	7.06902705708323	-7.07647519062161	0.51996244286248

C	4.69710400079394	-7.13203873849516	-0.38833753518421
C	8.04155313775859	-2.26530469814845	-1.54504483263376
C	5.81770129247503	-2.45791077420444	-2.77299947327204
C	2.88489096533485	-3.03400372054361	3.52232557854193
C	5.19621998093068	-2.47217047297578	4.39695716765150
H	4.61339310915943	-5.01726760792496	2.70795542133787
H	6.46575922277006	-4.74845489855302	-1.17398703804814
H	4.05216496621407	-1.32223648458453	2.97067225237529
H	6.33609947338360	-1.00662354497383	-1.28321170915504
H	5.26031074582719	-6.95617696251821	1.68351700976065
H	7.10838057122674	-8.18511163373935	0.53686343286369
H	7.73471253192435	-6.69462201903547	1.31969933997508
H	7.48836638221674	-6.74450424446242	-0.45253539861884
H	4.70967423458523	-8.24160251112994	-0.39456261825976
H	5.01405236746004	-6.78619064210883	-1.39421159273581
H	3.65179673854769	-6.79744647396857	-0.23530647975999
H	8.45810734488520	-1.66175993138689	-2.37784154747987
H	8.31556230778729	-3.32515463488558	-1.72796959484774
H	8.53943069378065	-1.94819188822706	-0.60654510101858
H	4.72186051880927	-2.32371154555509	-2.69153069020901
H	6.01580469568272	-3.51279075930657	-3.05584103965682
H	6.18626845467074	-1.81746450271342	-3.60070216175965
H	2.22491666951909	-3.05678200857694	2.63371285509772
H	2.36505920593871	-2.45835860559645	4.31564811761949
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H	6.14752270065818	-1.93723734469076	4.20364881743440
H	5.45086337304885	-3.52694149348758	4.62944815752432
H	4.73326162651314	-2.02893556593634	5.30200226446576
H	-5.42275244494557	-8.23316684896279	0.96445992100865
H	3.00096916640794	-0.61370444816196	5.66137988582048
H	-4.65872835434870	-6.69353551911430	1.49060334770151
H	3.70318191616931	0.60993500192794	7.73092233292369
H	5.16954710865079	0.55491230033306	5.60610122144498
C	-5.22675655868678	-7.18050154078181	0.67320772032083
H	-2.66597673468531	-3.38969419887600	-3.67620830486718
H	-2.62675058647616	-3.47135786062282	-1.88616608035901
H	-4.57315587588613	-7.19420855444858	-0.22383191994664
C	-3.24386361335970	-3.69389771251509	-2.77870054615975
H	1.91331460261159	0.57823058372873	7.57715007868633
C	2.84672719047924	0.96111038134571	7.11865093929864
C	2.98666612969277	0.49930940463478	5.65534002999757
C	4.30905581618193	0.98118287774521	5.05196059434196
H	-3.38503048786681	-4.79316986822933	-2.83321938101881
H	4.40567735356260	0.68466154819344	3.98966649034649
H	0.57968341260733	-0.74638751919812	5.59022143405327
H	-6.39742921356393	-2.66600206578688	-3.94192651848891
H	-6.79267316169744	-7.17103888189214	-1.66986301863067
C	-6.54133050853973	-6.43337093242761	0.38647235687547
H	-5.32274699836888	-5.36835453725155	-1.83802662434567
H	-2.50759278005978	-0.19900846919436	3.64503550821455

C	1.75765605325295	0.91243142271498	4.85663547419885
H	-7.14810286930256	-6.45165763240071	1.31841665409188
C	0.56991968358959	0.16266700877222	4.96926620666845
H	-4.92070957504435	-3.05194089763766	-4.88654574307728
H	2.81667835608507	2.06928120336653	7.17419033905987
S	-1.22721570850553	-2.37221098648059	1.32735683541558
C	-5.46390527555047	-3.26532181311996	-3.94429466329409
C	-7.35522694082546	-7.13242851113271	-0.71392905547965
H	4.40603309979674	2.08519674837729	5.09978285722284
C	-4.58831286101701	-2.94846475509519	-2.71993880261779
H	-8.31031569604271	-6.60451937979533	-0.90790827808945
H	-0.83607677062935	-1.07027314650537	-1.54593469372285
C	-5.62651714044963	-4.58987533914805	-1.12059431883342
H	-4.35632303290418	-1.86467383376418	-2.73536781164759
C	-1.91431397836138	-0.23751363255439	4.58254781092876
C	-6.27369154481991	-4.97023073692417	0.06532889625338
S	-2.10341847313549	-0.48374343157167	-1.46419322458698
H	-3.71753190075321	-0.11018066099304	5.82445545865300
C	1.73694224198765	2.05487158283436	4.04618500742036
C	-0.62562812011232	0.54754265098070	4.34148515775332
H	2.65696797415293	2.64227316873444	3.91320229434253
H	-1.24912284063323	-1.85783550785680	5.91862073101388
H	-1.03894570347455	-2.20769844415717	4.16448211111495
C	-5.33168772639259	-3.24849130493442	-1.42219025823696
P	-2.17316951465957	-0.83877924282584	0.60259567742140
C	-2.75848410760502	0.43049985475979	5.68576002202325
C	-1.69375073970983	-1.71897934491918	4.91125678456022
H	-2.99493092147132	1.48457609204889	5.44418828031308
H	-5.75875342900403	-4.33508458270594	-3.96104748298034
H	-7.58991545339553	-8.17801380109346	-0.42684614732945
H	1.68456566782932	4.40418470838611	0.68839816858273
C	0.57001742591702	2.47309544518538	3.37761491342031
C	-0.62349636670852	1.72973908414010	3.54502884022814
C	-6.63170742147627	-3.95585636171451	0.96604927147684
O	-3.79336846525361	-0.84313661822384	0.99936726650922
O	-1.69239350969908	0.61532785003933	1.24550506350257
H	-2.21228167898288	0.41625947606629	6.65177690135425
C	-5.71019758516003	-2.23790145812311	-0.49603943858946
H	-2.66541699491826	-2.25288500044280	4.90697669929458
H	-7.14044087045584	-4.23800239652356	1.90233841223517
C	1.72528200317979	3.55896474059789	1.40662226130789
H	0.01238875907260	5.12827291154429	4.04075011687217
C	-6.36245913127265	-2.59889536386041	0.71824493132852
C	-1.90811966448159	2.21865168749479	2.95254133529228
C	0.63557506508669	3.70379213920144	2.48126561494794
C	-2.49784597107857	1.58841729411266	1.80932933241834
C	-4.55733283553417	-0.08140510209101	0.11551531578187
H	1.60568199403327	2.61677322122194	0.83871980112743
C	0.82439363675369	4.99276326916156	3.29801490663436
C	-5.43113030494905	-0.79395403685685	-0.76044537216170

H	2.74031948289945	3.55505233129561	1.85288211974016
H	0.83299275175651	5.88162204222434	2.63355808981413
C	-2.58172760983868	3.28299676791398	3.53350120731022
C	-3.74401418680937	1.96987583074493	1.28603270756202
H	-8.65447975385779	-0.76739935828581	2.62085396691168
H	-2.12764664741246	3.79131372899603	4.39800451664748
H	-0.33858597530793	3.78202360658818	1.95885874770114
C	-4.38942571852161	1.30565257200604	0.11614284445635
C	-6.80765366920323	-1.57296125935697	1.75884824056659
H	1.78573493564363	4.97883305786199	3.85276889746999
C	-8.33953231358829	-1.55040081289434	1.90057179081952
H	-8.83008687575114	-1.34217924622499	0.92843002676792
C	-6.02304980788309	-0.06394796854430	-1.78318867023502
H	-6.50879691673468	-0.56694798732135	1.40319578835168
C	-3.86959680409952	3.68986053949680	3.09203950423390
C	-4.48962876035278	2.99257850560210	1.99369029588675
H	-6.71089206969061	-0.56969247252133	-2.47782361444032
C	-6.11592520525454	-1.79951563960960	3.11540272368039
C	-4.93851526074419	2.03173522469833	-1.00327521305525
H	-6.38519558118597	-0.99349802080637	3.82890615950949
C	-4.58040615474914	4.72880850158099	3.76175329036944
C	-5.84389794603444	3.32279757749596	1.68223701361097
C	-5.74284038989668	1.32199985788012	-1.97080367509228
H	-5.01455226754743	-1.80903215979395	3.00128529174253
H	-8.72728728288081	-2.52206942268099	2.27077869767791
H	-4.07854739059344	5.25656020453003	4.58768311615149
H	-6.36656349399898	2.76528646534969	0.89477599667096
C	-5.87868647329949	5.05254563170970	3.40209551648841
C	-6.51842356953823	4.32462755135146	2.36610849683812
C	-4.67593881300073	3.41579858580885	-1.22481316320277
H	-6.42378039022072	-2.76423935927928	3.56928305403127
H	-4.06324431639598	3.96398686868753	-0.49688596307472
C	-6.25337865721482	2.02947772501194	-3.09937808345475
H	-6.41961867115580	5.85208475760478	3.93004384503439
H	-7.56363616240567	4.54878415843070	2.10461826139093
H	-6.86780898616452	1.47885048840995	-3.82836482965859
C	-5.16741157309590	4.06727154604513	-2.34763765282241
C	-5.96851814004227	3.37259907233048	-3.29145369523335
H	-4.93242268619490	5.13065730349927	-2.50577147698442
H	-6.35604329218542	3.89899542680272	-4.17635345502486

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DSI Monomer

C	5.33459797437620	-0.50065913279362	0.22180373730871
C	4.03295662986088	-0.18332771069204	-0.20185699864197
C	6.30715219653385	0.50583146820276	0.32641496795632
C	3.00155443078487	-1.24174859795970	-0.38530863510036
C	3.72020366556639	1.14711374148385	-0.54048205620744
C	5.98997065203110	1.83517447470694	0.01067752730638
C	7.71795923407456	0.14456452745480	0.73091580619146
C	1.73104836129718	-1.23295570704588	0.27090613213749

C	3.22670290995120	-2.23828850813493	-1.32911891634023
C	4.69464130161694	2.14785385838991	-0.42651432322062
S	1.38704582321017	-0.09327599033522	1.62877789374141
C	0.67636594650028	-2.06787197027403	-0.10924898262798
H	4.20136591874787	-2.27448728486800	-1.83952292366964
C	2.21246596475858	-3.15206205172812	-1.72195055866673
C	4.31106726712168	3.57486075622780	-0.74939154957727
N	0.43251682360902	1.05977945542343	0.72888279033474
C	0.89487437557421	-3.03555344414675	-1.14891843702103
C	-0.69650267387192	-1.95708145098879	0.47958037302293
C	2.45169940982030	-4.14002933027759	-2.72182849137541
S	-0.73320245833980	0.62312290401878	-0.49324953120116
C	-0.14131619769962	-3.88398633806165	-1.64164306646583
C	-1.18838334682310	-3.01812851968565	1.31177849770218
C	-1.52573938128676	-0.86121253932689	0.20015464604537
H	3.46267659082301	-4.22332498446972	-3.14886989470111
C	1.42932680916716	-4.96629473546691	-3.15969130957297
C	0.12181477987722	-4.82807422461842	-2.62211205566486
H	-1.15724266862249	-3.78315460592230	-1.23698693134725
C	-0.36528888166539	-4.11043069299875	1.71316912263905
C	-2.53967190523048	-2.95126146424482	1.80185459491100
C	-2.89569789144772	-0.81654200170357	0.62061871610422
H	1.62452808185251	-5.72242140309356	-3.93474773885999
H	-0.69022411881326	-5.47269515973095	-2.99000318745522
H	0.67706070923364	-4.15026652158716	1.36845398407592
C	-0.86266445732429	-5.10048455811396	2.54650456748648
C	-3.02558099049015	-3.99153996661972	2.64676908899090
C	-3.36331870992371	-1.86154068832089	1.41347165245332
H	-0.21163173555855	-5.93160414151435	2.85578649705976
C	-2.20398655346084	-5.04632434407632	3.01150480080056
H	-4.06310266881307	-3.93601195716450	3.00996802823222
H	-4.42034286310659	-1.85993356570909	1.72110789835108
H	-2.58613217080190	-5.84109249758320	3.66944869619734
H	0.01274422260912	1.75582980159494	1.36664889424608
C	-3.87083794087719	0.21214884047202	0.16689463594761
C	-4.06086501470463	0.45718999303805	-1.20969210940562
C	-5.03380011103677	1.36499485343528	-1.63879252811382
C	-5.82859820098009	2.05298744195728	-0.70527996282126
C	-5.64625135915140	1.80909987441325	0.66023907687288
C	-4.67640391923868	0.88954026965381	1.09673208026100
C	-5.27785529154733	1.57668496161229	-3.11634093887975
C	-6.48607733390768	2.52153510028287	1.69603302321610
O	2.57663437390162	0.63824244510191	2.08604404811937
O	-1.64397657821739	1.77957281660376	-0.47147657291230
O	0.54524387439029	-0.78664056031943	2.62409912896795
O	0.01147422782740	0.24641643892396	-1.70469713329701
H	5.58622168422642	-1.53521180583913	0.49556012026374
H	2.70690660532853	1.39561630638673	-0.88973644266718
H	6.74732988681773	2.62450465386977	0.10455480795255
H	-3.43957457134988	-0.06434795321842	-1.95170933552053

H	-6.58084962700352	2.77887738118659	-1.04151332286734
H	-4.52883400166283	0.71725005176647	2.17306878217686
F	-4.20542952892391	1.22826857000335	-3.86128709220531
F	-5.57300078064312	2.86843406904620	-3.38983791892662
F	-6.32654123967493	0.82951007745581	-3.54648767411458
F	-5.70966035253092	3.17894636081321	2.59059400699987
F	-7.23708518484774	1.63866411359133	2.40225631776837
F	-7.32810493760768	3.42146357701362	1.14292264790977
F	8.46841459831391	-0.18415846544244	-0.35187382163079
F	7.74191082767855	-0.92113889546312	1.56633420513062
F	8.34251535795043	1.17104194985072	1.35135244635131
F	5.38723007873667	4.39458516444226	-0.78591364484408
F	3.45311151188367	4.07134759685875	0.17385603152607
F	3.69077568673215	3.65618771735714	-1.95047869213576

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DSI Dimer

C	-5.74289766192854	1.43610565559275	-2.65499538163474
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C	-6.62604734717415	0.41679008800690	-3.04002781683773
C	-3.96536666085092	2.33529165339691	-1.10640486975287
C	-5.09394740680093	0.12479933561976	-0.72316284641772
C	-6.71244505070327	-0.77333912823855	-2.29944247318723
C	-7.51963357329939	0.60323345053721	-4.24560785978317
C	-2.57550381280577	2.02685235329315	-0.89677572521314
C	-4.39347858436405	3.63381889373930	-0.87827032956500
C	-5.94029272765733	-0.91143217537251	-1.13775783901341
S	-2.06339347862346	0.39848562371232	-1.52532923842713
C	-1.67086515722147	2.95728002065827	-0.37198302508061
H	-5.45781483084700	3.87888450058413	-1.01535886712838
C	-3.50143544788940	4.65157047517433	-0.44874465088397
C	-5.93602703988309	-2.21483952213345	-0.37299824351278
N	-0.39193168123885	0.46402716253092	-1.77190334578483
C	-2.12684335656879	4.31595930353096	-0.17873548068981
C	-0.25812532390561	2.69445864947433	0.08046986847193
C	-3.94708484706665	5.99213499617902	-0.26070421568441
S	0.41508651395523	1.85379254919248	-2.41837186921931
C	-1.25137095826118	5.35861319932503	0.25138785402512
C	0.00845289682430	2.68412534469734	1.49255951220134
C	0.82285647990963	2.56292916041185	-0.79891328986798
H	-5.00270907239223	6.22806866489025	-0.46442899795978
C	-3.07111735603482	6.97852064861151	0.16262814284407
C	-1.71158789031326	6.65688250524453	0.41229041514121
H	-0.19505308075165	5.13023223638690	0.44473970532536
C	-1.03126233107491	2.75724427246925	2.46551675169682
C	1.37203017516945	2.54298724019360	1.94800801304263
C	2.18628106312504	2.56507772877454	-0.36778088828929
H	-3.42500923664383	8.01105343531592	0.30074799714757
H	-1.01444016639615	7.44427526195488	0.73531601396891
H	-2.06990997587532	2.86924832329529	2.13200514577476
C	-0.74521804571178	2.65591029313131	3.81722046047215

C	1.63198635212358	2.44540306500930	3.34614102042315
C	2.43147469173838	2.54227074891368	1.00175668778326
H	-1.56888705236938	2.68475663255003	4.54441475173072
C	0.59316598982399	2.49339599366080	4.26160794078448
H	2.67194066357653	2.31668048350994	3.67932080489816
H	3.47027806868452	2.54550394612885	1.36239408686463
H	0.80343162451933	2.40347857665369	5.33781572957076
H	0.09828504563328	0.06101998248108	-0.94137834832919
C	3.30203902106095	2.68570130896761	-1.34031304490487
C	3.24561326733040	3.68083893432098	-2.33864993690035
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C	5.38738767040211	2.95069458602002	-3.22971847408340
C	5.44881414686110	1.96489825713395	-2.23632537625976
C	4.42310059117593	1.84030354875807	-1.28443072862188
C	4.23800787212088	4.93656891408278	-4.28305009399737
C	6.59452975248055	0.98106352306867	-2.20318809767108
O	-2.70493708752141	0.22744952072740	-2.83649053986250
O	1.62947582330044	1.33190674882331	-3.06352987592886
O	-2.21478142474764	-0.63084734310306	-0.46254102348995
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H	-5.63740943083007	2.33331694397110	-3.28073720729592
H	-4.52182362343136	0.01301717371235	0.20211825646983
H	-7.37722563613316	-1.58410709228850	-2.62725363787641
H	2.37244893387969	4.34738427651502	-2.39635079615744
H	6.19103564347832	3.04102724716431	-3.97217806866695
H	4.48126695879069	1.05811157587209	-0.51505284705909
F	2.96869799452460	5.24058978945128	-4.63660449012319
F	4.91832969788576	4.61905237925229	-5.40878973593116
F	4.79561327978852	6.06905455746188	-3.78467938200292
F	7.57962863473951	1.30290001487078	-3.06558455900046
F	6.16735158010586	-0.27286202470690	-2.53047737458692
F	7.13965952295848	0.90018055489835	-0.96550876552116
F	-7.72208583030650	-0.56359825210406	-4.90172872303648
F	-7.00344966969614	1.48938829204221	-5.12687905501513
F	-8.74042584232850	1.06834262610375	-3.87744177277617
F	-5.70679328887059	-2.02496708663307	0.95192765537169
F	-4.95790033655725	-3.04569040157707	-0.82320829383935
F	-7.10686203878526	-2.88087300141455	-0.49481802649456
C	5.61616831672685	-2.43186741813533	-0.31964867280227
C	4.38290062077296	-1.91132501142628	0.10278318474296
C	6.80788395828620	-2.01738825770460	0.29624986084738
C	3.11084865409222	-2.28886881912213	-0.57688859147549
C	4.35735447192012	-0.95152052534975	1.13501617710210
C	6.78180622629897	-1.08278640237761	1.33810268471158
C	8.12893338032069	-2.52412787014879	-0.23537474412074
C	2.00573485634054	-2.90169054099163	0.09318126479738
C	2.93011399059438	-1.91916168696450	-1.90604603753741
C	5.55081306064420	-0.54689960921566	1.74720519541708
S	2.15288979480599	-3.45309652336736	1.80057168924883
C	0.73360912350578	-3.00596745102134	-0.48357090286339

H	3.75827359693814	-1.42510408994933	-2.43670044237277
C	1.68503717353180	-2.07806496349389	-2.57323993455917
C	5.51372277598335	0.52777756486581	2.80458032700398
N	1.44708894664004	-2.02282856377655	2.56621334216130
C	0.55007061111420	-2.59716590983250	-1.84945357168371
C	-0.47937605944256	-3.38418614613715	0.30678877254105
C	1.51375780170391	-1.64942355064364	-3.92059825943497
S	0.09049026615622	-1.19525253111491	1.88010324909862
C	-0.71987586102617	-2.63406587452001	-2.50107317873034
C	-1.18770787831130	-4.58782678255778	-0.01530074608579
C	-0.98493471243177	-2.53485824225228	1.30289589430439
H	2.37987543460547	-1.23255373619791	-4.45429468431756
C	0.27268165735465	-1.72145451645282	-4.53101533124085
C	-0.85010938567000	-2.20839618958791	-3.81299405136878
H	-1.60796199280344	-2.95900177819563	-1.94537952959528
C	-0.68142831208856	-5.53601160976261	-0.95173876649185
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H	-1.84150262666419	-2.21301437251264	-4.28730832221915
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C	-3.16580895817494	-6.03357256073523	0.29240112052899
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H	-3.90707046776701	-4.12482057820875	2.06448678381307
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C	-3.29250119817672	-0.59895824685998	2.63491081319416
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C	-3.94075750358526	-1.64175404148707	5.15620707324064
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O	1.27137186235689	-4.61429983991580	2.02465504946253
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IDP Monomer

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C	-2.11455996660405	-4.24157765930842	2.23002178863653
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IDP Dimer

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IDPi Monomer

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C	-8.86525371746706	-1.50198845173315	-2.72755133307566
H	-13.20317861085541	1.81314681056505	0.44287531344030
C	-10.88513837109872	1.65362046302797	-2.04872882029263
C	-6.71392648684294	0.52790175540175	-6.80460141425478
C	-9.99550966665311	0.76217331621889	-2.67282309126663
C	-7.13052501625479	-3.54318643869082	-3.76931309888052
H	-6.47938306985003	-0.28265848363544	-6.08448669067086
C	-8.13656645336134	2.17881218989138	-3.64421395027420
H	-13.02320959891935	2.89982018095564	-0.95472457912718
C	-6.36667448074592	-4.67100279018327	-4.19717272292181
H	-4.72781950551872	0.71902998254326	-7.66267513198443
H	-11.05845081645085	2.63842411849427	-2.51383397855678
H	-10.01792302629605	1.68543381992490	-4.60696394619182
H	-7.67328177362489	2.54536117455271	-4.57999989478327
C	-9.28046990466350	1.19874853323455	-3.93228228525526
C	-5.46335279750233	1.35873074095490	-7.12975776934791
H	-3.50280937849860	-2.29635527836830	-7.01526099774771
H	-5.33082733307669	-2.08638359085931	-5.34338511726061
H	-7.33755269118028	1.70881052458404	-3.03913096345699
H	-7.50200126497409	1.15318360697059	-6.34157769471787
H	-5.73758080884846	2.17204938985455	-7.83508693543073
C	-7.46108956297203	-1.50663944961927	-2.48145058205874
C	-6.57191078139074	-2.45556198054985	-2.99405701739072
C	-3.29954494422709	-2.50317121721698	-5.95366094311382
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H	-5.30793170250776	-4.74224000251862	-3.91924221431890
O	-7.73759825652290	-0.44086682738790	3.41566670783111
H	-8.89562319953762	0.31525945651053	-4.48130428876387
C	-4.80170289856438	1.95276566217274	-5.90486551261849
O	-6.96146734971301	-0.43875253862440	-1.72916437291473
F	-6.97968477301522	-3.73532562805521	3.27636054899962
H	-3.46341143654993	0.27069584847425	-5.61918283989129
C	-1.99117803198941	-2.87117162854295	-5.54317836834548
H	-5.91011067461655	3.81708977907182	-5.95666867217630
C	-4.08421173898799	-2.62430108142790	-3.64012408921968
C	-5.11890153586140	-2.47811394948698	-2.64660875822223
H	-1.18588425615743	-2.95633669372489	-6.28794161034661
C	-3.79457885925196	1.24469098353005	-5.22635013819570
C	-5.16375409021055	3.21637704171594	-5.40977734341702
F	-8.95486552220092	-2.88436737017832	2.90836401725687
S	-6.92918889363389	-1.20989249550026	2.46263031746403
C	-7.69861414507481	-2.96359510919493	2.45931224056057
O	-7.88460688479067	3.49671512994924	-0.65077541746853
F	-7.10798031734623	4.80043269285030	2.37235301279555
O	-5.47601536570347	-1.40043642569323	2.56098290485625
F	-9.01601644962054	5.06449257738090	1.35842806459442

C	-1.72710752221307	-3.11793974413720	-4.20406779717029
C	-2.75385413745984	-2.99822646890147	-3.22227219063941
P	-6.16431446737266	-0.61799289604478	-0.33038987235947
C	-4.72439113891025	-2.54859952369538	-1.30739865872561
O	-5.64073259358145	-2.16135209403813	-0.31077704539662
N	-7.32654403396868	-0.66168159748432	0.89804442096234
C	-3.15801547004858	1.75567000886831	-4.08220207356243
C	-4.57002663715941	3.76564672265599	-4.25678179803258
H	-4.11023279205491	5.61785917101889	-3.25514034792220
C	-8.20889932414299	4.17530002918966	1.94734817604925
H	-1.13833372601609	1.63772843102782	-3.32487565362663
N	-6.27794763800321	2.46833302457107	1.13919554816964
S	-7.76000407176332	2.83121212033854	0.66199965851727
H	-2.54042306373084	1.02845286637904	-1.33502080656182
F	-7.69333611312614	-3.49092905176925	1.23509329013942
H	-7.98205194386687	0.19165637442346	0.92743169576266
C	-2.01595832743693	0.97228935319322	-3.46800484943344
C	-4.95162569516712	5.16771808021883	-3.82030429957934
H	-6.83781580465787	-5.77099780326482	0.40363054711716
C	-3.58311838685370	3.01051706735328	-3.56982037057196
H	-0.71628407509388	-3.39984622928042	-3.87563356308073
H	-4.58348326824216	-6.74553137905500	-0.26122098510577
C	-2.51174019539479	-3.30871743944473	-1.85197158720218
N	-5.04540293642050	0.48496508605805	-0.30142649213873
H	-6.60587274109360	-4.45969262696036	-0.78377467496711
C	-3.48373587877753	-3.11036709617217	-0.87785122166398
C	-2.35144394697330	0.29489694805604	-2.13952076720112
C	-6.32349781022784	-5.50022093471163	-0.53962807574119
P	-5.00342804179823	1.96901568042736	0.31263204228800
H	-5.07386617704788	5.78993799567472	-4.73306886856151
F	-8.84535106074346	3.62635574444358	2.98926155124659
C	-4.80422560765310	-5.66700954716625	-0.41384957094681
H	-6.43664788003543	6.30629801382862	-2.68777918245162
O	-4.61805925064618	3.01026996738660	-0.89618937593205
O	-8.68699807156630	1.68573024810858	0.95508599579535
C	-6.23247686811651	5.25561880879898	-2.97915225629743
H	-1.69339741376565	0.19897283990972	-4.19536622935117
H	-1.51878211074179	-0.35651280616264	-1.81177519582177
H	-1.54737259851211	-3.75424774285959	-1.56331869408904
H	-4.32866523102345	-5.39886243774765	-1.37907899174568
H	-3.26232062097030	-0.32458994547841	-2.22690769003490
C	-2.86917559909083	3.63125122833145	-2.41157059119247
H	-4.52258325643350	-1.72107928796662	7.39817831598618
H	-7.11006149144515	4.88792675460019	-3.54588680275006
H	-6.7181192228522	-6.14935681027111	-1.34714893758071
C	-3.38642937519359	-3.70442974333383	0.49236926444542
C	-3.39627923771014	3.65422181706062	-1.08041131994784
C	-4.11483584389981	-4.91039294578773	0.71289594336256
H	-0.88570786528353	-1.96027916441670	2.07326796168437
O	-3.71621612749484	2.02698731881079	1.32383366547095

H	-3.17073381457442	-2.36188583580107	6.43735925726545
H	0.42305013206265	2.41995812949971	4.70453543216846
C	-4.18048681800127	-1.90571310503580	6.35554354034498
H	-6.17130806500274	4.64923857655140	-2.05637112308557
H	-1.25816532265575	4.28560538267993	-3.66811949804318
C	-1.66313127065801	4.27858169694589	-2.64447886950742
H	-0.82467514008696	0.60544319471090	3.50938761357113
C	-4.06967809741853	-0.58446382649139	5.62606334128760
H	-1.97176572385137	-0.80748804836683	5.13491970940392
C	-2.86747297243132	-0.17056020420386	5.03906154026438
C	-1.66531781863261	-1.98260724931287	1.28238791027659
C	-2.54805967102715	-3.18719280824301	1.51111731757654
H	-6.78776973060412	2.06621087291951	3.56904253589747
C	-0.59895243755487	2.14233708570240	5.02662289133686
C	-5.19076077963232	0.25501362663436	5.49547096978454
H	-6.14120656901729	-0.05362033119652	5.95408343867588
H	-1.11195045567141	3.05889471148848	5.38409815654474
C	-2.76010522656268	1.04662018546136	4.33901566971477
C	-1.38590081985803	1.48680035066026	3.88295321479215
C	-3.61798897895792	3.22347305162265	2.04942279120047
C	-4.08234768326443	-5.49512211059715	1.99148974685330
H	-6.15959820406403	-2.46349330574198	5.59707191989362
C	-2.77334494233994	4.34210344125679	-0.03069912316800
H	-1.12389510783018	-2.08771381271353	0.31947963599160
C	-5.14805670027788	1.46017675022563	4.77608438708226
C	-5.13844425811022	-2.88856182443900	5.67143940115620
C	-3.91219216706604	1.85885732453895	4.18971473948337
C	-6.40504828630725	2.28624045564373	4.58743804263625
H	-1.80423402438778	0.19869134346466	1.13933645999745
C	-2.45621079039501	-0.68036814304923	1.28381898343424
H	-4.64730838372331	-6.42791945810294	2.15812756148337
H	-3.19290299123966	-0.67183355577441	0.46384789173993
C	-3.33175028186183	4.39861508729686	1.34993100910409
C	-0.93978444398267	4.93251666553056	-1.61360517852339
H	-6.13860947971519	3.36080332975613	4.55937728993240
H	-4.80356028763327	-3.11193276095643	4.64058979001831
C	-3.79699090001789	3.16191949702674	3.46360088115865
H	-0.51662330096507	1.45375293629638	5.89305978487371
C	-2.53388954394953	-3.82225975531315	2.76664662247305
C	-1.48552643097708	4.95600050154990	-0.28098370931932
H	-1.44964131167465	2.18979410219190	3.02990014282809
C	-3.30891445892088	-4.96210073900912	3.03771795504175
H	-5.20985767527950	-3.84178139672357	6.23361926432770
H	0.71215374730012	5.52585996564161	-2.90522274544294
C	0.31561746499115	5.55447126340553	-1.87898438519361
C	-7.52490884338142	2.05642355945113	5.60009753650725
H	-7.17375933450117	2.19736860906902	6.64353998269547
C	-3.48695282834116	5.64713448082980	2.05192157363121
H	-3.01709983046397	-0.54797450376945	2.22632684938320
H	-3.29730588755054	6.93067529816783	0.29945029871518

H	-1.87769045685633	-3.41847990835833	3.55467243598639
H	-7.95083609082969	1.03791665614772	5.51253129484012
C	-3.80389423210962	4.37303881326612	4.14836265524592
C	-3.44225248578354	6.90848881348425	1.38871675700691
C	-0.69493761843094	5.55593015708524	0.74550516880913
C	-3.23516801348649	-5.65942936843549	4.37795594264942
H	-2.40633890857321	-7.46622731706351	5.31374049561867
C	-3.71963800007493	5.62388799540922	3.47465603394833
H	-4.26454936120150	-5.84469710920220	4.75352265554785
H	-8.35277969282040	2.76904777892296	5.41816256487904
C	1.03105389210321	6.17092300353502	-0.86616416030168
H	-3.91138864915198	4.36209916397183	5.24404078884949
C	-2.46399480630416	-6.98555130644705	4.31553643357876
H	-1.05304094481673	5.53839577124608	1.78229079432709
H	-2.94979694233829	-7.70280980380664	3.62301501188215
C	0.52484921747003	6.15267203950935	0.45903203198546
C	-3.59628260863030	8.09100078646213	2.09712903768648
H	-2.75187984426297	-4.98251894145170	5.11255529048983
C	-3.85078164129788	6.85900747978192	4.17605713374064
H	1.99584648178968	6.65113216088989	-1.08538968847180
H	-3.57373661469213	9.05299997425868	1.56331891261031
C	-3.78877939965769	8.06977819608134	3.50424379590854
H	-1.43070074331616	-6.82057080211637	3.95036261680033
H	-4.01773568074074	6.82893319760173	5.26394539293804
H	1.10600453383812	6.60973172732187	1.27378606947818
H	-3.90138305806670	9.01509751602165	4.05616684718387

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X-TBS (xTB)

P	-0.66901539166255	-0.04435863068277	-1.29576850442843
N	-1.13487422275255	-1.04259435796603	-2.45249252184694
S	-0.91496876166070	-0.65362802518258	-3.95829416151606
O	0.42710963701308	-0.30752083207831	-4.33411127313939
O	-1.96267640203079	0.12884506269674	-4.55615990129256
C	-1.17170650565818	-2.37516402037546	-4.69353348504435
F	-0.40059436984061	-3.29645117677720	-4.10973974749045
F	-2.43574009025005	-2.79005330454325	-4.57467368328492
F	-0.87710081363281	-2.38954093042984	-6.00202027089528
N	-0.14380304739480	-0.90903463425118	-0.05408061775529
P	0.70831182157828	-0.35164738243157	1.15131613887654
N	1.02538923451504	-1.56409846145650	2.19508726648320
S	-0.18275193628142	-2.18331087107953	2.89960733261013
O	-1.13342886207040	-1.35042935832655	3.54116136801508
O	-0.83216314565812	-3.34344441725654	2.21769255414360
Si	-0.66029541747152	-4.41057202487463	0.85504288769246
C	1.17176005046643	-4.33505975195807	0.40549039456650
H	1.81637019888472	-4.55917219078099	1.25210375402298
H	1.39870661424710	-3.32104677461101	0.08301191865970
H	1.43429891426851	-5.01112073715166	-0.40307318693808
C	-1.83776808207931	-3.80293608676485	-0.49316065064678
H	-2.88398822980388	-3.86330933300783	-0.20677252905271

H	-1.62009520406607	-2.76973768809061	-0.75876456263884
H	-1.71359722436324	-4.39724384012413	-1.39375835983026
C	-1.20155255931664	-6.10075212028344	1.64405680335051
C	-0.08793353980069	-6.69616728254322	2.51941686422864
H	0.15413099422866	-6.03272738899778	3.34521132408054
H	0.81240820986596	-6.87045310939776	1.93625236956237
H	-0.41597821011348	-7.64782382715267	2.93506058122294
C	-2.46504992810479	-5.94791348785992	2.50295630831330
H	-2.29378932702399	-5.24437657506779	3.31464252279609
H	-3.30145681286370	-5.59438087797542	1.90471172059819
H	-2.73978458516249	-6.91041784725598	2.93234176301559
C	-1.50248249925795	-7.09122657309550	0.51137768747068
H	-2.32332685880879	-6.73499368518417	-0.10411728636967
H	-0.63151287868787	-7.22316128309129	-0.12442632282947
H	-1.77847782782289	-8.05971496864285	0.92386767368505
C	0.70748537328432	-3.09865487986673	4.28535506067435
F	-0.13615201851811	-3.82860252957181	5.01692246836398
F	1.30602564156549	-2.22976179964854	5.09845151282706
F	1.63870020385104	-3.91867141473162	3.80745290036847
O	2.09690643444300	0.25390092708980	0.70424129769626
C	2.94293431939683	0.50332462234382	1.80368758994322
C	2.68804784691542	1.61439020055108	2.57354272010848
C	3.45411116324539	1.83016416341621	3.75967951170141
C	3.14871180665633	2.83333309876857	4.70521627223732
C	3.93586311356663	3.02114296518769	5.80816117486313
C	5.06570415644576	2.21807649734761	6.02612227185394
C	5.35561262848243	1.20203952371950	5.16027022919034
C	4.54617600304614	0.96346320782739	4.02759604086117
C	4.77534084777628	-0.14154542324416	3.18863393856670
C	3.96073040705692	-0.42684650245647	2.11476830100356
C	4.11562067103355	-1.69162237148578	1.38370042282288
C	4.37029416124726	-2.84391997733932	2.13362810301623
C	4.49752448008458	-4.08132793388304	1.53393499680099
C	4.33776069430628	-4.17120386064562	0.16032569221872
C	4.08222433627828	-3.02284852617593	-0.60366912913532
C	3.99463839501883	-1.78354538324797	-0.00518637098148
H	3.83075059012417	-0.89409332768473	-0.59478072193536
C	3.91642185550893	-3.38398980438207	-2.05918863119489
C	4.00276160725177	-4.89217553857301	-2.01588327422578
C	3.83151160426328	-5.81567784446416	-3.02677288965020
C	3.98487518356400	-7.16643058852618	-2.73913793254393
C	4.30092223202047	-7.59273842785576	-1.45820348645633
C	4.45420922597487	-6.67646689538231	-0.43043183387378
C	4.30011050570477	-5.32923162032791	-0.71468132859215
H	4.68574202290779	-7.00637239600989	0.57146139657825
H	4.41911418466109	-8.64825674686636	-1.26020312620654
H	3.85408992468452	-7.89505216915995	-3.52636924568640
H	3.56926291317531	-5.50875507850889	-4.02693841757464
C	2.62552396635500	-2.85055234474297	-2.70866354636713
H	1.79160057064668	-3.53605735695922	-2.56364203714470

H	2.34698447790783	-1.89908968356976	-2.25229018250477
C	2.93826730149148	-2.64647697420047	-4.20058059169504
H	2.57681257858980	-1.67028660849405	-4.52245852406281
H	2.42291760474672	-3.39078564517863	-4.80839858874449
C	4.46387849066420	-2.77786354626432	-4.35513745207967
H	4.88313835165509	-1.97027067095968	-4.95623440852152
H	4.72042595753043	-3.71322831218275	-4.85379427132467
C	5.02745174591634	-2.77417765235388	-2.93457188242481
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F	1.33291927258099	-0.28415562074301	-3.61536990697474
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C	-3.60596688633433	-6.06356448747791	4.11341772552361
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H	-0.48263432770606	-3.32595596766025	3.39951156983352
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H	1.20152752472092	-6.15762736379919	-1.03743689159732
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H	0.03787866302805	-9.45767446582171	-3.10326221762320
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H	-2.90132974918725	-3.46301375187452	-5.78757117752214
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TS-1 (r²SCAN-3c/xTB)

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H	2.25320127764883	-3.45754085120588	2.73435914028601
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H	2.86246877129937	-6.02344017484205	3.75878769978027
H	2.32486318215481	-7.02829560314705	1.43136116659971
H	2.52666307572187	-4.58471889377955	1.38574927135644
H	0.71970321189545	-7.72829457311878	1.13936374564802
H	1.06527231695040	-6.02285706579813	-0.55610962084446
H	-0.99962902392285	-7.90992328437015	-2.06147609262934
C	1.66024389569943	-5.49090044636989	-1.29970938558638
H	2.70851784063533	-5.77434904378270	-1.15737873272155
H	1.56381238806427	-4.41882540525314	-1.08190444988092
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H	0.57770318641657	-8.31515305426435	-1.36464491187573
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H	-2.99102513400941	-3.69152429787936	-5.53512654627463
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C	2.02380808648924	-8.33451746420506	-3.71981239293319
C	0.68379838669637	-7.61681400963822	-3.44205406707833
C	-2.05916506453828	-3.92937812105802	-5.02259598748653
C	-1.91646292663502	-5.31002788521581	-1.64125226190744
C	-1.53629041433303	-4.86926534557446	-2.87974315427469
O	-2.47535364881378	-4.41807141769430	-3.72346700990653
O	-0.30744968519107	-4.84459161552978	-3.36095657854268
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H	-1.44202556104759	-3.03328288790270	-4.91612586364609
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H	-1.50768102558362	-4.70317008984605	-5.56295932922329
C	-0.20189924492233	-7.69900608947420	-4.69946363488813
C	2.30305434841873	-5.09111989129819	-4.27916715363227
H	0.24949322747745	-7.17644719215225	-5.54982537160668
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P-1 (r²SCAN-3c/xTB)

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C	5.88141543611248	2.51773577972630	4.34090063665425
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C	3.44739327448054	5.34403081991463	1.77250515299608
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C	5.07634546768192	6.96681490474629	1.02704504789534
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C	2.40910858124726	6.26446425229362	1.47783509417144
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P	0.04330034268720	1.64853132907136	-0.90057041712424
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H	7.05685694725928	0.01400538805843	-4.60327488620228
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H	6.56259291419971	4.98960679051602	-0.89768193415522
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H	6.96835025547082	1.39898767266838	0.54015245807088
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H	8.21138125256199	5.37549493425431	0.70351850395715
H	9.40081169834644	4.39839409289425	-0.14124776861133
C	8.03340545242210	3.23055915170727	1.08556649117632
H	7.74700389963820	3.54544384466630	2.09013438910166
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C	6.88660698336012	-2.76250530166528	-0.94660612739824
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RC-2 (r²SCAN-3c/xTB)

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C	-9.85409677013532	-3.44247459690718	2.11542147709644
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TS-2 (r²SCAN-3c/xTB)

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2 (r²SCAN-3c)

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