Supporting Information for

Excited-State Dynamics of C_3-symmetric Heptazine-based Thermally Activated Delayed Fluorescence Emitters

Katrina Bergmann and Zachary M. Hudson*

Department of Chemistry, The University of British Columbia, 2036 Main Mall, Vancouver, BC, Canada, V6T 1Z1

Tel: +1-604-822-3266; Fax: +1-604-822-2847; Email: zhudson@chem.ubc.ca

A. General Information

Optimal tuning of the range separation parameter: The optimally tuned LC-ωPBE/6-31G(d) level of theory was used for all calculations.[1–3] In range-separated (RS) functionals such as LC-ωPBE, a general expression for the separation of the exchange term into short- and long-range domains is defined by the interelectronic distance *r*.

$$\frac{1}{r} = \frac{\alpha + \beta erf(\omega r)}{r} + \frac{1 - \big(\alpha + \beta erf(\omega r)\big)}{r} \tag{S1}$$

In this expression, α, β and ω are tunable parameters. By using Fock exchange for the first term on the right-hand side of equation S1 but semilocal exchange (such as the Perdew-Burke-Ernzerhof (PBE) functional)[4] for the second term, the exchange functional can be written as

$$E_X = \alpha E_F^{SR} + (1 - \alpha) E_{PBE}^{S} + (\alpha + \beta) E_F^{LR} + (1 - \alpha - \beta) E_{PBE}^{LR} \tag{S2}$$

where subscripts 'F' and 'PBE' denote Fock and PBE exchange, and superscripts 'SR' and 'LR' denote short- and long-range, respectively. In this expression, α determines the fraction of Fock exchange in the short-range, $\alpha + \beta$ determines the fraction of Fock exchange in the long-range, and ω is the range-separation parameter that determines the transition from short- to long-range.

The value of ω must be non-empirically tuned such that the functional fulfills Koopmans' theorem, a fundamental property of exact Kohn-Sham theory. This theorem equates the vertical ionization potential (IP) of an *N*-electron system to the negative of the highest occupied molecular orbital energy (ε_{HOMO}). In donor-acceptor systems, it is also useful to include the electron affinity, which can be equated to the ionization potential of the anionic ($N + 1$ electron) system.[1] Using default values of α and β where $\alpha + \beta = 1$, ω is optimized in the gas phase to minimize the error measure $J(\omega)$:

$$J^2(\omega) = \sum_{i=0}^{1} \left[\varepsilon_{HOMO}^{N+i}(\omega) + \mathrm{IP}^{\mathrm{N+i}}(\omega)\right]^2 \tag{S3}$$

$$\mathrm{IP}(N) = E_{GS}(N-1) - E_{GS}(N) \tag{S4}$$

For each ω value tested, single point energy calculations were carried out on the N, $N - 1$ and $N + 1$ electron systems in order to calculate $J(\omega)$, and minimization of $J(\omega)$ was conducted using a golden section search. Possible ω values for the minimization were limited between 0.0050 and 0.5000, with a tolerance criterion of 0.0010.

Table S1. Optimally tuned range separation parameters (ω) for heptazine-based molecules.

	HAP-3MeOCz	**HAP-3MeOTPA**	**HAP-3Cz**	**HAP-3HMAT**
ω (bohr^{-1})	0.1515	0.1458	0.1579	0.1374

Image-dependent pair potential method: Rather than a linear interpolation in Cartesian coordinates, which may result in overlap of atoms when generating a path between two states, the image-dependent pair potential (IDPP) method was used. The IDPP method interpolates pairwise distances between neighbouring atoms in the initial and final states and a path is generated to match those distances.[5] Since the number of pairwise distances exceeds the number of atomic coordinates, the path is generated by minimizing the objective function:

$$S_K^{IDPP}(r_i) = \sum_A^M \sum_{B>A}^M w(d_{AB})\left(d_{AB}^K - d_{AB}\right)^2$$

Where d_{AB} is the pairwise distance between atoms A and B for intermediate image *i*, d_{AB}^K is the ideal interpolated distance between atoms A and B of the same image, and *w* is a weight function to give shorter bond distances more weight and make unnecessary bond-breaking unfavourable. The weight function is given as $w = (d_{AB})^{-4}$. Eight intermediate images were generated between each state in this study.

B. Cartesian coordinates of critical points

Table S2. FC Cartesian coordinates of **HAP-3MeOCz**.

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y(Å)	Z(Å)
C	-2.031015	-1.687992	1.658038	O	2.339985	2.797008	-2.946962
N	-2.343015	-0.379992	1.649038	O	-3.592015	0.628008	-2.946962
C	-1.321015	0.489008	1.650038	C	1.033985	-4.113992	-4.166962
N	-0.000015	0.000008	1.666038	H	1.695985	-3.744992	-4.973962
C	0.235985	-1.388992	1.650038	H	1.179985	-5.205992	-4.054962
N	-0.799015	-2.232992	1.640038	H	-0.012015	-3.916992	-4.439962
N	-1.534015	1.808008	1.640038	C	3.045985	2.953008	-4.166962
C	-0.447015	2.603008	1.658038	H	2.395985	3.341008	-4.973962
N	0.841985	2.219008	1.649038	H	3.917985	3.625008	-4.054962
C	1.083985	0.899008	1.650038	H	3.397985	1.948008	-4.439962
N	2.332985	0.425008	1.640038	C	-4.080015	1.161008	-4.166962
C	2.476985	-0.914992	1.658038	H	-4.091015	0.404008	-4.973962
N	1.500985	-1.838992	1.649038	H	-5.098015	1.581008	-4.054962
C	-0.707015	4.070008	1.703038	H	-3.386015	1.969008	-4.439962
C	-1.459015	4.589008	2.781038	O	4.108985	-0.249992	3.735038
C	-0.226015	4.964008	0.721038	O	-1.838015	3.683008	3.735038
C	-1.737015	5.968008	2.871038	O	-2.271015	-3.433992	3.735038
C	-0.551015	6.346008	0.820038	C	-2.243015	-4.388992	4.785038
C	0.554985	4.813008	-0.502962	H	-2.151015	-5.419992	4.396038
C	-1.288015	6.856008	1.892038	H	-1.353015	-4.147992	5.382038
H	-2.303015	6.359008	3.717038	H	-3.141015	-4.320992	5.428038
C	0.670985	6.111008	-1.074962	C	4.922985	0.252008	4.785038
C	1.133985	3.722008	-1.162962	H	5.769985	0.847008	4.396038
H	-1.504015	7.923008	1.973038	H	4.268985	0.902008	5.382038
C	1.328985	6.319008	-2.289962	H	5.312985	-0.559992	5.428038
C	1.803985	3.927008	-2.375962	C	-2.680015	4.137008	4.785038
H	1.096985	2.713008	-0.753962	H	-3.618015	4.573008	4.396038
C	1.896985	5.218008	-2.937962	H	-2.916015	3.246008	5.382038
H	1.392985	7.314008	-2.735962	H	-2.172015	4.881008	5.428038
H	2.412985	5.375008	-3.887962	N	-0.000015	7.037008	-0.265962
C	-3.171015	-2.646992	1.703038	N	-6.094015	-3.517992	-0.265962
C	-3.245015	-3.557992	2.781038	N	6.093985	-3.517992	-0.265962
C	-4.185015	-2.677992	0.721038	C	7.356985	-4.114992	-0.511962
C	-4.300015	-4.487992	2.871038	C	7.449985	-5.500992	-0.726962
C	-5.221015	-3.650992	0.820038	C	8.518985	-3.324992	-0.545962
C	-4.445015	-1.925992	-0.502962	C	8.693985	-6.085992	-0.982962
C	-5.293015	-4.542992	1.892038	H	6.542985	-6.110992	-0.678962
H	-4.356015	-5.173992	3.717038	C	9.761985	-3.921992	-0.780962
C	-5.628015	-2.474992	-1.074962	H	8.435985	-2.244992	-0.401962
C	-3.790015	-0.878992	-1.162962	C	9.853985	-5.301992	-1.004962
H	-6.110015	-5.263992	1.973038	H	8.757985	-7.164992	-1.150962
C	-6.137015	-2.007992	-2.289962	H	10.661985	-3.300992	-0.803962
C	-4.302015	-0.400992	-2.375962	H	10.825985	-5.763992	-1.195962
H	-2.898015	-0.405992	-0.753962	C	-7.243015	-4.313992	-0.511962
C	-5.467015	-0.965992	-2.937962	C	-8.489015	-3.700992	-0.726962
H	-7.031015	-2.450992	-2.735962	C	-7.139015	-5.714992	-0.545962
H	-5.861015	-0.596992	-3.887962	C	-9.617015	-4.485992	-0.982962
C	3.877985	-1.422992	1.703038	H	-8.564015	-2.610992	-0.678962

C	4.703985	-1.030992	2.781038	C	-8.278015	-6.492992	-0.780962
C	4.411985	-2.285992	0.721038	H	-6.162015	-6.182992	-0.401962
C	6.036985	-1.479992	2.871038	C	-9.518015	-5.882992	-1.004962
C	5.771985	-2.695992	0.820038	H	-10.584015	-4.001992	-1.150962
C	3.890985	-2.886992	-0.502962	H	-8.190015	-7.582992	-0.803962
C	6.580985	-2.311992	1.892038	H	-10.405015	-6.493992	-1.195962
H	6.658985	-1.184992	3.717038	C	-0.114015	8.429008	-0.511962
C	4.956985	-3.635992	-1.074962	C	1.038985	9.202008	-0.726962
C	2.655985	-2.842992	-1.162962	C	-1.380015	9.040008	-0.545962
H	7.613985	-2.658992	1.973038	C	0.923985	10.572008	-0.982962
C	4.807985	-4.309992	-2.289962	H	2.019985	8.722008	-0.678962
C	2.498985	-3.525992	-2.375962	C	-1.484015	10.415008	-0.780962
H	1.800985	-2.306992	-0.753962	H	-2.274015	8.428008	-0.401962
C	3.569985	-4.251992	-2.937962	C	-0.336015	11.184008	-1.004962
H	5.637985	-4.863992	-2.735962	H	1.825985	11.167008	-1.150962
H	3.447985	-4.776992	-3.887962	H	-2.472015	10.884008	-0.803962
O	1.251985	-3.424992	-2.946962	H	-0.422015	12.258008	-1.195962

Table S3. $S_{1,min}$ Cartesian coordinates of **HAP-3MeOCz**.

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y(Å)	Z(Å)
C	-2.200178	-1.484903	2.585058	O	1.401446	2.457552	-2.934121
N	-2.478132	-0.154604	2.585175	O	-1.27229	-0.20361	-2.223074
C	-1.448198	0.664601	2.433419	C	-0.08635	-3.987952	-3.734343
N	-0.12225	0.118167	2.300197	H	0.356704	-3.734709	-4.717387
C	0.053013	-1.309795	2.269249	H	0.144948	-5.045869	-3.505036
N	-0.996669	-2.099546	2.422216	H	-1.178111	-3.861567	-3.791912
N	-1.598603	1.998498	2.36489	C	2.225212	2.55918	-4.087227
C	-0.502723	2.723388	2.121707	H	1.662255	2.899865	-4.978029
N	0.759741	2.287839	1.890488	H	3.072501	3.24852	-3.916804
C	0.957981	0.967407	1.966471	H	2.612081	1.54737	-4.274695
N	2.163602	0.442054	1.73985	C	-0.906649	0.066867	-3.586208
C	2.261013	-0.904549	1.83374	H	-0.507036	-0.849694	-4.047656
N	1.292986	-1.796518	2.060422	H	-1.770079	0.451989	-4.153864
C	-0.699202	4.211302	2.090885	H	-0.126966	0.83735	-3.51167
C	-1.176092	4.860501	3.25154	O	4.17213	-0.437213	3.712839
C	-0.430561	5.001981	0.954252	O	-1.365643	4.059699	4.349403
C	-1.401522	6.25203	3.270446	O	-3.579079	-2.763197	4.72556
C	-0.691435	6.401123	0.990325	C	-4.193269	-3.370571	5.862981
C	0.091313	4.719315	-0.382732	H	-4.129803	-4.471657	5.810061
C	-1.164981	7.035487	2.139416	H	-3.622572	-3.011355	6.72808
H	-1.759063	6.737591	4.179873	H	-5.247635	-3.060003	5.960255
C	0.122103	5.959892	-1.082999	C	5.124993	-0.039766	4.683587
C	0.534529	3.558907	-1.033787	H	5.93509	0.567649	4.238502
H	-1.333552	8.113812	2.166585	H	4.571767	0.572059	5.409391
C	0.552501	6.045317	-2.409484	H	5.571225	-0.908528	5.206951
C	0.980024	3.647379	-2.357481	C	-1.870006	4.661873	5.526208
H	0.583179	2.600649	-0.51577	H	-2.862969	5.121993	5.363088
C	0.983695	4.876587	-3.045902	H	-1.968507	3.847965	6.258372
H	0.550205	6.996967	-2.945658	H	-1.180206	5.429587	5.929817
H	1.323953	4.934403	-4.082521	N	-0.357453	6.974368	-0.247293
C	-3.387651	-2.387362	2.427268	N	-5.192189	-3.584268	-0.46358

C	-4.067925	-3.031882	3.49872	N	5.536012	-3.419148	-0.745377
C	-3.864831	-2.646645	1.149629	C	6.737038	-4.008908	-1.210393
C	-5.178066	-3.88688	3.263494	C	6.767184	-5.370086	-1.561547
C	-4.959302	-3.51938	0.913499	C	7.906938	-3.236665	-1.323085
C	-3.431775	-2.16308	-0.154078	C	7.952208	-5.944622	-2.031869
C	-5.636732	-4.140503	1.973399	H	5.860872	-5.970155	-1.447108
H	-5.689477	-4.360129	4.103015	C	9.092116	-3.826009	-1.773415
C	-4.279749	-2.777477	-1.122817	H	7.871462	-2.173909	-1.067283
C	-2.4329	-1.301331	-0.560493	C	9.119532	-5.178484	-2.134708
H	-6.493209	-4.796326	1.802462	H	7.964858	-7.004925	-2.303385
C	-4.104712	-2.557743	-2.504507	H	9.997447	-3.217619	-1.856874
C	-2.256895	-1.06398	-1.946949	H	10.046481	-5.633313	-2.493813
H	-1.771723	-0.797182	0.137753	C	-6.212348	-4.368576	-1.091112
C	-3.089551	-1.699495	-2.912791	C	-7.187772	-3.735562	-1.874344
H	-4.747151	-3.049133	-3.238866	C	-6.221324	-5.758575	-0.9136
H	-2.935869	-1.515057	-3.976678	C	-8.177656	-4.508283	-2.489827
C	3.648569	-1.452021	1.656107	H	-7.174687	-2.64755	-1.980106
C	4.618652	-1.163943	2.638797	C	-7.222117	-6.519382	-1.526075
C	4.038469	-2.230144	0.550337	H	-5.439489	-6.232029	-0.312603
C	5.943258	-1.629892	2.517032	C	-8.197022	-5.897894	-2.315298
C	5.387252	-2.669283	0.433338	H	-8.942514	-4.019566	-3.099356
C	3.338054	-2.737428	-0.628063	H	-7.231909	-7.60451	-1.392192
C	6.340325	-2.386343	1.412253	H	-8.975775	-6.497338	-2.79481
H	6.676967	-1.40845	3.293929	C	-0.479296	8.344164	-0.586917
C	4.295466	-3.462834	-1.393249	C	0.621529	9.043522	-1.112751
C	2.018897	-2.643548	-1.091202	C	-1.70188	9.013608	-0.400794
H	7.366896	-2.751971	1.330533	C	0.493039	10.393041	-1.45734
C	3.959432	-4.057749	-2.612161	H	1.576248	8.524873	-1.23063
C	1.678572	-3.253299	-2.305813	C	-1.814164	10.368067	-0.728443
H	1.248465	-2.130794	-0.515133	H	-2.559148	8.459317	-0.010432
C	2.640982	-3.949661	-3.06418	C	-0.721645	11.061435	-1.263001
H	4.70472	-4.590102	-3.207455	H	1.355373	10.928258	-1.86682
H	2.373363	-4.411759	-4.016377	H	-2.769489	10.880892	-0.578709
O	0.354727	-3.120189	-2.702944	H	-0.815862	12.119715	-1.52586

Table S4. $T_{1,min}$ Cartesian coordinates of **HAP-3MeOCz**.

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y(Å)	Z(Å)
C	-1.064244	-2.473544	1.461805	O	0.864933	3.014685	-3.190056
N	-1.827736	-1.341775	1.503081	O	-5.450062	0.006577	-0.951147
C	-1.208124	-0.176768	1.567221	C	2.807151	-2.925928	-4.495628
N	0.207059	-0.127793	1.618366	H	3.268063	-2.225139	-5.218572
C	0.938636	-1.346115	1.551201	H	3.377672	-3.874957	-4.507097
N	0.306105	-2.497421	1.464331	H	1.770319	-3.126274	-4.801532
N	-1.899008	0.983405	1.582524	C	1.372646	3.353104	-4.469256
C	-1.180023	2.109005	1.650394	H	0.567818	3.439224	-5.225029
N	0.162056	2.243892	1.675372	H	1.945787	4.299849	-4.44809
C	0.876591	1.107511	1.655812	H	2.045509	2.531288	-4.752094
N	2.21202	1.13394	1.674157	C	-6.539324	0.544485	-1.694432
C	2.83718	-0.064865	1.652165	H	-6.506293	0.220737	-2.750493
N	2.291679	-1.281346	1.574508	H	-7.51073	0.256976	-1.252658
C	-1.966775	3.383632	1.714992	H	-6.421697	1.634794	-1.642878

C	-2.736605	3.653307	2.865706	O	4.063092	0.924737	3.876736
C	-1.961458	4.333195	0.677119	O	-2.670044	2.707981	3.858871
C	-3.484906	4.842482	2.973934	O	-0.110226	-4.67556	2.814499
C	-2.749171	5.513064	0.792518	C	0.626459	-5.749681	3.395131
C	-1.29856	4.403694	-0.619851	H	1.074233	-6.388455	2.614946
C	-3.498717	5.781911	1.939278	H	1.422164	-5.270245	3.979095
H	-4.061445	5.048365	3.877428	H	-0.010831	-6.360202	4.059612
C	-1.71094	5.623653	-1.22555	C	4.601829	1.599055	5.001265
C	-0.428298	3.552003	-1.309122	H	5.148834	2.514154	4.706619
H	-4.074264	6.704956	2.039866	H	3.739182	1.878681	5.622044
C	-1.286358	5.978066	-2.508747	H	5.27654	0.948447	5.59079
C	0.011144	3.910951	-2.590409	C	-3.443343	2.924511	5.026413
H	-0.064275	2.622854	-0.870855	H	-4.523843	2.993709	4.797475
C	-0.420105	5.113696	-3.188258	H	-3.266679	2.04944	5.667466
H	-1.624725	6.902268	-2.983243	H	-3.130319	3.838804	5.566427
H	-0.084286	5.388015	-4.190197	N	-2.591078	6.293689	-0.362563
C	-1.750222	-3.754089	1.376987	N	-4.579412	-5.356958	-0.215739
C	-1.120997	-4.943987	1.967199	N	7.209271	-0.833176	-0.325416
C	-2.994634	-3.985966	0.730875	C	8.604088	-0.850582	-0.573868
C	-1.583378	-6.251552	1.747576	C	9.238041	-2.046702	-0.953417
C	-3.418785	-5.343235	0.52353	C	9.361827	0.326802	-0.445727
C	-4.010516	-3.152309	0.06458	C	10.612501	-2.058343	-1.210831
C	-2.737902	-6.482275	1.000814	H	8.646589	-2.962814	-1.03024
H	-1.067208	-7.095529	2.206774	C	10.739607	0.300416	-0.68356
C	-4.964684	-4.045709	-0.509422	H	8.859241	1.258672	-0.173828
C	-4.229152	-1.785389	-0.100745	C	11.369485	-0.888522	-1.071682
H	-3.121035	-7.488959	0.830355	H	11.096813	-2.993626	-1.506981
C	-6.063372	-3.624037	-1.256853	H	11.321155	1.221303	-0.580043
C	-5.347144	-1.3447	-0.851156	H	12.445799	-0.903215	-1.265215
H	-3.570373	-1.050005	0.361608	C	-5.279013	-6.529218	-0.641975
C	-6.257656	-2.249907	-1.433822	C	-6.596197	-6.742333	-0.210865
H	-6.753738	-4.346142	-1.69951	C	-4.645493	-7.446182	-1.492923
H	-7.10858	-1.89964	-2.01926	C	-7.281651	-7.884091	-0.638484
C	4.332314	-0.006449	1.729568	H	-7.066076	-6.020551	0.462211
C	4.929467	0.545779	2.883376	C	-5.337688	-8.589111	-1.90647
C	5.172735	-0.471226	0.698817	H	-3.623905	-7.251495	-1.829141
C	6.330088	0.647174	2.9985	C	-6.654269	-8.808402	-1.48294
C	6.58382	-0.327206	0.823274	H	-8.307979	-8.054627	-0.302275
C	4.936392	-1.09391	-0.600374	H	-4.846775	-9.306067	-2.570106
C	7.169077	0.215114	1.968886	H	-7.192773	-9.701281	-1.812079
H	6.777742	1.063071	3.902751	C	-3.206477	7.544956	-0.610989
C	6.213647	-1.297008	-1.195935	C	-2.428977	8.649064	-1.002905
C	3.785495	-1.472594	-1.301925	C	-4.59773	7.691495	-0.469139
H	8.253941	0.294111	2.070021	C	-3.041303	9.8798	-1.258997
C	6.343594	-1.83618	-2.478361	H	-1.345283	8.534995	-1.088987
C	3.913006	-2.025958	-2.582812	C	-5.198175	8.932087	-0.705757
H	2.790135	-1.366415	-0.871475	H	-5.200019	6.824133	-0.186533
C	5.183178	-2.200781	-3.170271	C	-4.42534	10.028818	-1.10655
H	7.324388	-1.963334	-2.942728	H	-2.427691	10.732655	-1.564048
H	5.280618	-2.622978	-4.172364	H	-6.28118	9.036605	-0.590566
O	2.727961	-2.370495	-3.195053	H	-4.899402	10.995456	-1.298798

Table S5. FC Cartesian coordinates of **HAP-3MeOTPA**.

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y(Å)	Z(Å)
C	6.312985	9.094029	-1.413779	C	2.361985	-4.396971	0.205221
C	5.899985	9.574029	-0.155779	C	9.530985	-5.640971	1.778221
C	4.671985	9.190029	0.374221	C	3.843985	-11.449971	-3.101779
C	3.815985	8.332029	-0.344779	C	11.901985	-5.845971	1.677221
C	4.225985	7.871029	-1.604779	C	-11.838015	2.396029	-3.101779
C	5.469985	8.234029	-2.135779	C	-11.014015	-7.383971	1.677221
N	2.544985	7.964029	0.195221	C	-0.888015	13.231029	1.677221
C	2.117985	6.627029	0.193221	C	7.993985	9.054029	-3.101779
C	0.738985	6.307029	0.176221	H	6.568985	10.239029	0.394221
C	1.104985	8.863029	1.986221	H	4.359985	9.557029	1.356221
C	1.714985	9.001029	0.722221	H	3.565985	7.212029	-2.174779
C	1.517985	10.189029	0.004221	H	5.759985	7.851029	-3.115779
C	3.054985	5.566029	0.209221	H	-0.000015	7.111029	0.150221
C	2.626985	4.244029	0.205221	H	1.258985	7.946029	2.560221
C	0.319985	4.981029	0.178221	H	1.990985	10.306029	-0.974779
C	0.307985	9.881029	2.501221	H	4.122985	5.793029	0.236221
C	0.119985	11.074029	1.778221	H	3.351985	3.426029	0.228221
C	0.735985	11.227029	0.526221	H	-0.744015	4.736029	0.155221
C	1.253985	3.925029	0.191221	H	-0.170015	9.782029	3.479221
C	0.805985	2.524029	0.189221	H	0.607985	12.140029	-0.057779
N	-0.529015	2.312029	0.192221	H	-3.729015	-3.011971	0.155221
C	-0.949015	1.044029	0.189221	H	-6.158015	-3.555971	0.150221
N	-0.000015	0.000029	0.189221	H	-7.079015	0.674029	0.236221
C	1.377985	0.300029	0.189221	H	-4.643015	1.190029	0.228221
N	1.770985	1.577029	0.185221	H	-10.457015	-1.002971	1.356221
N	-2.251015	0.745029	0.185221	H	-9.920015	-3.428971	-0.974779
C	-2.588015	-0.563971	0.189221	H	-7.510015	-2.881971	2.560221
N	-1.738015	-1.613971	0.192221	H	-8.028015	-0.517971	-2.174779
C	-0.429015	-1.343971	0.189221	H	-9.679015	1.063029	-3.115779
N	0.479985	-2.321971	0.185221	H	-12.152015	0.570029	0.394221
C	1.781985	-1.959971	0.189221	H	-10.818015	-5.543971	-0.057779
N	2.265985	-0.697971	0.192221	H	-8.386015	-5.038971	3.479221
C	-4.026015	-0.876971	0.191221	H	5.582985	-10.808971	0.394221
C	-4.474015	-2.212971	0.178221	H	6.096985	-8.554971	1.356221
C	-5.831015	-2.513971	0.176221	H	4.461985	-6.693971	-2.174779
C	-6.798015	-1.479971	0.193221	H	3.918985	-8.913971	-3.115779
C	-6.348015	-0.136971	0.209221	H	6.251985	-5.062971	2.560221
C	-4.989015	0.153029	0.205221	H	6.157985	-3.555971	0.150221
N	-8.170015	-1.777971	0.195221	H	2.954985	-6.467971	0.236221
C	-9.124015	-0.860971	-0.344779	H	7.929985	-6.876971	-0.974779
C	-10.295015	-0.548971	0.374221	H	10.209985	-6.596971	-0.057779
C	-9.583015	-3.779971	0.004221	H	8.556985	-4.742971	3.479221
C	-8.652015	-3.015971	0.722221	H	4.472985	-1.722971	0.155221
C	-8.229015	-3.474971	1.986221	H	1.290985	-4.615971	0.228221
C	-8.929015	-0.275971	-1.604779	H	3.733985	-12.532971	-3.250779
C	-9.866015	0.620029	-2.135779	H	4.458985	-11.029971	-3.919779
C	-11.241015	0.322029	-0.155779	H	2.844985	-10.975971	-3.119779
C	-10.091015	-4.975971	0.526221	H	12.753985	-5.586971	2.321221
C	-9.650015	-5.432971	1.778221	H	12.003985	-5.322971	0.708221
C	-8.711015	-4.673971	2.501221	H	11.897985	-6.937971	1.499221

C	-11.032015	0.920029	-1.413779	H	-11.782015	1.654029	-3.919779
C	4.718985	-10.013971	-1.413779	H	-12.721015	3.033029	-3.250779
C	5.340985	-9.895971	-0.155779	H	-10.928015	3.024029	-3.119779
C	5.622985	-8.640971	0.374221	H	-11.216015	-8.251971	2.321221
C	5.307985	-7.470971	-0.344779	H	-10.612015	-7.734971	0.708221
C	4.703985	-7.594971	-1.604779	H	-11.958015	-6.834971	1.499221
C	4.395985	-8.853971	-2.135779	H	-1.393015	13.057029	0.708221
N	5.624985	-6.185971	0.195221	H	-1.538015	13.839029	2.321221
C	6.937985	-5.984971	0.722221	H	0.058985	13.773029	1.499221
C	7.122985	-5.388971	1.986221	H	8.986985	9.501029	-3.250779
C	5.092985	-3.792971	0.176221	H	7.322985	9.376029	-3.919779
C	4.679985	-5.146971	0.193221	H	8.082985	7.952029	-3.119779
C	3.292985	-5.428971	0.209221	O	4.475985	-11.292971	-1.836779
C	8.063985	-6.408971	0.004221	O	10.740985	-5.424971	2.381221
C	9.354985	-6.250971	0.526221	O	7.541985	9.523029	-1.836779
C	8.402985	-5.207971	2.501221	O	-0.672015	12.014029	2.381221
C	4.153985	-2.767971	0.178221	O	-10.069015	-6.588971	2.381221
C	2.772985	-3.048971	0.191221	O	-12.018015	1.770029	-1.836779

Table S6. $S_{1,min}$ Cartesian coordinates of **HAP-3MeOTPA**.

Atom	**X (Å)**	**Y (Å)**	**Z (Å)**	**Atom**	**X (Å)**	**Y(Å)**	**Z(Å)**
C	6.312985	9.094029	-1.413779	C	2.361985	-4.396971	0.205221
C	5.899985	9.574029	-0.155779	C	9.530985	-5.640971	1.778221
C	4.671985	9.190029	0.374221	C	3.843985	-11.449971	-3.101779
C	3.815985	8.332029	-0.344779	C	11.901985	-5.845971	1.677221
C	4.225985	7.871029	-1.604779	C	-11.838015	2.396029	-3.101779
C	5.469985	8.234029	-2.135779	C	-11.014015	-7.383971	1.677221
N	2.544985	7.964029	0.195221	C	-0.888015	13.231029	1.677221
C	2.117985	6.627029	0.193221	C	7.993985	9.054029	-3.101779
C	0.738985	6.307029	0.176221	H	6.568985	10.239029	0.394221
C	1.104985	8.863029	1.986221	H	4.359985	9.557029	1.356221
C	1.714985	9.001029	0.722221	H	3.565985	7.212029	-2.174779
C	1.517985	10.189029	0.004221	H	5.759985	7.851029	-3.115779
C	3.054985	5.566029	0.209221	H	-0.000015	7.111029	0.150221
C	2.626985	4.244029	0.205221	H	1.258985	7.946029	2.560221
C	0.319985	4.981029	0.178221	H	1.990985	10.306029	-0.974779
C	0.307985	9.881029	2.501221	H	4.122985	5.793029	0.236221
C	0.119985	11.074029	1.778221	H	3.351985	3.426029	0.228221
C	0.735985	11.227029	0.526221	H	-0.744015	4.736029	0.155221
C	1.253985	3.925029	0.191221	H	-0.170015	9.782029	3.479221
C	0.805985	2.524029	0.189221	H	0.607985	12.140029	-0.057779
N	-0.529015	2.312029	0.192221	H	-3.729015	-3.011971	0.155221
C	-0.949015	1.044029	0.189221	H	-6.158015	-3.555971	0.150221
N	-0.000015	0.000029	0.189221	H	-7.079015	0.674029	0.236221
C	1.377985	0.300029	0.189221	H	-4.643015	1.190029	0.228221
N	1.770985	1.577029	0.185221	H	-10.457015	-1.002971	1.356221
N	-2.251015	0.745029	0.185221	H	-9.920015	-3.428971	-0.974779
C	-2.588015	-0.563971	0.189221	H	-7.510015	-2.881971	2.560221
N	-1.738015	-1.613971	0.192221	H	-8.028015	-0.517971	-2.174779
C	-0.429015	-1.343971	0.189221	H	-9.679015	1.063029	-3.115779
N	0.479985	-2.321971	0.185221	H	-12.152015	0.570029	0.394221

C	1.781985	-1.959971	0.189221	H	-10.818015	-5.543971	-0.057779
N	2.265985	-0.697971	0.192221	H	-8.386015	-5.038971	3.479221
C	-4.026015	-0.876971	0.191221	H	5.582985	-10.808971	0.394221
C	-4.474015	-2.212971	0.178221	H	6.096985	-8.554971	1.356221
C	-5.831015	-2.513971	0.176221	H	4.461985	-6.693971	-2.174779
C	-6.798015	-1.479971	0.193221	H	3.918985	-8.913971	-3.115779
C	-6.348015	-0.136971	0.209221	H	6.251985	-5.062971	2.560221
C	-4.989015	0.153029	0.205221	H	6.157985	-3.555971	0.150221
N	-8.170015	-1.777971	0.195221	H	2.954985	-6.467971	0.236221
C	-9.124015	-0.860971	-0.344779	H	7.929985	-6.876971	-0.974779
C	-10.295015	-0.548971	0.374221	H	10.209985	-6.596971	-0.057779
C	-9.583015	-3.779971	0.004221	H	8.556985	-4.742971	3.479221
C	-8.652015	-3.015971	0.722221	H	4.472985	-1.722971	0.155221
C	-8.229015	-3.474971	1.986221	H	1.290985	-4.615971	0.228221
C	-8.929015	-0.275971	-1.604779	H	3.733985	-12.532971	-3.250779
C	-9.866015	0.620029	-2.135779	H	4.458985	-11.029971	-3.919779
C	-11.241015	0.322029	-0.155779	H	2.844985	-10.975971	-3.119779
C	-10.091015	-4.975971	0.526221	H	12.753985	-5.586971	2.321221
C	-9.650015	-5.432971	1.778221	H	12.003985	-5.322971	0.708221
C	-8.711015	-4.673971	2.501221	H	11.897985	-6.937971	1.499221
C	-11.032015	0.920029	-1.413779	H	-11.782015	1.654029	-3.919779
C	4.718985	-10.013971	-1.413779	H	-12.721015	3.033029	-3.250779
C	5.340985	-9.895971	-0.155779	H	-10.928015	3.024029	-3.119779
C	5.622985	-8.640971	0.374221	H	-11.216015	-8.251971	2.321221
C	5.307985	-7.470971	-0.344779	H	-10.612015	-7.734971	0.708221
C	4.703985	-7.594971	-1.604779	H	-11.958015	-6.834971	1.499221
C	4.395985	-8.853971	-2.135779	H	-1.393015	13.057029	0.708221
N	5.624985	-6.185971	0.195221	H	-1.538015	13.839029	2.321221
C	6.937985	-5.984971	0.722221	H	0.058985	13.773029	1.499221
C	7.122985	-5.388971	1.986221	H	8.986985	9.501029	-3.250779
C	5.092985	-3.792971	0.176221	H	7.322985	9.376029	-3.919779
C	4.679985	-5.146971	0.193221	H	8.082985	7.952029	-3.119779
C	3.292985	-5.428971	0.209221	O	4.475985	-11.292971	-1.836779
C	8.063985	-6.408971	0.004221	O	10.740985	-5.424971	2.381221
C	9.354985	-6.250971	0.526221	O	7.541985	9.523029	-1.836779
C	8.402985	-5.207971	2.501221	O	-0.672015	12.014029	2.381221
C	4.153985	-2.767971	0.178221	O	-10.069015	-6.588971	2.381221
C	2.772985	-3.048971	0.191221	O	-12.018015	1.770029	-1.836779

Table S7. $T_{1,min}$ Cartesian coordinates of **HAP-3MeOTPA**.

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y(Å)	Z(Å)
C	-2.7376	-10.639802	1.800025	C	4.917924	1.174953	-0.201472
C	-3.328736	-10.741855	0.527246	C	10.45155	-2.859803	-2.630063
C	-3.806284	-9.606741	-0.121236	C	10.658788	3.927935	4.335487
C	-3.727042	-8.339729	0.492489	C	12.225818	-4.384574	-3.100606
C	-3.150085	-8.248171	1.768697	C	-9.389499	7.224646	3.443375
C	-2.644599	-9.382348	2.416937	C	-1.943192	13.068381	-2.138094
N	-4.237205	-7.184366	-0.167693	C	-10.311416	-8.134438	-2.146665
C	-3.508428	-5.973357	-0.168004	C	-1.687116	-11.745702	3.629556
C	-4.175646	-4.728818	-0.167597	H	-3.388594	-11.726753	0.05675
C	-5.714553	-6.719525	-2.085214	H	-4.253275	-9.692591	-1.115259

C	-5.512675	-7.263378	-0.799589	H	-3.08638	-7.27299	2.25884
C	-6.588266	-7.90339	-0.165708	H	-2.196411	-9.270676	3.406423
C	-2.095551	-5.982566	-0.172218	H	-5.268182	-4.704527	-0.154144
C	-1.380992	-4.78782	-0.170253	H	-4.884216	-6.222072	-2.593396
C	-3.452257	-3.538439	-0.176004	H	-6.445094	-8.329222	0.831087
C	-6.958206	-6.803214	-2.703782	H	-1.564941	-6.937989	-0.184195
C	-8.029776	-7.455423	-2.065745	H	-0.288227	-4.791474	-0.180295
C	-7.83636	-8.013317	-0.792438	H	-3.96583	-2.573964	-0.169866
C	-2.045183	-3.546739	-0.174263	H	-7.121862	-6.380149	-3.698283
C	-1.280043	-2.277242	-0.177294	H	-8.648786	-8.522948	-0.270251
N	-2.01364	-1.139004	-0.189735	H	-0.178301	4.797762	-0.171186
C	-1.339762	0.015696	-0.192501	H	-1.405638	6.972449	-0.167982
N	0.065996	-0.000628	-0.188079	H	-5.157788	4.824248	-0.273433
C	0.76894	-1.237676	-0.174118	H	-3.904593	2.664694	-0.25278
N	0.057504	-2.381821	-0.16639	H	-6.242156	8.50114	-1.223452
N	-1.98664	1.185673	-0.198882	H	-4.041341	9.76187	0.77998
C	-1.226766	2.306689	-0.203461	H	-2.855479	7.389994	-2.621678
N	0.11283	2.380273	-0.202766	H	-4.760741	6.311542	2.184172
C	0.797497	1.219876	-0.194779	H	-6.966636	6.490451	3.280764
N	2.117953	1.196735	-0.194374	H	-8.468223	8.720279	-0.102632
C	2.72637	-0.031499	-0.181714	H	-3.123887	11.790319	-0.292074
N	2.089655	-1.245264	-0.168024	H	-1.890183	9.431034	-3.69585
C	-1.962456	3.593416	-0.210364	H	11.942553	2.732735	0.788187
C	-1.270631	4.818779	-0.196177	H	10.757057	1.126021	-0.71239
C	-1.958078	6.029824	-0.195305	H	7.627402	0.707457	2.245795
C	-3.370322	6.052819	-0.220989	H	8.791716	2.309619	3.724644
C	-4.065367	4.823374	-0.241999	H	7.675342	-0.858843	-2.61059
C	-3.369573	3.61721	-0.230961	H	6.812016	-2.253127	-0.129418
N	-4.073233	7.278927	-0.226291	H	6.860158	2.096534	-0.235728
C	-5.34677	7.388622	0.405238	H	10.686604	-1.397861	0.448342
C	-6.404652	8.067961	-0.232881	H	11.879037	-3.012789	-0.986953
C	-3.572525	9.685265	-0.204771	H	8.877189	-2.505627	-4.063035
C	-3.511835	8.435888	-0.840482	H	4.311945	-2.213564	-0.137697
C	-2.904618	8.355416	-2.111119	H	4.359695	2.112669	-0.234787
C	-5.573225	6.837821	1.676028	H	11.385773	4.647205	4.73461
C	-6.8255	6.939091	2.295291	H	10.563723	3.076402	5.03253
C	-7.644294	8.194631	0.387025	H	9.677804	4.421541	4.219079
C	-3.052997	10.8343	-0.81503	H	12.504261	-5.033905	-3.940868
C	-2.43783	10.739379	-2.072923	H	12.073808	-4.999998	-2.195978
C	-2.364286	9.488022	-2.71257	H	13.033109	-3.652774	-2.918368
C	-7.868774	7.625669	1.654285	H	-8.741039	7.658688	4.227678
C	10.455794	2.622161	2.349227	H	-10.438668	7.460469	3.670049
C	11.003063	2.267412	1.095361	H	-9.256436	6.126502	3.433708
C	10.344577	1.371093	0.269176	H	-1.458571	13.764881	-2.836565
C	9.115078	0.796137	0.675934	H	-1.398296	13.079998	-1.17526
C	8.569918	1.157048	1.926173	H	-2.986423	13.393545	-1.964496
C	9.232059	2.058827	2.758251	H	-10.593427	-7.637057	-1.199579
N	8.416683	-0.094499	-0.165229	H	-11.144952	-8.056453	-2.858615
C	9.111297	-1.005467	-0.989967	H	-10.103843	-9.202222	-1.944233
C	8.593177	-1.339148	-2.264795	H	-1.395533	-12.774645	3.882752
C	6.268057	-1.304729	-0.169245	H	-2.394251	-11.369357	4.39268
C	6.999973	-0.080196	-0.177613	H	-0.787112	-11.102286	3.625387
C	6.295015	1.160756	-0.193026	O	11.183234	3.510859	3.073571

C	10.300602	-1.622039	-0.549053	O	11.016931	-3.737542	-3.498529
C	10.969152	-2.539016	-1.359322	O	-2.288783	-11.816486	2.344143
C	9.257532	-2.249254	-3.071666	O	-9.206705	-7.492665	-2.768685
C	4.890914	-1.288362	-0.165223	O	-1.88667	11.791683	-2.759019
C	4.167382	-0.048164	-0.182422	O	-9.128463	7.796795	2.168767

Table S8. FC Cartesian coordinates of **HAP-3Cz**.

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y(Å)	Z(Å)
C	-2.291	1.322009	0	H	1.791	-7.770991	2.165
N	-1.164	2.064009	-0.003	C	1.097	-11.547991	1.286
C	0	1.409009	0	C	-1.968	-11.201991	-2.321
N	0	0.000009	0	H	-2.887	-9.597991	-3.452
C	-1.22	-0.703991	0	H	-0.895	-12.598991	-1.057
N	-2.369	-0.023991	0.003	C	1.968	-11.201991	2.321
N	1.164	2.064009	0.003	H	2.887	-9.597991	3.452
C	2.291	1.322009	0	H	0.895	-12.598991	1.057
N	2.369	-0.023991	-0.003	H	-2.459	-11.985991	-2.904
C	1.22	-0.703991	0	H	2.459	-11.985991	2.904
N	1.205	-2.039991	0.003	C	-8.318	3.935009	0.857
C	0	-2.644991	0	C	-7.567	5.236009	-0.857
N	-1.205	-2.039991	-0.003	C	-8.439	3.016009	1.908
C	-3.572	2.062009	0	C	-9.358	4.852009	0.547
C	-3.58	3.469009	0.012	C	-6.831	5.801009	-1.908
C	-4.795	1.366009	-0.012	C	-8.88	5.678009	-0.547
C	-4.786	4.168009	0.02	C	-9.636	3.009009	2.628
H	-2.626	4.000009	0.033	H	-7.625	2.334009	2.165
C	-6.002	2.060009	-0.02	C	-10.55	4.824009	1.286
H	-4.777	0.274009	-0.033	C	-7.424	6.840009	-2.628
C	-6.006	3.468009	0	H	-5.834	5.437009	-2.165
H	-4.793	5.260009	0.063	C	-9.452	6.724009	-1.286
H	-6.952	1.521009	-0.063	C	-10.685	3.897009	2.321
C	0	-4.123991	0	H	-9.755	2.299009	3.452
C	-1.214	-4.834991	0.012	H	-11.358	5.524009	1.057
C	1.214	-4.834991	-0.012	C	-8.717	7.305009	-2.321
C	-1.217	-6.227991	0.02	H	-6.868	7.299009	-3.452
H	-2.151	-4.273991	0.033	H	-10.463	7.074009	-1.057
C	1.217	-6.227991	-0.02	H	-11.609	3.863009	2.904
H	2.151	-4.273991	-0.033	H	-9.15	8.122009	-2.904
C	0	-6.934991	0	C	8.318	3.935009	-0.857
H	-2.158	-6.780991	0.063	C	7.567	5.236009	0.857
H	2.158	-6.780991	-0.063	C	8.439	3.016009	-1.908
C	3.572	2.062009	0	C	9.358	4.852009	-0.547
C	3.58	3.469009	-0.012	C	6.831	5.801009	1.908
C	4.795	1.366009	0.012	C	8.88	5.678009	0.547
C	4.786	4.168009	-0.02	C	9.636	3.009009	-2.628
H	2.626	4.000009	-0.033	H	7.625	2.334009	-2.165
C	6.002	2.060009	0.02	C	10.55	4.824009	-1.286
H	4.777	0.274009	0.033	C	7.424	6.840009	2.628
C	6.006	3.468009	0	H	5.834	5.437009	2.165
H	4.793	5.260009	-0.063	C	9.452	6.724009	1.286
H	6.952	1.521009	0.063	C	10.685	3.897009	-2.321

C	-0.751	-9.170991	-0.857	H	9.755	2.299009	-3.452
C	0.751	-9.170991	0.857	H	11.358	5.524009	-1.057
C	-1.608	-8.815991	-1.908	C	8.717	7.305009	2.321
C	-0.477	-10.529991	-0.547	H	6.868	7.299009	3.452
C	1.608	-8.815991	1.908	H	10.463	7.074009	1.057
C	0.477	-10.529991	0.547	H	11.609	3.863009	-2.904
C	-2.212	-9.848991	-2.628	H	9.15	8.122009	2.904
H	-1.791	-7.770991	-2.165	N	0	-8.349991	0
C	-1.097	-11.547991	-1.286	N	-7.231	4.175009	0
C	2.212	-9.848991	2.628	N	7.231	4.175009	0

Table S9. $S_{1,min}$ Cartesian coordinates of **HAP-3Cz**.

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y(Å)	Z(Å)
C	-2.309943	1.324679	0.499246	H	1.783431	-7.967678	2.195235
N	-1.162259	2.042252	0.614247	C	1.113304	-11.64193	0.940229
C	-0.003447	1.400041	0.492247	C	-1.905445	-10.944106	-2.656772
N	0.000031	-0.000036	0.196245	H	-2.815696	-9.237361	-3.63377
C	-1.21001	-0.703165	0.492243	H	-0.847442	-12.458637	-1.523774
N	-2.349726	-0.029262	0.614244	C	1.968893	-11.39749	2.01523
N	1.149901	2.048883	0.614249	H	2.868913	-9.910582	3.310233
C	2.302226	1.338511	0.499249	H	0.9187	-12.664884	0.605227
N	2.349538	-0.014742	0.614247	H	-2.388297	-11.666682	-3.320774
C	1.214737	-0.696217	0.492245	H	2.45487	-12.233464	2.524229
N	1.199706	-2.020708	0.614243	C	-8.380199	3.955871	0.742245
C	0.00802	-2.662321	0.499241	C	-7.496995	5.150784	-0.982753
N	-1.187187	-2.02762	0.614241	C	-8.582753	3.100336	1.834244
C	-3.577354	2.051639	0.376246	C	-9.392603	4.845823	0.296246
C	-3.5913	3.460107	0.320248	C	-6.678604	5.654868	-2.003751
C	-4.797938	1.351803	0.293244	C	-8.830165	5.605486	-0.805753
C	-4.79393	4.15062	0.192248	C	-9.833265	3.131154	2.457243
H	-2.646041	4.002348	0.399249	H	-7.792171	2.439181	2.195243
C	-6.00022	2.039173	0.149244	C	-10.639293	4.856383	0.940245
H	-4.78545	0.259725	0.331242	C	-7.210955	6.646077	-2.83075
C	-6.007324	3.446167	0.101246	H	-5.663775	5.279938	-2.157751
H	-4.80523	5.243465	0.182249	C	-9.340649	6.603239	-1.649752
H	-6.94199	1.494134	0.054242	C	-10.854705	3.993386	2.015243
C	0.011582	-4.12379	0.376239	H	-10.017273	2.471093	3.310242
C	-1.201194	-4.839628	0.320237	H	-11.427621	5.53751	0.605245
C	1.229073	-4.8308	0.293239	C	-8.525179	7.122272	-2.65675
C	-1.197914	-6.226365	0.192235	H	-6.591632	7.056961	-3.633749
H	-2.14309	-4.292181	0.399237	H	-10.365898	6.963024	-1.523752
C	1.233752	-6.215791	0.149237	H	-11.821894	3.990842	2.524242
H	2.167291	-4.273745	0.331241	H	-8.909795	7.901652	-3.32075
C	0.019305	-6.925132	0.101235	C	8.210078	3.917132	-0.982743
H	-2.138298	-6.783976	0.182234	C	7.615483	5.279749	0.742259
H	2.176489	-6.759328	0.054237	C	8.236655	2.957047	-2.003744
C	3.565864	2.072043	0.376251	C	9.26981	4.843895	-0.805741
C	3.568957	3.478889	0.293253	C	6.976268	5.883772	1.834259
C	4.791609	1.379623	0.320251	C	8.892745	5.710639	0.29626
C	4.766561	4.176511	0.149255	C	9.361376	2.921594	-2.830744
H	2.617273	4.014122	0.331253	H	7.404336	2.26468	-2.157746

C	5.991936	2.075637	0.192253	C	10.388924	4.787145	-1.64974
H	4.788245	0.289935	0.399249	C	7.628313	6.95045	2.457261
C	5.988322	3.479835	0.101255	H	6.007851	5.528591	2.195258
H	4.764616	5.265297	0.054257	C	9.52608	6.785436	0.940262
H	6.94341	1.539426	0.182253	C	10.430723	3.821738	-2.656741
C	-0.712989	-9.068019	-0.982769	H	9.407429	2.180309	-3.633745
C	0.764807	-9.23573	0.742232	H	11.213436	5.495513	-1.523738
C	-1.557744	-8.611036	-2.003769	C	8.8859	7.403987	2.015263
C	-0.439761	-10.450461	-0.80577	H	7.148446	7.439367	3.310261
C	1.606784	-8.983245	1.834233	H	10.509012	7.127264	0.605263
C	0.49974	-10.557547	0.29623	H	11.298192	3.764937	-3.320741
C	-2.150322	-9.567765	-2.83077	H	9.367322	8.243482	2.524264
H	-1.740673	-7.545693	-2.157767	N	0.023823	-8.334639	-0.039767
C	-1.048178	-11.390484	-1.649772	N	-7.230198	4.147175	-0.039754
C	2.20525	-10.080744	2.457232	N	7.206679	4.188334	-0.039743

Table S10. $T_{1,min}$ Cartesian coordinates of **HAP-3Cz**.

Atom	**X (Å)**	**Y (Å)**	**Z (Å)**	**Atom**	**X (Å)**	**Y(Å)**	**Z(Å)**
C	0.807186	2.538187	0.408537	H	-7.386012	-3.418547	2.195443
N	1.757273	1.569094	0.503816	C	-11.139833	-3.542173	1.003803
C	1.371714	0.300048	0.403279	C	-11.154761	-0.455398	-2.603091
N	0	0	0.158643	H	-9.693988	0.790275	-3.608925
C	-0.945706	1.037915	0.403279	H	-12.392812	-1.80587	-1.444625
N	-0.528652	2.296358	0.503015	C	-10.702224	-4.323412	2.074248
N	2.253031	-0.690353	0.503015	H	-9.037504	-4.88512	3.343303
C	1.794542	-1.968137	0.408537	H	-12.186637	-3.568276	0.686833
N	0.480239	-2.30639	0.503816	H	-11.973679	-0.138702	-3.254597
C	-0.426008	-1.337963	0.403279	H	-11.408488	-4.973567	2.597573
N	-1.724379	-1.606005	0.503015	C	2.099339	9.023929	0.765654
C	-2.601728	-0.57005	0.408537	C	3.46334	8.440668	-0.962143
N	-2.237512	0.737296	0.503816	C	1.213831	9.024391	1.852455
C	1.251967	3.9332	0.309301	C	2.758616	10.20832	0.342259
C	2.626115	4.245007	0.268647	C	4.133494	7.763388	-1.990456
C	0.310972	4.98029	0.237128	C	3.62592	9.837047	-0.76128
C	3.04882	5.568143	0.165805	C	0.976587	10.242377	2.49385
H	3.354929	3.434469	0.339045	H	0.732458	8.105748	2.195443
C	0.731371	6.302747	0.117592	C	2.502304	11.418465	1.003803
H	-0.753749	4.737636	0.262463	C	4.995175	8.506118	-2.801007
C	2.10444	6.607758	0.084654	H	3.982633	6.695103	-2.161541
H	4.114443	5.810027	0.166958	C	4.497688	10.559423	-1.589533
H	0	7.109888	0.029948	C	1.606928	11.430104	2.074248
C	-4.032234	-0.882365	0.309301	H	0.288114	10.269269	3.343303
C	-4.989341	0.151779	0.268647	H	3.0031	12.338075	0.686833
C	-4.468544	-2.220836	0.237128	C	5.182994	9.888005	-2.603091
C	-6.346563	-0.143716	0.165805	H	5.531392	8.000103	-3.608925
H	-4.651802	1.18822	0.339045	H	4.632476	11.635425	-1.444625
C	-5.824025	-2.517987	0.117592	H	1.397009	12.366824	2.597573
H	-3.726039	-3.021584	0.262463	H	5.86672	10.438861	-3.254597
C	-6.774706	-1.48138	0.084654	C	5.578163	-7.219674	-0.962143
H	-7.088853	0.658199	0.166958	C	6.765282	-6.330045	0.765654
H	-6.157344	-3.554944	0.029948	C	4.656545	-7.461405	-1.990456

C	2.780268	-3.050835	0.309301	C	6.706173	-8.058663	-0.76128
C	4.157572	-2.759455	0.237128	C	7.208436	-5.563404	1.852455
C	2.363226	-4.396786	0.268647	C	7.461357	-7.493192	0.342259
C	5.092654	-3.78476	0.117592	C	4.868927	-8.579007	-2.801007
H	4.479787	-1.716052	0.262463	H	3.806813	-6.796613	-2.161541
C	3.297743	-5.424427	0.165805	C	6.895885	-9.174824	-1.589533
H	1.296873	-4.622689	0.339045	C	8.381865	-5.966938	2.49385
C	4.670266	-5.126378	0.084654	H	6.653555	-4.687201	2.195443
H	6.157344	-3.554944	0.029948	C	8.637529	-7.876292	1.003803
H	2.974409	-6.468226	0.166958	C	5.971767	-9.432607	-2.603091
C	-9.041503	-1.220994	-0.962143	H	4.162596	-8.790378	-3.608925
C	-8.864621	-2.693884	0.765654	H	7.760335	-9.829555	-1.444625
C	-8.790039	-0.301983	-1.990456	C	9.095296	-7.106692	2.074248
C	-10.332093	-1.778385	-0.76128	H	8.74939	-5.384148	3.343303
C	-8.422268	-3.460987	1.852455	H	9.183536	-8.769799	0.686833
C	-10.219973	-2.715129	0.342259	H	6.106959	-10.300159	-3.254597
C	-9.864102	0.072889	-2.801007	H	10.011479	-7.393257	2.597573
H	-7.789446	0.10151	-2.161541	N	-8.153897	-1.782821	-0.031288
C	-11.393573	-1.3846	-1.589533	N	2.53298	7.952893	-0.031288
C	-9.358452	-4.275439	2.49385	N	5.620917	-6.170072	-0.031288

Table S11. FC Cartesian coordinates of **HAP-3HMAT**.

Atom	**X (Å)**	**Y (Å)**	**Z (Å)**	**Atom**	**X (Å)**	**Y(Å)**	**Z(Å)**
C	0	4.121966	0.40672	H	-9.333	-0.157034	-0.88528
C	-1.205	4.839966	0.43272	H	-7.884	-2.690034	2.28072
C	-1.225	6.233966	0.40172	H	-7.062	-1.188034	2.78972
C	0	6.941966	0.27272	H	-8.776	-1.143034	2.26272
C	1.225	6.233966	0.40172	H	-6.511	0.607966	1.14172
C	1.205	4.839966	0.43272	H	-6.914	0.450966	-0.59228
N	0	8.340966	0.00972	H	-8.2	0.661966	0.63572
C	1.228	8.927966	-0.45128	H	-9.379	-5.415034	1.30172
C	2.45	8.224966	-0.31628	H	-11.072	-5.356034	0.73672
C	2.506	7.023966	0.61572	H	-10.175	-6.910034	0.73672
C	-2.507	7.023966	0.61572	H	-10.762	-7.231034	-1.66928
C	-2.45	8.224966	-0.31728	H	-11.643	-5.705034	-1.66928
C	-1.228	8.927966	-0.45128	H	-10.383	-5.995034	-2.90628
C	-1.226	10.208966	-1.05428	H	-6.271	-5.483034	2.28072
C	0	11.095966	-0.89228	H	-5.378	-7.029034	2.26272
C	1.226	10.208966	-1.05428	H	-4.56	-5.522034	2.78972
C	2.393	10.667966	-1.68028	H	-3.526	-7.432034	0.63472
C	3.595	8.718966	-0.95528	H	-3.066	-6.213034	-0.59228
C	-3.595	8.718966	-0.95628	H	-2.729	-5.943034	1.14172
C	-3.566	9.914966	-1.67228	C	6.804	-8.046034	-1.67128
C	-2.393	10.667966	-1.68028	C	5.754	-7.473034	-0.95528
C	0	11.647966	0.56372	C	5.898	-6.234034	-0.31628
C	0	12.298966	-1.84828	C	7.118	-5.527034	-0.45128
C	-2.503	7.553966	2.07972	C	8.228	-6.166034	-1.05428
C	-3.771	6.172966	0.42772	C	8.043	-7.406034	-1.68028
C	2.502	7.553966	2.07972	N	7.223	-4.170034	0.00972
C	3.771	6.172966	0.42772	C	8.346	-3.400034	-0.45128
C	3.566	9.914966	-1.67128	C	9.454	-4.043034	-1.05428

H	-2.133	4.268966	0.48472	C	9.61	-5.548034	-0.89228
H	2.133	4.268966	0.48472	C	4.83	-5.683034	0.61572
H	2.386	11.638966	-2.17928	C	4.786	-4.178034	0.40172
H	4.53	8.160966	-0.88528	C	6.012	-3.471034	0.27272
H	-4.53	8.160966	-0.88528	C	6.011	-2.056034	0.40172
H	-4.464	10.280966	-2.17828	C	7.336	-1.341034	0.61572
H	-2.386	11.638966	-2.17928	C	8.348	-1.990034	-0.31728
H	0	10.829966	1.30172	C	9.348	-1.246034	-0.95628
H	0.897	12.266966	0.73672	C	10.435	-3.262034	-1.68028
H	-0.897	12.266966	0.73672	C	3.589	-3.464034	0.43272
H	0.881	12.935966	-1.66928	C	3.57	-2.061034	0.40672
H	0	11.988966	-2.90628	C	4.794	-1.376034	0.43272
H	-0.881	12.935966	-1.66928	C	7.794	-1.610034	2.07972
H	-1.613	8.172966	2.28072	C	7.232	0.179966	0.42772
H	-3.398	8.171966	2.26272	C	5.291	-5.944034	2.07972
H	-2.502	6.709966	2.78972	C	3.46	-6.352034	0.42772
H	-3.782	5.334966	1.14172	C	10.088	-5.824034	0.56372
H	-4.673	6.769966	0.63472	C	10.651	-6.150034	-1.84828
H	-3.848	5.761966	-0.59228	C	10.37	-1.869034	-1.67228
H	1.613	8.172966	2.28072	H	4.802	-8.004034	-0.88528
H	2.502	6.709966	2.78972	H	8.887	-7.886034	-2.17928
H	3.398	8.171966	2.26272	H	9.332	-0.157034	-0.88528
H	3.782	5.333966	1.14172	H	11.273	-3.753034	-2.17928
H	3.848	5.762966	-0.59228	H	2.631	-3.982034	0.48472
H	4.673	6.769966	0.63572	H	4.764	-0.287034	0.48472
H	4.464	10.280966	-2.17828	H	7.884	-2.690034	2.28072
C	-6.804	-8.046034	-1.67228	H	8.776	-1.143034	2.26272
C	-8.043	-7.406034	-1.68028	H	7.062	-1.188034	2.78972
C	-8.228	-6.166034	-1.05428	H	8.2	0.661966	0.63472
C	-7.118	-5.527034	-0.45128	H	6.914	0.450966	-0.59228
C	-5.898	-6.234034	-0.31728	H	6.511	0.607966	1.14172
C	-5.754	-7.473034	-0.95628	H	6.272	-5.483034	2.28072
N	-7.223	-4.170034	0.00972	H	4.56	-5.522034	2.78972
C	-6.012	-3.471034	0.27272	H	5.378	-7.029034	2.26272
C	-4.786	-4.178034	0.40172	H	3.526	-7.432034	0.63572
C	-4.83	-5.683034	0.61572	H	2.729	-5.943034	1.14172
C	-9.61	-5.548034	-0.89228	H	3.067	-6.213034	-0.59228
C	-9.454	-4.043034	-1.05428	H	9.379	-5.415034	1.30172
C	-8.346	-3.400034	-0.45128	H	10.175	-6.910034	0.73672
C	-8.348	-1.990034	-0.31628	H	11.072	-5.356034	0.73672
C	-7.336	-1.341034	0.61572	H	10.762	-7.231034	-1.66928
C	-6.011	-2.056034	0.40172	H	10.383	-5.995034	-2.90628
C	-4.794	-1.376034	0.43272	H	11.643	-5.705034	-1.66928
C	-3.589	-3.464034	0.43272	H	11.136	-1.275034	-2.17828
C	-10.435	-3.262034	-1.68028	H	-6.672	-9.006034	-2.17828
C	-10.37	-1.869034	-1.67128	H	6.672	-9.006034	-2.17828
C	-9.349	-1.246034	-0.95528	C	0	2.648966	0.41072
C	-7.794	-1.610034	2.07972	C	1.222	0.704966	0.41072
C	-7.231	0.179966	0.42772	C	-1.222	0.704966	0.41072
C	-10.088	-5.824034	0.56372	C	0	-1.411034	0.41072
C	-10.651	-6.150034	-1.84828	C	2.294	-1.325034	0.41072
C	-5.291	-5.945034	2.07972	C	-2.294	-1.325034	0.41072
C	-3.46	-6.352034	0.42772	N	0	-0.000034	0.40872

C	-3.57	-2.061034	0.40672	N	1.207	2.041966	0.41272
H	-8.887	-7.886034	-2.17928	N	-1.207	2.041966	0.41272
H	-4.802	-8.004034	-0.88528	N	1.165	-2.066034	0.41272
H	-4.764	-0.287034	0.48472	N	2.372	0.024966	0.41272
H	-2.631	-3.982034	0.48472	N	-1.164	-2.066034	0.41272
H	-11.273	-3.753034	-2.17928	N	-2.372	0.024966	0.41272
H	-11.136	-1.275034	-2.17828				

Table S12. $S_{1,min}$ Cartesian coordinates of **HAP-3HMAT**.

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y(Å)	Z(Å)
C	-0.000624	4.12069	0.81605	H	-9.196102	-0.077291	-0.889937
C	-1.206481	4.840558	0.765051	H	-8.03537	-2.786744	2.251063
C	-1.225069	6.221994	0.583051	H	-7.267044	-1.318609	2.916061
C	-0.000582	6.913105	0.383049	H	-8.927074	-1.24043	2.238063
C	1.223638	6.22345	0.588048	H	-6.577395	0.568209	1.43006
C	1.205146	4.840256	0.770048	H	-6.819407	0.509454	-0.33994
N	-0.00075	8.278614	-0.026951	H	-8.212638	0.651447	0.774062
C	1.228204	8.811845	-0.546953	H	-9.428482	-5.447463	0.991065
C	2.449926	8.126521	-0.334954	H	-11.063023	-5.353431	0.278067
C	2.503352	7.032985	0.721046	H	-10.164591	-6.907409	0.274067
C	-2.506566	7.030994	0.711052	H	-10.530761	-7.093169	-2.188933
C	-2.448487	8.125341	-0.345948	H	-11.411342	-5.568144	-2.184932
C	-1.226333	8.81049	-0.55195	H	-10.043713	-5.791853	-3.315934
C	-1.223533	10.020717	-1.28895	H	-6.425573	-5.574309	2.244061
C	0.001994	10.920212	-1.218952	H	-5.530404	-7.118626	2.224061
C	1.227905	10.02144	-1.282953	H	-4.767806	-5.644559	2.906059
C	2.395532	10.410796	-1.952955	H	-3.537874	-7.439102	0.754058
C	3.595838	8.54953	-1.020956	H	-2.968143	-6.157059	-0.356943
C	-3.592271	8.547396	-1.036947	H	-2.792571	-5.983089	1.414057
C	-3.562172	9.660238	-1.876947	C	6.583973	-7.922303	-1.860955
C	-2.389012	10.408328	-1.962949	C	5.606954	-7.389076	-1.020953
C	-0.001765	11.623356	0.170048	C	5.813075	-6.185118	-0.334954
C	0.003139	12.015204	-2.296952	C	7.017245	-5.468783	-0.546956
C	-2.5038	7.714814	2.110052	C	8.064378	-6.073551	-1.282957
C	-3.771799	6.16632	0.614054	C	7.818079	-7.2799	-1.952956
C	2.494458	7.717008	2.120046	N	7.169286	-4.139018	-0.026956
C	3.770679	6.168486	0.630045	C	8.243277	-3.343069	-0.551958
C	3.569001	9.663017	-1.860956	C	9.289677	-3.950568	-1.288959
H	-2.138405	4.284681	0.883053	C	9.456624	-5.461162	-1.218959
H	2.136355	4.286382	0.890047	C	4.838914	-5.684872	0.721047
H	2.390578	11.322191	-2.552955	C	4.777509	-4.171134	0.588047
H	4.531112	8.002619	-0.889957	C	5.987143	-3.456267	0.383045
H	-4.527325	7.998949	-0.908945	C	6.001575	-2.050017	0.583044
H	-4.459048	9.968408	-2.420946	C	7.342601	-1.344803	0.711042
H	-2.381939	11.320886	-2.562949	C	8.260707	-1.942017	-0.345959
H	-0.00284	10.888565	0.991048	C	9.197704	-1.162732	-1.03696
H	0.895493	12.257363	0.278047	C	10.208425	-3.135633	-1.962961
H	-0.899177	12.256746	0.274049	C	3.58944	-3.464096	0.770048
H	0.88321	12.667004	-2.184954	C	3.569025	-2.059472	0.816047
H	0.005787	11.594237	-3.315952	C	4.794777	-1.374558	0.765046
H	-0.877845	12.666147	-2.188951	C	7.933375	-1.68866	2.110042

H	-1.614736	8.351021	2.244051	C	7.226563	0.183604	0.614042
H	-3.400345	8.348703	2.224053	C	5.435353	-6.018536	2.120046
H	-2.504514	6.951372	2.906053	C	3.457419	-6.349934	0.630049
H	-3.785937	5.410143	1.414055	C	10.067885	-5.81052	0.17004
H	-4.673611	6.78332	0.754055	C	10.40369	-6.010508	-2.29696
H	-3.848525	5.648789	-0.356945	C	10.147629	-1.74506	-1.876961
H	1.604109	8.352161	2.251047	H	4.664906	-7.925395	-0.889952
H	2.492012	6.952566	2.916046	H	8.610584	-7.73137	-2.552957
H	3.389484	8.350881	2.238045	H	9.191452	-0.078933	-0.90896
H	3.780728	5.412404	1.430045	H	10.995264	-3.597297	-2.562962
H	3.850733	5.651324	-0.339955	H	2.643396	-3.993485	0.890049
H	4.670234	6.786501	0.774043	H	4.779596	-0.29129	0.883045
H	4.467662	9.972303	-2.401957	H	8.039871	-2.778142	2.244042
C	-6.584678	-7.914746	-1.876938	H	8.930177	-1.229275	2.22404
C	-7.819001	-7.273629	-1.962936	H	7.27225	-1.306876	2.906043
C	-8.066229	-6.070216	-1.288936	H	8.211408	0.655717	0.754041
C	-7.017027	-5.467488	-0.551938	H	6.815719	0.507704	-0.356957
C	-5.812302	-6.183391	-0.345939	H	6.577933	0.573747	1.414043
C	-5.606884	-7.384364	-1.036939	H	6.431189	-5.565481	2.251045
N	-7.169117	-4.138796	-0.026938	H	4.774963	-5.634021	2.916047
C	-5.987507	-3.457404	0.38306	H	5.537518	-7.110516	2.238047
C	-4.775718	-4.171543	0.583059	H	3.541461	-7.438513	0.774049
C	-4.836113	-5.686257	0.711059	H	2.796592	-5.980677	1.43005
C	-9.457837	-5.458618	-1.218935	H	2.968592	-6.160845	-0.33995
C	-9.292369	-3.947956	-1.282935	H	9.431245	-5.441167	0.991041
C	-8.244665	-3.342629	-0.546937	H	10.167451	-6.903998	0.278041
C	-8.263082	-1.94147	-0.334937	H	11.064555	-5.348903	0.274039
C	-7.342344	-1.348178	0.721061	H	10.528043	-7.098928	-2.18496
C	-6.000359	-2.051882	0.58806	H	10.037832	-5.802453	-3.31596
C	-4.794664	-1.376225	0.770058	H	11.408517	-5.573046	-2.188961
C	-3.588007	-3.4647	0.765057	H	10.862352	-1.122812	-2.420962
C	-10.213699	-3.130964	-1.952935	H	-6.403394	-8.845665	-2.420938
C	-10.152196	-1.740282	-1.860935	H	6.401593	-8.85515	-2.401954
C	-9.202377	-1.161388	-1.020936	C	-0.000107	2.666497	0.955051
C	-7.930383	-1.69767	2.120062	C	1.213137	0.70072	0.95205
C	-7.227677	0.180517	0.630061	C	-1.212749	0.699725	0.952053
C	-10.0657	-5.813769	0.170066	C	0.000402	-1.400011	0.952052
C	-10.406918	-6.004764	-2.296933	C	2.309433	-1.332498	0.955049
C	-5.429647	-6.026219	2.11006	C	-2.309402	-1.334065	0.955055
C	-3.453976	-6.34949	0.614058	N	-0.000026	-0.000022	0.648051
C	-3.568478	-2.061283	0.816057	N	1.193539	2.023855	1.079049
H	-8.612549	-7.723159	-2.562935	N	-1.194768	2.023753	1.079052
H	-4.663712	-7.92095	-0.90894	N	1.156601	-2.045777	1.079051
H	-4.779828	-0.292963	0.890058	N	2.35024	0.022009	1.079048
H	-2.641269	-3.993457	0.883056	N	-1.155548	-2.045827	1.079054
H	-11.001252	-3.590889	-2.552933	N	-2.350216	0.021857	1.079054
H	-10.869843	-1.116355	-2.401934				

Table S13. $T_{1,min}$ Cartesian coordinates of **HAP-3HMAT**.

Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y(Å)	Z(Å)
C	-0.38981	-2.047727	3.570893	H	0.738686	8.237868	4.571114
C	-0.437921	-1.375305	4.799204	H	-2.293415	8.179092	1.611931
C	-0.407674	-2.065058	6.012392	H	-2.792957	6.720666	2.513774
C	-0.26404	-3.476865	6.004238	H	-2.268713	8.19118	3.398834
C	-0.359203	-4.173508	4.772049	H	-1.139466	5.342553	3.784966
C	-0.390935	-3.448697	3.579101	H	0.58709	5.78603	3.86719
N	-0.018145	-4.18662	7.220437	H	-0.660692	6.778416	4.68556
C	0.466626	-5.533259	7.110864	H	-1.197453	10.983785	0
C	0.372422	-6.229901	5.880806	H	-0.532231	12.37764	0.897186
C	-0.54453	-5.683352	4.796611	H	-0.532231	12.37764	-0.897186
C	-0.645876	-1.361876	7.340324	H	1.917169	12.884445	-0.877249
C	0.273655	-2.011936	8.363399	H	1.917169	12.884445	0.877249
C	0.417228	-3.421518	8.35341	H	3.085021	11.85091	0
C	1.000842	-4.066901	9.471462	H	-2.293415	8.179092	-1.611931
C	0.842908	-5.573777	9.611293	H	-2.268713	8.19118	-3.398834
C	1.050314	-6.176778	8.229737	H	-2.792957	6.720666	-2.513774
C	1.700442	-7.404867	8.047618	H	-0.660692	6.778416	-4.68556
C	1.035086	-7.456502	5.740483	H	0.58709	5.78603	-3.86719
C	0.889901	-1.271578	9.380967	H	-1.139466	5.342553	-3.784966
C	1.589907	-1.896521	10.412508	C	1.589907	-1.896521	-10.412508
C	1.604075	-3.289673	10.46945	C	0.889901	-1.271578	-9.380967
C	-0.624578	-5.863003	10.044464	C	0.273655	-2.011936	-8.363399
C	1.771897	-6.178196	10.67541	C	0.417228	-3.421518	-8.35341
C	-2.115264	-1.640795	7.773303	C	1.000842	-4.066901	-9.471462
C	-0.464381	0.16098	7.250013	C	1.604075	-3.289673	-10.46945
C	-2.013546	-5.978512	5.22008	N	-0.018145	-4.18662	-7.220437
C	-0.31107	-6.335694	3.425385	C	0.466626	-5.533259	-7.110864
C	1.733688	-8.030681	6.802029	C	1.050314	-6.176778	-8.229737
H	-0.505556	-0.286931	4.774336	C	0.842908	-5.573777	-9.611293
H	-0.422111	-3.957056	2.614652	C	-0.645876	-1.361876	-7.340324
H	2.184439	-7.886462	8.899514	C	-0.407674	-2.065058	-6.012392
H	0.997191	-7.977438	4.78188	C	-0.26404	-3.476865	-6.004238
H	0.813795	-0.182553	9.37031	C	-0.359203	-4.173508	-4.772049
H	2.078187	-1.303896	11.191356	C	-0.54453	-5.683352	-4.796611
H	2.088524	-3.784027	11.313744	C	0.372422	-6.229901	-5.880806
H	-1.343863	-5.452385	9.317834	C	1.035086	-7.456502	-5.740483
H	-0.792279	-6.951123	10.116969	C	1.700442	-7.404867	-8.047618
H	-0.828654	-5.404747	11.027227	C	-0.437921	-1.375305	-4.799204
H	1.597121	-7.26141	10.770939	C	-0.38981	-2.047727	-3.570893
H	2.836277	-6.014287	10.439248	C	-0.390935	-3.448697	-3.579101
H	1.561426	-5.742831	11.664991	C	-2.013546	-5.978512	-5.22008
H	-2.310749	-2.722329	7.853425	C	-0.31107	-6.335694	-3.425385
H	-2.31674	-1.181225	8.756066	C	-2.115264	-1.640795	-7.773303
H	-2.814992	-1.218819	7.032075	C	-0.464381	0.16098	-7.250013
H	-1.168245	0.59044	6.52053	C	-0.624578	-5.863003	-10.044464
H	-0.689013	0.635459	8.218577	C	1.771897	-6.178196	-10.67541
H	0.559171	0.438965	6.9497	C	1.733688	-8.030681	-6.802029
H	-2.245766	-5.531533	6.200283	H	0.813795	-0.182553	-9.37031
H	-2.713014	-5.560371	4.476504	H	2.088524	-3.784027	-11.313744
H	-2.177905	-7.067295	5.290902	H	0.997191	-7.977438	-4.78188

H	-1.014228	-5.931876	2.680858	H	2.184439	-7.886462	-8.899514
H	0.715013	-6.171854	3.057582	H	-0.505556	-0.286931	-4.774336
H	-0.498506	-7.420064	3.475832	H	-0.422111	-3.957056	-2.614652
H	2.258199	-8.981551	6.672084	H	-2.245766	-5.531533	-6.200283
C	1.57316	9.971518	-3.613474	H	-2.177905	-7.067295	-5.290902
C	1.654983	10.699103	-2.426167	H	-2.713014	-5.560371	-4.476504
C	1.102804	10.216467	-1.234702	H	-0.498506	-7.420064	-3.475832
C	0.495792	8.9316	-1.232387	H	0.715013	-6.171854	-3.057582
C	0.294856	8.246286	-2.462777	H	-1.014228	-5.931876	-2.680858
C	0.857732	8.775139	-3.62946	H	-2.310749	-2.722329	-7.853425
N	0.116591	8.312073	0	H	-2.814992	-1.218819	-7.032075
C	-0.276681	6.957681	0	H	-2.31674	-1.181225	-8.756066
C	-0.424146	6.236368	-1.241542	H	-0.689013	0.635459	-8.218577
C	-0.620219	7.033917	-2.514733	H	-1.168245	0.59044	-6.52053
C	1.01387	11.097952	0	H	0.559171	0.438965	-6.9497
C	1.102804	10.216467	1.234702	H	-1.343863	-5.452385	-9.317834
C	0.495792	8.9316	1.232387	H	-0.828654	-5.404747	-11.027227
C	0.294856	8.246286	2.462777	H	-0.792279	-6.951123	-10.116969
C	-0.620219	7.033917	2.514733	H	1.561426	-5.742831	-11.664991
C	-0.424146	6.236368	1.241542	H	2.836277	-6.014287	-10.439248
C	-0.489617	4.861649	1.2239	H	1.597121	-7.26141	-10.770939
C	-0.489617	4.861649	-1.2239	H	2.258199	-8.981551	-6.672084
C	1.654983	10.699103	2.426167	H	2.03269	10.353955	-4.528823
C	1.57316	9.971518	3.613474	H	2.078187	-1.303896	-11.191356
C	0.857732	8.775139	3.62946	C	-0.398117	-1.297512	2.293186
C	-2.089343	7.568779	2.506486	C	-0.39076	-1.38278	0
C	-0.435423	6.18753	3.784214	C	-0.419737	0.739544	1.231049
C	-0.404857	11.749248	0	C	-0.419737	0.739544	-1.231049
C	2.051792	12.233982	0	C	-0.398117	-1.297512	-2.293186
C	-2.089343	7.568779	-2.506486	C	-0.432822	2.679851	0
C	-0.435423	6.18753	-3.784214	N	-0.40486	0.02384	0
C	-0.447764	4.123036	0	N	-0.385147	-2.043021	1.162543
H	2.156795	11.667452	-2.432554	N	-0.417942	0.04241	2.382125
H	0.738686	8.237868	-4.571114	N	-0.417942	0.04241	-2.382125
H	-0.576672	4.279417	2.141085	N	-0.385147	-2.043021	-1.162543
H	-0.576672	4.279417	-2.141085	N	-0.433702	2.06202	-1.222434
H	2.156795	11.667452	2.432554	N	-0.433702	2.06202	1.222434
H	2.03269	10.353955	4.528823				

C. Electronic and vertical excitation energies

Table S14. Electronic energy (EE) and first 25 singlet and 25 triplet vertical excitation energies of **HAP-3MeOCz** at the FC geometry.

State	Symmetry	Energy	State	Symmetry	Energy
EE	-	-3539.4477088 hartrees			
T_1	E	2.2060 eV	S_8	A	3.2727 eV
T_2	E	2.2060 eV	S_9	E	3.2844 eV
T_3	A	2.2088 eV	S_{10}	E	3.2844 eV
S_1	E	2.4276 eV	S_{11}	E	3.4030 eV
S_2	E	2.4276 eV	S_{12}	E	3.4030 eV
T_4	A	2.4947 eV	S_{13}	A	3.4238 eV
S_3	A	2.5004 eV	T_{19}	A	3.4442 eV
S_4	A	2.6846 eV	T_{20}	E	3.4478 eV
T_5	E	2.9207 eV	T_{21}	E	3.4478 eV
T_6	E	2.9207 eV	S_{14}	A	3.4699 eV
T_7	A	2.9250 eV	S_{15}	E	3.4702 eV
T_8	A	3.0005 eV	S_{16}	E	3.4702 eV
T_9	E	3.0162 eV	T_{22}	A	3.5036 eV
T_{10}	E	3.0162 eV	T_{23}	E	3.5042 eV
T_{11}	A	3.0636 eV	T_{24}	E	3.5042 eV
S_5	A	3.1230 eV	S_{17}	E	3.5286 eV
T_{12}	E	3.1301 eV	S_{18}	E	3.5286 eV
T_{13}	E	3.1301 eV	S_{19}	A	3.5908 eV
T_{14}	A	3.2026 eV	T_{25}	A	3.5961 eV
S_6	E	3.2095 eV	S_{20}	E	3.8158 eV
S_7	E	3.2095 eV	S_{21}	E	3.8158 eV
T_{15}	E	3.2225 eV	S_{22}	A	3.8312 eV
T_{16}	E	3.2225 eV	S_{23}	E	3.9720 eV
T_{17}	E	3.2460 eV	S_{24}	E	3.9720 eV
T_{18}	E	3.2460 eV	S_{25}	A	3.9828 eV

Table S15. Electronic energy (EE) and first 25 singlet and 25 triplet vertical excitation energies of **HAP-3MeOCz** at the $S_{1,min}$ geometry.

State	Symmetry	Energy	State	Symmetry	Energy
EE	-	-3539.4363511 hartrees			
T_1	A	1.8313 eV	S_{11}	A	3.1893 eV
S_1	A	1.8406 eV	T_{16}	A	3.2087 eV
T_2	A	2.1982 eV	S_{12}	A	3.2226 eV
T_3	A	2.2162 eV	T_{17}	A	3.2298 eV
S_2	A	2.3351 eV	T_{18}	A	3.2589 eV
S_3	A	2.3989 eV	S_{13}	A	3.2818 eV
T_4	A	2.4257 eV	T_{19}	A	3.3115 eV
S_4	A	2.6204 eV	T_{20}	A	3.3378 eV
T_5	A	2.6498 eV	T_{21}	A	3.3467 eV
T_6	A	2.7518 eV	S_{14}	A	3.3782 eV
S_5	A	2.7619 eV	S_{15}	A	3.4031 eV
T_7	A	2.8513 eV	T_{22}	A	3.4236 eV
T_8	A	2.8930 eV	T_{23}	A	3.4312 eV

T_9	A	2.9574 eV	S_{16}	A	3.4521 eV
T_{10}	A	2.9807 eV	T_{24}	A	3.4601 eV
T_{11}	A	3.0110 eV	S_{17}	A	3.4628 eV
T_{12}	A	3.0168 eV	S_{18}	A	3.4752 eV
S_6	A	3.0186 eV	T_{25}	A	3.4807 eV
S_7	A	3.0335 eV	S_{19}	A	3.5076 eV
T_{13}	A	3.0595 eV	S_{20}	A	3.5528 eV
S_8	A	3.0883 eV	S_{21}	A	3.7368 eV
T_{14}	A	3.0915 eV	S_{22}	A	3.7643 eV
T_{15}	A	3.1108 eV	S_{23}	A	3.8221 eV
S_9	A	3.1308 eV	S_{24}	A	3.8408 eV
S_{10}	A	3.1489 eV	S_{25}	A	3.9895 eV

Table S16. Electronic energy (EE) and first 25 singlet and 25 triplet vertical excitation energies of **HAP-3MeOCz** at the $T_{1,min}$ geometry.

State	Symmetry	Energy	State	Symmetry	Energy
EE	-	-3539.4383488 hartrees			
T_1	A	1.6476 eV	T_{17}	A	3.2877 eV
S_1	A	2.1999 eV	S_{10}	A	3.2969 eV
T_2	A	2.3024 eV	S_{11}	A	3.3185 eV
T_3	A	2.3359 eV	T_{18}	A	3.3194 eV
T_4	A	2.4541 eV	S_{12}	A	3.3247 eV
S_2	A	2.4637 eV	S_{13}	A	3.3470 eV
S_3	A	2.4930 eV	T_{19}	A	3.4080 eV
T_5	A	2.6329 eV	S_{14}	A	3.4302 eV
S_4	A	2.6412 eV	T_{20}	A	3.4317 eV
T_6	A	2.8179 eV	T_{21}	A	3.4425 eV
T_7	A	2.8507 eV	T_{22}	A	3.4463 eV
T_8	A	2.8640 eV	T_{23}	A	3.4775 eV
T_9	A	2.8837 eV	T_{24}	A	3.4936 eV
S_5	A	2.9467 eV	S_{15}	A	3.5068 eV
T_{10}	A	3.0108 eV	T_{25}	A	3.5100 eV
T_{11}	A	3.0726 eV	S_{16}	A	3.5436 eV
S_6	A	3.0878 eV	S_{17}	A	3.5660 eV
T_{12}	A	3.1070 eV	S_{18}	A	3.5890 eV
T_{13}	A	3.1397 eV	S_{19}	A	3.6251 eV
T_{14}	A	3.1778 eV	S_{20}	A	3.7522 eV
S_7	A	3.1797 eV	S_{21}	A	3.7807 eV
T_{15}	A	3.1832 eV	S_{22}	A	3.8261 eV
S_8	A	3.2399 eV	S_{23}	A	3.8677 eV
T_{16}	A	3.2417 eV	S_{24}	A	3.9006 eV
S_9	A	3.2576 eV	S_{25}	A	3.9776 eV

Table S17. Electronic energy (EE) and first 25 singlet and 25 triplet vertical excitation energies of **HAP-3MeOTPA** at the FC geometry.

State	Symmetry	Energy	State	Symmetry	Energy
EE	-	-3542.9865401 hartrees			
T_1	E	2.3443 eV	T_{19}	A	3.6070 eV

T_2	E	2.3443 eV	T_{20}	E	3.6071 eV
T_3	A	2.3790 eV	T_{21}	E	3.6071 eV
T_4	A	2.6299 eV	T_{22}	A	3.6555 eV
S_1	E	2.7758 eV	T_{23}	E	3.6606 eV
S_2	E	2.7758 eV	T_{24}	E	3.6606 eV
S_3	A	2.7903 eV	S_8	A	3.6654 eV
T_5	A	3.0989 eV	S_9	A	3.6654 eV
S_4	A	3.1688 eV	S_{10}	A	3.7013 eV
T_6	E	3.2210 eV	T_{25}	A	3.7217 eV
T_7	E	3.2210 eV	S_{11}	E	3.7267 eV
S_5	A	3.2238 eV	S_{12}	E	3.7267 eV
T_8	E	3.2428 eV	S_{13}	A	3.7411 eV
T_9	E	3.2428 eV	S_{14}	A	3.8435 eV
T_{10}	A	3.2509 eV	S_{15}	E	3.8968 eV
T_{11}	E	3.2562 eV	S_{16}	E	3.8968 eV
T_{12}	E	3.2562 eV	S_{17}	E	4.1032 eV
S_6	E	3.3337 eV	S_{18}	E	4.1032 eV
S_7	E	3.3337 eV	S_{19}	A	4.1449 eV
T_{13}	A	3.4005 eV	S_{20}	E	4.1461 eV
T_{14}	E	3.4007 eV	S_{21}	E	4.1461 eV
T_{15}	E	3.4007 eV	S_{22}	E	4.1852 eV
T_{16}	A	3.4415 eV	S_{23}	E	4.1852 eV
T_{17}	E	3.4690 eV	S_{24}	A	4.1914 eV
T_{18}	E	3.4690 eV	S_{25}	A	4.2421 eV

Table S18. Electronic energy (EE) and first 25 singlet and 25 triplet vertical excitation energies of **HAP-3MeOTPA** at the $S_{1,min}$ geometry.

State	Symmetry	Energy	State	Symmetry	Energy
EE	-	-3542.9667997 hartrees			
T_1	A	1.8056 eV	S_{10}	A	3.3246 eV
S_1	A	1.8508 eV	T_{17}	A	3.3256 eV
T_2	A	2.2182 eV	S_{11}	A	3.3444 eV
T_3	A	2.2413 eV	T_{18}	A	3.3540 eV
T_4	A	2.4580 eV	T_{19}	A	3.3558 eV
S_2	A	2.5285 eV	T_{20}	A	3.3602 eV
S_3	A	2.6685 eV	T_{21}	A	3.3895 eV
S_4	A	2.7051 eV	T_{22}	A	3.4238 eV
T_5	A	2.9400 eV	S_{12}	A	3.4887 eV
T_6	A	2.9682 eV	T_{23}	A	3.5264 eV
T_7	A	3.0086 eV	T_{24}	A	3.5458 eV
T_8	A	3.0218 eV	T_{25}	A	3.5837 eV
T_9	A	3.0549 eV	S_{13}	A	3.6160 eV
S_5	A	3.0643 eV	S_{14}	A	3.6213 eV
T_{10}	A	3.0811 eV	S_{15}	A	3.6981 eV
S_6	A	3.1514 eV	S_{16}	A	3.7571 eV
T_{11}	A	3.1564 eV	S_{17}	A	3.7637 eV
T_{12}	A	3.1818 eV	S_{18}	A	3.8850 eV
T_{13}	A	3.1934 eV	S_{19}	A	3.9727 eV
T_{14}	A	3.2147 eV	S_{20}	A	3.9929 eV
T_{15}	A	3.2276 eV	S_{21}	A	4.0239 eV
S_7	A	3.2354 eV	S_{22}	A	4.0529 eV

S_8	A	3.2607 eV	S_{23}	A	4.0601 eV
T_{16}	A	3.2643 eV	S_{24}	A	4.0842 eV
S_9	A	3.3068 eV	S_{25}	A	4.1305 eV

Table S19. Electronic energy (EE) and first 25 singlet and 25 triplet vertical excitation energies of **HAP-3MeOTPA** at the $T_{1,min}$ geometry.

State	Symmetry	Energy	State	Symmetry	Energy
EE	-	-3542.9794545 hartrees			
T_1	A	1.9632 eV	S_8	A	3.4241 eV
T_2	A	2.3202 eV	T_{19}	A	3.4478 eV
T_3	A	2.3416 eV	T_{20}	A	3.4893 eV
S_1	A	2.4581 eV	S_9	A	3.5192 eV
T_4	A	2.5601 eV	S_{10}	A	3.5585 eV
S_2	A	2.6782 eV	T_{21}	A	3.5803 eV
S_3	A	2.7310 eV	T_{22}	A	3.5823 eV
S_4	A	2.9594 eV	S_{11}	A	3.5849 eV
T_5	A	3.0455 eV	T_{23}	A	3.6054 eV
T_6	A	3.1076 eV	T_{24}	A	3.6111 eV
T_7	A	3.1436 eV	T_{25}	A	3.6215 eV
S_5	A	3.1501 eV	S_{12}	A	3.6755 eV
T_8	A	3.1640 eV	S_{13}	A	3.6866 eV
T_9	A	3.2013 eV	S_{14}	A	3.7890 eV
T_{10}	A	3.2108 eV	S_{15}	A	3.8136 eV
T_{11}	A	3.2172 eV	S_{16}	A	3.8434 eV
T_{12}	A	3.2255 eV	S_{17}	A	3.9948 eV
T_{13}	A	3.2345 eV	S_{18}	A	4.0342 eV
S_6	A	3.2474 eV	S_{19}	A	4.0779 eV
T_{14}	A	3.2773 eV	S_{20}	A	4.1194 eV
T_{15}	A	3.2866 eV	S_{21}	A	4.1235 eV
S_7	A	3.3189 eV	S_{22}	A	4.1425 eV
T_{16}	A	3.3561 eV	S_{23}	A	4.1622 eV
T_{17}	A	3.3563 eV	S_{24}	A	4.1679 eV
T_{18}	A	3.3604 eV	S_{25}	A	4.1727 eV

Table S20. Electronic energy (EE) and first 25 singlet and 25 triplet vertical excitation energies of **HAP-3Cz** at the FC geometry.

State	Symmetry	Energy	State	Symmetry	Energy
EE	-	-2853.0088576 hartrees			
T_1	A_2	2.5870 eV	T_{19}	A_2	3.6905 eV
T_2	E	2.6845 eV	T_{20}	E	3.6990 eV
T_3	E	2.6845 eV	T_{21}	E	3.6990 eV
T_4	A_1	2.7040 eV	S_8	E	3.7125 eV
S_1	A_2	2.7646 eV	S_9	A_2	3.7125 eV
S_2	E	2.9808 eV	S_{10}	E	3.7125 eV
S_3	E	2.9808 eV	T_{22}	E	3.7207 eV
T_5	A_1	3.0878 eV	T_{23}	E	3.7207 eV
S_4	A_1	3.1444 eV	T_{24}	A_2	3.7224 eV
T_6	E	3.2028 eV	T_{25}	E	3.8238 eV

T_7	E	3.2028 eV	S_{11}	E	3.9538 eV
S_5	E	3.2427 eV	S_{12}	E	3.9538 eV
T_8	E	3.2538 eV	S_{13}	-	3.9816 e
T_9	E	3.2538 eV	S_{14}	-	4.0951 e
S_6	E	3.3274 eV	S_{15}	E	4.1117 eV
S_7	E	3.3274 eV	S_{16}	E	4.1117 eV
T_{10}	E	3.4244 eV	S_{17}	E	4.1214 eV
T_{11}	E	3.4244 eV	S_{18}	E	4.1214 eV
T_{12}	E	3.4244 e	S_{19}	-	4.1225 e
T_{13}	E	3.4485 e	S_{20}	E	4.1616 eV
T_{14}	E	3.4485 eV	S_{21}	E	4.1616 eV
T_{15}	E	3.4485 eV	S_{22}	A_2	4.2429 eV
T_{16}	E	3.6881 eV	S_{23}	E	4.2579 eV
T_{17}	E	3.6899 eV	S_{24}	E	4.2579 eV
T_{18}	E	3.6899 eV	S_{25}	E	4.2994 eV

Table S21. Electronic energy (EE) and first 25 singlet and 25 triplet vertical excitation energies of **HAP-3Cz** at the $S_{1,min}$ geometry.

State	Symmetry	Energy	State	Symmetry	Energy
EE	-	-2852.9914767 hartrees			
T_1	A	2.0263 eV	S_8	E	3.5417 eV
S_1	A	2.1246 eV	S_9	E	3.5417 eV
T_2	E	2.5396 eV	S_{10}	A	3.5417 eV
T_3	E	2.5396 eV	T_{19}	E	3.5622 eV
T_4	A	2.5903 eV	T_{20}	E	3.5622 eV
T_5	A	2.7293 eV	T_{21}	A	3.5622 eV
S_2	E	2.8081 eV	T_{22}	E	3.6207 eV
S_3	E	2.8081 eV	T_{23}	E	3.6207 eV
T_6	E	2.8304 eV	T_{24}	A	3.6235 eV
T_7	E	2.8304 eV	T_{25}	A	3.7221 eV
S_4	A	2.8677 eV	S_{11}	E	3.8468 eV
S_5	E	2.9787 eV	S_{12}	E	3.8468 eV
S_6	E	2.9787 eV	S_{13}	E	3.9467 eV
S_7	A	3.0626 eV	S_{14}	E	3.9467 eV
T_8	E	3.0863 eV	S_{15}	A	3.9714 eV
T_9	E	3.0863 eV	S_{16}	E	4.0386 eV
T_{10}	E	3.4191 eV	S_{17}	E	4.0386 eV
T_{11}	E	3.4191 eV	S_{18}	A	4.0914 eV
T_{12}	A	3.4191 eV	S_{19}	E	4.0966 eV
T_{13}	E	3.4320 eV	S_{20}	E	4.0966 eV
T_{14}	E	3.4320 eV	S_{21}	A	4.1324 eV
T_{15}	A	3.4321 eV	S_{22}	E	4.1370 eV
T_{16}	E	3.5207 eV	S_{23}	E	4.1370 eV
T_{17}	E	3.5207 eV	S_{24}	A	4.2305 eV
T_{18}	A	3.5407 eV	S_{25}	A	4.2588 eV

Table S22. Electronic energy (EE) and first 25 singlet and 25 triplet vertical excitation energies of **HAP-3Cz** at the $T_{1,min}$ geometry.

State	Symmetry	Energy	State	Symmetry	Energy
EE	-	-2852.9965468 hartrees			
T_1	A	2.1565 eV	S_8	E	3.5763 eV
S_1	A	2.2717 eV	S_9	E	3.5763 eV
T_2	E	2.5745 eV	S_{10}	A	3.5763 eV
T_3	E	2.5745 eV	T_{19}	E	3.5833 eV
T_4	A	2.6147 eV	T_{20}	E	3.5833 eV
T_5	A	2.7883 eV	T_{21}	A	3.5833 eV
S_2	E	2.8503 eV	T_{22}	E	3.6390 eV
S_3	E	2.8503 eV	T_{23}	E	3.6390 eV
T_6	E	2.8997 eV	T_{24}	A	3.6417 eV
T_7	E	2.8997 eV	T_{25}	A	3.7474 eV
S_4	A	2.9164 eV	S_{11}	E	3.8905 eV
S_5	E	3.0416 eV	S_{12}	E	3.8905 eV
S_6	E	3.0416 eV	S_{13}	E	3.9649 eV
S_7	A	3.0961 eV	S_{14}	E	3.9649 eV
T_8	E	3.1201 eV	S_{15}	A	3.9683 eV
T_9	E	3.1201 eV	S_{16}	E	4.0818 eV
T_{10}	E	3.4285 eV	S_{17}	E	4.0818 eV
T_{11}	E	3.4285 eV	S_{18}	A	4.1085 eV
T_{12}	A	3.4285 eV	S_{19}	E	4.1185 eV
T_{13}	E	3.4295 eV	S_{20}	E	4.1185 eV
T_{14}	E	3.4295 eV	S_{21}	A	4.1309 eV
T_{15}	A	3.4295 eV	S_{22}	E	4.1456 eV
T_{16}	E	3.5555 eV	S_{23}	E	4.1456 eV
T_{17}	E	3.5555 eV	S_{24}	A	4.2228 eV
T_{18}	A	3.5659 eV	S_{25}	A	4.2578 eV

Table S23. Electronic energy (EE) and first 25 singlet and 25 triplet vertical excitation energies of **HAP-3HMAT** at the FC geometry.

State	Symmetry	Energy	State	Symmetry	Energy
EE	-	-3906.0288704 hartrees			
T_1	E	2.4326 eV	T_{19}	E	3.6536 eV
T_2	E	2.4326 eV	T_{20}	E	3.6536 eV
T_3	A_1	2.4695 eV	T_{21}	A_1	3.6590 eV
T_4	A_2	2.5941 eV	T_{22}	-	3.6798 eV
S_1	A_2	2.7572 eV	S_8	E	3.6802 eV
S_2	E	2.7964 eV	S_9	E	3.6802 eV
S_3	E	2.7964 eV	T_{23}	E	3.7138 eV
T_5	A_2	3.0543 eV	T_{24}	E	3.7138 eV
S_4	A_2	3.1430 eV	S_{10}	-	3.7241 eV
S_5	A_1	3.1433 eV	S_{11}	A_2	3.7665 eV
T_6	E	3.1786 eV	S_{12}	E	3.7763 eV
T_7	E	3.1786 eV	S_{13}	E	3.7763 eV
T_8	E	3.2128 eV	T_{25}	-	3.8308 eV
T_9	E	3.2128 eV	S_{14}	A_2	3.8405 eV
S_6	E	3.2878 eV	S_{15}	E	3.8913 eV

S_7	E	3.2878 eV	S_{16}	E	3.8913 eV
T_{10}	A_2	3.3721 eV	S_{17}	E	4.0370 eV
T_{11}	E	3.3748 eV	S_{18}	E	4.0370 eV
T_{12}	E	3.3748 eV	S_{19}	E	4.1660 eV
T_{13}	A_1	3.4790 eV	S_{20}	E	4.1660 eV
T_{14}	E	3.4930 eV	S_{21}	-	4.1748 eV
T_{15}	E	3.4930 eV	S_{22}	-	4.2150 eV
T_{16}	-	3.4931 eV	S_{23}	-	4.2573 eV
T_{17}	E	3.5055 eV	S_{24}	-	4.2573 eV
T_{18}	E	3.5055 eV	S_{25}	-	4.2699 eV

Table S24. Electronic energy (EE) and first 25 singlet and 25 triplet vertical excitation energies of **HAP-3HMAT** at the $S_{1,min}$ geometry.

State	Symmetry	Energy	State	Symmetry	Energy
EE	-	-3906.0112511 hartrees			
T_1	A	2.0015 eV	T_{19}	A	3.5365 eV
S_1	A	2.0859 eV	T_{20}	A	3.5478 eV
T_2	A	2.2963 eV	T_{21}	A	3.5485 eV
T_3	A	2.2976 eV	S_8	A	3.6700 eV
T_4	A	2.3797 eV	S_9	A	3.6712 eV
S_2	A	2.6370 eV	S_{10}	A	3.6839 eV
S_3	A	2.6374 eV	S_{11}	A	3.6898 eV
T_5	A	2.7008 eV	S_{12}	A	3.6913 eV
T_6	A	2.8008 eV	S_{13}	A	3.7541 eV
T_7	A	2.8021 eV	S_{14}	A	3.7562 eV
S_4	A	2.8410 eV	S_{15}	A	3.7626 eV
S_5	A	2.9317 eV	T_{22}	A	3.7952 eV
S_6	A	2.9329 eV	T_{23}	A	3.8100 eV
S_7	A	3.0230 eV	T_{24}	A	3.8115 eV
T_8	A	3.0239 eV	T_{25}	A	3.8408 eV
T_9	A	3.0279 eV	S_{16}	A	3.9349 eV
T_{10}	A	3.2637 eV	S_{17}	A	3.9355 eV
T_{11}	A	3.2650 eV	S_{18}	A	3.9827 eV
T_{12}	A	3.2699 eV	S_{19}	A	4.0903 eV
T_{13}	A	3.4179 eV	S_{20}	A	4.0934 eV
T_{14}	A	3.4349 eV	S_{21}	A	4.1406 eV
T_{15}	A	3.4363 eV	S_{22}	A	4.1608 eV
T_{16}	A	3.4960 eV	S_{23}	A	4.2006 eV
T_{17}	A	3.4966 eV	S_{24}	A	4.2015 eV
T_{18}	A	3.4973 eV	S_{25}	A	4.2027 eV

Table S25. Electronic energy (EE) and first 25 singlet and 25 triplet vertical excitation energies of **HAP-3HMAT** at the $T_{1,min}$ geometry.

State	Symmetry	Energy	State	Symmetry	Energy
EE	-	-3906.0230631 hartrees			
T_1	A'	2.1113 eV	T_{19}	A'	3.5230 eV
T_2	A"	2.4801 eV	S_8	A"	3.5860 eV
T_3	A'	2.5046 eV	T_{20}	A"	3.6318 eV

T_4	A"	2.5574 eV	S_9	A'	3.6346 eV
S_1	A'	2.6479 eV	S_{10}	A'	3.6532 eV
S_2	A"	2.7202 eV	T_{21}	A"	3.6711 eV
S_3	A"	2.8104 eV	T_{22}	A'	3.6854 eV
T_5	A"	3.0388 eV	T_{23}	A'	3.7070 eV
S_4	A'	3.0999 eV	T_{24}	A"	3.7344 eV
S_5	A"	3.1278 eV	T_{25}	A'	3.7543 eV
T_6	A"	3.1346 eV	S_{11}	A"	3.7688 eV
T_7	A"	3.1777 eV	S_{12}	A'	3.7846 eV
T_8	A'	3.1815 eV	S_{13}	A"	3.7887 eV
T_9	A'	3.2372 eV	S_{14}	A"	3.8498 eV
S_6	A"	3.2409 eV	S_{15}	A'	3.8908 eV
S_7	A'	3.2871 eV	S_{16}	A"	3.9066 eV
T_{10}	A"	3.3271 eV	S_{17}	A"	4.0065 eV
T_{11}	A"	3.3577 eV	S_{18}	A'	4.0364 eV
T_{12}	A'	3.3930 eV	S_{19}	A'	4.0928 eV
T_{13}	A'	3.4025 eV	S_{20}	A"	4.1014 eV
T_{14}	A"	3.4044 eV	S_{21}	A"	4.1612 eV
T_{15}	A'	3.4091 eV	S_{22}	A'	4.1790 eV
T_{16}	A"	3.4161 eV	S_{23}	A"	4.1911 eV
T_{17}	A'	3.4874 eV	S_{24}	A'	4.2001 eV
T_{18}	A"	3.4874 eV	S_{25}	A"	4.2200 eV

D. Hole-electron analysis and spin-orbit coupling of low-lying T_n states

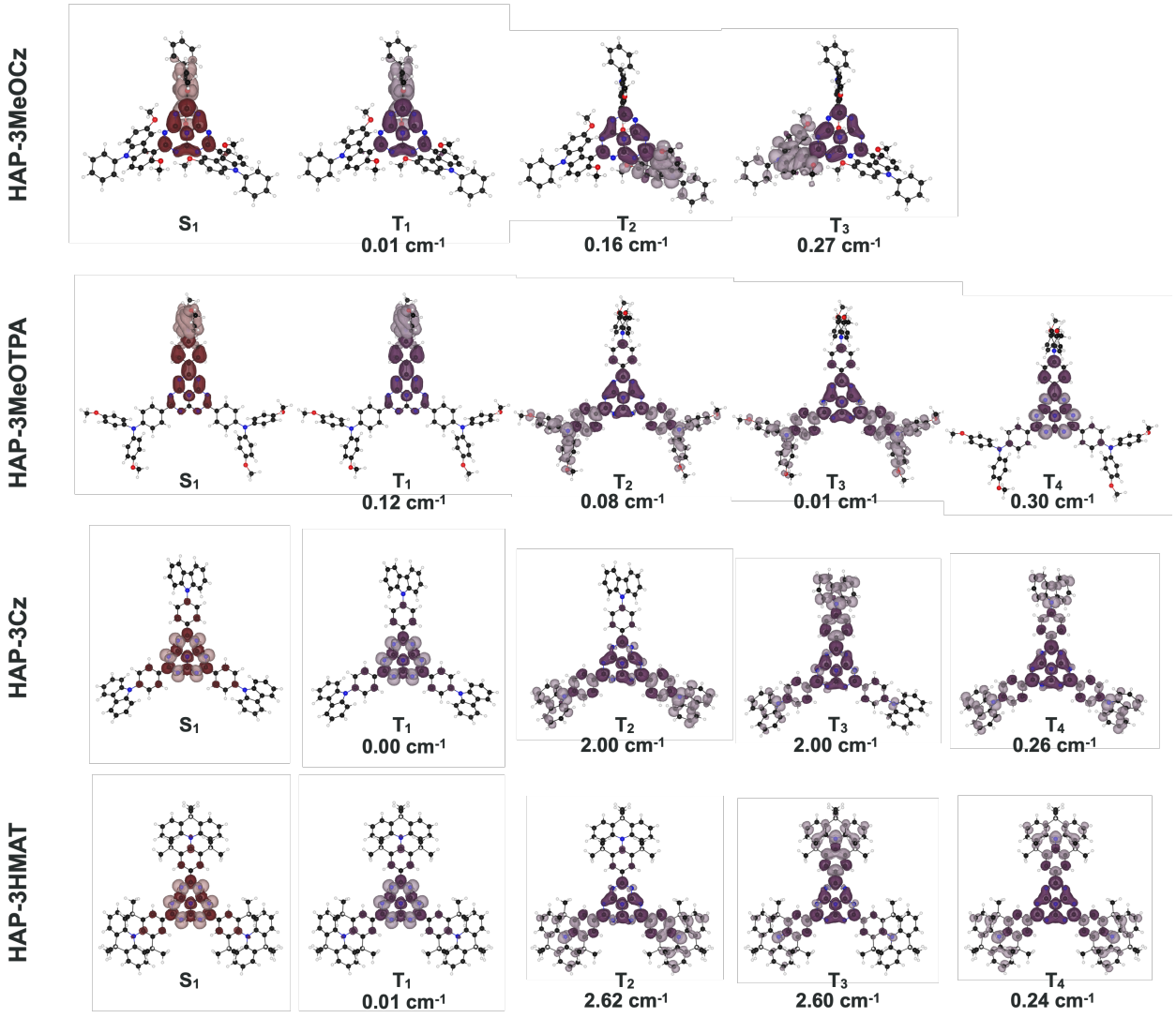

Figure S1. Hole (light) and electron (dark) analysis of the S_1 state and all low-lying T_n states at the $S_{1,min}$ geometry. Spin orbit coupling constants are shown for the coupling between S_1 and each T_n state.

E. Calculation of k_{rISC}

Experimental calculation: Experimental values for the rISC rate constant (k_{rISC}) were calculated according to equations 3 and 4. All data are from literature measurements in toluene solution with an optical density of 0.1 at λ_{exc} = 380 nm.

Table S26. Values used to calculate the experimental k_{rISC}.

	Φ_{N_2}	Φ_{air}	Φ_{ISC}	τ_{DF} (µs)	k_{rISC} (s^{-1})
HAP-3MeOCz	0.17	0.08	0.09	0.000139	**7.91E+03**
HAP-3MeOTPA	0.59	0.31	0.28	0.000082	**1.69E+04**
HAP-3Cz	1	0.57	0.43	0.00000186	**9.43E+05**
HAP-3HMAT	1	0.98	0.02	0.000021	**4.86E+04**

Computational calculation: Computational values for k_{rISC} were calculated according to equation 2. Superscripts in tables refer to the geometry at which the value was calculated at. All energies of the S_1 and T_n states are relative to the ground state at the FC geometry. For T_n states that could not be optimized to a minimum, the minimum T_n energy along the FC to $S_{1,min}$ to $T_{1,min}$ PES was taken as the T_n energy.

Table S27. Values used to calculate the computational k_{rISC} for **HAP-3MeOCz**.

	$H_{SO}^{S_1,min}$ (eV)	$S_1^{S_{1,min}}$ (eV)	$T_n^{T_n,min}$ (eV)	$S_1^{T_{n,min}}$ (eV)	ΔE_{ST_n}(eV)	λ_n(eV)	P_n (%)	Weighted k_{rISC} (s^{-1})
T_1	1.75E-06	2.1497	1.9023	2.4546	0.2474	0.3049	99.998538	5.51E+00
T_2	1.94E-05	2.1497	2.206	2.4276	-0.0563	0.2779	0.000731	1.58E+01
T_3	3.34E-05	2.1497	2.206	2.4276	-0.0563	0.2779	0.000731	4.64E+01
							Total k_{rISC}	**6.77E+01**

Table S28. Values used to calculate the computational k_{rISC} for **HAP-3MeOTPA**.

	$H_{SO}^{S_1,min}$ (eV)	$S_1^{S_{1,min}}$ (eV)	$T_n^{T_n,min}$ (eV)	$S_1^{T_{n,min}}$ (eV)	ΔE_{ST_n} (eV)	λ_n(ev)	P_n (%)	Weighted k_{rISC} (s^{-1})
T_1	1.50E-05	2.388	2.1560	2.6509	0.2320	0.2629	99.917754	8.46E+02
T_2	1.00E-05	2.388	2.3443	2.7758	0.0437	0.3878	0.065330	1.64E+01
T_3	1.75E-06	2.388	2.3790	2.7758	0.0090	0.3878	0.016915	2.69E-01
T_4	3.72E-05	2.388	2.6299	2.7758	-0.2419	0.3878	0.000001	2.11E-01
							Total k_{rISC}	**8.63E+02**

Table S29. Values used to calculate the computational k_{rISC} for **HAP-3Cz**.

	$H_{SO}^{S_1,min}$ (eV)	$S_1^{S_{1,min}}$ (eV)	$T_n^{T_n,min}$ (eV)	$S_1^{T_{n,min}}$ (eV)	ΔE_{ST_n} (eV)	λ_n(eV)	P_n (%)	Weighted k_{rISC} (s^{-1})
T_1	0	2.5976	2.4915	2.6067	0.1061	0.0091	99.865804	0.00E+00
T_2	2.48E-04	2.5976	2.6845	2.7646	-0.0869	0.167	0.054375	9.49E+05
T_3	2.48E-04	2.5976	2.6845	2.7646	-0.0869	0.167	0.054375	9.49E+05
T_4	3.23E-05	2.5976	2.704	2.7646	-0.1064	0.167	0.025446	8.79E+03
							Total k_{rISC}	**1.91E+06**

Table S30. Values used to calculate the computational k_{rISC} for **HAP-3HMAT**.

	$H_{SO}^{S_1,min}$ (eV)	$S_1^{S_1,min}$ (eV)	$T_n^{T_n,min}$ (eV)	$S_1^{T_n,min}$ (eV)	ΔE_{ST_n} (eV)	λ_n(eV)	P_n (%)	Weighted k_{rISC} (s^{-1})
T_1	3.25E-04	2.5653	2.2693	2.8782	0.2960	0.3129	99.757392	3.08E+04
T_2	3.23E-04	2.5653	2.4326	2.7572	0.1327	0.1919	0.172669	3.30E+04
T_3	2.98E-05	2.5653	2.4695	2.7572	0.0958	0.1919	0.041036	2.10E+02
T_4	1.24E-06	2.5653	2.4785	2.5711	0.0868	0.0065	0.028904	2.02E-04
							Total k_{rISC}	**6.40E+04**

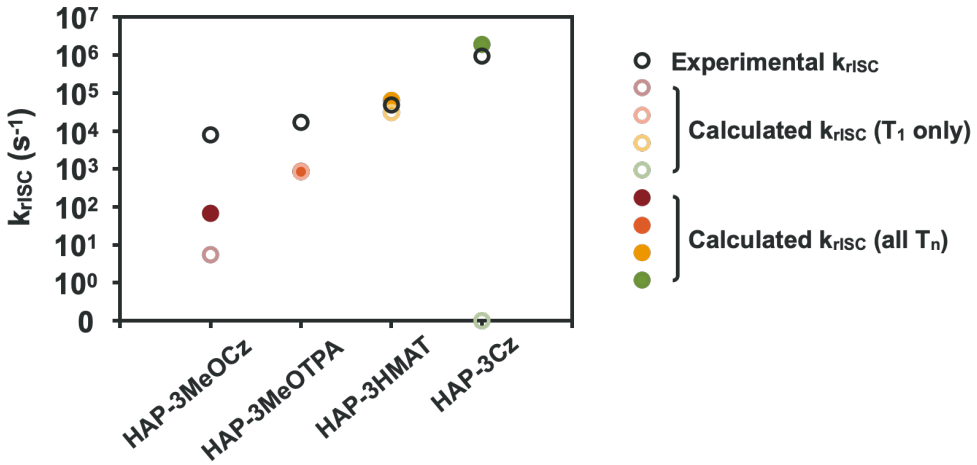

Figure S2. Comparison of experimental k_{risc} values with the computational values calculated by considering the T_1 states only (equation 1) or by considering all T_n states with energies below S_1 (equation 2).

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