Supplementary Information

Insights into Tautomerism and pH Effects on the Photoluminescence of Citric Acid-derived Molecular Fluorophores.

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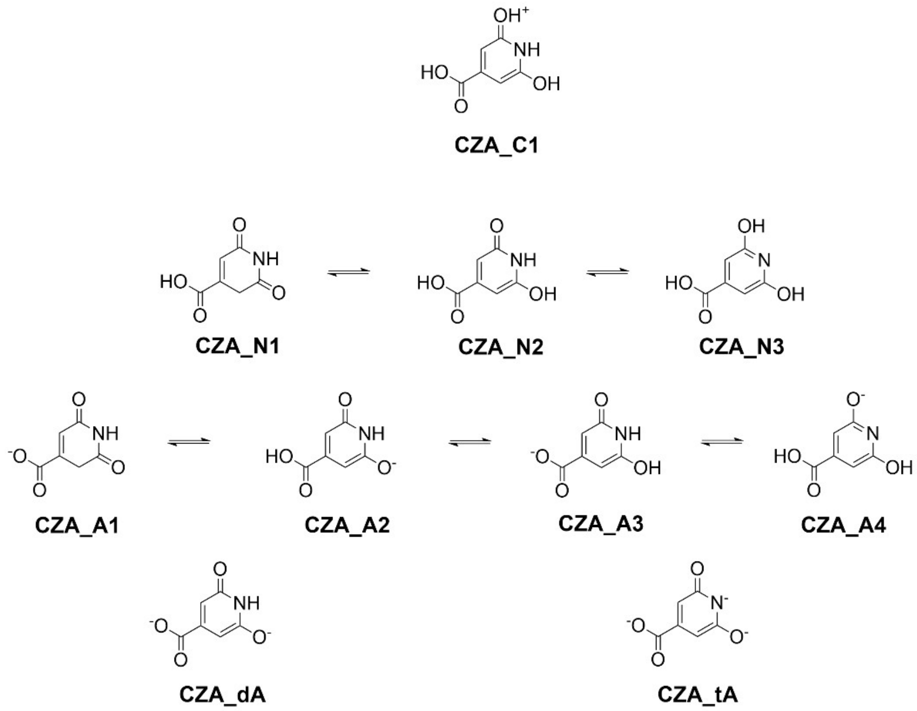
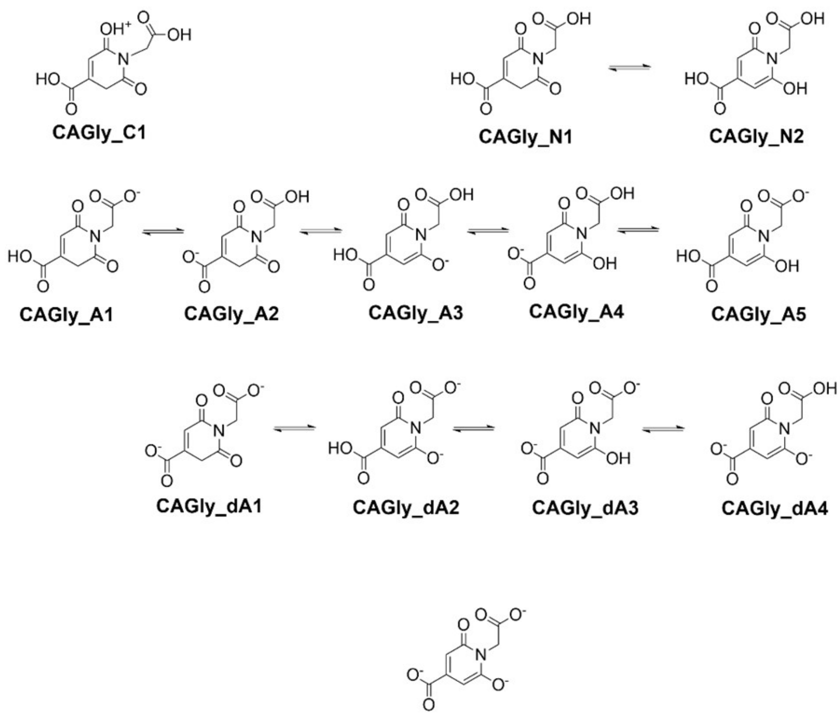
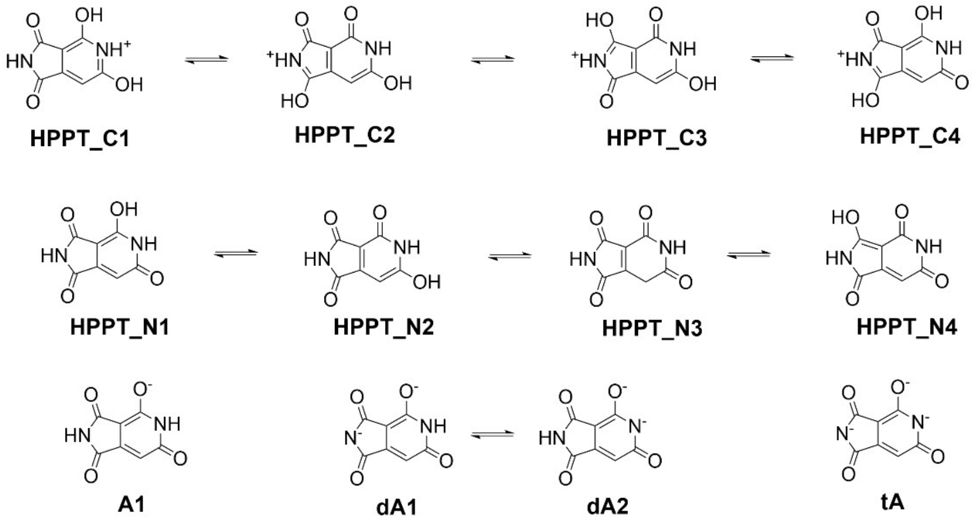
1. Tautomeric forms, relative population and optical properties:



Scheme S1. Tautomeric forms of CZA evaluated in this work: **C** (cation); **N** (neutral); **A** (anion); **dA** (dianion); **tA** (trianion). Relative populations in S_0 (those in S_1 shown in brackets).



Scheme S2. Tautomeric forms of CAGly evaluated in this work: **C** (cation); **N** (neutral); **A** (anion); **dA** (dianion); **tA** (trianion).



Scheme S3. Tautomeric forms of HPPT evaluated in this work: **C** (cation); **N** (neutral); **A** (anion); **dA** (dianion); **tA** (trianion).

Table S1. Gibbs absolute energies (in Hartree) in water implicit model solvent for the different tautomeric forms of CZA in the different pH-dependent species*; relative population in the ground state $N(S_0)$ and in the first single excited state $N(S_1)$, the longest absorption and emission from S_1 wavelengths (in nm), λ_{abs} and λ_{em}, respectively, together with the corresponding oscillator strength value, f_{abs} and f_{em}. See Scheme S1 for corresponding structures.

	G (S_0)	%N(S_0)	λ_{abs}	f_{abs}	G (S_1)	%N(S_1)	λ_{em}	f_{em}
CZA-**C**	587.89455	100.00	313.1	0.1498	-587.76896	100.00	378.1	0.2106
CZA-**N1**	-587.47594	99.70	311.1	0	-587.34455	0.00	383.6	0
CZA-**N2**	-587.46986	0.20	355.2	0.1246	-587.36078	100.00	446.1	0.1806
CZA-**N3**	-587.46935	0.1	319.9	0.0936	-587.34538	0.00	395.8	0.1425
CZA-**A1**	-587.03660	99.42	335.4	0	-586.93059	0.08	638.5	0
CZA-**A2**	-587.03150	0.44	400.5	0.1229	-586.93735	99.92	520.8	0.1681
CZA-**A3**	587.03025	0.12	316.6	0.1471	-586.90565	0.00	384.5	0.2245
CZA-**A4**	-587.02841	0.02	286.1	0.1001	-586.88593	0.00	341.3	0.1694
CZA-**dA**	-586.58690	100.0	346.2	0.1639	-586.47334	100	426.8	0.2374
CZA-**tA**	-586.10117	100.0	354.4	0.1101	-585.99203	100	450.3	0.1723

* C_i means tautomeric forms of the cationic form; N_i of neutral; A_i anionic; dA_i : dianionic and tA: trianionic.

Table S2. Gibbs absolute energies (in Hartree) in water implicit model solvent for the different tautomeric forms of CA-Gly in the different pH-dependent species*; relative population in the ground state $N(S_0)$ and in the first single excited state $N(S_1)$, the longest absorption and emission from S_1 wavelengths (in nm), λ_{abs} and λ_{em}, respectively, together with the corresponding oscillator strength value, f_{abs} and f_{em}. See Scheme S2 for corresponding structures.

	G (S_0)	%N(S_0)	λ_{abs}	f_{abs}	G (S_1)	%N(S_1)	λ_{em}	f_{em}
CA-Gly-**C**	-815.81585	100.00	317.2	0.1327	-815.69065	100.00	386.3	0.2004
CA-Gly-**N1**	-815.39956	99.80	308.2	0	-815.26762	0.00	385.6	0.0011
CA-Gly-**N2**	-815.39370	0.20	357.4	0.1133	-815.28441	100.00	448.1	0.1772
CA-Gly-**A1**	-814.96066	90.89	329.2	0	-814.85527	0.10	631.9	0
CA-Gly-**A2**	-814.95840	8.27	336.8	0.0083	-814.85252	0.01	599.6	0.0038
CA-Gly-**A3**	-814.95622	0.82	405.2	0.1099	-814.86181	99.90	524.8	0.1618
CA-Gly-**A4**	-814.95261	0.02	319.6	0.1303	-814.82914	0.00	393.0	0.2109
CA-Gly-**A5**	-814.95238	0.00	361.6	0.1061	-814.845141	0.00	454.1	0.1676
CA-Gly-**dA1**	-814.51801	99.90	324.9	0	-814.41021	0.04	615.4	0
CA-Gly-**dA2**	-814.51091	0.05	408.5	0.1031	-814.41765	99.96	530.3	0.1534
CA-Gly-**dA3**	-814.51073	0.04	321.1	0.1247	-814.25269	0.00	392.8	0.2050
CA-Gly-**dA4**	-814.50827	0.00	349.5	0.1408	-814.26265	0.00	433.0	0.2240
CA-Gly-**tA**	-814.06402	100.00	349.9	0.1376	-813.80672	100.00	435.9	0.2183

* C_i means tautomeric forms of the cationic form; N_i of neutral; A_i anionic; dA_i : dianionic and tA: trianionic.

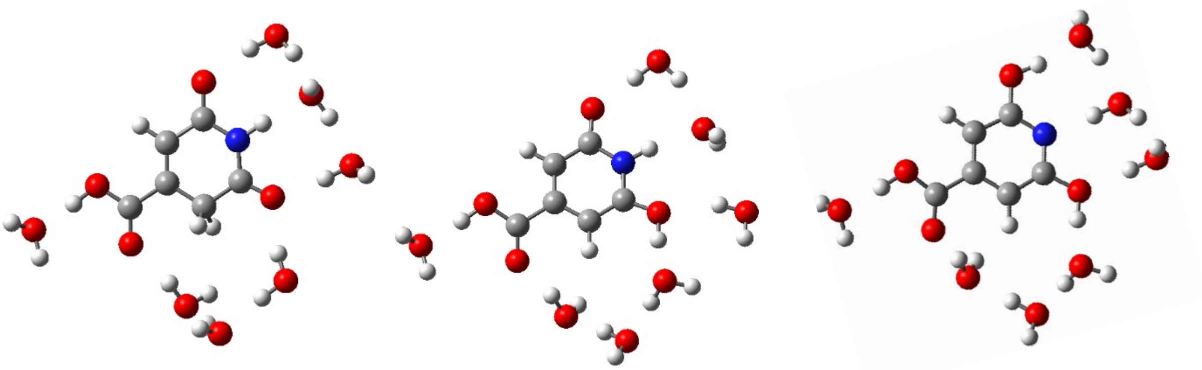
Table S3. Gibbs absolute energies (in Hartree) in water implicit model solvent for the different tautomeric forms of HPPT in the different pH-dependent species*; relative population in the ground state $N(S_0)$ and in the first single excited state $N(S_1)$, the longest absorption and emission from S_1 wavelengths (in nm), λ_{abs} and λ_{em}, respectively, together with the corresponding oscillator strength value, f_{abs} and f_{em}. See Scheme S3 for corresponding structures.

	$G(S_0)$	$\%N(S_0)$	λ_{abs}	f_{abs}	$G(S_1)$	$\%N(S_1)$	λ_{em}	f_{em}
HPPT-**C1**	-680.18301	100.00	333.3	0.1544	-680.06542	0.00	412.2	0.2060
HPPT-**C2**	-680.16746	0.00	470.2	0.1206	-680.08873	98.0	656.4	0.1285
HPPT-**C3**	-680.17507	0.00	431.4	0.1620	-680.08503	1.9	548.3	0.1882
HPPT-**C4**	-680.16927	0.00	412.6	0.1628	-680.08207	0.1	599.0	0.1751
HPPT-**N1**	-679.76860	94.87	357.0	0.1825	-679.66171	0.12	465.5	0.2386
HPPT-**N2**	-679.76609	4.87	395.4	0.1457	-679.66718	40.07	494.0	0.1843
HPPT-**N3**	-679.76331	0.26	371.8	0	-679.65444	0.00	453.6	0
HPPT-**N4**	-679.75957	0.00	410.6	0.1835	-679.66755	59.81	561.8	0.2129
HPPT-**A**	-679.33934	100.00	405.8	0.1755	-679.13077	100.00	535.0	0.1871
HPPT-**dA1**	-678.87543	100.00	403.8	0.1137	-678.78086	97.7	533.6	0.1313
HPPT-**dA2**	-678.86585	0.00	424.3	0.1562	-678.77732	2.30	577.0	0.1871
HPPT-**tA**	-678.21882	100.00	421.0	0.1167	-678.30429	100.00	568.4	0.1332

* C_i means tautomeric forms of the cationic form; N_i of neutral; A_i anionic; dA_i : dianionic and tA: trianionic.

2. ***MICROSOLVATION***

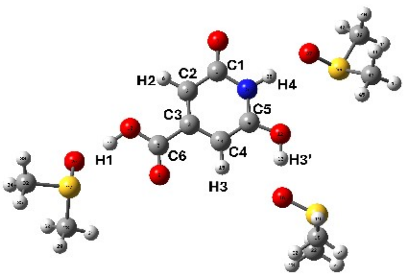
Although microsolvation narrows the Gibbs energy gap among the tautomers, the keto tautomer CZA_N1 continues to be the most stable form. In addition, the computed TS with three water molecules between CZA_N1 and CZA_N2 has been located at 18.7 kcal·mol^{-1} (without assisting water molecules the barrier results extremely high at 60.8 kcal·mol^{-1}) and this barrier slightly reduces to 17.2 kcal·mol^{-1} with 7 water molecules. Therefore, considering both thermodynamics and kinetics, tautomer CZA_N1 should be the dominant species in solution.



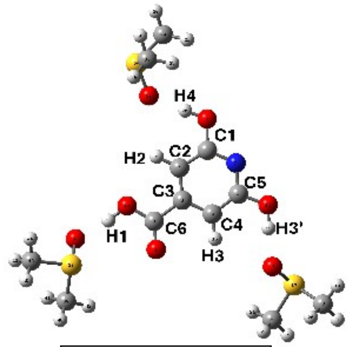
CZA_**N1**+7W **(79.4%)** **CZA_N2+7W (20.3%)** **CZA_N3+7W (0.3%)**

Fig. S1. B3LYP/6-311++g(2d,2p)/SMD(water) optimized geometries of tautomeric form of neutral CZA when solvated with seven water molecules. Relative population is also shown (in brackets).

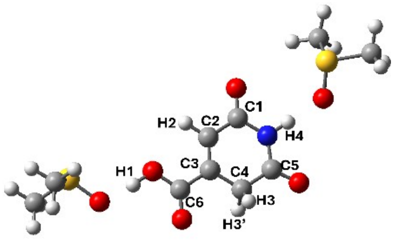
3. ^{13}C and ^{1}H NMR simulations for CZA in DMSO.



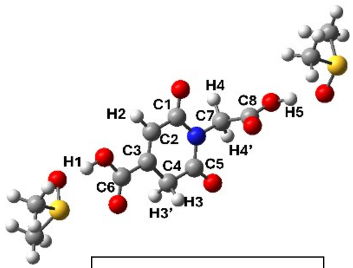
CZA-N2x3DMSO



CZA-N3x3DMSO



CZA-**N1**x2DMSO



CAGly-**N1**x2DMSO

Fig. S2. Representative B3LYP/6-311++g(2d,2p)/SMD(DMSO) optimized structures of the envisioned CZA···DMSO IHB complexes with one and up to three DMSO solvent molecules; based on the well-known IHB formation of DMSO with -OH or -NH groups. The optimized structures for CAGly-N1 with two DMSO molecules is also shown.

Experimental data NMR in DMSO

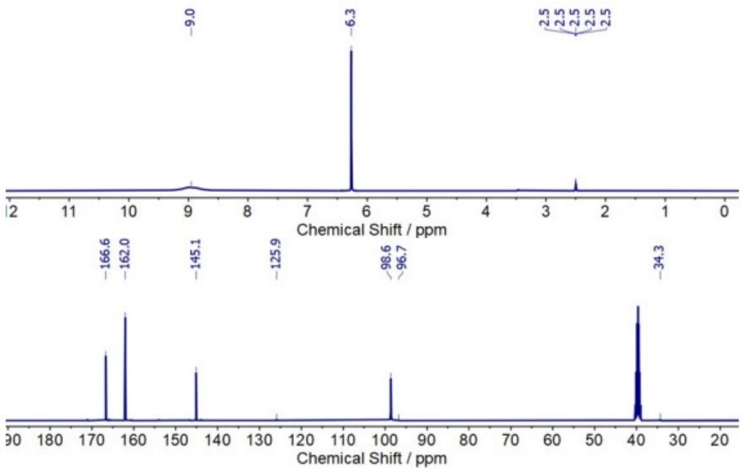


Fig. S3. ^{1}H-NMR (top) and ^{13}C-NMR (bottom) spectra of CZA (commercial) in DMSO-d6. *Reproduced from Chem. Sci.,2020, 11,8256*–8266.

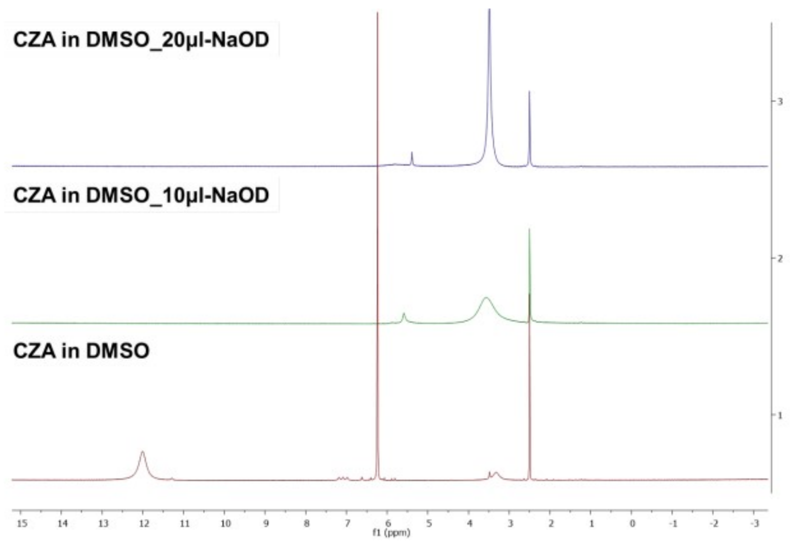


Fig. S4. ^{1}H-NMR spectra of CZA in DMSO. *Reproduced from* Stagi L., Mura S., Malfatti L., Carbonaro C.M., Ricci P.C., Porcu S., Secci F., Innocenzi P. Anomalous optical properties of citrazinic acid under extreme pH conditions. ACS Omega. 2020;5:10958–10964. doi: 10.1021/acsomega.0c00775

Table S4. List of calculated ^{13}C NMR chemical shifts (in ppm) for envisioned neutral (**N1**, **N2**, **N3**, see main text) CZA···DMSO species, regarding TMS computed at (B3LYP/6-311+G(2d,p)//B3LYP/6-311++g(2d,2p)/SMD(DMSO), level of theory. See **Fig. S2** for labelling.

	C1	**C2**	**C3**	**C4**	**C5**	**C6**
CZA-**N2**x3DMSO	168.26	116.64	148.19	84.82	163.38	174.98
CZA-**N3**x3DMSO	171.98	100.75	147.70	101.00	172.21	174.23
CZA-**N1**x2DMSO	173.18	132.22	150.65	36.58	175.01	171.56
CZA-**N2**x2DMSO	166.91	115.04	150.12	85.71	162.79	172.59
CZA-**N3**x2DMSO	169.6	97.74	149.0.5	104.33	172.88	171.20
CZA-**N1**x1DMSO	171.01	131.00	151.49	36.68	174.37	171.18
CZA-**N2**x1DMSO	166.40	116.34	146.13	85.69	163.42	172.38
CZA-**N3**x1DMSO	170.19	101.64	150.47	101.97	170.09	172.34

Table S5. List of calculated ^{13}C NMR chemical shifts (in ppm) for envisioned neutral (**N1** and **N2**, see main text) CAGly···DMSO species, regarding TMS computed at (B3LYP/6-311+G(2d,p)//B3LYP/6-311++g(2d,2p)/SMD(DMSO), level of theory. See **Fig. S2** for labelling.

	C1	**C2**	**C3**	**C4**	**C5**	**C6**	**C7**	**C8**
CAGly-**N2**x3DMSO	167.61	112.49	147.86	88.02	164.06	172.24	42.96	175.82
CAGly-**N1**x2DMSO	171.68	132.58	149.2	36.46	174.98	173.18	41.87	174.61

CAGly-**N2**x2DMSO	166.98	113.40	148.18	87.53	163.41	172.79	41.78	175.30

Table S6. List of calculated [1]H NMR chemical shifts (in ppm) for envisioned neutral (**N1**, **N2**, **N3**, see main text) CZA···DMSO species, regarding TMS computed at (B3LYP/6-311+G(2d,p)//B3LYP/6-311++g(2d,2p)/SMD(DMSO) level of theory. See **Fig. S2** for labelling.

	H1	H2	H3	H3'	H4
CZA-**N2**x3DMSO	12.94	6.62	5.87	11.68	11.57
CZA-**N3**x3DMSO	12.87	6.80	6.84	10.86	10.31
CZA-**N1**x2DMSO	13.33	6.93	3.29	3.29	11.82
CZA-**N2**x2DMSO	12.90	6.61	5.89	12.57	7.36
CZA-**N3**x2DMSO	12.92	6.34	7.07	11.4	4.12
CZA-**N1**x1DMSO	13.59	6.99	3.45	3.37	7.29
CZA-**N2**x1DMSO	5.68	6.64	5.95	12.92	7.46
CZA-**N3**x1DMSO	13.61	6.66	6.74	4.51	4.51

Table S7. List of calculated [1]H NMR chemical shifts (in ppm) for envisioned neutral (**N1** and **N2**, see main text) CAGly···DMSO species, regarding TMS computed at (B3LYP/6-311+G(2d,p)//B3LYP/6-311++g(2d,2p)/SMD(DMSO), level of theory. See **Fig. S2** for labelling.

	H1	H2	H3	H3'	H4	H4'	H5
CAGly-**N2**x3DMSO	12.32	6.63	6.21	12.70	5.34	4.11	12.19
CAGly-**N1**x2DMSO	13.77	7.11	3.56	3.40	4.66	4.38	12.43
CAGly-**N2**x2DMSO	12.54	6.77	6.20	12.94	5.65	4.12	5.58

4. ^{13}C and ^{1}H NMR simulations for CZA in $D_2O·NaOD$

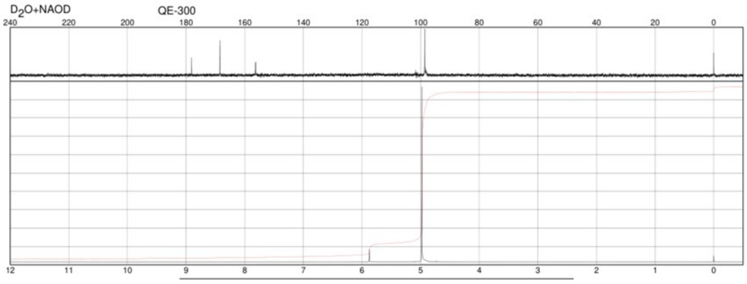


Fig. S5. ^{13}C and ^{1}H NMR of CZA in $D_2O·NaOD$ taken from https://m.chemicalbook.com/SpectrumEN_99-11-6_1HNMR.htm

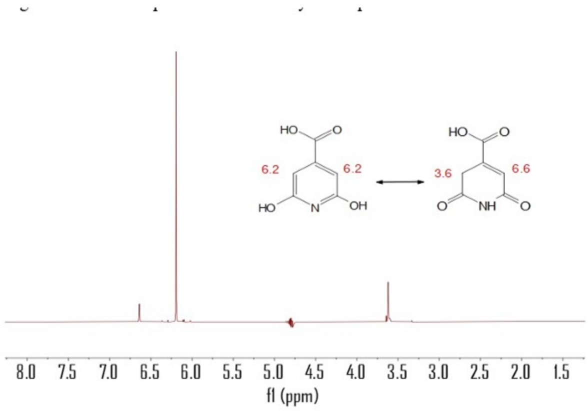


Fig. S6. ^{1}H NMR spectrum of citrazinic acid in 90% H_2O+10%D_2O in water suppression mode. Reproduced from ESI of the published research work *Unconventional aliphatic fluorophores discovered as the luminescence origin in citric acid-urea carbon dots.* X. Yao, Y. Wang, F. Li, J. J. Dalluge, G. Orr, R. Hernandez, Q. Cui, C. L. Haynes. *Nanoscale* **2022**, 14, 9516-9525.

Table S8. List of calculated ^{13}C and ^{1}H NMR chemical shifts (in ppm) of the different CZA species, regarding TMS computed at the (B3LYP/6-311+G(2d,p)//B3LYP/6-311++g(2d,2p)/SMD(water) level of theory. See Fig. 2 for labelling.

	C1	**C2**	**C3**	**C4**	**C5**	**C6**
CZA-**N1**	186.33	150.92	163.78	52.74	189.42	187.09
CZA-**N2**	167.66	117.06	147.83	88.38	161.57	172.60
CZA-**N3**	168.65(2)	103.75	147.38	105.23	168.65(2)	171.2
CZA-**A1**	175.04	121.70	165.36	40.63	181.07	171.87
CZA-**A2**	172.17	94.97	143.93	96.18	171.77	176.64
CZA-**dA**	171.5(2)	96.31	160.98	96.18	171.5(2)	176.47

	H1	**H2**	**H3**	**H3'**	**H4**
CZA-**N1**	5.92	7.10	3.42	3.42	7.38
CZA-**N2**	6.56	6.82	6.17	5.40	8.10

CZA-**N3**	6.01	7.02	7.22	4.76(2)	4.76(2)
CZA-**A1**	---	7.00	3.59	3.59	6.77
CZA-**A2**	4.78	5.48	5.64	---	7.27
CZA-**dA**	---	5.93(2)	5.93(2)	---	6.49

Conclusions from analysis of the experimental and computational NMR data of CZA and CAGly:

The experimental ^{1}H NMR spectrum in DMSO reported in the literature (Fig. S4) shows signals at approximately 12 ppm integrating for three protons. These resonances are attributed to the three strong intramolecular hydrogen bonds (IHBs) formed between DMSO and the proton-donor groups of CZA, consistent with the structural information in Fig. S2 and the analysis summarized in Tables S4 and S6.

Computationally, our results indicate that when up to two explicit DMSO molecules are included, the keto tautomer remains dominant: CZA_N1_2×DMSO is the most stable species (ΔG = 0.0 kcal·mol^{-1}), followed by CZA_N2_2×DMSO (ΔG = 0.9 kcal·mol^{-1}) and CZA_N3_2×DMSO (ΔG = 5.9 kcal·mol^{-1}). However, both CZA_N2 and CZA_N3 contain an additional proton-donor group capable of forming an extra intramolecular hydrogen bond with DMSO, suggesting that the presence of DMSO may shift the tautomeric equilibrium toward N2 and N3.

These findings are consistent with the experimental ^{1}H and ^{13}C NMR spectra of CZA in DMSO reported in the literature (Fig. S3), where a resonance near 35 ppm supports the presence of the keto tautomer, although only as a minority species.

Overall, while CZA_N1 is clearly predominant in aqueous solution, the tautomeric distribution shifts in DMSO in favor of CZA_N2 and CZA_N3 due to their ability to form additional hydrogen bonds with the solvent.

A similar analysis has been carried out with CAGly. When modelled the system with two DMSO molecules, CAGly_**N1**_2×DMSO is largely the most stable tautomer (ΔG = 0.0 kcal·mol^{-1}), followed by CAGly_**N2**_2×DMSO (ΔG = 6.4 kcal·mol^{-1}). However, similarly to the CZA system, CAGly_**N2** is also capable of forming an additional intramolecular hydrogen bond (IHB) with a DMSO molecule. This interaction provides extra stabilization and makes the coexistence of both tautomers compatible with the NMR spectra recorded under experimental conditions (Tables S5 and S7).

As expected under the strongly basic conditions of the NMR experiment in D_2O with added NaOD, both the ^{1}H (Fig. S5) and ^{13}C (Fig. S6) spectra are in good agreement with the dianionic form of CZA (CZA_dA) (Table S8). Notably, the ^{1}H NMR spectrum in D_2O with water suppression (Fig. S6) shows a resonance at approximately 3.6 ppm, which is consistent with the presence of the keto tautomer. However, the authors do not provide any additional analysis or complementary experiments to clarify the origin of this signal or to determine the tautomeric composition under these conditions.

5. pK_a estimation

a) The thermodynamic cycle method.[1]

Estimating pK_a values from computed Gibbs free energies (ΔG) is a standard workflow in computational chemistry, especially in solution-phase thermochemistry. The widely accepted way to do it, along with the key equations, assumptions, and practical tips.

-For an acid–base equilibrium:

$$HA \rightleftharpoons A^- + H^+$$

-The standard thermodynamic relation is:

$$\Delta G^\circ = -RT\ln K_a$$

-Using $pK_a = -\log K_a$, this becomes:

$$pK_a = \frac{\Delta G^\circ}{2.303RT}$$

-At T=298:

$$pK_a = \frac{\Delta G^\circ (kcal\cdot mol^{-1})}{1.364}$$

To compute ΔG° for the dissociation reaction, use:

$$\Delta G^\circ = G^\circ(\mathrm{A}^-) + G^\circ(\mathrm{H}^+) - G^\circ(\mathrm{HA})$$

But this must be corrected for solvation and standard-state conventions.

Where the convention value for the proton free energy in solution is taken from literature. The commonly used value in water at 298 K is:

$$G^\circ_{\mathrm{solv}}(\mathrm{H}^+) = -265.9 \pm 0.5 \text{ kcal/mol}$$

Quantum chemistry gives ΔG for a gas-phase 1 atm standard state.

Solution-phase pK_a uses 1 mol/L standard state. Thus,

$$\Delta G^\circ_{1\text{ atm}\rightarrow 1\text{ M}} = RT\ln(24.46) = 1.89 \text{ kcal/mol}$$

This applies to HA and the deprotonated A^-.

b) Isodesmic method[2]

An isodesmic reaction is a hypothetical reaction where the *number and type of bonds are conserved* on both sides.

In acid–base chemistry, we use a reference acid with a known experimental pK_a, and construct a reaction of the form:

$$\mathrm{HA} + \mathrm{B}^-_{\mathrm{ref}} \rightarrow \mathrm{A}^- + \mathrm{HB}_{\mathrm{ref}}$$

The reference should have similar functional groups, to bond changes are minimal; solvation environment is similar and cancel systematic errors.

Then:

$$pK_a(\mathrm{HA}) = pK_a(\mathrm{HB}_{\mathrm{ref}}) + \frac{\Delta G_{\mathrm{iso}}}{1.364}$$

Where:

$$\Delta G_{\mathrm{iso}} = G(A^-) + G(HB_{\mathrm{ref}}) - G(HA) - G(B^-_{\mathrm{ref}})$$

Table S9. Proton dissociation Gibbs energy (PDE) computed at the B3LYP/6-311++g(2d,2p)/SMD(water) level of theory as PDE = $G_{product}$ - $G_{reactant}$.

	CZA	HPPT	CAGly
$PDE_{C\rightarrow N}$	262.7	259.9	261.2
$PDE_{N\rightarrow A}$	275.7	269.5	275.4
$PDE_{A\rightarrow dA}$	282.2	291.1	277.8
$PDE_{dA\rightarrow tA}$	304.8	301.9	284.9

$PDE_{OH-\rightarrow H2O}$: -303.3 kcal·mol^{-1}

Table S10. Summary of estimated pK_a for CZA, HPPT and CAGly by using both methods. All Gibbs energies computed at the B3LYP/6-311++g(2d,2p) level of theory.

	Reference	CZA	HPPT	CAGly
Thermodynamic cycle		4.0	-0.5	3.7
Isodesmic Method	CACys[a] (pK_{a1}: 2.35; pK_{a2}: 3.41)[3]	3.9	-0.6	3.7
	CACystemaine (pK_a: 3.31)[4]	2.8	-1.7	2.6
	DHP (pK_a: 4.52)[5]	3.4	-1.1	3.2
	Salicylic acid (pK_{a1}: 3.97; pK_{a2}: 13.8)	2.6	-1.9	2.4

[a] By using the thermodynamic cycle, we have obtained a pka1 of 3.2

In agreement with $PDE_{N\rightarrow A}$ values (Table S8), the calculated pK_a values for CZA and CAGly are similar (Table S9). Depending on the method and the reference used (Table S10), the first deprotonation of CZA yields pK_a values in the range of 2.6-4, while CAGly shows values between 2.4 and 3.7. Attempts to compute a second pKa are considerably less reliable: the thermodynamic cycle introduces substantial uncertainty due to solvation errors and other limitations, and the isodesmic approach lacks appropriate reference acids for this purpose. Therefore, to infer the pH at which a second deprotonation may occur, we instead examine the PDE values.

Considering the $PDE_{A\rightarrow dA}$ trends, we can deduce that CAGly will undergo a second deprotonation at a lower pH than CZA. This is expected, as the anion of CA-Gly retains a second carboxylate site, making further deprotonation feasible below pH 7. In contrast, the second deprotonation of CZA would most likely require a higher pH value. Experimentally, the first pK_a of CZA has been reported between 2.24 and approximately 4, depending on measurement conditions, while the second pK_a has been estimated to be around 11.

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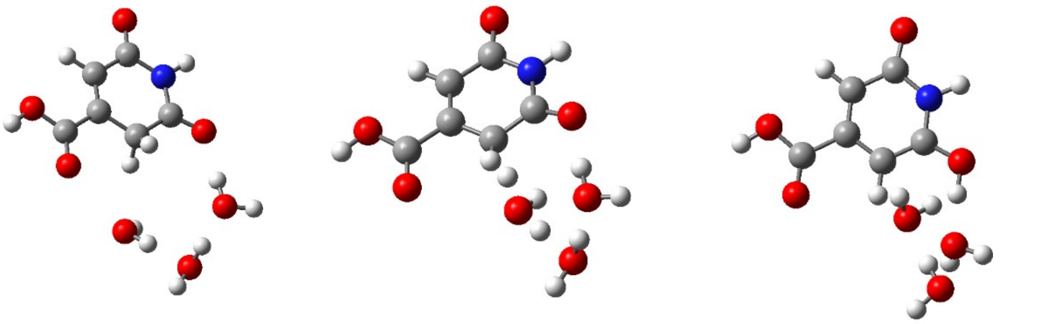
6. Keto to enol tautomerization in the ground state:

With up to three water molecules **TS**$_{\mathbf{CZA\_N1+3W \rightarrow CZA\_N2+3W}}$ is located at 18.7 kcal·mol^{-1}. In addition, the thermodynamics neither favored the process ($\Delta G_{\mathrm{CZA_}\mathbf{N1+3W}\rightarrow\mathrm{\ CZA_}\mathbf{N2+3W}}$ = 3.0 kcal·mol^{-1}). Therefore, considering both thermodynamics and kinetics, tautomer CZA_N1 should be the dominant species in solution.



CZA_N1+3W **TS**$_{\mathbf{CZA\_N1+3W \rightarrow CZA\_N2+3W}}$ **CZA_N2+3W**

Fig. S7. Molecular structures of CZA_N1+3W, CZA_N2+3W and the transition state for the keto to enol tautomerization with three water molecules, **TS**$_{\mathbf{CZA\_N1+3W \rightarrow CZA\_N2+3W}}$.

It is noted that, as expected, the corresponding TS without assisting water molecules is found much uphill (60.8 kcal·mol^{-1}).

7. Fluorescence mechanism HPPT.

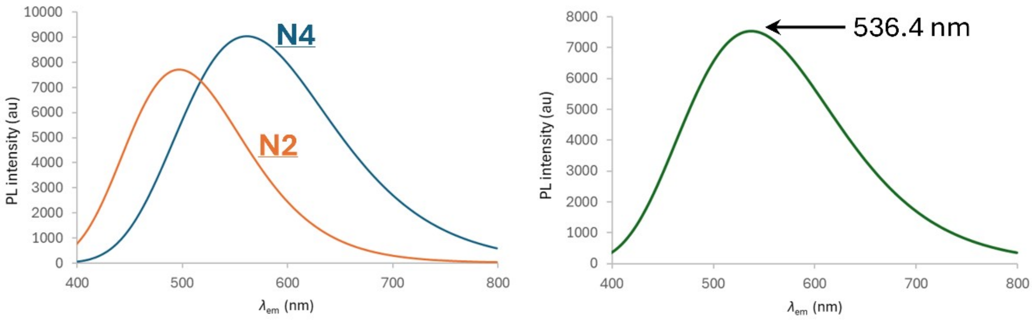


Fig. S8. Computed emission spectrum of HPPT_**N2** and HPPT_**N4** tautomeric forms of neutral HPPT a) as individual contributions and b) as a population weighted average (see Table S3).

Cartesian geometries

-Tautomeric forms in the ground state

CZA_C1

6	-1.271794	1.209522	0.000002
6	0.111108	1.193869	0.000010
6	0.751103	-0.041288	0.000009
6	0.033174	-1.231894	-0.000002
6	-1.346194	-1.163688	-0.000011
7	-1.955817	0.043335	-0.000009
1	0.649289	2.126951	0.000019
1	0.522535	-2.192182	-0.000004
8	-2.183373	-2.192223	-0.000022
8	-2.046565	2.285596	0.000002
1	-1.513503	3.094772	0.000008
6	2.251369	-0.135645	0.000019
8	2.847896	-1.190009	0.000005
8	2.846721	1.059227	0.000005
1	3.810001	0.932995	-0.000004
1	-2.972716	0.077565	-0.000016
1	-1.694917	-3.029422	-0.000022

CZA_N1

6	1.335504	1.298593	-0.000022
6	-0.126840	1.179918	-0.000018
6	-0.727474	-0.013354	0.000037
6	0.038811	-1.295031	0.000071
6	1.536198	-1.156467	0.000040
7	2.056721	0.118201	0.000001
1	-0.673019	2.109354	-0.000050
1	-0.232714	-1.899273	0.868941
8	2.280212	-2.126638	0.000113
8	1.913469	2.379133	-0.000096
6	-2.213404	-0.140647	0.000062
8	-2.780097	-1.215531	0.000082
8	-2.859512	1.032761	-0.000207
1	-3.815453	0.863482	-0.000287
1	-0.232730	-1.899320	-0.868762
1	3.067524	0.202472	-0.000007

CZA_N2

6	-1.365666	1.303473	0.000060
6	0.060786	1.261726	0.000048
6	0.725574	0.059927	-0.000003
6	0.039138	-1.172283	-0.000076
6	-1.330133	-1.129267	-0.000097
7	-1.984567	0.056424	-0.000037
1	0.593467	2.198480	0.000091
1	0.547133	-2.121275	-0.000127
8	-2.149835	-2.193112	-0.000173
1	-1.630652	-3.009686	-0.000189
8	-2.068969	2.334196	0.000073
6	2.223769	0.093086	0.000005
8	2.777927	-1.127871	0.000268
8	2.880332	1.114492	-0.000089
1	-2.998314	0.044870	-0.000057
1	3.743889	-1.028974	0.000285

CZA_N3

6	1.300990	1.160525	-0.000366
6	-0.089824	1.183148	-0.000113
6	-0.741909	-0.045848	0.000130
6	-0.008642	-1.227649	0.000381
6	1.376329	-1.114298	0.000694
7	2.025637	0.046446	0.000012
1	-0.619490	2.120717	-0.000296
1	-0.483702	-2.194855	0.000348
8	2.115030	-2.254071	0.000087
1	3.053856	-2.018466	-0.000150
8	1.961048	2.347553	-0.000439
1	2.913752	2.176145	-0.000028
6	-2.232442	-0.136712	-0.000066
8	-2.847406	-1.184815	-0.001281
8	-2.837704	1.060578	0.001056
1	-3.798630	0.922380	0.000696

CZA_A1

6	1.329978	1.275034	-0.000798
6	-0.127423	1.201916	-0.000107
6	-0.779504	0.034300	0.000104
6	-0.044191	-1.266037	0.000102
6	1.457140	-1.182338	0.000113
7	2.019429	0.071489	-0.000179
1	-0.649827	2.145630	0.000041
1	-0.335222	-1.865023	0.866312
8	2.169971	-2.179717	0.000431
8	1.954064	2.334196	0.000174
6	-2.306816	-0.011648	0.000282
8	-2.829487	-1.158597	-0.000625
8	-2.922347	1.085522	0.000366
1	-0.335254	-1.865103	-0.866033
1	3.031601	0.125479	-0.000017

CZA_A2

6	-1.342941	1.268105	-0.000405
6	0.069497	1.197004	-0.000258
6	0.694213	-0.046547	0.000222
6	-0.015504	-1.243402	0.000397
6	-1.428317	-1.218377	0.000360
7	-2.003260	0.046741	-0.000018
1	0.626273	2.118461	-0.000674
1	0.486093	-2.196895	0.000640
8	-2.189332	-2.227450	0.000752
8	-2.028991	2.329740	-0.000846
6	2.187841	-0.137025	-0.000022
8	2.812031	-1.181819	-0.002430
8	2.803127	1.059683	0.002212
1	3.761846	0.909930	0.000940
1	-3.014801	0.081523	-0.000052

CZA_A3

6	-1.279822	1.324917	0.000085
6	0.141291	1.233459	-0.000031
6	0.778922	0.015158	-0.000097
6	0.038379	-1.186382	-0.000022
6	-1.326728	-1.102089	0.000080
7	-1.945656	0.103330	0.000147
1	0.699679	2.155128	-0.000044
8	-2.184410	-2.142519	0.000107
8	-1.952462	2.382496	0.000153
6	2.311331	-0.049634	-0.000172
8	2.834777	-1.195937	-0.000688
8	2.935369	1.043995	0.000338
1	0.519964	-2.149808	0.000379
1	-1.688040	-2.972790	0.000062
1	-2.958451	0.127317	0.000244

CZA_A4

6	1.297467	1.134536	0.000428
6	-0.089744	1.199736	0.000199
6	-0.796465	0.000238	-0.000096
6	-0.090070	-1.199403	-0.000136
6	1.297186	-1.134656	-0.000028
7	1.991590	-0.000177	0.000217
1	-0.591289	2.153352	-0.000219
1	-0.591702	-2.152981	-0.000694
8	2.000144	-2.303860	-0.000742
1	2.945095	-2.095955	0.000338
8	2.000774	2.303507	0.000163
1	2.945681	2.095382	0.000953
6	-2.325154	0.000173	-0.000035
8	-2.900873	-1.121110	0.001412
8	-2.901075	1.121175	-0.001320

CZA_dA

6	1.344240	1.241019	0.000240
6	-0.066321	1.214274	0.000127
6	-0.748652	0.000163	-0.000036
6	-0.066396	-1.214093	-0.000181
6	1.344096	-1.241082	-0.000238

7	*1.966735*	*-0.000049*	*0.000022*
1	*-0.593807*	*2.153569*	*0.000201*
1	*-0.594203*	*-2.153227*	*-0.000306*
8	*2.072145*	*-2.281244*	*-0.000395*
8	*2.072349*	*2.281121*	*0.000416*
6	*-2.282063*	*-0.000110*	*-0.000110*
8	*-2.866249*	*-1.118955*	*0.001268*
8	*-2.866611*	*1.118958*	*-0.001155*
1	*2.978359*	*-0.000054*	*0.000065*

CZA_tA

6	*-1.401532*	*1.181312*	*0.025604*
6	*0.019752*	*1.199940*	*0.018247*
6	*0.724737*	*-0.000001*	*-0.000100*
6	*0.019743*	*-1.199937*	*-0.018488*
6	*-1.401539*	*-1.181292*	*-0.026087*
7	*-2.076693*	*0.000009*	*-0.000086*
1	*0.531375*	*2.150169*	*0.034219*
1	*0.531357*	*-2.150175*	*-0.034223*
8	*-2.082823*	*-2.294108*	*-0.056514*
8	*-2.082799*	*2.294111*	*0.057033*
6	*2.249778*	*-0.000007*	*0.000034*
8	*2.845824*	*-1.105633*	*0.161858*
8	*2.845860*	*1.105612*	*-0.161709*

CAGly_C1

6	-0.133082	1.203096	-0.366378
6	1.913645	0.033284	-0.022779
6	1.249069	-1.178357	-0.147696
6	-0.112667	-1.165287	-0.388150
1	1.750261	-2.127781	-0.055784
8	-0.872155	-2.244544	-0.506122
6	3.391260	0.090193	0.238986
8	4.005520	1.129866	0.338380
8	3.947312	-1.118392	0.347881
7	-0.787032	0.014153	-0.524833
6	-3.035549	-0.025331	0.493958
8	-2.564541	-0.027155	1.607172
8	-4.343349	-0.048660	0.222338
8	-0.911888	2.270929	-0.462658
6	-2.232723	0.003741	-0.790040
1	-2.476069	-0.866529	-1.390159
1	-2.494403	0.888488	-1.360562
1	4.899497	-1.014554	0.510723
1	-4.842117	-0.065859	1.056269
6	1.227024	1.233951	-0.128390
1	1.721477	2.185720	-0.018387
1	-0.396160	3.084516	-0.359567
1	-0.342317	-3.051172	-0.421688

CAGly_N1

6	0.241503	-1.269951	-0.356071
6	-1.927847	0.005295	-0.025459
6	-1.262671	1.153348	-0.161847
6	0.181008	1.186440	-0.417003
1	-1.737660	2.118408	-0.087477
8	0.793583	2.241971	-0.507042
6	-3.394876	-0.031620	0.233847
8	-4.016000	-1.070776	0.340716
8	-3.961059	1.177912	0.335517
7	0.847108	-0.034352	-0.561616
6	3.089332	0.066743	0.467444
8	2.631707	0.079115	1.587991
8	4.401597	0.112807	0.196843
8	0.904945	-2.294338	-0.378703
6	2.280936	-0.002797	-0.809179
1	2.520099	0.861303	-1.422059
1	2.568826	-0.896513	-1.355060
1	4.895317	0.153348	1.032493
1	-4.911771	1.063629	0.496510
6	-1.243178	-1.312472	-0.126573
1	-1.673077	-1.900089	-0.942253
1	-1.414914	-1.903063	0.775623

CAGly_N2

6	-0.139551	1.178870	-0.362148
6	1.906700	0.007980	-0.027721
6	1.264075	-1.195192	-0.166296
6	-0.140671	-1.251847	-0.406043
1	1.782678	-2.135571	-0.086005
8	-0.801548	-2.301754	-0.510181
6	3.377890	0.075766	0.235948
8	3.992768	1.118184	0.342071
8	3.959821	-1.126478	0.344748
7	-0.794418	-0.008674	-0.534801
6	-3.043402	-0.057960	0.483587
8	-2.592318	-0.037492	1.606393
8	-4.353748	-0.109736	0.205587
8	-0.931226	2.258840	-0.453271
6	-2.228652	-0.026224	-0.790876
1	-2.464162	-0.911915	-1.373486
1	-2.515765	0.845404	-1.370595
1	-4.853068	-0.126162	1.038722
6	1.207386	1.224444	-0.120779
1	1.697238	2.175942	0.004348
1	-0.406523	3.063042	-0.336179
1	4.907899	-0.997553	0.510005

CAGly_A1

6	-0.180010	1.257433	-0.357661
6	1.979265	-0.051865	-0.013053
6	1.282910	-1.183513	-0.145116
6	-0.152612	-1.197950	-0.403682
1	1.747286	-2.153469	-0.060688
8	-0.792446	-2.241302	-0.493789
6	3.482825	-0.070515	0.254968
8	4.044468	1.053178	0.352413
8	4.043929	-1.192704	0.354479
7	-0.805275	0.034250	-0.557167
6	-3.054602	-0.042784	0.460500
8	-2.606692	-0.052435	1.585144
8	-4.366047	-0.086197	0.181315
8	-0.826729	2.295881	-0.387922
6	-2.237182	0.021595	-0.810198
1	-2.486078	-0.835873	-1.428403
1	-2.512470	0.921602	-1.352624
6	1.304578	1.270923	-0.125009
1	1.745086	1.850112	-0.941133
1	1.484898	1.867887	0.771225
1	-4.864691	-0.121313	1.014175

CAGly_A2

6	-0.285050	1.270953	-0.353034
6	1.885007	-0.005383	-0.025287
6	1.212701	-1.148772	-0.163128
6	-0.233244	-1.173136	-0.414595
1	1.682967	-2.116723	-0.095737
8	-0.841654	-2.233894	-0.506375
6	3.352414	0.024823	0.224711
8	3.978800	1.060623	0.338389
8	3.917404	-1.187458	0.309623
7	-0.897802	0.043238	-0.557941
6	-3.198594	-0.080334	0.493241
8	-2.629248	-0.080707	1.612007
8	-4.440647	-0.147358	0.283393
8	-0.937021	2.305577	-0.380386
6	-2.343477	0.012511	-0.785341
1	-2.569944	-0.840436	-1.416292
1	-2.619948	0.915012	-1.320224
6	1.200278	1.312419	-0.117516
1	1.633040	1.908013	-0.925586
1	1.367948	1.894422	0.791139
1	4.869272	-1.075701	0.464780

CAGly_A3

6	-0.154714	1.287938	-0.364802
6	1.897150	0.031654	-0.029086
6	1.231879	-1.179929	-0.160574
6	-0.160447	-1.202813	-0.398881
1	1.738114	-2.125648	-0.070528
8	-0.851457	-2.252245	-0.504220
6	3.367956	0.065872	0.233772

8	4.014902	1.085992	0.382830
8	3.937019	-1.151555	0.292611
7	-0.794902	0.045201	-0.530176
6	-3.053265	-0.037497	0.469279
8	-2.628012	-0.039080	1.603677
8	-4.363631	-0.103225	0.174350
8	-0.838543	2.344645	-0.442905
6	-2.220735	0.046333	-0.789150
1	-2.478442	-0.795374	-1.425509
1	-2.490731	0.962507	-1.307330
1	-4.869035	-0.141895	1.002678
6	1.235658	1.248256	-0.125751
1	1.755426	2.184416	-0.008031
1	4.885866	-1.035549	0.460369

CAGly_A4

6	-0.093803	1.140120	-0.363667
6	1.961701	-0.025646	-0.010960
6	1.303752	-1.223059	-0.139961
6	-0.096009	-1.286372	-0.383598
1	1.826618	-2.160837	-0.046887
8	-0.760867	-2.340198	-0.483398
6	3.470225	0.005943	0.256170
8	4.017722	1.140185	0.300084
8	4.054023	-1.099313	0.408906
7	-0.753592	-0.046150	-0.525755
6	-3.014019	-0.023349	0.473326
8	-2.577301	-0.002766	1.601977
8	-4.323219	-0.018831	0.180541
8	-0.886160	2.224486	-0.469800
6	-2.184872	-0.059522	-0.791029
1	-2.426004	-0.970850	-1.330729
1	-2.459275	0.784161	-1.416666
1	-4.831357	-0.001219	1.008110
6	1.251437	1.184874	-0.119695
1	1.737010	2.139949	-0.005493
1	-0.355907	3.025403	-0.358047

CAGly_A5

6	-0.198046	1.151655	-0.375992
6	1.863398	0.012224	-0.029224
6	1.228861	-1.198014	-0.151670
6	-0.175700	-1.268696	-0.388241
1	1.755587	-2.133071	-0.061581
8	-0.819926	-2.334038	-0.477063
6	3.333456	0.096998	0.226996
8	3.939436	1.145907	0.326491
8	3.930898	-1.098523	0.337245
7	-0.843681	-0.038568	-0.534465
6	-3.151351	-0.045303	0.511837
8	-2.586186	0.026877	1.629770
8	-4.392838	-0.102885	0.298735
8	-0.993283	2.230677	-0.483040
6	-2.289908	-0.067035	-0.767286
1	-2.514378	-0.974834	-1.316143
1	-2.564889	0.780284	-1.385905
6	1.150358	1.217835	-0.135633
1	1.628720	2.176948	-0.024863
1	-0.468255	3.034993	-0.370369
1	4.877767	-0.956443	0.498282

CAGly_dA1

6	-0.225510	1.254293	-0.356159
6	1.937196	-0.051770	-0.014231
6	1.235850	-1.179802	-0.145659
6	-0.202287	-1.188438	-0.400712
1	1.696963	-2.151937	-0.066825
8	-0.835204	-2.238575	-0.492837
6	3.441029	-0.073705	0.244642
8	4.005637	1.048675	0.346647
8	4.002944	-1.196973	0.333745
7	-0.856168	0.038007	-0.552756
6	-3.165644	-0.052005	0.485767
8	-2.606498	-0.051424	1.609942
8	-4.407603	-0.107618	0.267755
8	-0.862379	2.301742	-0.392531
6	-2.300209	0.024933	-0.786094
1	-2.536110	-0.826365	-1.415884
1	-2.563515	0.929138	-1.325226
6	1.260058	1.269786	-0.119986
1	1.701248	1.855570	-0.930845
1	1.436510	1.861176	0.780898

CAGly_dA2

6	-0.206547	1.274268	-0.368653
6	1.855591	0.034254	-0.030705
6	1.191908	-1.178511	-0.156199
6	-0.201862	-1.204954	-0.392508
1	1.700283	-2.123182	-0.065716
8	-0.879230	-2.266929	-0.494921
6	3.325767	0.075240	0.225495
8	3.971423	1.097839	0.367472
8	3.901093	-1.140110	0.287153
7	-0.845717	0.034181	-0.526843
6	-3.167038	-0.039838	0.493154
8	-2.630327	-0.026916	1.629274
8	-4.408330	-0.100193	0.261100
8	-0.886803	2.336351	-0.452284
6	-2.283453	0.028366	-0.766289
1	-2.526759	-0.823617	-1.392678
1	-2.544018	0.933533	-1.305368
6	1.185477	1.245484	-0.131106
1	1.698953	2.186094	-0.020349
1	4.849891	-1.018286	0.450535

CAGly_dA3

C	-0.14814176	1.12209549	-0.37013540
C	1.91813142	-0.02270247	-0.01337100
C	1.26348457	-1.22352685	-0.13490422
C	-0.13655505	-1.29336245	-0.37690545
H	1.79008200	-2.15900953	-0.03851439
O	-0.78873591	-2.35944986	-0.46965268
C	3.42630462	0.01833078	0.24768726
O	3.97069566	1.15519438	0.27853267
O	4.01751139	-1.08238699	0.40905420
N	-0.80355204	-0.06295465	-0.52689408
C	-3.12122044	-0.01204688	0.50027511
O	-2.56792526	0.03099888	1.62599940
O	-4.36264764	-0.00892302	0.27429669
O	-0.93962370	2.20946774	-0.48317556
C	-2.24790653	-0.07913742	-0.76780579
H	-2.48088768	-0.99947725	-1.29218843
H	-2.50905125	0.75225728	-1.41366367
C	1.19908304	1.18033504	-0.12741428
H	1.67680030	2.14038389	-0.02081845
H	-0.40535467	3.00740771	-0.37155148

CAGly_dA4

C	-0.03015438	1.38528389	-0.31727593
C	1.92129745	-0.04918868	-0.02804072
C	1.14684614	-1.18855448	-0.21054239
C	-0.23837892	-1.08816924	-0.44660237
H	1.57884656	-2.17456819	-0.16238246
O	-1.02781689	-2.06720210	-0.59565045
C	3.42240183	-0.18667429	0.24060978
O	4.07430936	0.87015036	0.46944070
O	3.91821352	-1.34795538	0.21742171
N	-0.77471240	0.20784636	-0.51890599
C	-3.10235377	-0.10405512	0.35083430
O	-2.53620041	-0.02721520	1.56313562
O	-4.26118965	-0.42913166	0.18155965
O	-0.62147405	2.50350939	-0.36400121
C	-2.19793080	0.31478050	-0.78341347
H	-2.47078616	-0.27675465	-1.65193531
H	-2.41998066	1.35946110	-0.99229174
C	1.34858786	1.21585634	-0.07859269
H	1.94123265	2.10314736	0.07099544
H	-3.19495313	-0.27912687	2.23084873

CAGly_tA

6	-0.149226	1.251184	-0.371375
6	1.910909	-0.004733	-0.018622

6	1.219436	-1.203473	-0.137960
6	-0.170622	-1.221647	-0.377905
1	1.719489	-2.152776	-0.039262
8	-0.862323	-2.280917	-0.477160
6	3.419039	-0.019014	0.243007
8	4.003976	1.093902	0.364676
8	3.990372	-1.143146	0.318795
7	-0.806104	0.020570	-0.522406
6	-3.135833	-0.009557	0.484569
8	-2.609066	0.003545	1.625646
8	-4.377294	-0.048437	0.244694
8	-0.820813	2.323905	-0.464854
6	-2.242184	0.029203	-0.768111
1	-2.493854	-0.828697	-1.383267
1	-2.490282	0.928725	-1.322623
6	1.240334	1.206653	-0.131127
1	1.757434	2.146258	-0.027241

HPPT_C1

6	0.206290	-0.855181	0.000466
6	0.362748	0.529479	0.000560
6	-0.750320	1.337206	0.000143
6	-2.127719	-0.629584	-0.000057
6	-1.014096	-1.475545	0.000030
6	1.591808	-1.449335	0.000034
6	1.795349	0.859433	0.000071
1	-2.784903	1.317820	-0.000060
1	-1.150541	-2.544680	-0.000226
1	3.462059	-0.459302	0.000115
7	2.454341	-0.368278	-0.000472
7	-1.961516	0.717205	0.000015
8	-3.340242	-1.138033	-0.000064
8	1.899952	-2.619655	-0.000055
8	2.320209	1.954791	-0.000103
8	-0.804678	2.650902	-0.000134
1	-4.050787	-0.474690	-0.001205
1	0.088103	3.035485	-0.000046

HPPT_C2

6	0.201915	-0.750677	0.000357
6	0.327001	0.636190	0.000403
6	-0.822522	1.476581	0.000142
6	-2.135100	-0.606476	-0.000030
6	-0.995086	-1.421770	0.000287
6	1.587486	-1.291501	-0.000091
6	1.728062	0.990249	0.000130
1	-2.884144	1.276042	-0.000711
1	-1.090224	-2.495842	0.000417
1	3.443373	-0.380389	-0.000489
7	2.432727	-0.289250	-0.000053
7	-2.025325	0.732613	-0.000144
8	-3.377322	-1.052209	-0.000042
8	1.991198	-2.508716	-0.000239
8	2.316162	2.041509	-0.000157
8	-0.871528	2.705351	-0.000086
1	1.271005	-3.164418	0.000302
1	-3.410435	-2.022000	-0.001137

HPPT_C3

6	0.126948	-0.863735	0.000037
6	0.361237	0.515176	-0.000045
6	-0.695362	1.465169	0.000023
6	-2.184545	-0.484376	0.000277
6	-1.121122	-1.411306	0.000198
6	1.477146	-1.535623	-0.000098
6	1.757808	0.713476	-0.000204
1	-2.770595	1.456672	0.000263
1	-1.323431	-2.470605	0.000255
1	3.407742	-0.589955	-0.000438
7	2.401420	-0.475666	-0.000262
7	-1.961124	0.841917	0.000204
8	-3.455953	-0.820140	0.000391
8	1.752191	-2.705976	-0.000133
8	2.430579	1.815508	-0.000354
8	-0.600292	2.691302	-0.000014
1	1.831075	2.585728	-0.000327
1	-3.571731	-1.783846	0.000408

HPPT_C4

6	0.227420	-0.806637	0.000317
6	0.241624	0.613203	0.000300
6	-0.964062	1.283398	0.000109
6	-2.167042	-0.860656	-0.000069
6	-0.894127	-1.558516	0.000199
6	1.639676	-1.218843	0.000013
6	1.604157	1.076415	-0.000043
1	-2.982658	1.035348	0.000046
1	-0.896930	-2.636618	0.000398
1	3.416485	-0.145041	-0.000177
7	2.401119	-0.144369	-0.000088
7	-2.094617	0.542388	0.000021
8	-3.267620	-1.406784	-0.000319
8	2.013589	-2.446621	0.000045
8	2.104758	2.175244	-0.000147
8	-1.159114	2.588614	0.000023
1	-0.322649	3.081926	-0.000426
1	2.981453	-2.575564	-0.001144

HPPT_N1

6	-0.188338	-0.869398	0.000139
6	-0.306765	0.538089	0.000235
6	0.833106	1.302837	-0.000042
6	2.204843	-0.733674	-0.000330
6	0.996615	-1.523642	-0.000157
6	-1.588013	-1.414431	0.000402
6	-1.710665	0.904137	0.000606
1	2.868119	1.222788	-0.000436
1	1.085373	-2.598469	-0.000247
1	-3.423760	-0.364995	-0.000195
7	-2.414409	-0.307936	0.000125
7	2.023651	0.660053	-0.000277
8	3.355671	-1.184849	-0.000626
8	-1.945978	-2.576310	-0.000038
8	-2.225635	2.012639	0.000261
8	0.908630	2.627795	-0.000018
1	0.019370	3.018151	0.000189

HPPT_N2

6	0.196946	-0.800036	0.000009
6	0.371982	0.575068	-0.000058
6	-0.740582	1.456836	0.000091
6	-2.131438	-0.580246	0.000220
6	-1.028552	-1.428987	0.000148
6	1.564896	-1.429222	-0.000010
6	1.803129	0.869849	-0.000358
1	-2.795998	1.352527	0.000266
1	-1.159744	-2.498150	0.000208
1	3.455247	-0.484578	-0.000326
7	2.450314	-0.378396	-0.000227
7	-1.970726	0.760653	0.000200
8	-3.356612	-1.094471	0.000357
8	1.841940	-2.613247	-0.000032
8	2.388381	1.939087	-0.000376
8	-0.751350	2.692957	-0.000010
1	-4.053784	-0.419778	0.000265

HPPT_N3

6	0.212114	-0.784891	-0.000000
6	0.338379	0.545029	-0.000062
6	-0.820227	1.437337	0.000053
6	-2.270746	-0.590059	0.000277
6	-1.071349	-1.508014	0.000214
6	1.590834	-1.388302	-0.000160
6	1.789700	0.899777	-0.000284
1	-2.865732	1.365724	0.000263
1	-1.145482	-2.166830	-0.869433
1	3.469944	-0.405009	-0.000314
7	2.462915	-0.318137	-0.000246
7	-2.041435	0.773923	0.000217
8	-3.412923	-1.019162	0.000392
8	1.883633	-2.564358	-0.000120
8	2.312119	1.991902	-0.000322

8	-0.767333	2.656243	-0.000021
1	-1.145272	-2.166635	0.870031

HPPT_N4

6	0.130234	-0.886596	0.000027
6	0.300074	0.525397	-0.000013
6	-0.810017	1.414551	0.000127
6	-2.255647	-0.623641	0.000232
6	-1.077300	-1.482611	0.000158
6	1.508627	-1.484289	-0.000079
6	1.660089	0.783750	-0.000224
1	-2.863488	1.333511	0.000246
1	-1.224049	-2.551060	0.000191
1	3.380152	-0.446351	-0.000384
7	2.370840	-0.385255	-0.000225
7	-2.033857	0.751367	0.000209
8	-3.413070	-1.055011	0.000326
8	1.850727	-2.646042	-0.000101
8	2.306139	1.918354	-0.000377
8	-0.751341	2.653029	0.000036
1	1.672510	2.659109	-0.000368

HPPT_A1

6	-0.176715	-0.813469	-0.000030
6	-0.316307	0.587618	0.000033
6	0.828998	1.421157	-0.000099
6	2.210012	-0.676540	-0.000290
6	1.011835	-1.472770	-0.000181
6	-1.560802	-1.396840	0.000094
6	-1.717241	0.916615	0.000260
1	1.097407	-2.547768	-0.000212
1	-3.416356	-0.393181	0.000369
7	-2.409071	-0.320879	0.000248
7	2.029603	0.701853	-0.000214
8	3.369516	-1.139008	-0.000349
8	-1.885258	-2.575126	0.000095
8	-2.300053	1.997987	0.000364
8	0.868377	2.668841	0.000031
1	2.875878	1.257955	-0.000242

HPPT_dA1

6	-0.148087	-0.817681	-0.000176
6	-0.284657	0.586038	-0.000174
6	0.888602	1.405835	0.000014
6	2.233281	-0.566507	0.000384
6	1.061672	-1.429224	-0.000101
6	-1.520645	-1.410412	-0.000375
6	-1.677759	0.905411	-0.000373
1	1.185689	-2.502078	-0.000324
1	-3.380279	-0.415135	0.001168
7	-2.373792	-0.340641	0.000398
7	2.107553	0.785316	0.000080
8	3.396551	-1.098714	-0.000502
8	-1.847118	-2.594117	0.000163
8	-2.286207	1.981564	0.000544
8	0.829752	2.681733	-0.000127

HPPT_dA2

6	0.199566	-0.812456	-0.000050
6	0.352373	0.576568	-0.000140
6	-0.775865	1.419803	-0.000006
6	-2.185223	-0.659889	0.000233
6	-1.001235	-1.463357	0.000128
6	1.611305	-1.366281	-0.000183
6	1.794830	0.836836	-0.000380
1	-1.098031	-2.538105	0.000192
7	2.503697	-0.355228	-0.000139
7	-1.989233	0.715902	0.000170
8	-3.361122	-1.104527	0.000399
8	1.875217	-2.586079	0.000026
8	2.344059	1.956426	-0.000163
8	-0.814355	2.677194	-0.000048
1	-2.828114	1.281936	0.000255

HPPT_tA

6	0.168824	-0.817406	0.000058
6	0.320230	0.572856	0.000031
6	-0.833164	1.405057	0.000161
6	-2.208341	-0.546967	0.000201
6	-1.053161	-1.418671	0.000193
6	1.570838	-1.381323	-0.000114
6	1.755463	0.822886	-0.000149
1	-1.190960	-2.490787	0.000228
7	2.468871	-0.377430	-0.000274
7	-2.066007	0.803497	0.000174
8	-3.391329	-1.060860	0.000303
8	1.835631	-2.607282	-0.000079
8	2.328892	1.937528	-0.000372
8	-0.767347	2.691829	-0.000080

-Explicitly DMSO solvation

N1_1DMSO

6	3.295779	1.549890	0.103973
6	1.919544	1.043972	0.000122
6	1.652168	-0.262604	-0.078360
6	2.732755	-1.295588	-0.066992
6	4.144499	-0.774216	0.039319
7	4.303186	0.595126	0.117161
1	1.144270	1.793627	-0.008510
1	2.580116	-1.992518	0.760340
8	5.112068	-1.512579	0.057251
8	3.564580	2.738242	0.176377
6	0.246567	-0.778127	-0.189016
8	0.015481	-1.967571	-0.296599
8	-0.675255	0.169190	-0.157810
1	-1.614417	-0.205655	-0.225003
1	2.678308	-1.909244	-0.968871
1	5.253791	0.940396	0.187404
8	-3.154342	-0.582110	-0.322931
16	-4.158824	0.457652	0.205109
6	-5.336937	0.727171	-1.140450
1	-4.796927	1.225054	-1.942642
1	-5.727409	-0.232684	-1.472560
1	-6.134539	1.371868	-0.773319
6	-5.244088	-0.445320	1.334988
1	-6.047926	0.221569	1.643702
1	-5.634822	-1.325850	0.828880
1	-4.643534	-0.727332	2.196909

N2_1DMSO

6	2.984280	-1.697632	-0.175728
6	3.252326	-0.289264	-0.108397
6	2.226971	0.609052	0.063551
6	0.609232	-1.144740	0.117926
7	1.629921	-2.027348	-0.053301
1	4.278813	0.024267	-0.197532
8	3.820187	-2.595463	-0.326455
6	2.499263	2.080105	0.134344
8	1.642856	2.922826	0.276277
8	3.804106	2.389960	0.024007
1	3.881089	3.356599	0.080409
1	1.399374	-3.012592	-0.095050
8	-0.581244	-1.713051	0.209155
1	-1.326611	-1.035617	0.330361
6	0.880897	0.203251	0.181207
1	0.086807	0.916799	0.317150
8	-2.511751	-0.060527	0.565681
16	-3.726975	-0.166089	-0.377489
6	-5.150442	-0.450668	0.699353
1	-5.028519	-1.440469	1.133554
1	-5.173355	0.314106	1.473116
1	-6.051455	-0.421467	0.088175
6	-4.095496	1.531736	-0.874366
1	-4.186510	2.152463	0.014609
1	-3.271853	1.867545	-1.500268
1	-5.021063	1.526233	-1.448268

N3_1DMSO

6	3.576796	1.180513	-0.054578
6	2.183116	1.160999	-0.112245

6	1.558054	-0.079046	-0.035087
6	3.708837	-1.079643	0.145996
7	4.325283	0.093162	0.071775
1	1.616223	2.073177	-0.213689
8	4.283851	2.334639	-0.125328
6	0.061360	-0.212376	-0.095063
8	-0.498108	-1.291603	-0.054686
8	-0.564554	0.948903	-0.194492
1	-1.568935	0.824226	-0.252766
8	4.546248	-2.137325	0.275668
1	4.029858	-2.953412	0.322923
6	2.324757	-1.231406	0.096321
1	1.860342	-2.203995	0.156883
1	3.675428	3.080704	-0.215573
8	-3.141655	0.889712	-0.425504
16	-4.005911	-0.123184	0.345842
6	-4.731345	-1.206677	-0.907910
1	-5.446721	-1.866723	-0.419287
1	-5.213010	-0.599137	-1.671547
1	-3.917713	-1.790063	-1.332536
6	-5.498171	0.787473	0.807366
1	-5.201889	1.535429	1.539364
1	-5.920155	1.257175	-0.078837
1	-6.202507	0.087808	1.255101

N1_2DMSO

6	1.464956	-0.473524	0.143555
6	0.006994	-0.273387	0.113734
6	-0.537882	0.945026	0.076601
6	0.302791	2.179608	0.065937
6	1.798230	1.962817	0.089869
7	2.256090	0.662692	0.124333
1	-0.589459	-1.171834	0.121806
1	0.074623	2.784406	-0.814541
8	2.576741	2.900876	0.079883
8	1.968017	-1.587459	0.181486
6	-2.023525	1.148822	0.040890
8	-2.511038	2.263035	0.004782
8	-2.719721	0.023581	0.050876
1	-3.717219	0.191553	0.015160
1	0.052179	2.814186	0.919181
1	3.279037	0.516214	0.145713
8	-5.308481	0.241380	-0.053131
16	-6.057325	-1.102474	-0.016070
6	-7.386728	-0.883388	1.190038
1	-6.918368	-0.779870	2.166255
1	-7.956648	0.008189	0.936139
1	-8.015885	-1.772234	1.171473
6	-7.063911	-1.142553	-1.518332
1	-7.700301	-2.025728	-1.482077
1	-7.656468	-0.231745	-1.575751
1	-6.378270	-1.213239	-2.359788
8	5.079731	0.240898	0.247411
16	5.701056	-1.009601	-0.375937
6	7.343276	-0.509167	-0.956552
1	7.882137	-0.031568	-0.140435
1	7.870085	-1.393900	-1.311640
1	7.192364	0.187024	-1.778668
6	6.234714	-2.055905	1.005082
1	6.854209	-1.468647	1.680427
1	5.334766	-2.401079	1.508974
1	6.785418	-2.905945	0.604169

N2_2DMSO

6	-0.592738	3.516435	0.275747
6	0.411926	2.503597	0.128672
6	0.062479	1.199863	-0.127552
6	-2.260512	1.756831	-0.111599
7	-1.903633	3.045067	0.140536
1	1.441160	2.806035	0.224887
8	-0.398196	4.717044	0.502447
6	1.115284	0.133310	-0.288224
8	0.835299	-1.021353	-0.546467
8	2.351577	0.579293	-0.121782
1	3.036250	-0.153860	-0.230854
8	-3.569146	1.570054	-0.192369

1	-3.812697	0.605168	-0.377179
6	-1.284168	0.798303	-0.254796
1	-1.544413	-0.225715	-0.458346
8	-4.307041	-0.836885	-0.725401
16	-4.753787	-1.756180	0.428134
6	-6.438025	-2.266938	0.015135
1	-7.067125	-1.382629	0.086924
1	-6.451348	-2.672498	-0.994516
1	-6.757295	-3.010988	0.743627
6	-3.916724	-3.331244	0.135993
1	-4.107955	-3.651478	-0.886201
1	-2.854319	-3.164902	0.298484
1	-4.294539	-4.057585	0.854093
8	4.294150	-1.148949	-0.380625
16	5.608890	-0.746347	0.307794
6	6.203758	-2.244415	1.127997
1	7.194851	-2.044576	1.533010
1	5.509128	-2.462597	1.935950
1	6.229698	-3.060040	0.407960
6	6.845575	-0.654053	-1.009514
1	6.832753	-1.581483	-1.578507
1	6.577209	0.191180	-1.639553
1	7.820467	-0.483676	-0.554551
1	-2.642302	3.730836	0.238617

N3_2DMSO

6	-0.541644	3.398059	0.166615
6	0.488443	2.460611	0.112637
6	0.123405	1.127969	-0.063724
6	-2.164696	1.816620	-0.109713
7	-1.827467	3.096264	0.059749
1	1.521205	2.758479	0.203941
8	-0.296527	4.723359	0.337584
6	1.151315	0.032893	-0.134165
8	0.852231	-1.137332	-0.271079
8	2.395862	0.477214	-0.031731
1	3.071003	-0.272046	-0.079634
8	-3.478695	1.589390	-0.211495
1	-3.680410	0.618494	-0.321541
6	-1.217583	0.787665	-0.178007
1	-1.520683	-0.237739	-0.315080
8	-4.102489	-0.952101	-0.540488
16	-5.216881	-1.540118	0.339880
6	-6.424535	-2.247176	-0.806653
1	-6.879888	-1.417358	-1.342317
1	-5.914574	-2.919521	-1.493665
1	-7.180695	-2.774819	-0.226946
6	-4.550467	-3.085051	1.005339
1	-4.172727	-3.693465	0.185925
1	-3.749761	-2.818873	1.691614
1	-5.346089	-3.598818	1.543174
8	4.301838	-1.304794	-0.129954
16	5.721296	-0.733724	0.025683
6	6.478156	-1.667070	1.377962
1	7.524471	-1.374239	1.453851
1	5.949150	-1.394563	2.288477
1	6.380788	-2.732020	1.176281
6	6.677365	-1.428133	-1.343651
1	6.558704	-2.509807	-1.349049
1	6.286871	-0.990621	-2.259637
1	7.721048	-1.146186	-1.211776
1	0.656916	4.866519	0.406588

N2_3DMSO

6	-0.584252	-2.823442	0.121920
6	0.793195	-2.431143	0.021826
6	1.145523	-1.104903	-0.030660
6	-1.146679	-0.447928	0.102978
7	-1.493511	-1.760186	0.153502
1	1.531382	-3.215096	-0.009757
8	-0.996649	-3.990045	0.179381
6	2.588456	-0.688323	-0.137911
8	2.928582	0.480029	-0.169970
8	3.435928	-1.705303	-0.195188
1	4.389535	-1.382410	-0.281644
8	-2.176777	0.388176	0.148421

1	-1.879471	1.349251	0.110869
6	0.177663	-0.080834	0.010976
1	0.458396	0.957473	-0.030096
8	-1.441689	2.876022	0.050002
16	-2.535493	3.959342	0.034651
6	-2.067830	5.137314	1.324343
1	-2.178003	4.626639	2.278317
1	-1.037165	5.448731	1.167029
1	-2.748398	5.986291	1.276031
6	-2.180454	4.986787	-1.410461
1	-1.143532	5.314157	-1.369544
1	-2.359843	4.372815	-2.290207
1	-2.863022	5.835589	-1.403509
8	5.959285	-1.136818	-0.483114
16	6.613829	-0.008415	0.331079
6	7.066314	1.269863	-0.867096
1	7.642557	2.035872	-0.349905
1	7.643844	0.818710	-1.671568
1	6.139441	1.694304	-1.245699
6	8.276255	-0.605466	0.718297
1	8.165421	-1.437563	1.409953
1	8.763684	-0.927041	-0.199863
1	8.828354	0.203266	1.194951
1	-2.496660	-1.991753	0.221734
8	-4.290549	-2.368943	0.397271
16	-5.357534	-1.571018	-0.350964
6	-6.641982	-2.766514	-0.806326
1	-6.949817	-3.316029	0.081364
1	-7.479978	-2.227248	-1.245805
1	-6.205862	-3.437725	-1.542908
6	-6.298857	-0.668821	0.909022
1	-6.635803	-1.367752	1.672452
1	-5.630028	0.075398	1.335241
1	-7.142450	-0.177613	0.425938

N3_3DMSO

6	-1.026714	-2.286131	0.121135
6	-1.102742	-0.890210	0.202138
6	0.083326	-0.173831	0.081697
6	1.245979	-2.242761	-0.173783
7	0.117327	-2.943155	-0.061167
1	-2.050180	-0.399456	0.350949
8	-2.113325	-3.066555	0.223594
6	0.105996	1.326848	0.153822
8	1.131366	1.973671	0.047336
8	-1.090976	1.864949	0.341848
1	-1.036675	2.872086	0.395369
8	2.350148	-2.981663	-0.355673
1	3.166475	-2.416203	-0.422872
6	1.285003	-0.845993	-0.110378
1	2.214694	-0.308848	-0.206295
8	4.582207	-1.572284	-0.589679
16	5.786451	-1.981575	0.271750
6	7.118537	-2.362545	-0.892696
1	6.823582	-3.259427	-1.432913
1	7.248547	-1.524337	-1.574498
1	8.027796	-2.553398	-0.324128
6	6.456851	-0.439350	0.939603
1	6.628320	0.258688	0.122522
1	5.720757	-0.046425	1.637307
1	7.383296	-0.666329	1.465455
1	-2.939506	-2.530402	0.356317
8	-4.339422	-1.669932	0.645998
16	-5.770878	-1.983817	0.195894
6	-6.105178	-3.698186	0.677976
1	-7.092033	-3.969574	0.305058
1	-5.338792	-4.351481	0.265889
1	-6.098260	-3.729946	1.765274
6	-5.711054	-2.227877	-1.598663
1	-5.452248	-1.269127	-2.042770
1	-4.964159	-2.981470	-1.839780
1	-6.700968	-2.536181	-1.932631
8	-1.217927	4.455798	0.569468
16	-0.447561	5.374067	-0.393557
6	0.707225	6.312672	0.635619
1	1.192149	7.062569	0.011913
1	0.162391	6.775338	1.456195
1	1.445251	5.606848	1.009708
6	-1.594937	6.713562	-0.794201
1	-2.399643	6.279038	-1.383169
1	-1.978565	7.145022	0.128176
1	-1.062024	7.457230	-1.385038

-Microsolvation

N1_7W

6	1.000228	0.506345	-0.132054
6	-1.007974	-1.036400	-0.111050
6	-0.187767	-2.089431	-0.153147
6	1.267975	-1.922640	-0.175933
1	-0.543161	-3.107152	-0.167240
8	2.031667	-2.883456	-0.199627
6	-2.492973	-1.203322	-0.070794
8	-3.245762	-0.250780	0.082414
8	-2.910323	-2.447616	-0.212730
7	1.763728	-0.629132	-0.174082
8	1.529334	1.616709	-0.132612
6	-0.492855	0.362786	-0.081565
1	-0.835886	0.874909	0.821159
1	-3.914932	-2.493547	-0.159148
1	-3.158152	1.402023	0.980341
8	-3.241715	2.258132	1.436836
1	-2.489448	2.289340	2.039524
1	-2.833895	3.474291	0.156888
1	0.572136	3.277892	-0.352869
8	0.248326	4.183527	-0.487456
8	-2.582170	4.154845	-0.503473
1	-0.726119	4.117455	-0.500405
1	-2.873480	3.802622	-1.351797
1	3.847978	-2.918565	0.489564
8	4.760937	-2.756887	0.777542
1	4.927973	-1.858122	0.445481
1	2.783866	-0.515932	-0.240826
8	4.711266	-0.198225	-0.431605
1	4.973907	-0.156426	-1.357850
1	3.260473	2.165739	0.287845
8	4.187918	2.339521	0.534947
1	4.483348	3.034565	-0.064209
8	-5.531542	-2.688320	-0.048835
1	-5.851487	-3.173480	-0.819766
1	-5.918296	-1.807349	-0.130504
1	4.670712	0.731623	-0.121207
1	-0.904922	0.940398	-0.912338

N2_7W

6	0.913016	0.223305	-0.242142
6	-1.172698	-0.921182	-0.158198
6	-0.536190	-2.119216	0.072987
6	0.883114	-2.171678	0.166381
1	-1.080726	-3.039414	0.202581
8	1.547950	-3.214990	0.385605
6	-2.669200	-0.856152	-0.216802
8	-3.288593	0.193468	-0.098810
8	-3.257331	-2.024441	-0.403159
7	1.537666	-0.960226	-0.003942
8	1.740851	1.253573	-0.375418
6	-0.459360	0.278758	-0.321302
1	-0.956010	1.215827	-0.505216
1	-4.258178	-1.923522	-0.398562
1	-2.855128	1.608506	1.051811
8	-2.789150	2.375196	1.650375
1	-2.229973	2.079231	2.377803
1	-1.897837	3.687562	0.821046
1	1.265956	2.117803	-0.594726
8	0.757967	3.566171	-1.020776
1	1.476299	4.175801	-0.812415
8	-1.395569	4.430259	0.418676
1	-0.013638	3.869233	-0.484774
1	-2.004781	4.843670	-0.203480
1	3.347206	-3.397568	0.325700
8	4.320394	-3.496338	0.293257

1	4.625928	-2.576516	0.256783
1	2.560439	-0.944277	0.065514
8	4.506841	-0.629619	0.218372
1	4.785719	-0.040624	-0.493154
1	3.686177	2.043262	-0.210325
8	4.362329	2.734644	-0.224773
1	3.874561	3.538090	-0.439834
8	-5.897733	-1.898241	-0.362015
1	-6.236696	-2.343763	-1.148444
1	-6.150308	-0.972565	-0.469690
1	4.681585	-0.139621	1.030759

N3_7W

6	0.912918	0.403990	-0.143285
6	-1.064889	-0.920382	-0.151369
6	-0.285619	-2.042932	0.092740
6	1.090833	-1.853917	0.222669
1	-0.707068	-3.029723	0.187502
8	1.852259	-2.937856	0.470321
6	-2.550580	-1.024189	-0.283493
8	-3.295384	-0.056943	-0.185303
8	-2.987208	-2.250059	-0.519884
7	1.677799	-0.661456	0.115544
8	1.588370	1.565652	-0.258368
6	-0.471177	0.332289	-0.273740
1	-1.055284	1.215922	-0.472059
1	-3.989542	-2.263107	-0.586205
1	-3.041105	1.323577	1.056330
8	-3.075160	2.041845	1.714965
1	-2.506111	1.749027	2.435991
1	-2.306110	3.511222	1.042507
1	0.990499	2.330491	-0.497284
8	0.186671	3.692401	-0.981419
1	0.809530	4.426068	-0.921886
8	-1.866785	4.329840	0.722476
1	-0.548490	3.921672	-0.366105
1	-2.537897	4.796344	0.211721
1	2.824678	-2.745716	0.424391
8	4.556550	-2.759727	0.283942
1	4.910850	-3.227216	1.049088
1	4.714119	-1.807309	0.463054
1	3.478525	-0.238745	0.617755
8	4.426619	-0.068961	0.808441
1	4.665590	0.605097	0.148025
1	3.395264	1.887022	-0.973887
8	4.340262	2.040547	-1.141838
1	4.493876	1.700911	-2.030720
8	-5.622882	-2.406325	-0.754045
1	-5.973722	-2.903271	-0.004407
1	-5.977604	-1.514529	-0.648058