Electronic Supplementary Information

# Trifluoroacetic Acid Prompted Unexpected Visible to NIR Switching of Ketoenamine-substituted Triphenylamines

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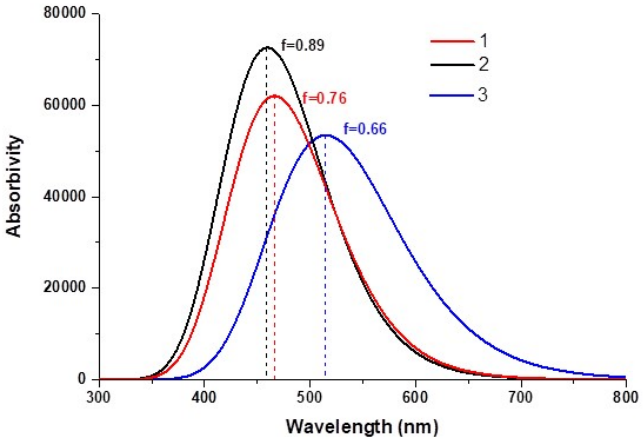


**Fig. S1** Calculated TD-DFT (B3LYP, 6-31G (d)) UV-Vis spectra. Vertical lines indicate the position of the calculated transition. Spectra were generated in Gauss view 5.0, using 0.3 eV line broadening.

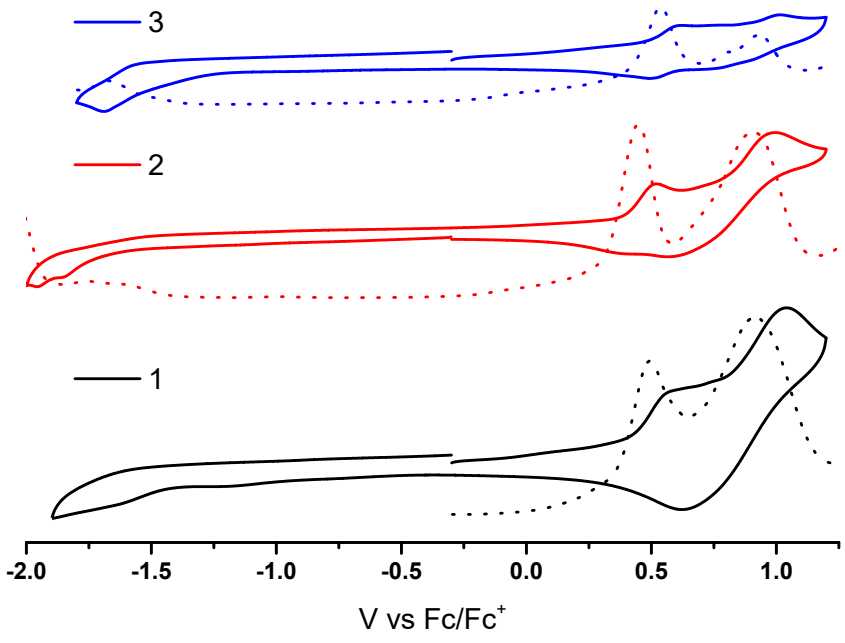


**Fig. S2** Cyclic Voltammogram and Differential Pulse Voltammogram of compounds **1-3** measured in $CH_2Cl_2$ using 0.1 M tetrabutylammonium perchlorate (TBAP) as supporting electrolyte, saturated calomel electrode as a reference.

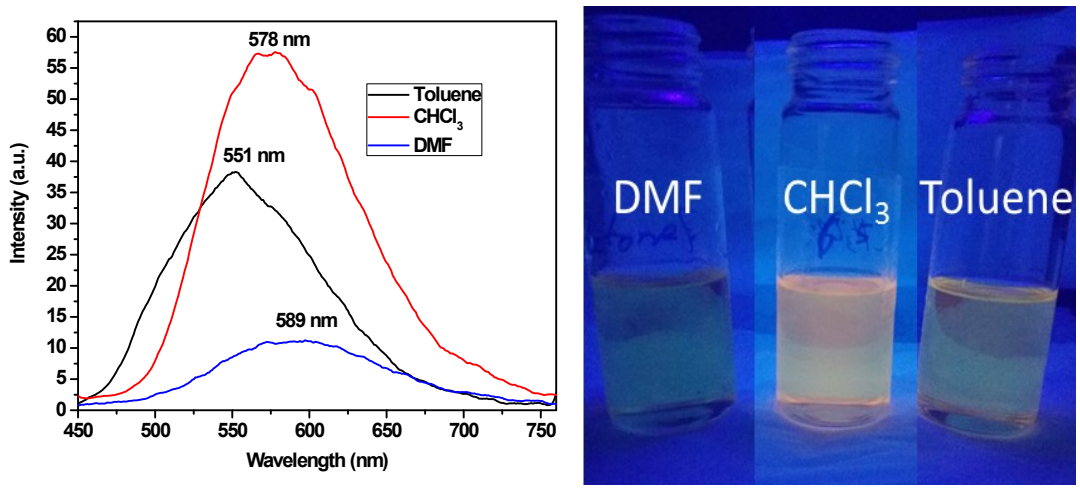


**Fig. S3** Fluorescence spectra of compound **1** in different solvents and a corresponding image of solutions under illumination with 365 nm light.

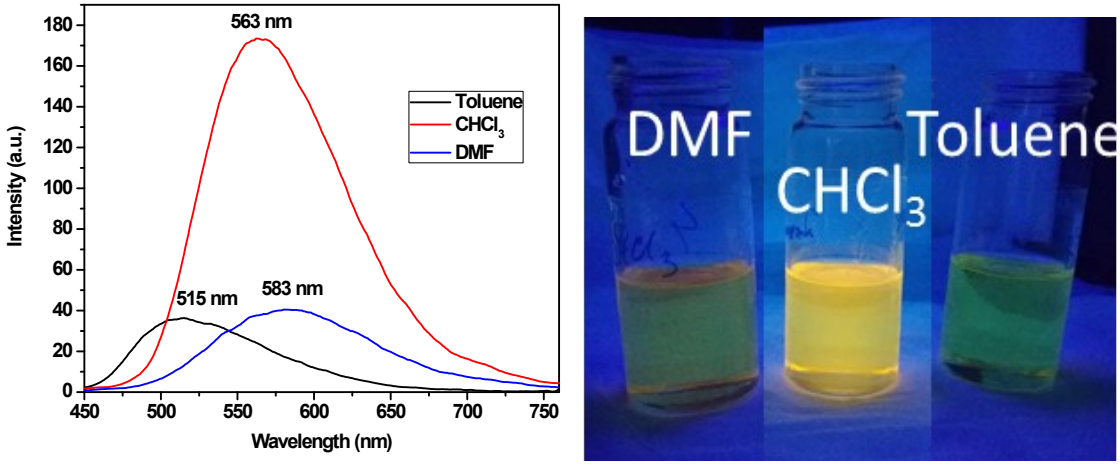


**Fig. S4** Fluorescence spectra of compound **2** in different solvents and a corresponding image of solutions under illumination with 365 nm light.

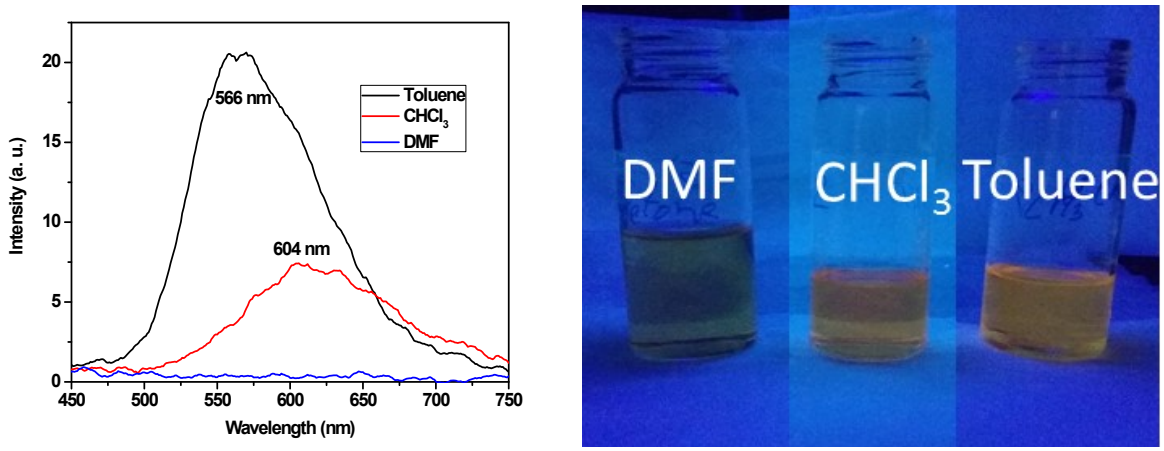


**Fig. S5** Fluorescence spectra of compound **3** in different solvents and a corresponding image of solutions under illumination with 365 nm light.

**Table S1** Fluorescence data of compounds **1-3** in various solvents.

| Compound | Fluorescence $\lambda_{em}$ ($\varphi_f$) in nm | | |
|---|---|---|---|
| | **Toluene** | **$CHCl_3$** | **DMF** |
| **1** | 551 (0.08%) | 578 (0.1%) | 589 (0.02%) |
| **2** | 515 (2.2%) | 563 (1.5%) | 583 (0.95%) |
| **3** | 566 (1.9%) | 604 (1.6%) | -- |

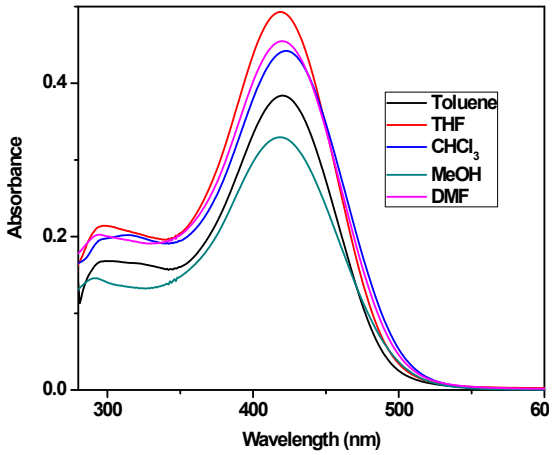


**Fig. S6** UV-Vis absorption spectra of compound **1 (**~1x10$^{-5}$ M) in different solvents.

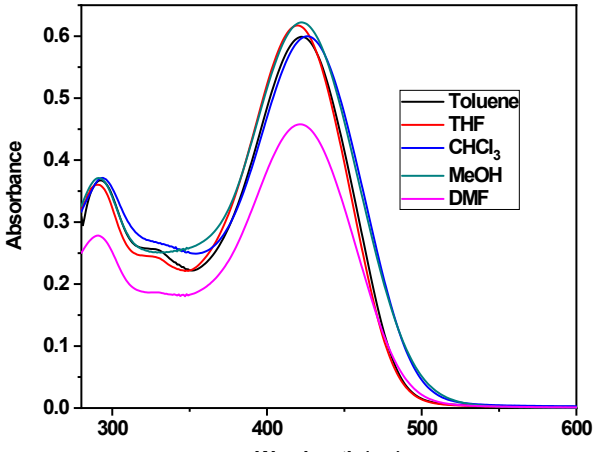


**Fig. S7** UV-Vis absorption spectra of compound **2 (**1x10$^{-5}$ M) in different solvents.

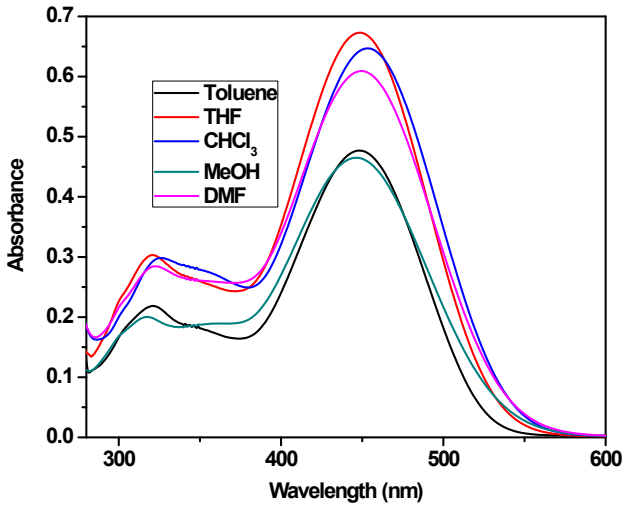


**Fig. S8** UV-Vis absorption spectra of compound **3 (**~1x10$^{-5}$ M) in different solvents**.**

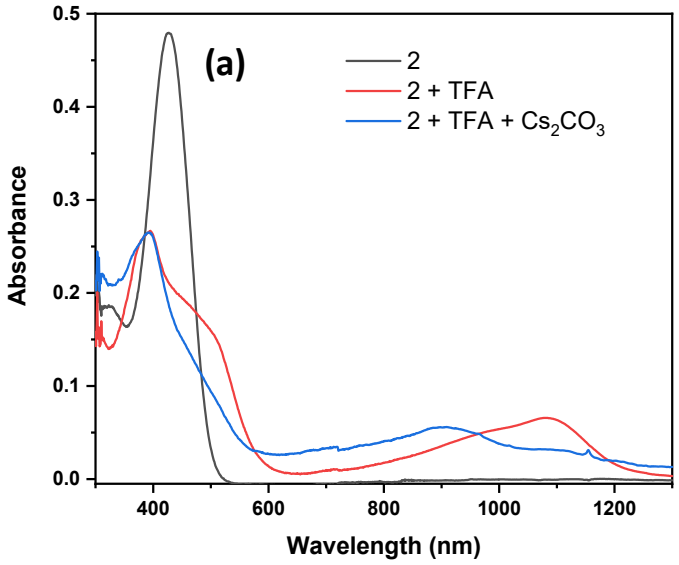


**Fig. S9** UV-Vis absorption spectra of compound **2** after treating acid and neutralization with anhydrous $Cs_2CO_3$ (excess). Clear colour change was observed with blue shifted NIR absorption

## Titration of Compounds **1-3** with TFA

A stock solution of $1\times10^{-3}$ M of compounds **1-3** in chloroform was diluted with chloroform to $1\times10^{-5}$ M concentration. The UV-Vis titration curves were obtained by adding progressive amounts of TFA (in µL, as indicated on the Figures) to 10 mL of the above solution.

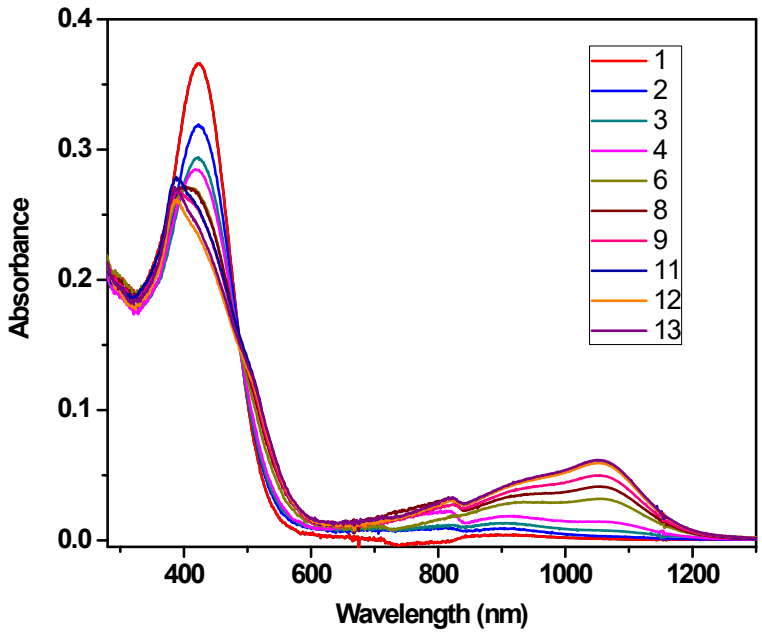


**Fig. S10** Protonation titration of compound **1** in $CHCl_3$ with TFA (in % v/v)

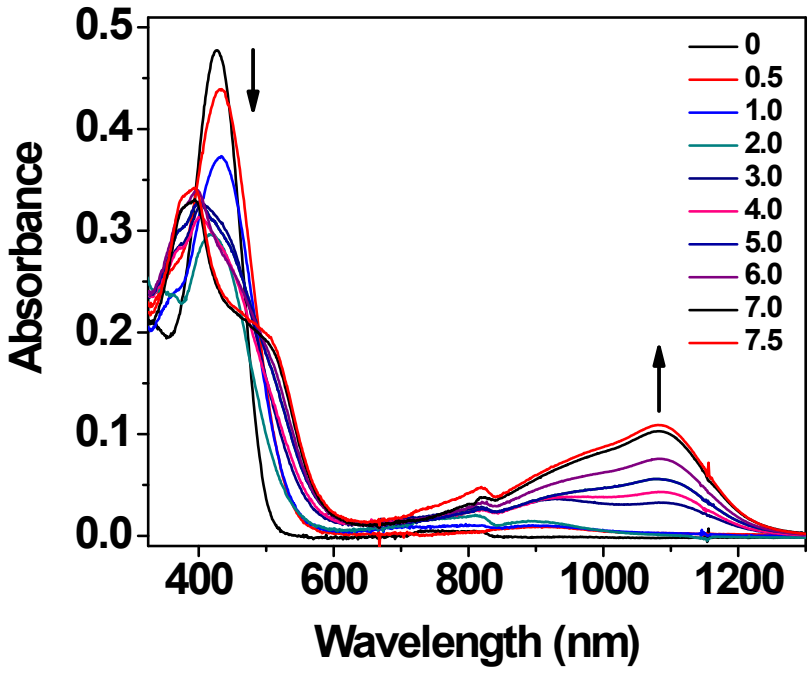


**Fig. S11** Protonation titration of compound **2** in $CHCl_3$ with TFA (in % v/v)

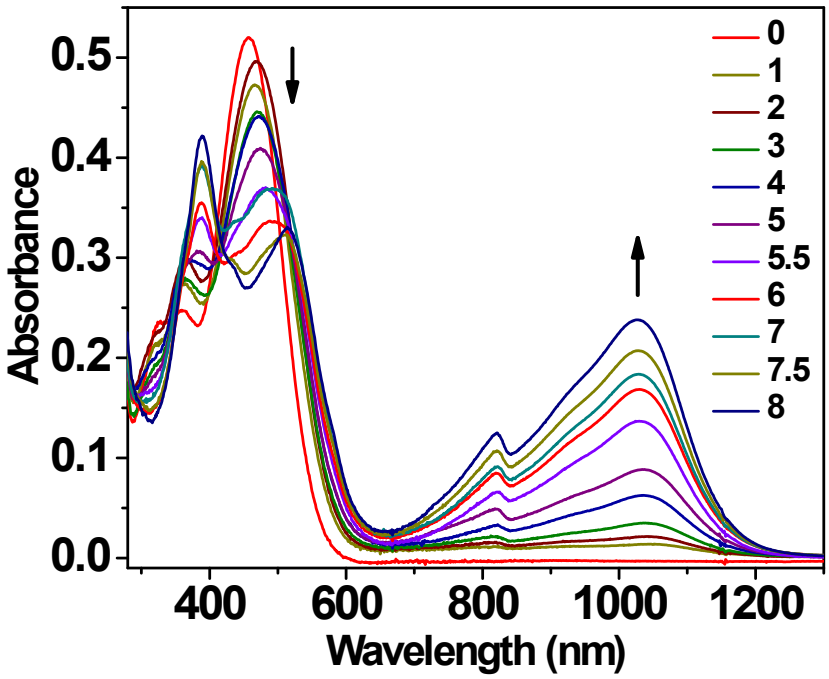


**Fig. S12** Protonation titration of compound **3** in $CHCl_3$ with TFA (in % v/v).

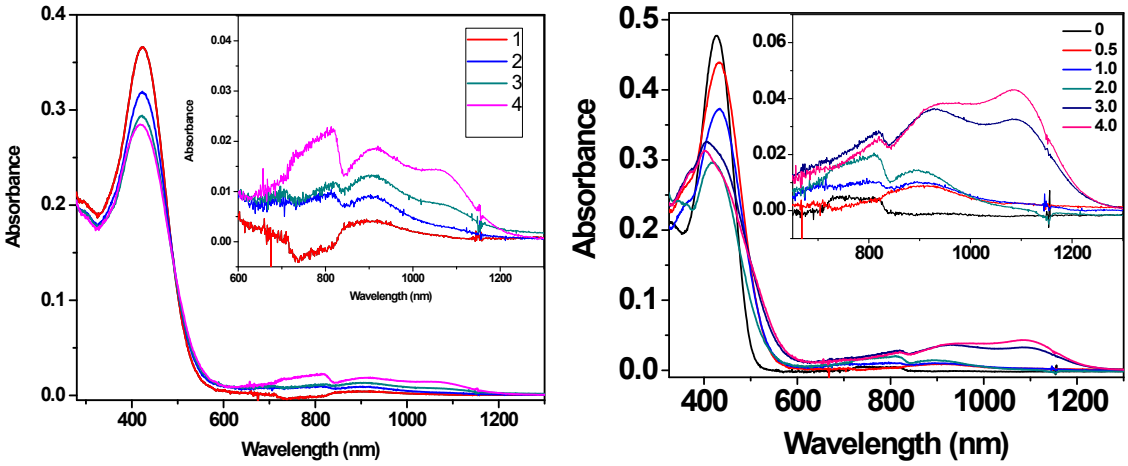


**Fig. S13** Protonation titration of compound **1** and **2** with TFA (up to 4%)

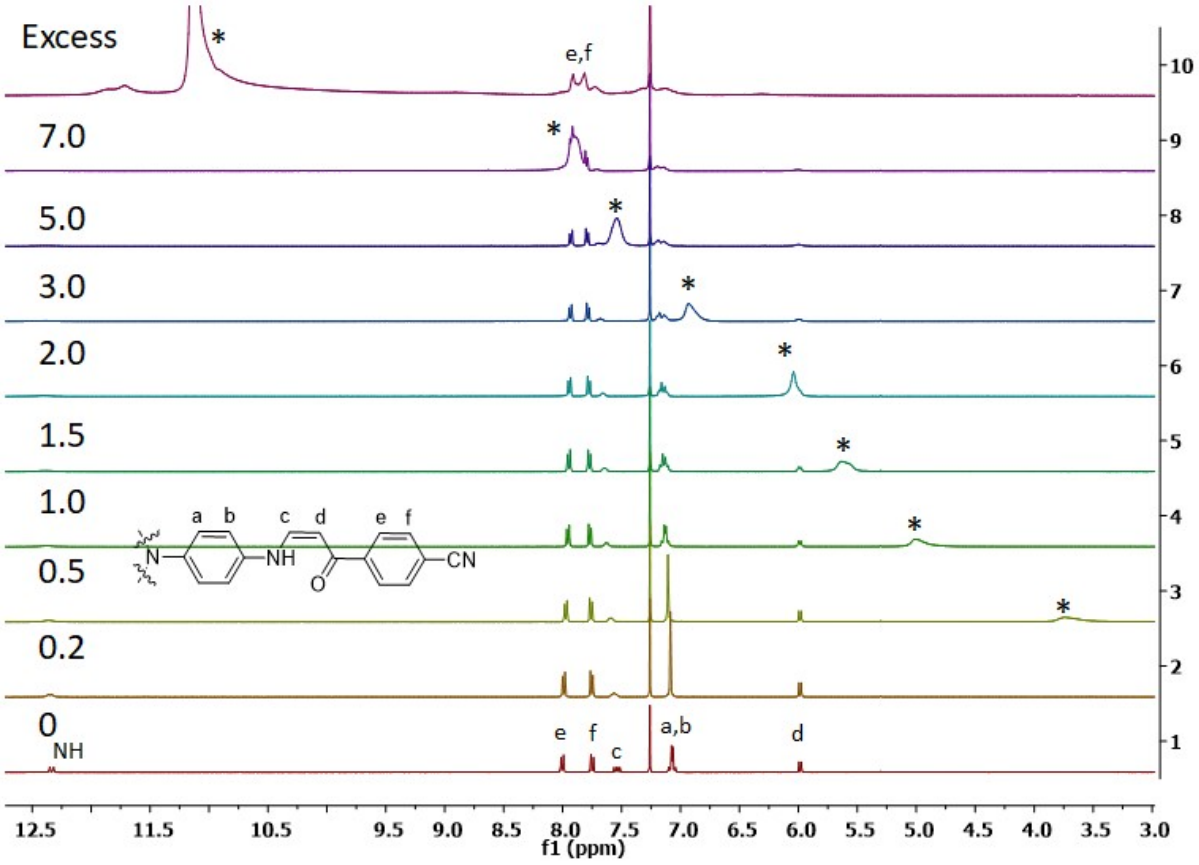


**Fig. S14** $^{1}$H NMR of compound **3** in presence of TFA (no of equivalents is specified).

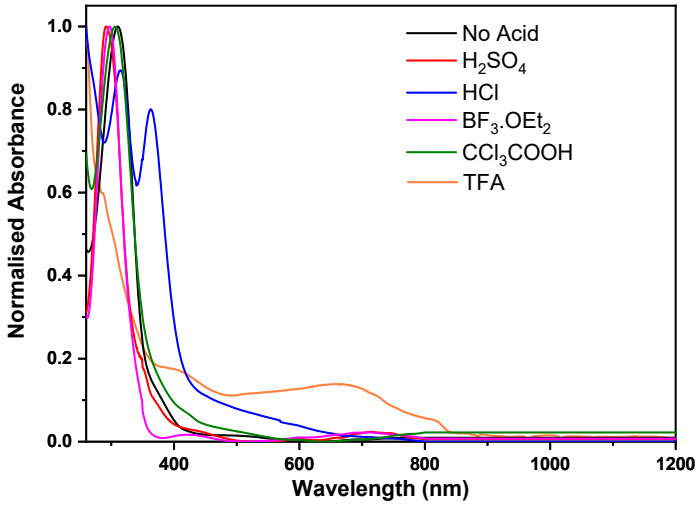


**Fig. S15** UV-Vis absorption spectra of Tris-(*p*-aminophenyl)amine **7** with different acids.

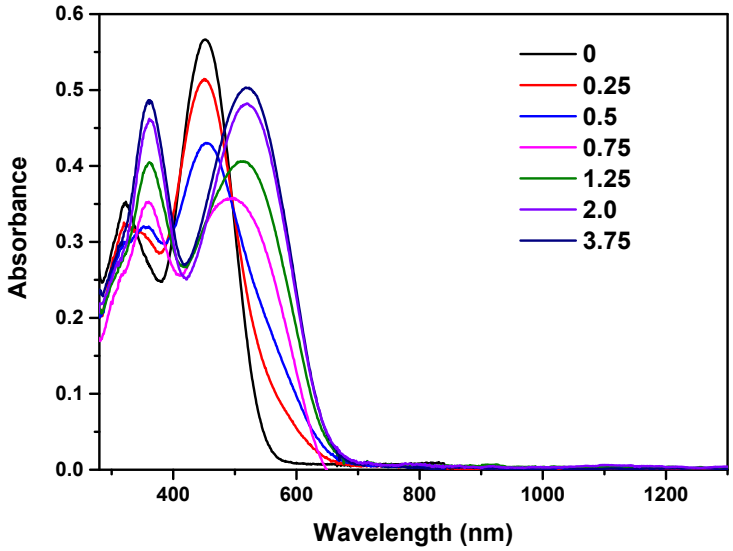


**Fig. S16** Titration of compound **1 (**$CHCl_3$ solution) with *p*-TSA (0 to 3.75% v/v)**.**

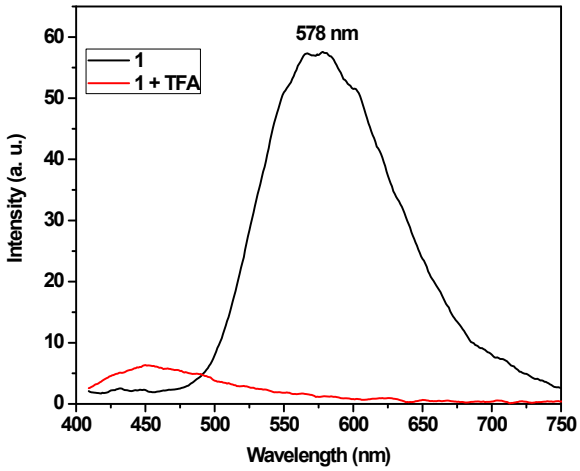


**Fig. S17** Quenching of the fluorescence of **1** (in chloroform) after addition of TFA.

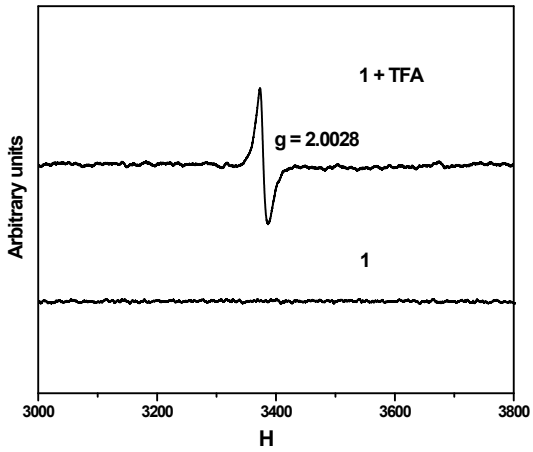


**Fig. S18** EPR spectrum of compound **1** after addition of TFA in toluene.

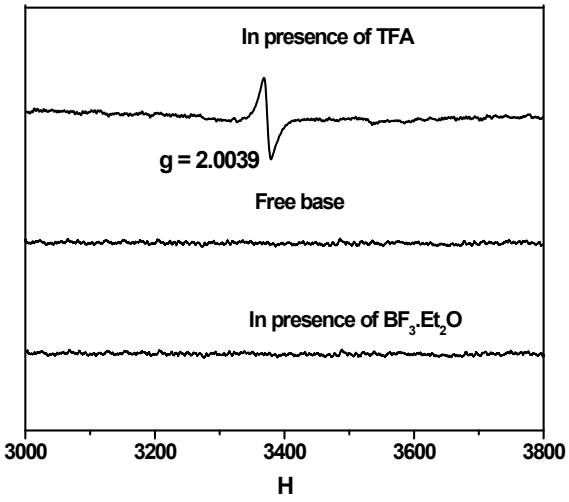


**Fig. S19** ESR spectra of Tris-(p-aminophenyl)amine **7** in presence and absence of TFA in toluene.

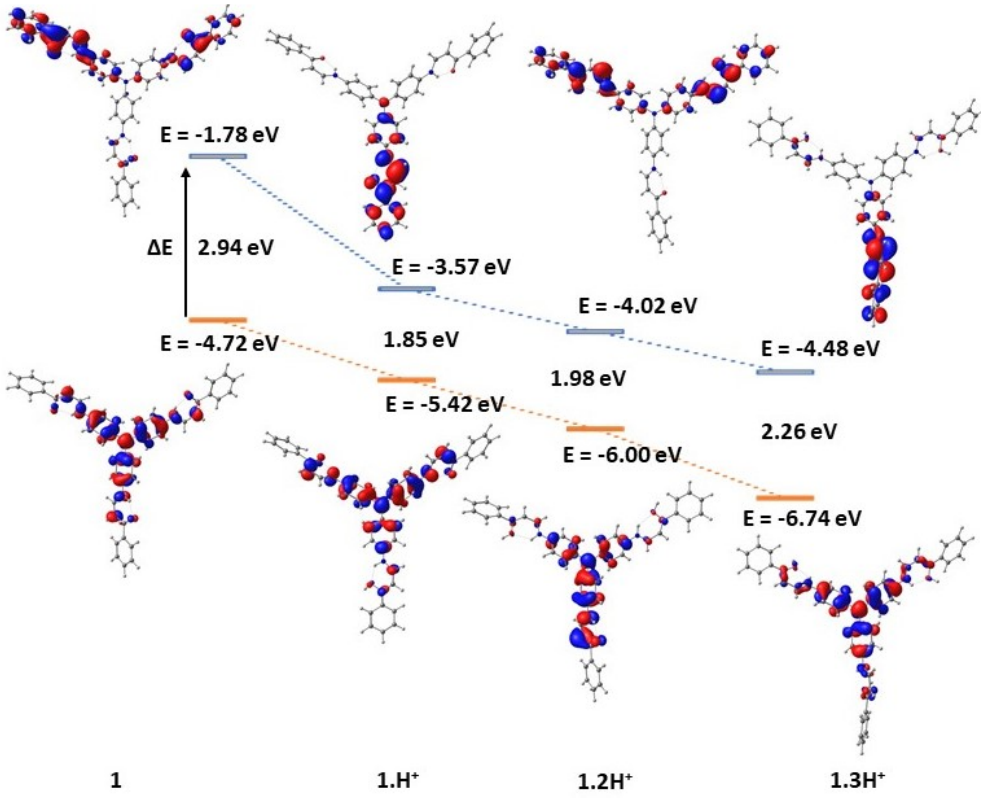


**Fig. S20** DFT calculated HOMO/LUMO frontier orbital topologies and their HOMO-LUMO (H-L) gaps; (B3LYP/6-31G(d), CPCM solvent model; Chloroform).

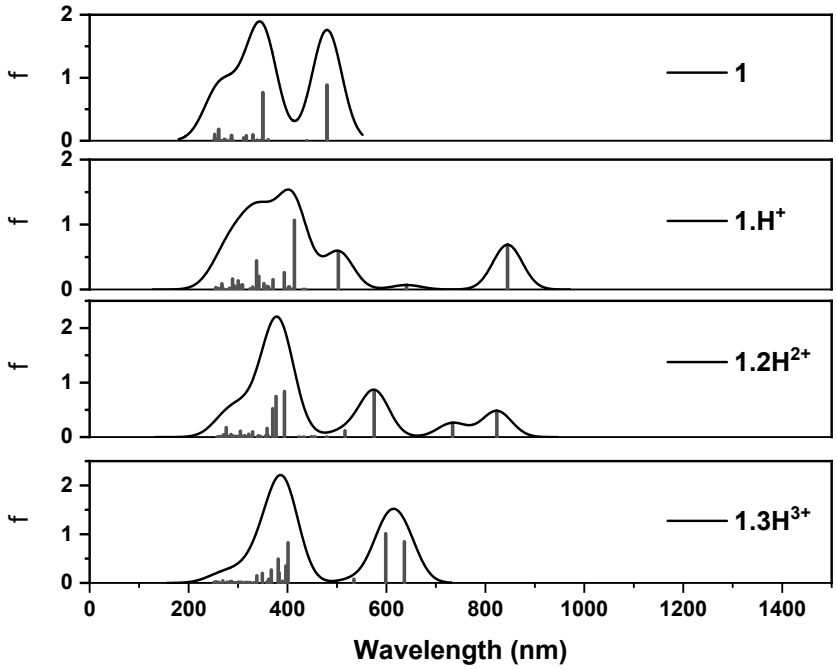


**Fig. S21** TD-DFT spectra of **1**, protonated species **1-H**$^{+}$, **1-2H**$^{+}$ and **1-3H**$^{+}$ in toluene (Using B3LYP/6-31G(d), CPCM solvent model; Chloroform).

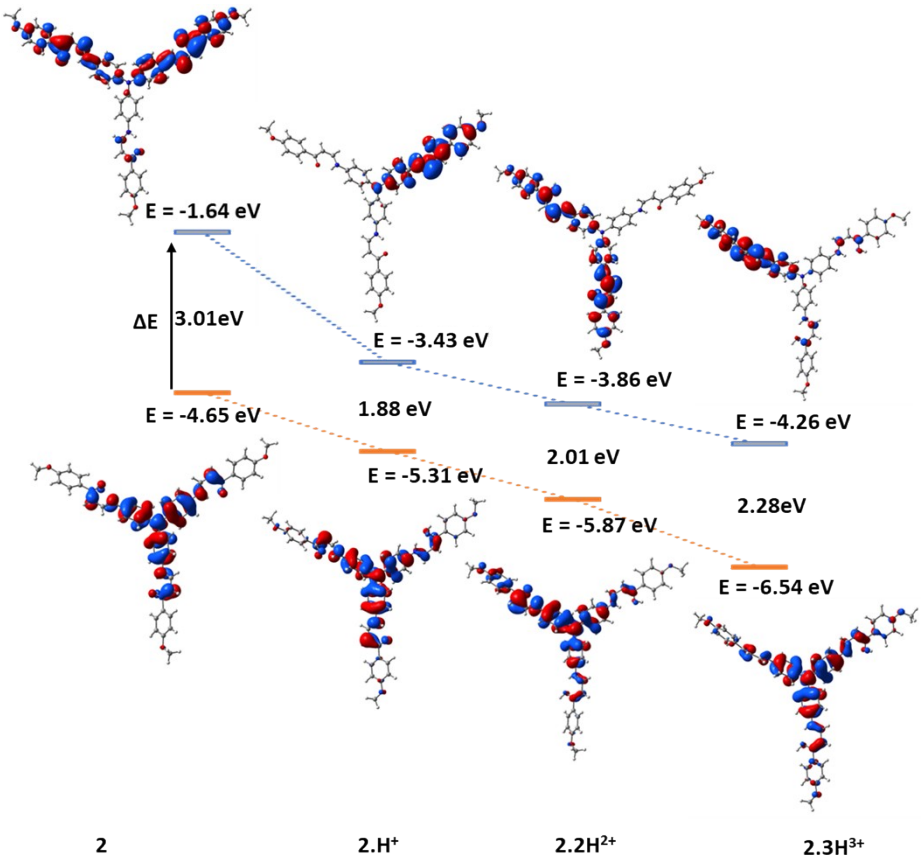


**Fig. S22** DFT calculated HOMO/LUMO frontier orbital topologies and their HOMO-LUMO (H-L) gaps; (Using B3LYP/6-31G(d), CPCM solvent model; Chloroform).

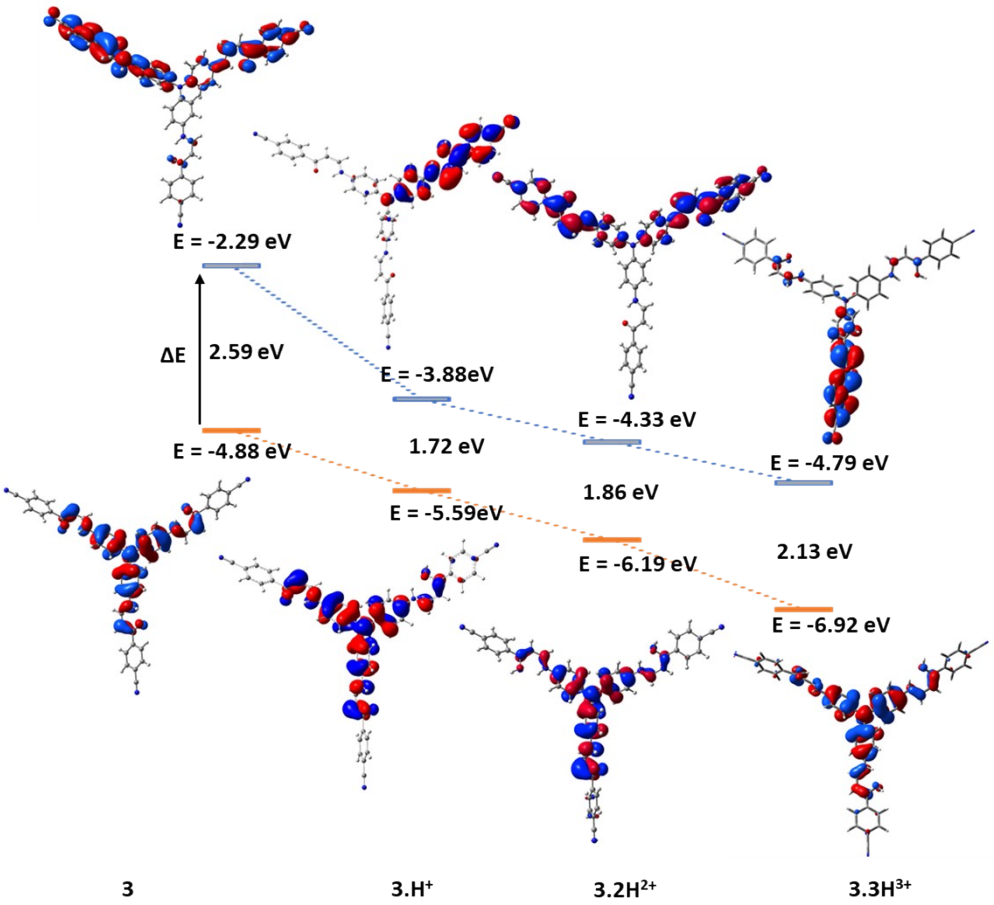


**Fig. S23** DFT calculated HOMO/LUMO frontier orbital topologies and their HOMO-LUMO (H-L) gaps; (Using B3LYP/6-31G(d), CPCM solvent model; Chloroform).

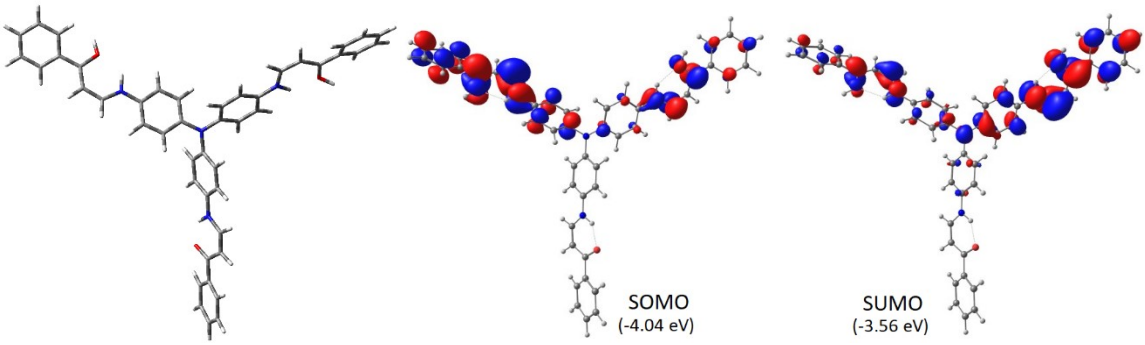


**Fig. S24** DFT geometry optimised structure of **1-2H**$^{+\bullet}$ (B3LYP/6-31G(d), CPCM solvent model; Chloroform).

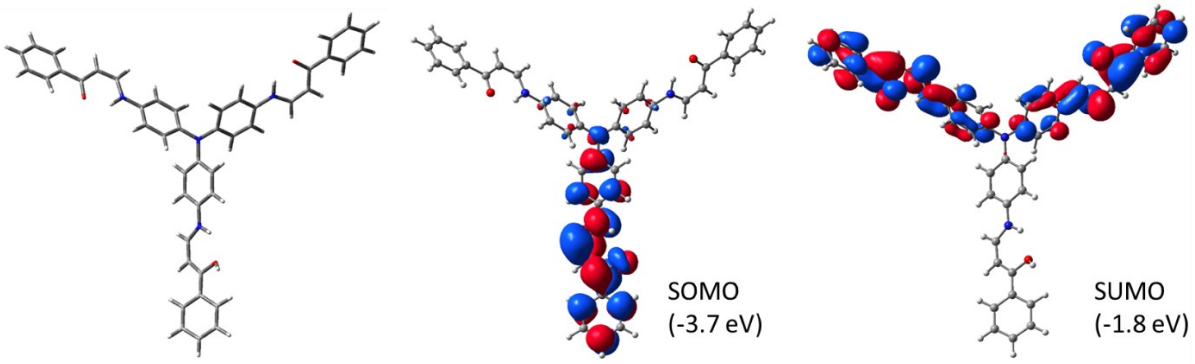


**Fig. S25** DFT geometry optimised structure of **1-H**• (B3LYP/6-31G(d), CPCM solvent model; Chloroform).

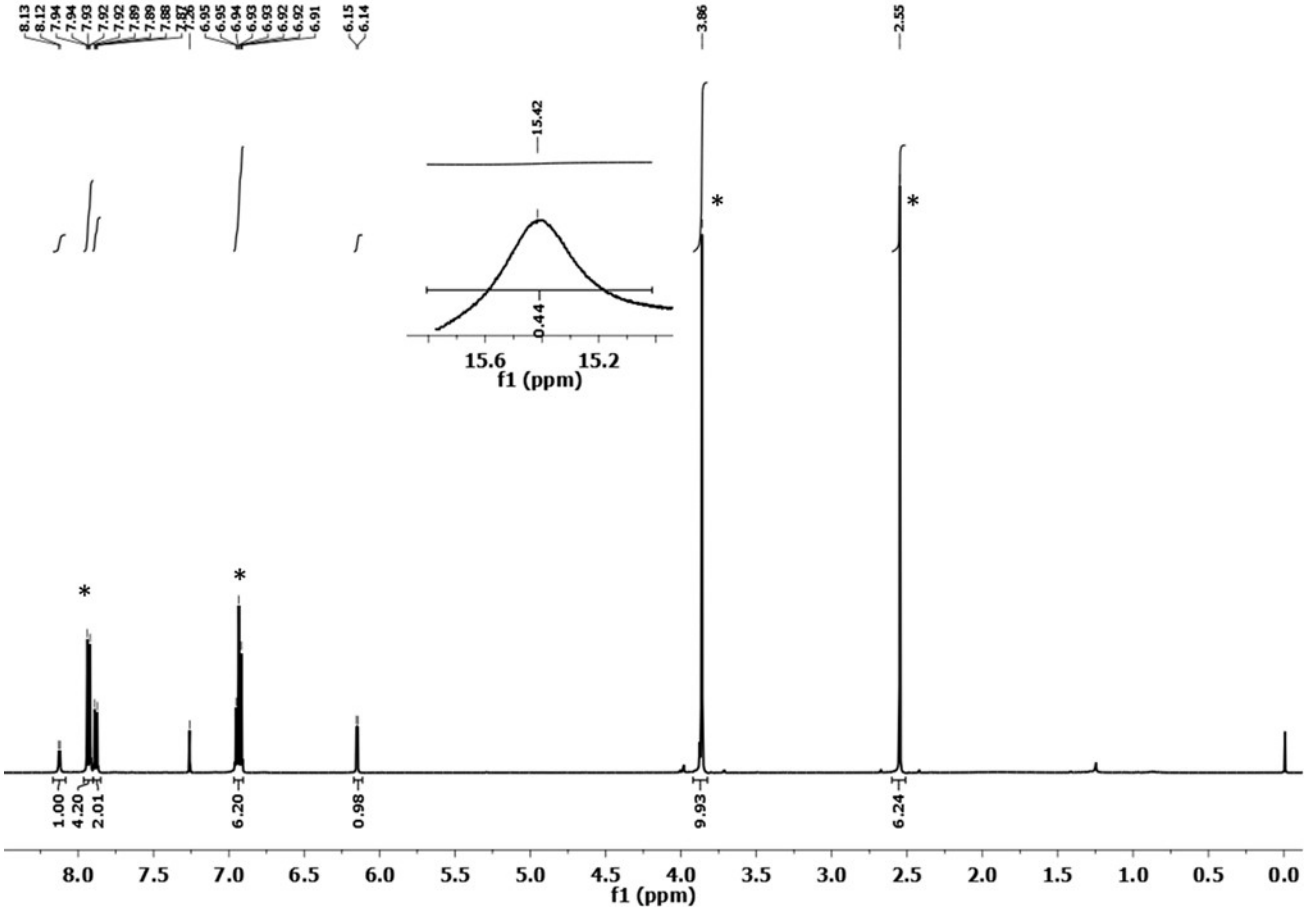


**Fig. S26** $^{1}$H NMR of compound **5.** The * indicate the signals belong to the unreacted starting material.

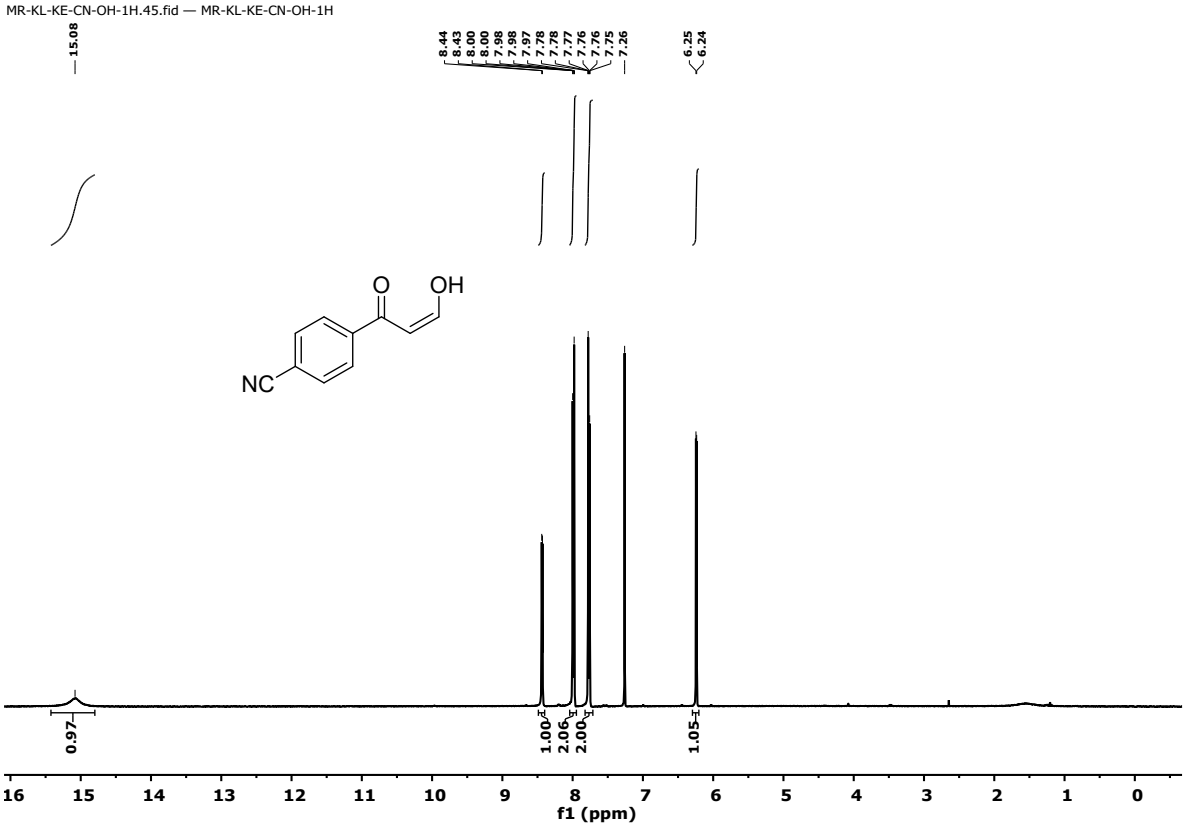


**Fig. S27** $^{1}$H NMR of compound **6**

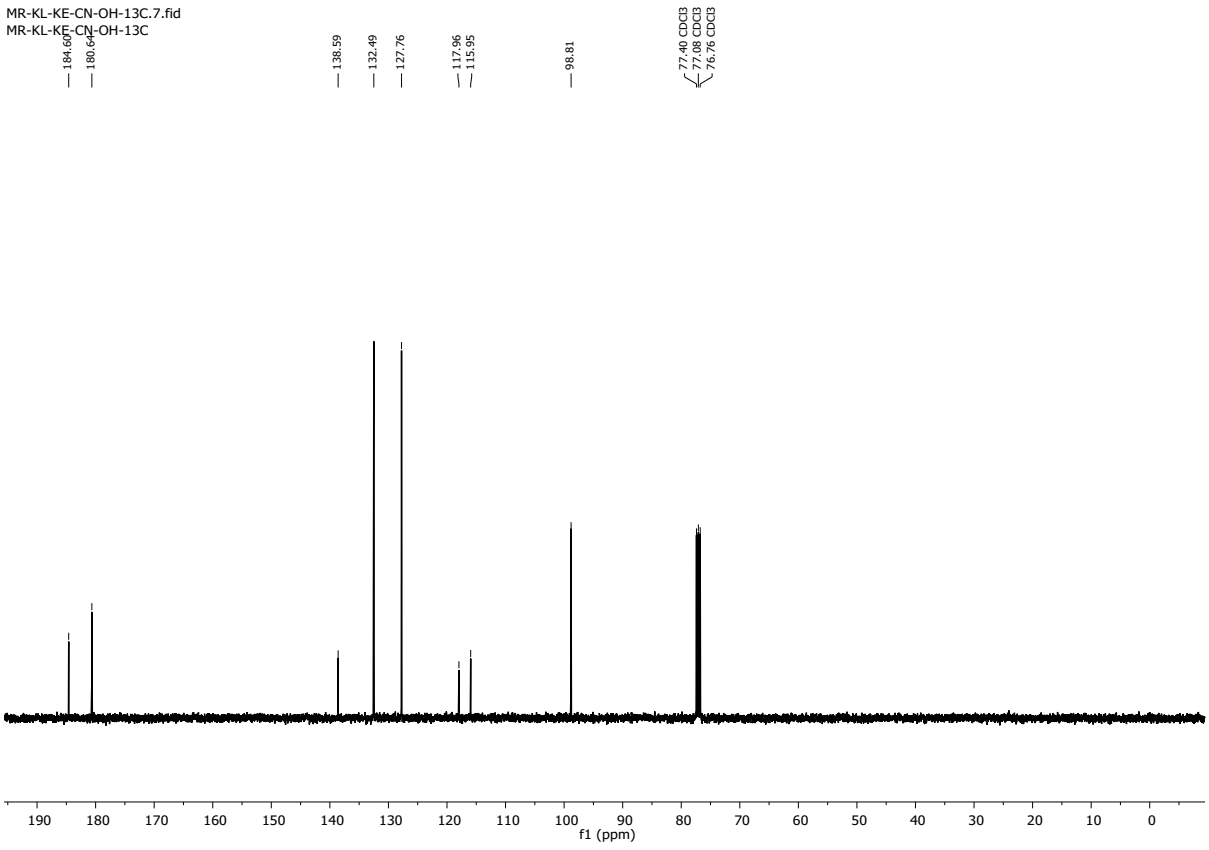


**Fig. S28** $^{13}$C NMR of compound **6**

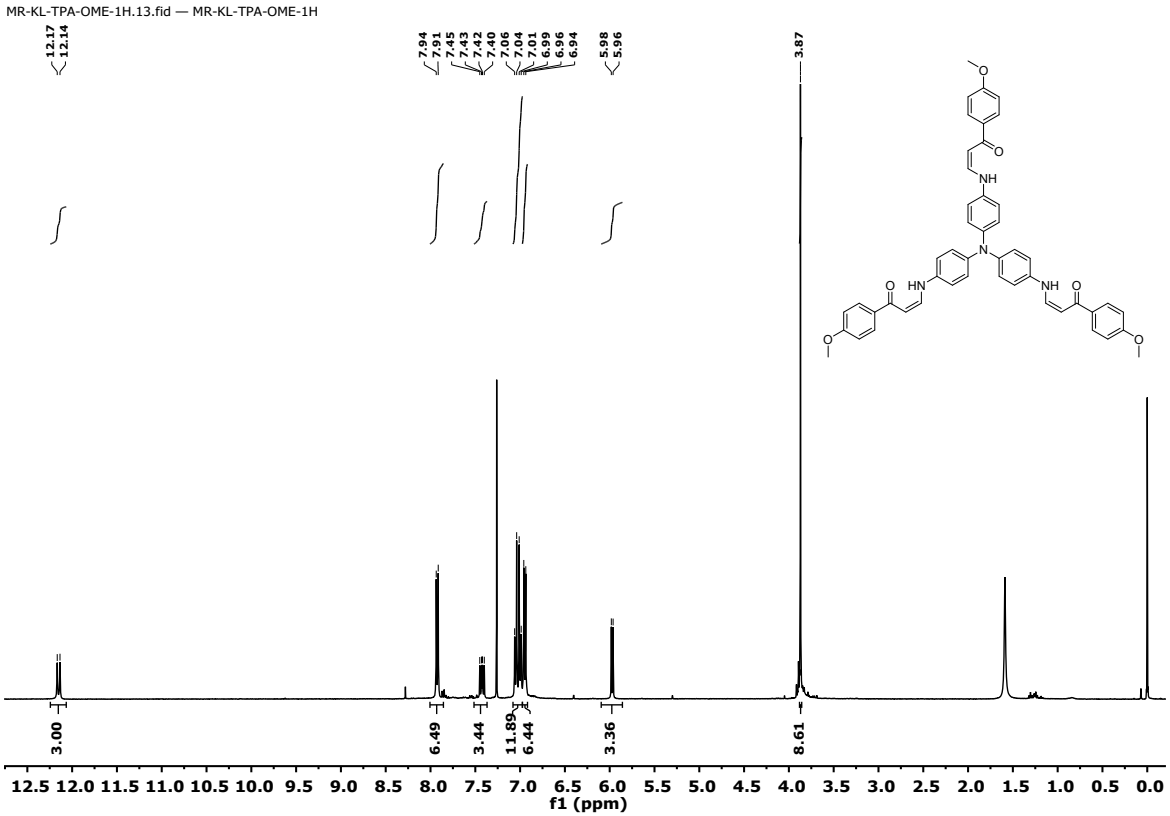


**Figure S29** $^{1}$H NMR of compound **2**

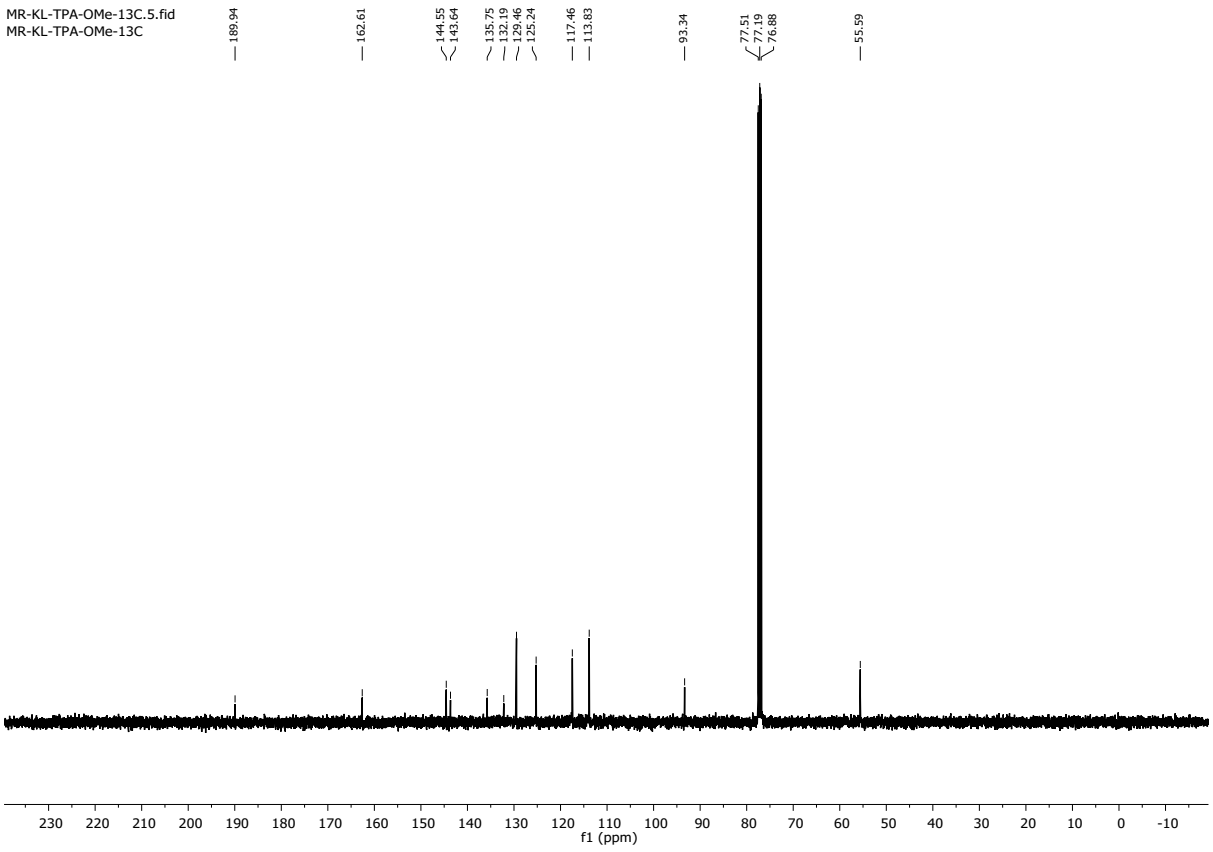


**Fig. S30** $^{13}$C NMR of compound **2**

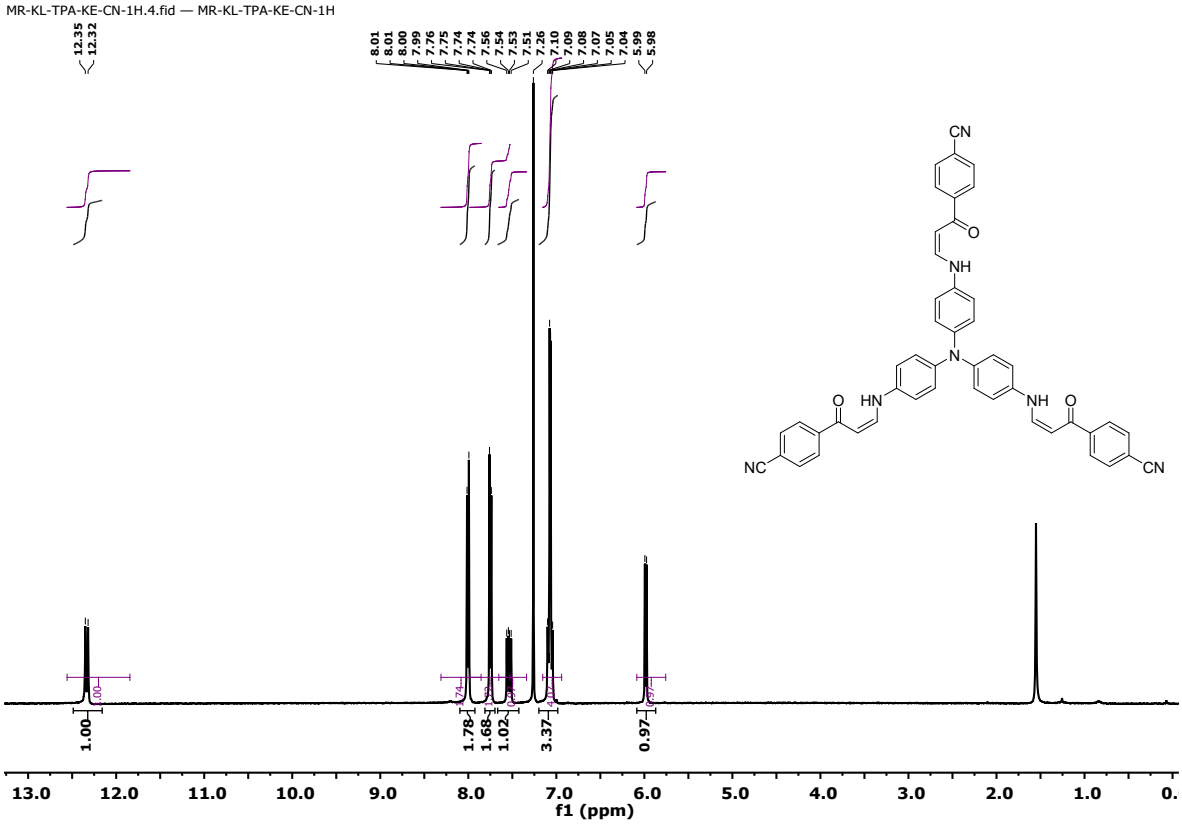


**Fig. S31** $^{1}$H NMR of compound **3**

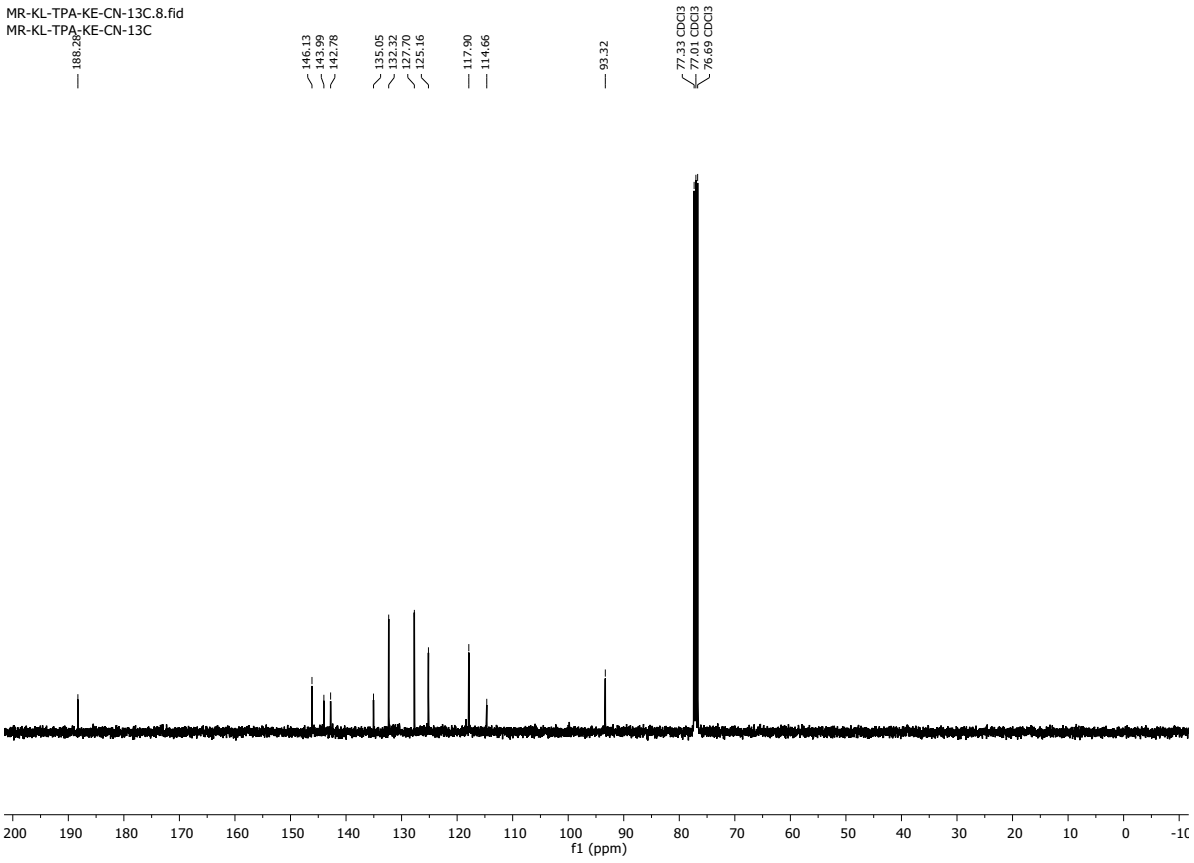


**Fig. S32** $^{13}$C NMR of compound **3**

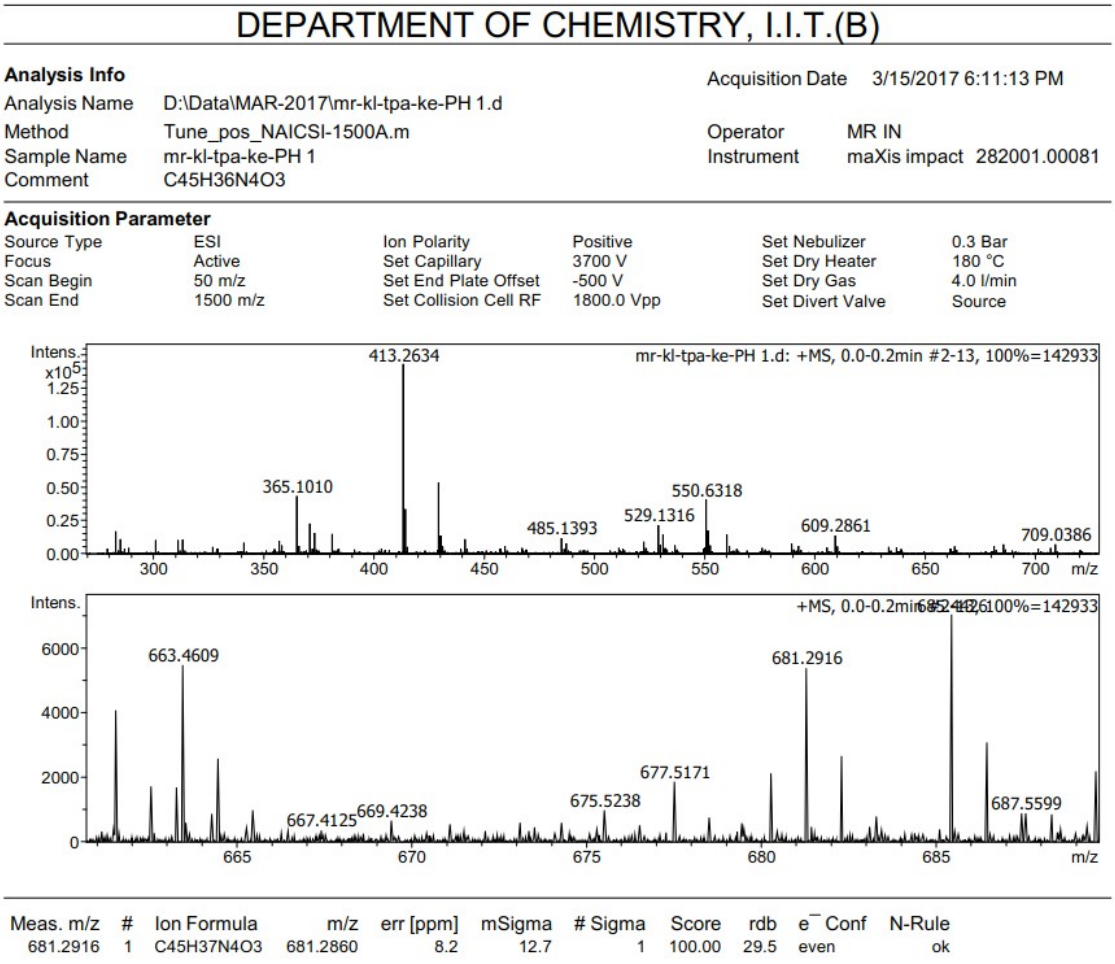


**Fig. S33** HRMS of compound **1**

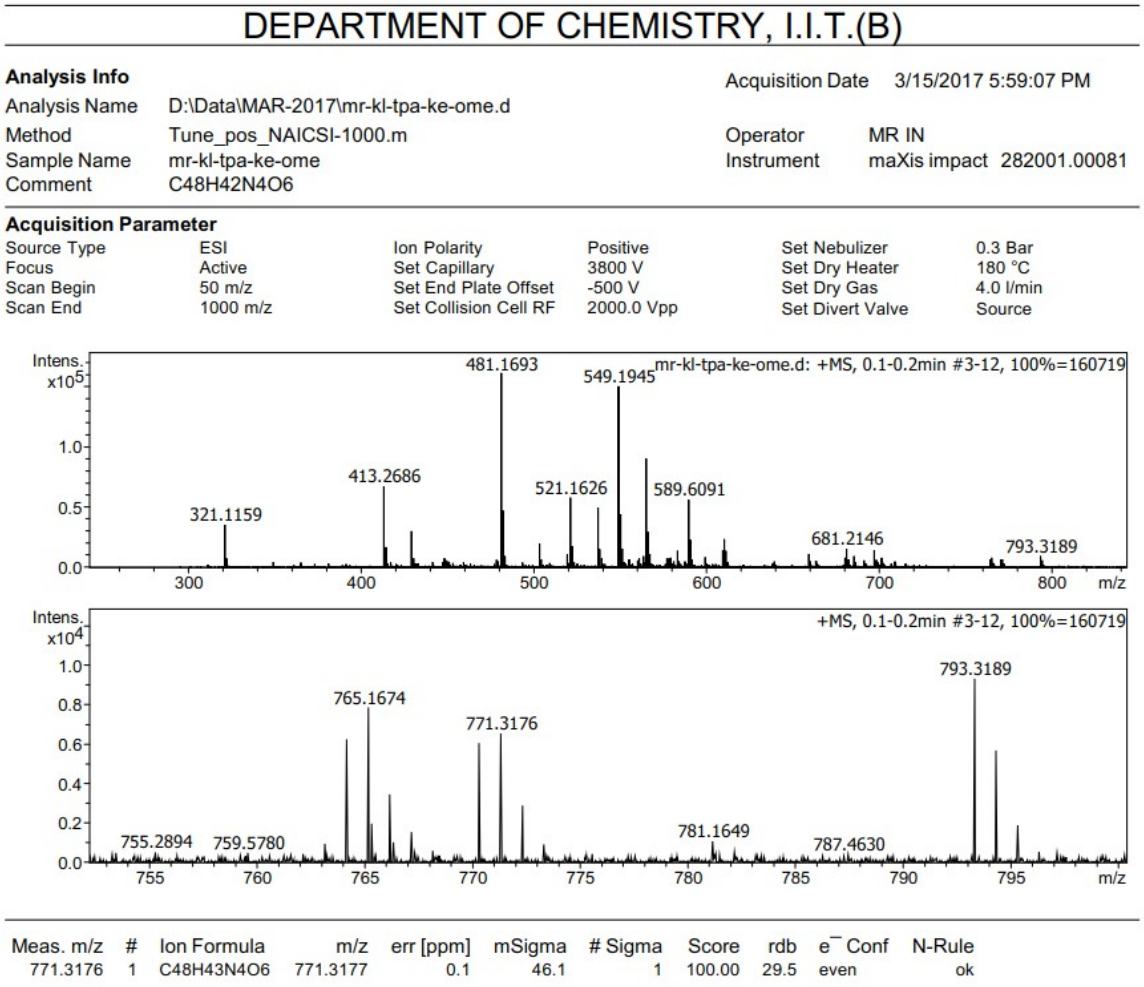


**Fig. S34** HRMS of compound **2**

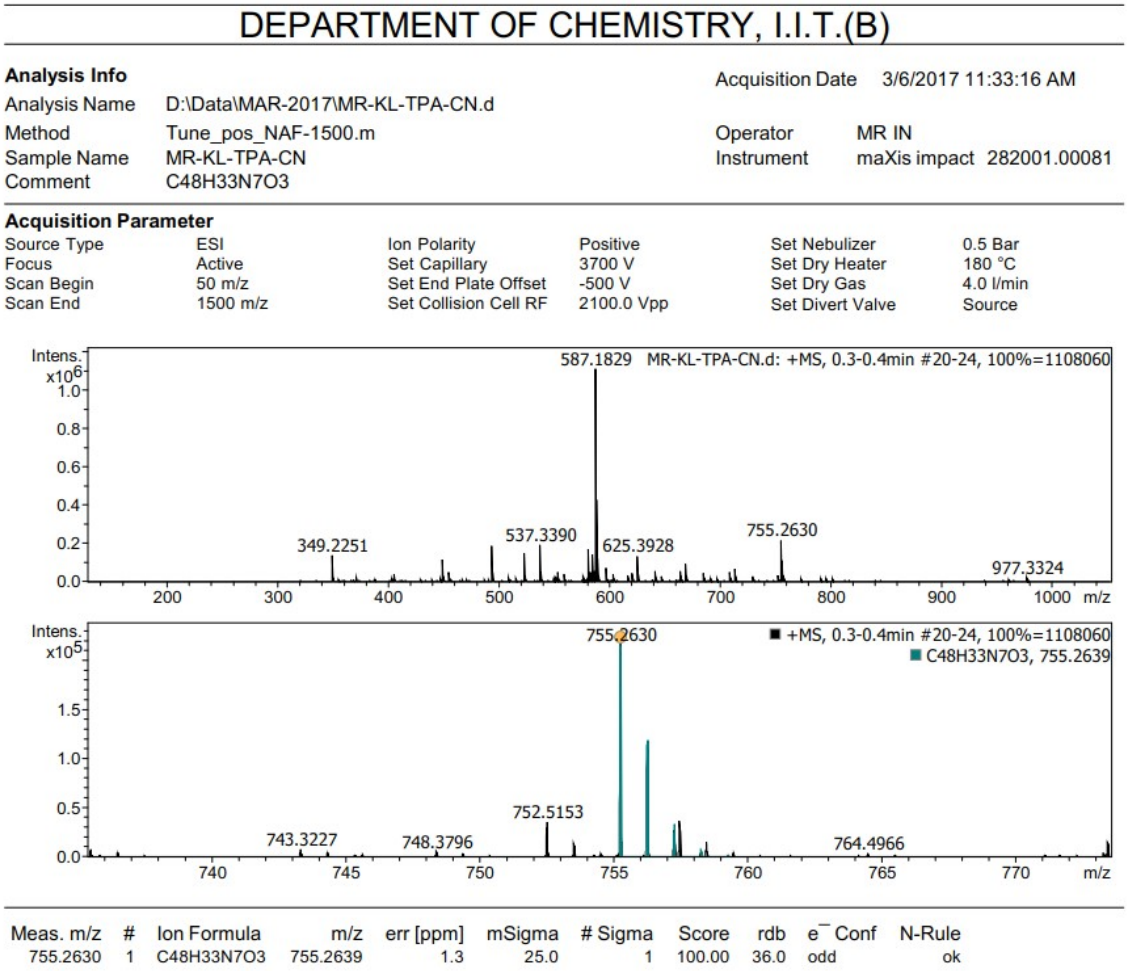


**Fig. S35** HRMS of compound **3.**

**Table S2** S0 optimized geometry of the compound **1** at B3LYP/6-31G(d) level of theory

| Symbol | X | Y | Z |
|---|---|---|---|
| N | -0.00415 | 0.001316 | -0.12289 |
| C | 0.518908 | -1.31916 | -0.12338 |
| C | -1.40905 | 0.208349 | -0.12169 |
| C | 0.878426 | 1.113794 | -0.12024 |
| C | 0.62339 | 2.237068 | 0.683603 |
| C | 1.487395 | 3.325145 | 0.678621 |
| C | 2.644901 | 3.322629 | -0.11686 |
| C | 2.901758 | 2.203817 | -0.92514 |
| C | 2.028212 | 1.121575 | -0.92677 |
| C | 1.615708 | -1.66131 | 0.684511 |
| C | 2.128897 | -2.95231 | 0.675905 |
| C | 1.554065 | -3.951 | -0.12726 |
| C | 0.459218 | -3.613 | -0.93855 |
| C | -0.04403 | -2.3163 | -0.93652 |
| C | -2.25358 | -0.57615 | 0.680888 |
| C | -3.62815 | -0.37433 | 0.674765 |

| | | | |
|---|---|---|---|
| C | -4.20564 | 0.629199 | -0.12027 |
| C | -3.36583 | 1.413554 | -0.9269 |
| C | -1.99142 | 1.200104 | -0.92781 |
| N | 2.113632 | -5.23656 | -0.08349 |
| N | 3.481666 | 4.447663 | -0.07013 |
| N | -5.59859 | 0.788501 | -0.0738 |
| C | 4.719868 | 4.584551 | -0.58866 |
| C | 5.466754 | 5.738011 | -0.52475 |
| C | 4.992767 | 6.93824 | 0.120451 |
| O | 3.875329 | 6.987667 | 0.689204 |
| C | -6.33898 | 1.789196 | -0.59454 |
| C | -7.71147 | 1.856194 | -0.52984 |
| C | -8.51147 | 0.845422 | 0.118363 |
| C | -10.0072 | 0.981134 | 0.137038 |
| C | 1.624754 | -6.37584 | -0.61615 |
| C | 2.254209 | -7.59733 | -0.54994 |
| C | 3.521603 | -7.78575 | 0.113462 |
| C | 4.154325 | -9.14776 | 0.134397 |
| O | 4.112193 | -6.84304 | 0.694245 |
| C | 5.859348 | 8.164894 | 0.136665 |
| O | -7.99352 | -0.14554 | 0.687835 |
| C | 5.526276 | 9.195388 | 1.031149 |
| C | 6.288047 | 10.35953 | 1.092736 |
| C | 7.392201 | 10.51875 | 0.249933 |
| C | 7.7264 | 9.506947 | -0.65312 |
| C | 6.968153 | 8.337131 | -0.7081 |
| C | 5.201091 | -9.37391 | 1.043355 |
| C | 5.830289 | -10.6144 | 1.111667 |
| C | 5.430262 | -11.6497 | 0.261534 |
| C | 4.399261 | -11.4339 | -0.65581 |
| C | 3.763494 | -10.1936 | -0.71776 |
| C | -10.7309 | 0.177676 | 1.033539 |
| C | -12.1198 | 0.255174 | 1.098596 |
| C | -12.812 | 1.131502 | 0.257378 |
| C | -12.1052 | 1.926461 | -0.64778 |
| C | -10.7131 | 1.854704 | -0.70635 |
| H | -0.25583 | 2.254994 | 1.319306 |
| H | 1.276749 | 4.180412 | 1.31537 |
| H | 3.764893 | 2.176741 | -1.58172 |
| H | 2.23562 | 0.272661 | -1.57017 |
| H | 2.065939 | -0.91056 | 1.325726 |
| H | 2.972524 | -3.19863 | 1.315373 |
| H | 0.007971 | -4.3456 | -1.59928 |
| H | -0.8809 | -2.07016 | -1.58213 |
| H | -1.82843 | -1.34608 | 1.316427 |
| H | -4.26342 | -0.98573 | 1.310335 |

| | | | |
|---|---|---|---|
| H | -3.77483 | 2.174928 | -1.58256 |
| H | -1.36007 | 1.805623 | -1.57002 |
| H | 5.13714 | 3.707912 | -1.07444 |
| H | 6.458994 | 5.703178 | -0.95384 |
| H | -5.79057 | 2.589054 | -1.08241 |
| H | -8.17969 | 2.731017 | -0.96029 |
| H | 0.66389 | -6.29954 | -1.11563 |
| H | 1.737571 | -8.43881 | -0.9914 |
| H | 4.662388 | 9.060548 | 1.673334 |
| H | 6.022033 | 11.14413 | 1.795938 |
| H | 7.986439 | 11.42744 | 0.294445 |
| H | 8.576772 | 9.628873 | -1.31835 |
| H | 7.23427 | 7.571766 | -1.42971 |
| H | 5.505088 | -8.55906 | 1.69178 |
| H | 6.633109 | -10.7756 | 1.826049 |
| H | 5.921466 | -12.6177 | 0.31138 |
| H | 4.090761 | -12.2309 | -1.32681 |
| H | 2.977666 | -10.0421 | -1.45039 |
| H | -10.1807 | -0.50257 | 1.674959 |
| H | -12.6643 | -0.36726 | 1.803526 |
| H | -13.896 | 1.191783 | 0.304649 |
| H | -12.6376 | 2.601718 | -1.31192 |
| H | -10.1855 | 2.46785 | -1.42956 |
| H | -6.16445 | 0.087588 | 0.415059 |
| H | 2.998302 | -5.37861 | 0.414383 |
| H | 3.159308 | 5.289226 | 0.41803 |

**Table S3** S0 optimized geometry of the compound **1-H**$^+$ at B3LYP/6-31G(d) level of theory

| Symbol | X | Y | Z |
|---|---|---|---|
| N | -0.07826 | -0.04475 | -0.24431 |
| C | -1.46529 | -0.20299 | -0.23971 |
| C | 0.514612 | 1.255791 | -0.23828 |
| C | 0.79172 | -1.17924 | -0.22374 |
| C | 1.824519 | -1.26427 | 0.720099 |
| C | 2.688163 | -2.35193 | 0.723745 |
| C | 2.538733 | -3.39357 | -0.20897 |
| C | 1.504675 | -3.30713 | -1.15684 |
| C | 0.650468 | -2.20934 | -1.16407 |
| C | -2.06893 | -1.35933 | 0.300763 |
| C | -3.44647 | -1.50332 | 0.304228 |
| C | -4.27436 | -0.50108 | -0.22414 |
| C | -3.68865 | 0.65013 | -0.77368 |
| C | -2.31168 | 0.792578 | -0.78235 |
| C | 0.11173 | 2.227572 | 0.689415 |
| C | 0.703407 | 3.484181 | 0.695782 |

| | | | |
|---|---|---|---|
| C | 1.728953 | 3.80134 | -0.21222 |
| C | 2.136203 | 2.825891 | -1.1382 |
| C | 1.531963 | 1.573202 | -1.14846 |
| N | -5.66766 | -0.71167 | -0.17189 |
| N | 3.43884 | -4.46153 | -0.14441 |
| N | 2.287015 | 5.081979 | -0.14763 |
| C | 3.449609 | -5.59453 | -0.88385 |
| C | 4.386724 | -6.58985 | -0.75988 |
| C | 5.470944 | -6.52919 | 0.196037 |
| O | 5.598675 | -5.56353 | 0.98493 |
| C | 3.369801 | 5.555867 | -0.80612 |
| C | 3.836407 | 6.842511 | -0.70161 |
| C | 3.207763 | 7.83733 | 0.13932 |
| C | 3.766686 | 9.228942 | 0.18948 |
| C | -6.64271 | 0.102891 | -0.54113 |
| C | -8.0274 | -0.15255 | -0.44874 |
| C | -8.62335 | -1.28448 | 0.065865 |
| C | -10.071 | -1.46796 | 0.195984 |
| O | -7.81199 | -2.29403 | 0.446058 |
| C | 6.463687 | -7.65202 | 0.268299 |
| O | 2.208586 | 7.565586 | 0.846008 |
| C | 7.312566 | -7.70819 | 1.386398 |
| C | 8.257608 | -8.7227 | 1.513098 |
| C | 8.377916 | -9.69519 | 0.515707 |
| C | 7.547995 | -9.64407 | -0.60658 |
| C | 6.595465 | -8.63225 | -0.72927 |
| C | -10.6298 | -2.75911 | 0.114008 |
| C | -12.0044 | -2.93868 | 0.242316 |
| C | -12.8374 | -1.83809 | 0.45835 |
| C | -12.2919 | -0.55314 | 0.542035 |
| C | -10.9199 | -0.36493 | 0.411403 |
| C | 3.331556 | 10.07626 | 1.222252 |
| C | 3.810455 | 11.37965 | 1.323832 |
| C | 4.726861 | 11.8635 | 0.385177 |
| C | 5.158233 | 11.03523 | -0.65347 |
| C | 4.684738 | 9.726586 | -0.75009 |
| H | 1.950124 | -0.47378 | 1.453116 |
| H | 3.481565 | -2.40605 | 1.464091 |
| H | 1.368959 | -4.07723 | -1.90803 |
| H | -0.132 | -2.14782 | -1.91412 |
| H | -1.45244 | -2.13943 | 0.731179 |
| H | -3.88675 | -2.39641 | 0.740279 |
| H | -4.29219 | 1.435037 | -1.21654 |
| H | -1.87736 | 1.680703 | -1.22576 |
| H | -0.66388 | 1.995468 | 1.412442 |
| H | 0.386556 | 4.224504 | 1.425201 |

| | | | |
|---|---|---|---|
| H | 2.906876 | 3.039041 | -1.87063 |
| H | 1.848724 | 0.832808 | -1.87618 |
| H | 2.652306 | -5.70399 | -1.61192 |
| H | 4.267147 | -7.45643 | -1.39576 |
| H | 3.892813 | 4.850945 | -1.44437 |
| H | 4.731114 | 7.084903 | -1.25866 |
| H | -6.33914 | 1.059127 | -0.95134 |
| H | -8.67369 | 0.625143 | -0.83239 |
| H | 7.212344 | -6.9435 | 2.149202 |
| H | 8.901726 | -8.75659 | 2.387494 |
| H | 9.116376 | -10.4865 | 0.611253 |
| H | 7.643415 | -10.391 | -1.38971 |
| H | 5.973989 | -8.60219 | -1.61804 |
| H | -10.0022 | -3.62048 | -0.09931 |
| H | -12.4254 | -3.936 | 0.163297 |
| H | -13.9089 | -1.98054 | 0.561032 |
| H | -12.9364 | 0.302098 | 0.719735 |
| H | -10.5004 | 0.630734 | 0.510997 |
| H | 2.615736 | 9.689319 | 1.939652 |
| H | 3.470282 | 12.01998 | 2.133095 |
| H | 5.100193 | 12.88107 | 0.461113 |
| H | 5.862539 | 11.40834 | -1.39174 |
| H | 5.020606 | 9.107419 | -1.57531 |
| H | 1.863095 | 5.780115 | 0.471922 |
| H | -5.96123 | -1.60828 | 0.213463 |
| H | 4.200025 | -4.4299 | 0.541732 |
| H | -8.2976 | -2.96507 | 0.957967 |

**Table S4** S0 optimized geometry of the compound **1-2H$^{2+}$** at B3LYP/6-31G(d) level of theory

| Symbol | X | Y | Z |
|---|---|---|---|
| N | -0.05061 | -0.11452 | 0.154137 |
| C | 1.106809 | -0.91983 | 0.17142 |
| C | 0.096609 | 1.312219 | 0.166148 |
| C | -1.34503 | -0.67 | 0.09951 |
| C | -2.37364 | -0.01413 | -0.60182 |
| C | -3.65491 | -0.54428 | -0.63532 |
| C | -3.94375 | -1.74771 | 0.02296 |
| C | -2.93193 | -2.40259 | 0.73965 |
| C | -1.65267 | -1.86782 | 0.776471 |
| C | 1.170805 | -2.12947 | -0.54484 |
| C | 2.327976 | -2.89492 | -0.5341 |
| C | 3.457349 | -2.46807 | 0.178322 |
| C | 3.403973 | -1.26746 | 0.900777 |
| C | 2.243782 | -0.50814 | 0.895263 |

| | | | |
|---|---|---|---|
| C | 0.876773 | 1.954594 | -0.80451 |
| C | 1.023391 | 3.335427 | -0.78638 |
| C | 0.382644 | 4.114083 | 0.194953 |
| C | -0.39931 | 3.466706 | 1.168225 |
| C | -0.53399 | 2.082525 | 1.151369 |
| N | 4.606735 | -3.28946 | 0.130782 |
| N | -5.26686 | -2.23792 | -0.06105 |
| N | 0.566672 | 5.496683 | 0.152765 |
| C | -5.71714 | -3.43599 | 0.277498 |
| C | -7.05276 | -3.87727 | 0.220111 |
| C | -8.14835 | -3.13045 | -0.17072 |
| O | -7.91525 | -1.88227 | -0.61684 |
| C | -0.03854 | 6.445667 | 0.908037 |
| C | 0.224215 | 7.787806 | 0.816263 |
| C | 1.191034 | 8.336839 | -0.11289 |
| C | 1.437479 | 9.815576 | -0.1444 |
| C | 5.825597 | -3.01918 | 0.571053 |
| C | 6.948194 | -3.86622 | 0.507402 |
| C | 6.992695 | -5.13244 | -0.04453 |
| C | 8.203832 | -5.94968 | -0.12974 |
| O | 5.83667 | -5.64645 | -0.50405 |
| C | -9.52656 | -3.62261 | -0.15774 |
| O | 1.823386 | 7.603694 | -0.90808 |
| C | -10.4607 | -3.12891 | -1.09099 |
| C | -11.7731 | -3.59169 | -1.08046 |
| C | -12.1722 | -4.54414 | -0.13907 |
| C | -11.2527 | -5.03889 | 0.791335 |
| C | -9.9377 | -4.58617 | 0.784182 |
| C | 8.110924 | -7.3557 | -0.08642 |
| C | 9.260088 | -8.13637 | -0.16925 |
| C | 10.51136 | -7.52879 | -0.30331 |
| C | 10.61291 | -6.13482 | -0.34902 |
| C | 9.470241 | -5.34687 | -0.26032 |
| C | 2.173469 | 10.33673 | -1.22207 |
| C | 2.438377 | 11.70058 | -1.31003 |
| C | 1.979214 | 12.56802 | -0.31406 |
| C | 1.256022 | 12.0614 | 0.768069 |
| C | 0.98419 | 10.69585 | 0.852346 |
| H | -2.16377 | 0.909657 | -1.12825 |
| H | -4.43133 | -0.03115 | -1.19613 |
| H | -3.13551 | -3.30518 | 1.305482 |
| H | -0.88763 | -2.36926 | 1.358501 |
| H | 0.318423 | -2.46287 | -1.12569 |
| H | 2.363979 | -3.81775 | -1.10674 |
| H | 4.245326 | -0.92556 | 1.493426 |
| H | 2.209072 | 0.411375 | 1.46817 |

| | | | |
|---|---|---|---|
| H | 1.365671 | 1.370266 | -1.57781 |
| H | 1.625004 | 3.823773 | -1.5479 |
| H | -0.88732 | 4.028765 | 1.956467 |
| H | -1.1288 | 1.593057 | 1.916475 |
| H | -4.97257 | -4.14319 | 0.62584 |
| H | -7.22027 | -4.90882 | 0.497735 |
| H | -0.78234 | 6.09704 | 1.617182 |
| H | -0.34943 | 8.442429 | 1.457881 |
| H | 5.96415 | -2.04353 | 1.022795 |
| H | 7.855705 | -3.47772 | 0.948918 |
| H | -10.156 | -2.42403 | -1.86009 |
| H | -12.4809 | -3.21708 | -1.81308 |
| H | -13.1975 | -4.90131 | -0.13071 |
| H | -11.5645 | -5.77162 | 1.528941 |
| H | -9.23845 | -4.95044 | 1.529511 |
| H | 7.151365 | -7.84336 | 0.064768 |
| H | 9.180004 | -9.21759 | -0.11889 |
| H | 11.40605 | -8.14012 | -0.37114 |
| H | 11.58346 | -5.66239 | -0.46295 |
| H | 9.553439 | -4.26729 | -0.32866 |
| H | 2.527779 | 9.650963 | -1.98418 |
| H | 3.002735 | 12.08941 | -2.1531 |
| H | 2.186502 | 13.63254 | -0.37978 |
| H | 0.904606 | 12.72915 | 1.549556 |
| H | 0.434881 | 10.32429 | 1.710873 |
| H | 1.2275 | 5.892454 | -0.5239 |
| H | 4.481555 | -4.19881 | -0.31084 |
| H | -5.95809 | -1.58799 | -0.4317 |
| H | 5.988715 | -6.45924 | -1.01918 |
| H | -8.74118 | -1.37271 | -0.70271 |

**Table S5** S0 optimized geometry of the compound **1-3H**$^{3+}$ at B3LYP/6-31G(d) level of theory

| Symbol | X | Y | Z |
|---|---|---|---|
| N | 0.000484 | -0.01477 | 0.047734 |
| C | -0.98817 | -1.03212 | 0.061128 |
| C | 1.375493 | -0.36318 | 0.03985 |
| C | -0.38912 | 1.34937 | 0.033543 |
| C | 0.281274 | 2.279716 | -0.77745 |
| C | -0.10198 | 3.614476 | -0.782 |
| C | -1.17353 | 4.045279 | 0.011757 |
| C | -1.84125 | 3.127085 | 0.833751 |
| C | -1.45 | 1.795061 | 0.841803 |
| C | -2.14322 | -0.91976 | -0.7297 |
| C | -3.11202 | -1.91404 | -0.70476 |

| | | | |
|---|---|---|---|
| C | -2.94194 | -3.04975 | 0.098641 |
| C | -1.79487 | -3.16888 | 0.895752 |
| C | -0.83322 | -2.16778 | 0.87611 |
| C | 1.838483 | -1.4299 | -0.7496 |
| C | 3.182594 | -1.77705 | -0.74771 |
| C | 4.09504 | -1.05504 | 0.032773 |
| C | 3.650651 | 0.029639 | 0.799785 |
| C | 2.300854 | 0.358434 | 0.81347 |
| N | -3.96437 | -4.02727 | 0.069296 |
| N | -1.5272 | 5.414495 | -0.04747 |
| N | 5.457131 | -1.44801 | 0.002418 |
| C | -2.64993 | 5.9776 | 0.375579 |
| C | -2.96844 | 7.34558 | 0.34836 |
| C | -2.15185 | 8.371046 | -0.09793 |
| O | -0.96774 | 8.024588 | -0.62937 |
| C | 6.377066 | -1.2083 | 0.938707 |
| C | 7.730353 | -1.55793 | 0.910064 |
| C | 8.474535 | -1.99155 | -0.18838 |
| C | 9.785541 | -2.61007 | -0.08894 |
| C | -3.93739 | -5.25176 | 0.5753 |
| C | -4.97262 | -6.20099 | 0.536798 |
| C | -6.2158 | -6.04054 | -0.05187 |
| C | -7.23795 | -7.0846 | -0.10722 |
| O | -6.4942 | -4.83616 | -0.57818 |
| C | -2.51227 | 9.7871 | -0.04943 |
| O | 8.030377 | -1.84756 | -1.44889 |
| C | -1.99968 | 10.67978 | -1.0133 |
| C | -2.33866 | 12.02841 | -0.96805 |
| C | -3.18335 | 12.50447 | 0.038603 |
| C | -3.69542 | 11.62683 | 0.999551 |
| C | -3.36793 | 10.27605 | 0.957749 |
| C | -8.60393 | -6.73498 | -0.13068 |
| C | -9.5791 | -7.72572 | -0.18585 |
| C | -9.20738 | -9.07239 | -0.22632 |
| C | -7.85519 | -9.42875 | -0.20525 |
| C | -6.87393 | -8.44546 | -0.14257 |
| C | 10.62459 | -2.66009 | -1.22368 |
| C | 11.88129 | -3.24656 | -1.13643 |
| C | 12.31638 | -3.79485 | 0.074609 |
| C | 11.489 | -3.76 | 1.202998 |
| C | 10.23198 | -3.17453 | 1.126092 |
| H | 1.097248 | 1.955571 | -1.41387 |
| H | 0.415807 | 4.318557 | -1.42726 |
| H | -2.63731 | 3.442348 | 1.499358 |
| H | -1.95747 | 1.096206 | 1.497667 |
| H | -2.27885 | -0.05701 | -1.37243 |

| | | | |
|---|---|---|---|
| H | -3.99328 | -1.81878 | -1.33286 |
| H | -1.65328 | -4.01351 | 1.560773 |
| H | 0.039316 | -2.25776 | 1.513815 |
| H | 1.14391 | -1.98657 | -1.36886 |
| H | 3.52267 | -2.60912 | -1.35817 |
| H | 4.344193 | 0.62817 | 1.380322 |
| H | 1.963496 | 1.18937 | 1.423026 |
| H | -3.3981 | 5.300772 | 0.773338 |
| H | -3.95783 | 7.606123 | 0.698201 |
| H | 6.002972 | -0.72625 | 1.836127 |
| H | 8.248264 | -1.46438 | 1.855473 |
| H | -3.01521 | -5.54406 | 1.064775 |
| H | -4.76807 | -7.14053 | 1.031221 |
| H | -1.38086 | 10.31901 | -1.83073 |
| H | -1.95293 | 12.70537 | -1.72349 |
| H | -3.44362 | 13.55791 | 0.073616 |
| H | -4.34376 | 11.99839 | 1.786647 |
| H | -3.74313 | 9.606774 | 1.724722 |
| H | -8.91305 | -5.69601 | -0.05171 |
| H | -10.6282 | -7.44794 | -0.18681 |
| H | -9.97026 | -9.84345 | -0.2729 |
| H | -7.56628 | -10.4741 | -0.24632 |
| H | -5.82674 | -8.7282 | -0.1592 |
| H | 10.28856 | -2.22405 | -2.1571 |
| H | 12.52556 | -3.27381 | -2.00942 |
| H | 13.29887 | -4.25274 | 0.139166 |
| H | 11.82363 | -4.19785 | 2.137917 |
| H | 9.585601 | -3.18052 | 1.997057 |
| H | 5.704391 | -2.0754 | -0.75855 |
| H | -4.82142 | -3.75829 | -0.41076 |
| H | -0.84197 | 6.036679 | -0.47205 |
| H | -7.31498 | -4.85453 | -1.10309 |
| H | -0.39361 | 8.800872 | -0.76225 |
| H | 7.395799 | -1.11148 | -1.52173 |

**Table S6** S0 optimized geometry of the compound **2** at B3LYP/6-31G(d) level of theory

| Symbol | X | Y | Z |
|---|---|---|---|
| N | 0.004098 | 0.003285 | -0.11774 |
| C | -0.47858 | -1.33232 | -0.11789 |
| C | -0.91092 | 1.089509 | -0.11515 |
| C | 1.402324 | 0.252957 | -0.118 |
| C | 1.956762 | 1.259969 | 0.689083 |
| C | 3.324388 | 1.504536 | 0.680979 |
| C | 4.189276 | 0.740693 | -0.12029 |
| C | 3.638888 | -0.26504 | -0.93101 |

| | | | |
|---|---|---|---|
| C | 2.267531 | -0.49789 | -0.93032 |
| C | 0.122484 | -2.31843 | 0.681665 |
| C | -0.34899 | -3.6253 | 0.672995 |
| C | -1.44873 | -3.99075 | -0.12099 |
| C | -2.05137 | -3.0086 | -0.9235 |
| C | -1.56781 | -1.70434 | -0.92264 |
| C | -2.05927 | 1.064964 | 0.693326 |
| C | -2.95636 | 2.125726 | 0.685819 |
| C | -2.73026 | 3.256677 | -0.11657 |
| C | -1.58372 | 3.285092 | -0.92681 |
| C | -0.69456 | 2.215305 | -0.92626 |
| N | -1.88169 | -5.32346 | -0.07634 |
| N | 5.559847 | 1.031383 | -0.07456 |
| N | -3.67055 | 4.295671 | -0.07242 |
| C | 6.579198 | 0.329936 | -0.61682 |
| C | 7.901157 | 0.699127 | -0.54882 |
| C | 8.344965 | 1.898948 | 0.1243 |
| O | 7.535328 | 2.660728 | 0.709233 |
| C | -3.57769 | 5.527959 | -0.61819 |
| C | -4.56172 | 6.485022 | -0.55116 |
| C | -5.82018 | 6.26759 | 0.126 |
| C | -6.85172 | 7.349439 | 0.146914 |
| C | -3.00227 | -5.85384 | -0.61303 |
| C | -3.34362 | -7.18335 | -0.54553 |
| C | -2.52336 | -8.16895 | 0.121726 |
| C | -2.94971 | -9.60176 | 0.144496 |
| O | -1.4553 | -7.85036 | 0.701157 |
| C | 9.798571 | 2.247671 | 0.146121 |
| O | -6.07023 | 5.187137 | 0.716045 |
| C | 10.21556 | 3.309217 | 0.973388 |
| C | 11.54494 | 3.688971 | 1.043557 |
| C | 12.51127 | 3.017434 | 0.273574 |
| C | 12.11757 | 1.964616 | -0.56385 |
| C | 10.77439 | 1.591377 | -0.61781 |
| C | -2.24562 | -10.4928 | 0.978501 |
| C | -2.58416 | -11.8332 | 1.049614 |
| C | -3.64433 | -12.3345 | 0.273398 |
| C | -4.35147 | -11.4683 | -0.57171 |
| C | -4.00083 | -10.1191 | -0.62622 |
| C | -7.9665 | 7.189858 | 0.993592 |
| C | -8.96098 | 8.150271 | 1.064352 |
| C | -8.87711 | 9.311095 | 0.274973 |
| C | -7.78231 | 9.485599 | -0.58278 |
| C | -6.78588 | 8.510582 | -0.63659 |
| H | 1.310857 | 1.85228 | 1.329097 |
| H | 3.734176 | 2.283063 | 1.319244 |

| | | | |
|---|---|---|---|
| H | 4.266556 | -0.85565 | -1.58985 |
| H | 1.85952 | -1.26932 | -1.57545 |
| H | 0.963084 | -2.05721 | 1.316279 |
| H | 0.1258 | -4.37077 | 1.305567 |
| H | -2.8822 | -3.25473 | -1.57616 |
| H | -2.03738 | -0.96367 | -1.56189 |
| H | -2.24764 | 0.20927 | 1.333541 |
| H | -3.83472 | 2.090169 | 1.324976 |
| H | -1.38747 | 4.124205 | -1.58579 |
| H | 0.17727 | 2.249006 | -1.57169 |
| H | 6.311147 | -0.58983 | -1.12742 |
| H | 8.617171 | 0.029096 | -1.00516 |
| H | -2.64836 | 5.75735 | -1.13038 |
| H | -4.3436 | 7.440336 | -1.00913 |
| H | -3.66785 | -5.16038 | -1.11772 |
| H | -4.28535 | -7.46727 | -0.99536 |
| H | 9.465861 | 3.826821 | 1.562049 |
| H | 11.86586 | 4.503095 | 1.686354 |
| H | 12.84031 | 1.435594 | -1.17375 |
| H | 10.50055 | 0.781981 | -1.2862 |
| H | -1.42604 | -10.1023 | 1.572141 |
| H | -2.04545 | -12.5173 | 1.69823 |
| H | -5.16619 | -11.8303 | -1.18766 |
| H | -4.5581 | -9.47794 | -1.30092 |
| H | -8.02883 | 6.290918 | 1.597386 |
| H | -9.81598 | 8.029452 | 1.722651 |
| H | -7.69762 | 10.36615 | -1.20868 |
| H | -5.95906 | 8.668484 | -1.32104 |
| H | -4.5498 | 4.152074 | 0.434323 |
| H | -1.31571 | -6.01626 | 0.423876 |
| H | 5.876548 | 1.864516 | 0.431275 |
| O | 13.78878 | 3.461813 | 0.408839 |
| O | -3.9018 | -13.6622 | 0.410895 |
| O | -9.90037 | 10.19527 | 0.412953 |
| C | 14.81568 | 2.820671 | -0.34479 |
| H | 14.63986 | 2.91923 | -1.42256 |
| H | 15.74174 | 3.332546 | -0.0798 |
| H | 14.89775 | 1.758845 | -0.08399 |
| C | -4.97029 | -14.2303 | -0.34348 |
| H | -4.79176 | -14.136 | -1.42123 |
| H | -4.99721 | -15.2861 | -0.07087 |
| H | -5.92941 | -13.7632 | -0.09008 |
| C | -9.87163 | 11.39503 | -0.35723 |
| H | -9.88704 | 11.17921 | -1.43211 |
| H | -10.7736 | 11.94439 | -0.08439 |
| H | -8.98903 | 12.00049 | -0.11914 |

**Table S7** S0 optimized geometry of the compound **2-H**$^{+}$ at B3LYP/6-31G(d) level of theory

| Symbol | X | Y | Z |
|---|---|---|---|
| N | 0.101822 | -0.01594 | -0.25008 |
| C | 1.493014 | -0.14743 | -0.25361 |
| C | -0.74797 | -1.16468 | -0.24482 |
| C | -0.51243 | 1.274815 | -0.22882 |
| C | -1.49998 | 1.576182 | 0.719367 |
| C | -2.11537 | 2.821375 | 0.725896 |
| C | -1.75464 | 3.808472 | -0.20875 |
| C | -0.76833 | 3.504314 | -1.16297 |
| C | -0.16349 | 2.251665 | -1.17191 |
| C | 2.323366 | 0.856319 | 0.289763 |
| C | 3.701892 | 0.718522 | 0.279613 |
| C | 4.305567 | -0.42502 | -0.26478 |
| C | 3.492971 | -1.43052 | -0.81078 |
| C | 2.114774 | -1.29047 | -0.80712 |
| C | -0.55218 | -2.20431 | 0.676283 |
| C | -1.39415 | -3.30911 | 0.683172 |
| C | -2.47018 | -3.40061 | -0.21777 |
| C | -2.66824 | -2.35707 | -1.13819 |
| C | -1.81475 | -1.25895 | -1.14895 |
| N | 5.714174 | -0.49632 | -0.23264 |
| N | -2.40733 | 5.042434 | -0.1422 |
| N | -3.28534 | -4.53401 | -0.152 |
| C | -2.152 | 6.164501 | -0.85682 |
| C | -2.8578 | 7.334367 | -0.74002 |
| C | -3.96715 | 7.494791 | 0.178876 |
| O | -4.32459 | 6.561453 | 0.937948 |
| C | -4.44382 | -4.77074 | -0.81271 |
| C | -5.17303 | -5.92734 | -0.70658 |
| C | -4.7724 | -7.03449 | 0.138239 |
| C | -5.60857 | -8.27024 | 0.194923 |
| C | 6.504997 | -1.47706 | -0.64409 |
| C | 7.910287 | -1.508 | -0.57303 |
| C | 8.733103 | -0.53356 | -0.03613 |
| C | 10.17882 | -0.64708 | 0.082798 |
| O | 8.136625 | 0.607376 | 0.376761 |
| C | -4.69889 | 8.794523 | 0.244305 |
| O | -3.73292 | -6.97616 | 0.839529 |
| C | -5.64341 | 8.975061 | 1.274751 |
| C | -6.35951 | 10.15288 | 1.396997 |
| C | -6.15903 | 11.19854 | 0.477588 |
| C | -5.23136 | 11.03692 | -0.56117 |
| C | -4.51379 | 9.845603 | -0.66599 |

| | | | |
|---|---|---|---|
| C | 10.99075 | 0.504508 | 0.107167 |
| C | 12.37254 | 0.415458 | 0.219539 |
| C | 12.98092 | -0.84753 | 0.31751 |
| C | 12.1815 | -2.00877 | 0.294674 |
| C | 10.80973 | -1.90985 | 0.177431 |
| C | -5.27944 | -9.25292 | 1.15021 |
| C | -6.00878 | -10.4238 | 1.259861 |
| C | -7.10011 | -10.6574 | 0.403526 |
| C | -7.44015 | -9.69737 | -0.55994 |
| C | -6.69746 | -8.5206 | -0.65326 |
| H | -1.7849 | 0.830362 | 1.454667 |
| H | -2.87461 | 3.042447 | 1.471225 |
| H | -0.48209 | 4.226271 | -1.91976 |
| H | 0.58389 | 2.025758 | -1.92628 |
| H | 1.881435 | 1.741907 | 0.730688 |
| H | 4.31755 | 1.501456 | 0.715175 |
| H | 3.920115 | -2.32069 | -1.25981 |
| H | 1.505382 | -2.07023 | -1.24858 |
| H | 0.259804 | -2.14361 | 1.394161 |
| H | -1.23396 | -4.10282 | 1.407901 |
| H | -3.47126 | -2.39986 | -1.86567 |
| H | -1.97477 | -0.46511 | -1.87172 |
| H | -1.32343 | 6.112244 | -1.55581 |
| H | -2.53301 | 8.161753 | -1.3561 |
| H | -4.8036 | -3.97322 | -1.45493 |
| H | -6.09347 | -5.97466 | -1.27232 |
| H | 6.010542 | -2.33888 | -1.07733 |
| H | 8.379618 | -2.38643 | -0.99451 |
| H | -5.79778 | 8.164714 | 1.97895 |
| H | -7.08249 | 10.2934 | 2.194714 |
| H | -5.06402 | 11.82314 | -1.28772 |
| H | -3.81372 | 9.748025 | -1.48887 |
| H | 10.55322 | 1.491936 | -0.01441 |
| H | 12.96457 | 1.322172 | 0.216124 |
| H | 12.66716 | -2.97476 | 0.383508 |
| H | 10.2123 | -2.81512 | 0.195116 |
| H | -4.43535 | -9.07018 | 1.806346 |
| H | -5.75791 | -11.1777 | 1.999835 |
| H | -8.27121 | -9.85563 | -1.23698 |
| H | -6.97972 | -7.80453 | -1.41759 |
| H | -3.02021 | -5.3061 | 0.467977 |
| H | 6.185685 | 0.312677 | 0.168115 |
| H | -3.17802 | 5.164955 | 0.522584 |
| H | 8.736947 | 1.142375 | 0.92485 |
| O | -7.75353 | -11.8336 | 0.586678 |
| O | -6.90729 | 12.31364 | 0.678753 |

| | | | |
|---|---|---|---|
| O | 14.30657 | -1.05333 | 0.434802 |
| C | -8.87293 | -12.1294 | -0.24693 |
| H | -8.58087 | -12.1803 | -1.30242 |
| H | -9.23405 | -13.1061 | 0.077671 |
| H | -9.66882 | -11.3857 | -0.12299 |
| C | -6.75117 | 13.4115 | -0.21887 |
| H | -7.01523 | 13.12778 | -1.24443 |
| H | -7.43806 | 14.18202 | 0.133319 |
| H | -5.7258 | 13.79908 | -0.19898 |
| C | 15.18595 | 0.0762 | 0.476508 |
| H | 14.96085 | 0.717196 | 1.335636 |
| H | 16.18838 | -0.3384 | 0.580903 |
| H | 15.12269 | 0.657507 | -0.44963 |

**Table S8** S0 optimized geometry of the compound **2-H$^{2+}$** at B3LYP/6-31G(d) level of theory

| Symbol | X | Y | Z |
|---|---|---|---|
| N | 0.049973 | 0.099477 | 0.176592 |
| C | -1.102 | 0.912918 | 0.208452 |
| C | -0.10568 | -1.32605 | 0.188894 |
| C | 1.347816 | 0.647544 | 0.109104 |
| C | 2.363333 | -0.00988 | -0.60927 |
| C | 3.647547 | 0.512902 | -0.65696 |
| C | 3.953598 | 1.710645 | 0.003781 |
| C | 2.954857 | 2.366001 | 0.737988 |
| C | 1.672307 | 1.83867 | 0.788734 |
| C | -1.16667 | 2.123922 | -0.50524 |
| C | -2.31703 | 2.899457 | -0.47695 |
| C | -3.44094 | 2.483542 | 0.250836 |
| C | -3.38982 | 1.276028 | 0.961813 |
| C | -2.23506 | 0.507872 | 0.941385 |
| C | -0.89515 | -1.96428 | -0.77713 |
| C | -1.05111 | -3.34399 | -0.7577 |
| C | -0.41022 | -4.12814 | 0.219831 |
| C | 0.385542 | -3.48532 | 1.185229 |
| C | 0.527021 | -2.10165 | 1.168588 |
| N | -4.57924 | 3.320128 | 0.223583 |
| N | 5.277426 | 2.19538 | -0.09673 |
| N | -0.60521 | -5.50829 | 0.177113 |
| C | 5.732953 | 3.398017 | 0.231302 |
| C | 7.061233 | 3.844072 | 0.15887 |
| C | 8.162691 | 3.100782 | -0.24209 |
| O | 7.918528 | 1.852897 | -0.69017 |
| C | -0.05787 | -6.46007 | 0.974464 |
| C | -0.3203 | -7.79997 | 0.866997 |
| C | -1.2236 | -8.34893 | -0.12808 |

| | | | |
|---|---|---|---|
| C | -1.47183 | -9.81869 | -0.17992 |
| C | -5.75606 | 3.1288 | 0.805927 |
| C | -6.87214 | 3.977553 | 0.747475 |
| C | -6.97034 | 5.170703 | 0.046239 |
| C | -8.17422 | 5.978919 | -0.03478 |
| O | -5.85226 | 5.603056 | -0.57218 |
| C | 9.530623 | 3.587799 | -0.23842 |
| O | -1.7993 | -7.60755 | -0.96064 |
| C | 10.49417 | 3.041969 | -1.12111 |
| C | 11.7963 | 3.500378 | -1.12113 |
| C | 12.19008 | 4.52015 | -0.23087 |
| C | 11.24606 | 5.072805 | 0.654773 |
| C | 9.938534 | 4.61063 | 0.642016 |
| C | -8.09391 | 7.367468 | -0.26785 |
| C | -9.23374 | 8.155705 | -0.34626 |
| C | -10.5 | 7.561823 | -0.19869 |
| C | -10.5961 | 6.173879 | 0.034888 |
| C | -9.45703 | 5.400296 | 0.118857 |
| C | -2.22377 | -10.3285 | -1.258 |
| C | -2.49458 | -11.6805 | -1.37112 |
| C | -2.02371 | -12.5782 | -0.39525 |
| C | -1.28075 | -12.0918 | 0.690075 |
| C | -1.01236 | -10.7269 | 0.78583 |
| H | 2.140974 | -0.92969 | -1.13778 |
| H | 4.413172 | -0.00164 | -1.23124 |
| H | 3.171578 | 3.264415 | 1.305739 |
| H | 0.917759 | 2.342027 | 1.382814 |
| H | -0.31859 | 2.452435 | -1.09528 |
| H | -2.34997 | 3.826622 | -1.0429 |
| H | -4.23296 | 0.926908 | 1.547362 |
| H | -2.20519 | -0.41804 | 1.504215 |
| H | -1.38618 | -1.37672 | -1.54673 |
| H | -1.66312 | -3.82785 | -1.51388 |
| H | 0.884334 | -4.05072 | 1.964294 |
| H | 1.132684 | -1.6167 | 1.928099 |
| H | 4.989152 | 4.105318 | 0.581239 |
| H | 7.223544 | 4.878774 | 0.427284 |
| H | 0.632933 | -6.11337 | 1.736062 |
| H | 0.198149 | -8.45333 | 1.555318 |
| H | -5.85611 | 2.219973 | 1.388156 |
| H | -7.73019 | 3.661524 | 1.324498 |
| H | 10.21342 | 2.289641 | -1.85352 |
| H | 12.53165 | 3.099039 | -1.81009 |
| H | 11.52802 | 5.847731 | 1.356715 |
| H | 9.233271 | 5.025625 | 1.354278 |
| H | -7.12834 | 7.861718 | -0.33754 |

| | | | |
|---|---|---|---|
| H | -9.13233 | 9.221827 | -0.50612 |
| H | -11.5817 | 5.731952 | 0.134507 |
| H | -9.55639 | 4.330384 | 0.266729 |
| H | -2.58767 | -9.63295 | -2.00639 |
| H | -3.0689 | -12.0731 | -2.20458 |
| H | -0.91252 | -12.7605 | 1.459016 |
| H | -0.44545 | -10.3831 | 1.644336 |
| H | -1.23076 | -5.90324 | -0.53303 |
| H | -4.48391 | 4.176804 | -0.31817 |
| H | 5.963045 | 1.543732 | -0.4729 |
| H | -6.04669 | 6.324986 | -1.19577 |
| H | 8.738682 | 1.333874 | -0.76692 |
| O | -2.34016 | -13.8828 | -0.59205 |
| O | 13.47902 | 4.893457 | -0.30636 |
| O | -11.6679 | 8.224254 | -0.26152 |
| C | -1.89189 | -14.8467 | 0.360199 |
| H | -2.30816 | -14.6467 | 1.354402 |
| H | -2.25626 | -15.8096 | 0.000314 |
| H | -0.79742 | -14.8684 | 0.418635 |
| C | -11.6597 | 9.636447 | -0.50598 |
| H | -11.197 | 9.863464 | -1.47214 |
| H | -12.7075 | 9.935016 | -0.52111 |
| H | -11.136 | 10.16915 | 0.29478 |
| C | 13.95778 | 5.937166 | 0.551529 |
| H | 15.00973 | 6.062882 | 0.296867 |
| H | 13.41882 | 6.872453 | 0.367678 |
| H | 13.86491 | 5.651715 | 1.6046 |

**Table S9** S0 optimized geometry of the compound **2-3H**$^{3+}$ at B3LYP/6-31G(d) level of theory

| Symbol | X | Y | Z |
|---|---|---|---|
| N | 0.021831 | -0.00312 | 0.071443 |
| C | -0.70265 | 1.216074 | 0.093701 |
| C | -0.67401 | -1.24052 | 0.062837 |
| C | 1.440267 | 0.014544 | 0.052373 |
| C | 2.159068 | -0.87071 | -0.76766 |
| C | 3.547733 | -0.85233 | -0.7772 |
| C | 4.250153 | 0.0603 | 0.021674 |
| C | 3.541894 | 0.939131 | 0.852944 |
| C | 2.153484 | 0.91323 | 0.865044 |
| C | -0.29023 | 2.311368 | -0.68275 |
| C | -1.00013 | 3.504448 | -0.65138 |
| C | -2.14842 | 3.627337 | 0.143109 |
| C | -2.56397 | 2.541803 | 0.92713 |
| C | -1.845 | 1.35409 | 0.902072 |

| | | | |
|---|---|---|---|
| C | -1.81881 | -1.41259 | -0.73371 |
| C | -2.50754 | -2.61824 | -0.72848 |
| C | -2.05644 | -3.68538 | 0.059883 |
| C | -0.89693 | -3.536 | 0.831641 |
| C | -0.22592 | -2.3188 | 0.844006 |
| N | -2.83032 | 4.865957 | 0.119917 |
| N | 5.662996 | 0.039898 | -0.04177 |
| N | -2.79233 | -4.89567 | 0.032779 |
| C | 6.505445 | 0.968477 | 0.399114 |
| C | 7.904443 | 0.919106 | 0.377621 |
| C | 8.690163 | -0.13004 | -0.08728 |
| O | 8.038645 | -1.15976 | -0.66053 |
| C | -2.81185 | -5.83746 | 0.985014 |
| C | -3.50224 | -7.04601 | 0.969979 |
| C | -4.1469 | -7.64419 | -0.12377 |
| C | -5.10796 | -8.7074 | -0.02 |
| C | -4.03599 | 5.142589 | 0.605249 |
| C | -4.69475 | 6.377804 | 0.574412 |
| C | -4.21785 | 7.558436 | 0.015253 |
| C | -4.97175 | 8.795066 | -0.0539 |
| O | -2.95988 | 7.53019 | -0.46461 |
| C | 10.13788 | -0.16204 | -0.01639 |
| O | -3.88255 | -7.24712 | -1.38632 |
| C | 10.88757 | -0.94149 | -0.92301 |
| C | 12.273 | -0.9821 | -0.86912 |
| C | 12.95186 | -0.23873 | 0.114273 |
| C | 12.21574 | 0.545725 | 1.027905 |
| C | 10.83929 | 0.586438 | 0.960497 |
| C | -4.31052 | 10.03917 | -0.13434 |
| C | -5.01636 | 11.23145 | -0.19919 |
| C | -6.42339 | 11.20678 | -0.19403 |
| C | -7.09896 | 9.970104 | -0.11531 |
| C | -6.38824 | 8.790903 | -0.04211 |
| C | -5.47254 | -9.45151 | -1.16695 |
| C | -6.39441 | -10.481 | -1.0941 |
| C | -6.9889 | -10.7957 | 0.144702 |
| C | -6.64247 | -10.0559 | 1.29861 |
| C | -5.7243 | -9.034 | 1.216999 |
| H | 1.629034 | -1.56807 | -1.40708 |
| H | 4.0884 | -1.53231 | -1.42961 |
| H | 4.057681 | 1.618941 | 1.522261 |
| H | 1.615412 | 1.582506 | 1.527433 |
| H | 0.583316 | 2.226025 | -1.31961 |
| H | -0.67451 | 4.336986 | -1.26901 |
| H | -3.42061 | 2.61712 | 1.587693 |
| H | -2.16243 | 0.528782 | 1.529951 |

| | | | |
|---|---|---|---|
| H | -2.17018 | -0.59885 | -1.35856 |
| H | -3.39703 | -2.73103 | -1.34231 |
| H | -0.50413 | -4.35978 | 1.417779 |
| H | 0.660997 | -2.20796 | 1.458196 |
| H | 6.047121 | 1.86097 | 0.810775 |
| H | 8.410022 | 1.800099 | 0.747835 |
| H | -2.25303 | -5.59041 | 1.88185 |
| H | -3.53331 | -7.57045 | 1.915697 |
| H | -4.5601 | 4.314202 | 1.068395 |
| H | -5.66623 | 6.402016 | 1.048086 |
| H | 10.39509 | -1.48699 | -1.7236 |
| H | 12.81589 | -1.57461 | -1.59478 |
| H | 12.75632 | 1.102666 | 1.785597 |
| H | 10.29344 | 1.170818 | 1.693194 |
| H | -3.22593 | 10.09443 | -0.09114 |
| H | -4.47469 | 12.16815 | -0.23851 |
| H | -8.18358 | 9.970766 | -0.12469 |
| H | -6.9293 | 7.851329 | -0.01463 |
| H | -5.00867 | -9.22059 | -2.1187 |
| H | -6.64431 | -11.0382 | -1.98826 |
| H | -7.12378 | -10.3068 | 2.237582 |
| H | -5.49722 | -8.46162 | 2.109625 |
| H | -3.45958 | -4.97771 | -0.72934 |
| H | -2.34439 | 5.634096 | -0.33787 |
| H | 6.081686 | -0.77727 | -0.48049 |
| H | -2.76127 | 8.321799 | -0.9955 |
| H | 8.623618 | -1.9276 | -0.78902 |
| H | -2.98168 | -6.88225 | -1.45623 |
| O | 14.28524 | -0.20749 | 0.2638 |
| O | -7.8898 | -11.7683 | 0.331899 |
| O | -7.2069 | 12.29469 | -0.25862 |
| C | 15.11034 | -0.98042 | -0.61886 |
| H | 16.13378 | -0.79872 | -0.29238 |
| H | 14.87914 | -2.04726 | -0.53463 |
| H | 14.98928 | -0.64995 | -1.65565 |
| C | -8.30964 | -12.5701 | -0.7829 |
| H | -9.03652 | -13.2722 | -0.37618 |
| H | -8.78222 | -11.9503 | -1.55134 |
| H | -7.46279 | -13.118 | -1.20786 |
| C | -6.60238 | 13.5925 | -0.34573 |
| H | -5.99225 | 13.67877 | -1.25073 |
| H | -7.4325 | 14.29656 | -0.39292 |
| H | -5.99274 | 13.79918 | 0.539898 |

**Table S10** S0 optimized geometry of the compound **3** at B3LYP/6-31G(d) level of theory

| Symbol | X | Y | Z |
|---|---|---|---|
| N | -0.0047 | -2.9E-05 | 0.146858 |
| C | 0.627633 | 1.271334 | 0.146233 |
| C | -1.42184 | -0.08826 | 0.146988 |
| C | 0.780626 | -1.18299 | 0.147462 |
| C | 0.43135 | -2.28187 | -0.6545 |
| C | 1.199332 | -3.43957 | -0.64522 |
| C | 2.351133 | -3.53235 | 0.152517 |
| C | 2.702572 | -2.4383 | 0.958614 |
| C | 1.924541 | -1.28579 | 0.956125 |
| C | 1.753206 | 1.516815 | -0.65715 |
| C | 2.373947 | 2.75965 | -0.64818 |
| C | 1.881329 | 3.804024 | 0.150731 |
| C | 0.758007 | 3.563232 | 0.957228 |
| C | 0.146845 | 2.314152 | 0.955165 |
| C | -2.198 | 0.764918 | -0.6545 |
| C | -3.58463 | 0.679926 | -0.64547 |
| C | -4.2418 | -0.27113 | 0.151507 |
| C | -3.47099 | -1.1239 | 0.957031 |
| C | -2.08374 | -1.02763 | 0.954798 |
| N | 2.549582 | 5.038095 | 0.108699 |
| N | 3.088579 | -4.72632 | 0.109696 |
| N | -5.64455 | -0.31125 | 0.108437 |
| C | 4.305374 | -4.97029 | 0.632555 |
| C | 4.949215 | -6.18714 | 0.569368 |
| C | 4.373576 | -7.33338 | -0.08075 |
| O | 3.259188 | -7.29346 | -0.65468 |
| C | -6.46515 | -1.2435 | 0.628968 |
| C | -7.84085 | -1.19078 | 0.566473 |
| C | -8.54445 | -0.11608 | -0.07994 |
| C | -10.0504 | -0.12073 | -0.09931 |
| C | 2.157644 | 6.213463 | 0.636299 |
| C | 2.89261 | 7.377575 | 0.573369 |
| C | 4.170895 | 7.449965 | -0.08132 |
| C | 4.922216 | 8.755035 | -0.10037 |
| O | 4.68837 | 6.464692 | -0.65954 |
| C | 5.132566 | -8.63404 | -0.10041 |
| O | -7.95141 | 0.829832 | -0.65128 |
| C | 4.722644 | -9.61719 | -1.0156 |
| C | 5.372044 | -10.8423 | -1.08783 |
| C | 6.448925 | -11.1092 | -0.22362 |
| C | 6.860401 | -10.1398 | 0.706318 |
| C | 6.205525 | -8.91386 | 0.760973 |
| C | 5.976536 | 8.889426 | -1.0183 |
| C | 6.71685 | 10.0618 | -1.0906 |
| C | 6.415803 | 11.12744 | -0.22364 |
| C | 5.372706 | 11.00118 | 0.709016 |
| C | 4.634402 | 9.823607 | 0.763792 |

| | | | |
|---|---|---|---|
| C | -10.6956 | 0.731423 | -1.01018 |
| C | -12.0812 | 0.783815 | -1.08232 |
| C | -12.852 | -0.01885 | -0.22244 |
| C | -12.2195 | -0.86548 | 0.703262 |
| C | -10.8304 | -0.91334 | 0.757956 |
| H | -0.44495 | -2.22596 | -1.29189 |
| H | 0.917865 | -4.27542 | -1.28029 |
| H | 3.563963 | -2.48344 | 1.616433 |
| H | 2.201962 | -0.45619 | 1.598202 |
| H | 2.141 | 0.729426 | -1.29505 |
| H | 3.238435 | 2.932155 | -1.28384 |
| H | 0.367698 | 4.33256 | 1.614882 |
| H | -0.71012 | 2.140982 | 1.597884 |
| H | -1.71066 | 1.495975 | -1.29117 |
| H | -4.16721 | 1.342716 | -1.27988 |
| H | -3.94161 | -1.84729 | 1.614317 |
| H | -1.50466 | -1.6836 | 1.596532 |
| H | 4.796102 | -4.13527 | 1.12257 |
| H | 5.938398 | -6.24139 | 1.003245 |
| H | -5.98803 | -2.08792 | 1.116329 |
| H | -8.3833 | -2.02112 | 0.997743 |
| H | 1.191208 | 6.222259 | 1.130356 |
| H | 2.449133 | 8.261487 | 1.011246 |
| H | 3.884998 | -9.39853 | -1.66823 |
| H | 5.054847 | -11.5937 | -1.80333 |
| H | 7.684001 | -10.3521 | 1.379733 |
| H | 6.526358 | -8.18619 | 1.497927 |
| H | 6.201036 | 8.054825 | -1.67288 |
| H | 7.524508 | 10.16114 | -1.80826 |
| H | 5.149475 | 11.82031 | 1.384367 |
| H | 3.84581 | 9.739314 | 1.503071 |
| H | -10.0865 | 1.35 | -1.65956 |
| H | -12.5724 | 1.43844 | -1.79463 |
| H | -12.8161 | -1.47542 | 1.373295 |
| H | -10.3617 | -1.5595 | 1.491631 |
| H | -6.1467 | 0.437509 | -0.37907 |
| H | 3.446511 | 5.099455 | -0.38354 |
| H | 2.693496 | -5.53522 | -0.38024 |
| C | -14.2831 | 0.029296 | -0.28661 |
| C | 7.124593 | -12.3716 | -0.28745 |
| C | 7.175516 | 12.34118 | -0.28737 |
| N | -15.445 | 0.06808 | -0.33927 |
| N | 7.67348 | -13.3966 | -0.3395 |
| N | 7.792142 | 13.32681 | -0.33949 |

**Table S11** S0 optimized geometry of the compound **3-H**$^+$ at B3LYP/6-31G(d) level of theory

| Symbol | X | Y | Z |
|---|---|---|---|
| N | 0.107792 | -0.03992 | 0.265122 |
| C | 1.499271 | -0.13218 | 0.248849 |
| C | -0.54677 | 1.230836 | 0.275347 |
| C | -0.70866 | -1.21362 | 0.250263 |
| C | -1.75216 | -1.33869 | -0.67707 |
| C | -2.56497 | -2.46481 | -0.6743 |
| C | -2.35131 | -3.50327 | 0.248745 |
| C | -1.3072 | -3.37694 | 1.180344 |
| C | -0.50366 | -2.2418 | 1.181113 |
| C | 2.151997 | -1.25947 | -0.29769 |
| C | 3.533824 | -1.33955 | -0.31022 |
| C | 4.317363 | -0.29969 | 0.215014 |
| C | 3.682853 | 0.823198 | 0.770936 |
| C | 2.301785 | 0.902303 | 0.78741 |
| C | -0.20377 | 2.225297 | -0.65202 |
| C | -0.8562 | 3.451427 | -0.64281 |
| C | -1.88315 | 3.712259 | 0.280906 |
| C | -2.23151 | 2.71339 | 1.205566 |
| C | -1.56665 | 1.492144 | 1.200526 |
| N | 5.716755 | -0.44627 | 0.157702 |
| N | -3.20403 | -4.61166 | 0.192143 |
| N | -2.5042 | 4.965488 | 0.228654 |
| C | -3.14664 | -5.74887 | 0.918137 |
| C | -4.04308 | -6.78512 | 0.805511 |
| C | -5.1473 | -6.7597 | -0.12157 |
| O | -5.34441 | -5.79861 | -0.90005 |
| C | -3.56517 | 5.403133 | 0.94029 |
| C | -4.10015 | 6.665186 | 0.834072 |
| C | -3.57447 | 7.658252 | -0.06935 |
| C | -4.20857 | 9.021947 | -0.12404 |
| C | 6.655888 | 0.416633 | 0.505364 |
| C | 8.052075 | 0.20837 | 0.420797 |
| C | 8.687079 | -0.91616 | -0.05346 |
| C | 10.14578 | -1.05466 | -0.14817 |
| O | 7.918578 | -1.96624 | -0.41397 |
| C | -6.0939 | -7.92816 | -0.1822 |
| O | -2.60867 | 7.424761 | -0.83211 |
| C | -6.94734 | -8.02099 | -1.29372 |
| C | -7.8494 | -9.06918 | -1.4165 |
| C | -7.91884 | -10.0467 | -0.40793 |
| C | -7.0804 | -9.95846 | 0.715699 |
| C | -6.17579 | -8.90709 | 0.821012 |
| C | 10.74475 | -2.31861 | 0.016952 |
| C | 12.12341 | -2.46276 | -0.06904 |
| C | 12.92602 | -1.33965 | -0.32901 |

| | | | |
|---|---|---|---|
| C | 12.33738 | -0.07383 | -0.49777 |
| C | 10.95958 | 0.064358 | -0.40719 |
| C | -3.90465 | 9.840705 | -1.22386 |
| C | -4.4488 | 11.1127 | -1.33973 |
| C | -5.30743 | 11.59427 | -0.33548 |
| C | -5.60926 | 10.79067 | 0.776499 |
| C | -5.06363 | 9.51491 | 0.874588 |
| H | -1.92579 | -0.55047 | -1.40253 |
| H | -3.36738 | -2.55081 | -1.40174 |
| H | -1.12501 | -4.14398 | 1.924678 |
| H | 0.287078 | -2.14857 | 1.918919 |
| H | 1.56921 | -2.06621 | -0.72562 |
| H | 4.012568 | -2.21004 | -0.7512 |
| H | 4.25285 | 1.631567 | 1.215951 |
| H | 1.829092 | 1.76719 | 1.237278 |
| H | 0.572129 | 2.035177 | -1.38679 |
| H | -0.58417 | 4.210605 | -1.37086 |
| H | -3.00586 | 2.881023 | 1.945775 |
| H | -1.83893 | 0.732423 | 1.926173 |
| H | -2.32847 | -5.83106 | 1.626084 |
| H | -3.86985 | -7.6522 | 1.428131 |
| H | -4.01232 | 4.694113 | 1.629176 |
| H | -4.96843 | 6.881965 | 1.441154 |
| H | 6.315452 | 1.370967 | 0.889804 |
| H | 8.668577 | 1.019212 | 0.784855 |
| H | -6.8868 | -7.25467 | -2.05818 |
| H | -8.50005 | -9.13876 | -2.28189 |
| H | -7.14337 | -10.708 | 1.497406 |
| H | -5.55043 | -8.84829 | 1.704642 |
| H | 10.14285 | -3.18958 | 0.258864 |
| H | 12.58095 | -3.4354 | 0.073134 |
| H | 12.96005 | 0.788468 | -0.70854 |
| H | 10.51094 | 1.038065 | -0.57003 |
| H | -3.23445 | 9.457368 | -1.98489 |
| H | -4.21623 | 11.73645 | -2.19644 |
| H | -6.26349 | 11.16847 | 1.554972 |
| H | -5.29557 | 8.917843 | 1.749315 |
| H | -2.14718 | 5.667598 | -0.42739 |
| H | 6.04896 | -1.33779 | -0.2089 |
| H | -3.98044 | -4.60431 | -0.47714 |
| H | 8.425998 | -2.62868 | -0.91561 |
| C | -5.872 | 12.90754 | -0.44362 |
| C | -8.84798 | -11.1323 | -0.52355 |
| C | 14.34925 | -1.48424 | -0.42281 |
| N | -6.33017 | 13.97356 | -0.53196 |
| N | -9.60166 | -12.0138 | -0.61795 |

| | | | |
|---|---|---|---|
| N | 15.50388 | -1.60127 | -0.49868 |

**Table S12** S0 optimized geometry of the compound **3-2H**$^{2+}$ at B3LYP/6-31G(d) level of theory

| Symbol | X | Y | Z |
|---|---|---|---|
| N | -0.0353 | -0.1525 | 0.206307 |
| C | 1.1634 | -0.89326 | 0.218344 |
| C | 0.034496 | 1.280449 | 0.229686 |
| C | -1.29872 | -0.77373 | 0.14579 |
| C | -2.35919 | -0.16346 | -0.54968 |
| C | -3.61168 | -0.75692 | -0.58774 |
| C | -3.83878 | -1.97899 | 0.060817 |
| C | -2.79482 | -2.58998 | 0.771071 |
| C | -1.5445 | -1.99222 | 0.812008 |
| C | 1.290085 | -2.09885 | -0.49732 |
| C | 2.487608 | -2.79867 | -0.49185 |
| C | 3.594885 | -2.30804 | 0.214659 |
| C | 3.478765 | -1.11244 | 0.938751 |
| C | 2.279265 | -0.41832 | 0.937549 |
| C | 0.76889 | 1.971778 | -0.7427 |
| C | 0.836905 | 3.358586 | -0.71507 |
| C | 0.16185 | 4.09131 | 0.278027 |
| C | -0.57349 | 3.395049 | 1.25324 |
| C | -0.62972 | 2.005764 | 1.226853 |
| N | 4.7887 | -3.0618 | 0.159867 |
| N | -5.13572 | -2.53215 | -0.0281 |
| N | 0.265379 | 5.483927 | 0.24171 |
| C | -5.53451 | -3.74353 | 0.31986 |
| C | -6.85246 | -4.24339 | 0.250774 |
| C | -7.96967 | -3.55079 | -0.1652 |
| O | -7.79166 | -2.29844 | -0.62387 |
| C | -0.35895 | 6.390776 | 1.027874 |
| C | -0.18368 | 7.748731 | 0.927376 |
| C | 0.692996 | 8.350671 | -0.04995 |
| C | 0.838322 | 9.846876 | -0.09507 |
| C | 5.994605 | -2.71686 | 0.5773 |
| C | 7.162953 | -3.50554 | 0.507191 |
| C | 7.264974 | -4.77238 | -0.02638 |
| C | 8.521191 | -5.52784 | -0.10537 |
| O | 6.136159 | -5.35731 | -0.46736 |
| C | -9.32545 | -4.11383 | -0.17088 |
| O | 1.331612 | 7.667796 | -0.8822 |
| C | -10.2564 | -3.69929 | -1.14318 |
| C | -11.5417 | -4.22508 | -1.15686 |

| | | | |
|---|---|---|---|
| C | -11.9166 | -5.17211 | -0.18957 |
| C | -10.9949 | -5.59087 | 0.786071 |
| C | -9.71051 | -5.06562 | 0.792085 |
| C | 8.50443 | -6.93318 | -0.01194 |
| C | 9.686859 | -7.65773 | -0.08585 |
| C | 10.90649 | -6.98352 | -0.26256 |
| C | 10.93302 | -5.58119 | -0.35924 |
| C | 9.748975 | -4.86186 | -0.27928 |
| C | 1.413213 | 10.41387 | -1.24424 |
| C | 1.582093 | 11.78744 | -1.35458 |
| C | 1.183562 | 12.62275 | -0.29582 |
| C | 0.619933 | 12.06745 | 0.864777 |
| C | 0.448279 | 10.6902 | 0.95759 |
| H | -2.19627 | 0.774173 | -1.06805 |
| H | -4.41308 | -0.27856 | -1.14397 |
| H | -2.95165 | -3.50786 | 1.327109 |
| H | -0.75477 | -2.45972 | 1.389133 |
| H | 0.455249 | -2.47913 | -1.07471 |
| H | 2.571959 | -3.71787 | -1.06504 |
| H | 4.302176 | -0.7265 | 1.529531 |
| H | 2.195937 | 0.497102 | 1.511759 |
| H | 1.282948 | 1.421575 | -1.52457 |
| H | 1.403749 | 3.885356 | -1.47753 |
| H | -1.08902 | 3.922567 | 2.047682 |
| H | -1.18949 | 1.477829 | 1.992682 |
| H | -4.76537 | -4.41323 | 0.687658 |
| H | -6.97808 | -5.27764 | 0.540741 |
| H | -1.04201 | 5.997501 | 1.773479 |
| H | -0.76245 | 8.36876 | 1.598208 |
| H | 6.086924 | -1.72847 | 1.012684 |
| H | 8.054047 | -3.06234 | 0.930571 |
| H | -9.9717 | -3.00035 | -1.92412 |
| H | -12.2509 | -3.9143 | -1.91572 |
| H | -11.2922 | -6.31475 | 1.53649 |
| H | -9.01578 | -5.37068 | 1.566739 |
| H | 7.576329 | -7.46833 | 0.166935 |
| H | 9.67159 | -8.73828 | 0.001668 |
| H | 11.87589 | -5.06627 | -0.50549 |
| H | 9.774705 | -3.7831 | -0.38603 |
| H | 1.722287 | 9.755505 | -2.0482 |
| H | 2.018772 | 12.21979 | -2.24866 |
| H | 0.323613 | 12.71354 | 1.684194 |
| H | 0.027373 | 10.28075 | 1.868964 |
| H | 0.871854 | 5.917612 | -0.46197 |
| H | 4.70944 | -3.98306 | -0.26874 |
| H | -5.85233 | -1.91749 | -0.41211 |

| | | | |
|---|---|---|---|
| H | 6.323186 | -6.16264 | -0.98235 |
| H | -8.6356 | -1.82118 | -0.7183 |
| C | 12.12897 | -7.72851 | -0.3439 |
| C | 1.355681 | 14.04231 | -0.39861 |
| C | -13.2441 | -5.71426 | -0.19767 |
| N | 13.12029 | -8.33279 | -0.4096 |
| N | 1.495058 | 15.19442 | -0.48276 |
| N | -14.3203 | -6.15444 | -0.20407 |

**Fig.S13** S0 optimized geometry of the compound **3-H**$^{3+}$ at B3LYP/6-31G(d) level of theory

| Symbol | X | Y | Z |
|---|---|---|---|
| N | -0.00532 | -0.00766 | -0.04969 |
| C | 0.33091 | 1.370175 | -0.06091 |
| C | 1.020713 | -0.98672 | -0.03419 |
| C | -1.36741 | -0.40421 | -0.04467 |
| C | -1.80249 | -1.465 | 0.766688 |
| C | -3.13622 | -1.85074 | 0.763636 |
| C | -4.0651 | -1.17471 | -0.03882 |
| C | -3.63905 | -0.12335 | -0.8623 |
| C | -2.30352 | 0.254439 | -0.86226 |
| C | -0.39104 | 2.29096 | 0.716172 |
| C | -0.06198 | 3.639599 | 0.694411 |
| C | 1.005395 | 4.094698 | -0.09177 |
| C | 1.726591 | 3.185136 | -0.87798 |
| C | 1.388341 | 1.839376 | -0.86136 |
| C | 2.164502 | -0.81094 | 0.763718 |
| C | 3.173572 | -1.76391 | 0.767838 |
| C | 3.053509 | -2.91824 | -0.01726 |
| C | 1.904388 | -3.11981 | -0.79292 |
| C | 0.906812 | -2.15371 | -0.81 |
| N | 1.296214 | 5.479288 | -0.0603 |
| N | -5.41291 | -1.60322 | 0.016855 |
| N | 4.114699 | -3.85857 | 0.015657 |
| C | -6.48476 | -0.95856 | -0.41399 |
| C | -7.815 | -1.421 | -0.37895 |
| C | -8.24287 | -2.64908 | 0.085104 |
| O | -7.32228 | -3.46564 | 0.622717 |
| C | 4.405537 | -4.76626 | -0.91328 |
| C | 5.43462 | -5.71876 | -0.87915 |
| C | 6.185712 | -6.12004 | 0.219978 |
| C | 7.405602 | -6.91669 | 0.120551 |
| C | 2.370651 | 6.095447 | -0.52485 |
| C | 2.623893 | 7.480971 | -0.49281 |
| C | 1.802115 | 8.452133 | 0.043817 |
| C | 2.139828 | 9.879753 | 0.072623 |

| | | | |
|---|---|---|---|
| O | 0.614507 | 8.060746 | 0.53339 |
| C | -9.64241 | -3.08875 | 0.056285 |
| O | 5.836228 | -5.82551 | 1.482385 |
| C | -10.1308 | -3.94697 | 1.060926 |
| C | -11.4535 | -4.36907 | 1.042946 |
| C | -12.3058 | -3.94228 | 0.011184 |
| C | -11.827 | -3.08695 | -0.99663 |
| C | -10.506 | -2.66281 | -0.97057 |
| C | 1.118462 | 10.84602 | -0.01334 |
| C | 1.42681 | 12.19957 | 0.01105 |
| C | 2.766254 | 12.6057 | 0.130227 |
| C | 3.792362 | 11.64876 | 0.218671 |
| C | 3.479291 | 10.29724 | 0.187055 |
| C | 7.868132 | -7.62534 | 1.248201 |
| C | 9.023373 | -8.38959 | 1.171611 |
| C | 9.738921 | -8.45022 | -0.03674 |
| C | 9.292672 | -7.73846 | -1.16482 |
| C | 8.136679 | -6.97731 | -1.08343 |
| H | -1.09828 | -1.98029 | 1.410378 |
| H | -3.46194 | -2.66062 | 1.410242 |
| H | -4.32512 | 0.380249 | -1.53448 |
| H | -1.97728 | 1.053318 | -1.51896 |
| H | -1.20427 | 1.949473 | 1.346783 |
| H | -0.62077 | 4.336674 | 1.312491 |
| H | 2.525263 | 3.513779 | -1.53356 |
| H | 1.93578 | 1.146898 | -1.49114 |
| H | 2.261279 | 0.072061 | 1.385419 |
| H | 4.054102 | -1.60979 | 1.385409 |
| H | 1.771506 | -4.02378 | -1.37718 |
| H | 0.028132 | -2.30963 | -1.42583 |
| H | -6.31271 | 0.029801 | -0.82553 |
| H | -8.56378 | -0.7273 | -0.73604 |
| H | 3.796806 | -4.72005 | -1.81032 |
| H | 5.640996 | -6.20106 | -1.82568 |
| H | 3.129041 | 5.462574 | -0.97188 |
| H | 3.548998 | 7.800503 | -0.95262 |
| H | -9.49811 | -4.25179 | 1.889386 |
| H | -11.831 | -5.01703 | 1.825864 |
| H | -12.4874 | -2.7684 | -1.79535 |
| H | -10.1361 | -2.02788 | -1.76793 |
| H | 0.082191 | 10.55068 | -0.14889 |
| H | 0.639807 | 12.94071 | -0.07087 |
| H | 4.823445 | 11.96834 | 0.31973 |
| H | 4.273558 | 9.565783 | 0.286091 |
| H | 7.30997 | -7.58442 | 2.175563 |
| H | 9.373549 | -8.94169 | 2.036499 |

| | | | |
|---|---|---|---|
| H | 9.85756 | -7.77961 | -2.08919 |
| H | 7.820477 | -6.40739 | -1.94965 |
| H | 4.775377 | -3.72733 | 0.777997 |
| H | 0.595415 | 6.070446 | 0.384401 |
| H | -5.57485 | -2.51049 | 0.451236 |
| H | 0.172981 | 8.771165 | 1.033415 |
| H | -7.6674 | -4.36705 | 0.758013 |
| H | 4.87803 | -5.66655 | 1.56329 |
| C | 3.088105 | 14.00282 | 0.160961 |
| C | -13.6711 | -4.38046 | -0.0132 |
| C | 10.93397 | -9.23828 | -0.11958 |
| N | 3.349067 | 15.13557 | 0.185923 |
| N | -14.778 | -4.73576 | -0.03303 |
| N | 11.90298 | -9.87747 | -0.18719 |