Experimental

General Methods

Thermogravimetric analysis (TGA) was carried out by using Pyris 1 TGA Perkin-Elmer.

Differential Scanning Calorimetry (DSC) was recorded on a Du Pont 1090B apparatus with a heating rate of 20 ºC/min under nitrogen.

The emission and excitation spectra were measured for chloroform solutions on the FLS-980 spectrophotometer in ambient temperature using 450 W Xe arc lamp as a light source and PMT (Hamamatsu, R928P) in cooled housing as a detector.

The quantum yields of fluorescence were determined by the absolute method at room temperature, using the integrating sphere with solvent as a blank. Compounds are excited in the wavelength corresponding to the absorption wavelength of the compounds. The time-resolved measurement has been prepared at optically diluted solutions at room temperature using the time-correlated single photon counting methods on the FLS-980 spectrophotometer. Excitation wavelengths were obtained using the picosecond pulsed diode EPLED–475 nm with 100 ns pulse period as light sources. PMT (Hamamatsu, R928P) in cooled housing was used as a detector. The system was alignment at emission wavelengths. Additionally, for the analysis of a fluorescence decay, an instrument response function needs to be obtained. The IRF contains information about the time response of the overall optical and electronic system. The IRF was designate using LUDOX solution as a standard at 475 nm. The influences of the Raman scattering of the solvent on the emission of the sample was avoided using a filter. The IRF contains information about the time response of the overall optical and electronic system.

The electrochemical experiments were performed at room temperature (20 ºC). Electroanalytical experiments were performed on PARSTAT 2273 potentiostat – galvanostat model and results were analyzed using PAR (Princeton Applied Research) program. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) were utilized as a measurement method. The measurements were done in a three-electrode cell with 2.0 mL volume of the sample solution. Pt (the surface area equals 13.0 mm^2 was used as a working electrode. Ag wire served as a pseudoreference electrode and platinum spiral was employed as an auxiliary electrode. Potentials were referenced to the redox potential of the ferrocene (Fc/Fc^+) couple as an internal standard. The measurements were recorded with a moderate scan rate equal to

0.05 V s^{-1}. To prepare electrolyte solution tetrabutylammonium hexafluorophosphate Bu_4NPF_6 salt ($TBAPF_6$) (Sigma Aldrich, 99 %) was dissolved in chloroform ($CHCl_3$) (Sigma Aldrich, for HPLC, ≥99.9%).

The TiO_2 and Pt electrodes were prepared according to the description included in the paper [1]. For electrodes fabrication, the FTO glasses were cleaned with distilled water, acetone, isopropyl alcohol and ethanol alcohol by ultrasonication. Next TiO_2 layer was screen-printed on FTO and coated glasses were dried at 120 °C for 5 minutes and then other layers were printed until three layers were obtained. Then coated FTO glasses were fired at 500 °C (with a temperature ramp - 30 °C per minute) under an inert atmosphere and maintain for 30 minutes. Platinum-based counter electrodes were prepared also by screen printing method following by thermal treatment at 500 °C for 30 minutes. The photoanodes were immersed in dye-solution for dyes **2a** and **2b** ($3 \cdot 10^{-4}$ M in MeOH) and for commercial dye (**N719**) it was the same concentration ($3 \cdot 10^{-4}$ M) but in $CHCl_3$, for 24h to ensure dye uptake, after the removal TiO_2 electrodes with adsorbed dyes, they were rinsed with MeOH. The next step was drying the TiO_2 electrodes in the air. The prepared devices were sandwich-type structure, with an active area of 0.49 cm^2, where between the TiO_2 and Pt electrodes the EL-HSE electrolyte was placed. The ready devices were tested by a PV Test Solutions Solar Simulator and a Keithley 2400 (Tektronix, Inc., Beaverton, OR, USA) in a glove box.

[1] A. Drygala, L.A. Dobrzanski, M. Szindler, M. Prokopiuk vel Prokopowicz, M. Pawlyta, K. Lukaszkowicz, *Arch Metal Mater*, 2016, **61**, 803.

Thermal properties

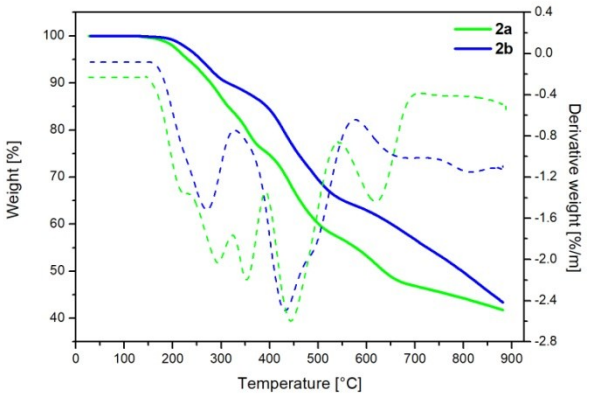


Figure S1. TGA and DTG curves of the phenothiazine derivatives **2a** and **2b**.

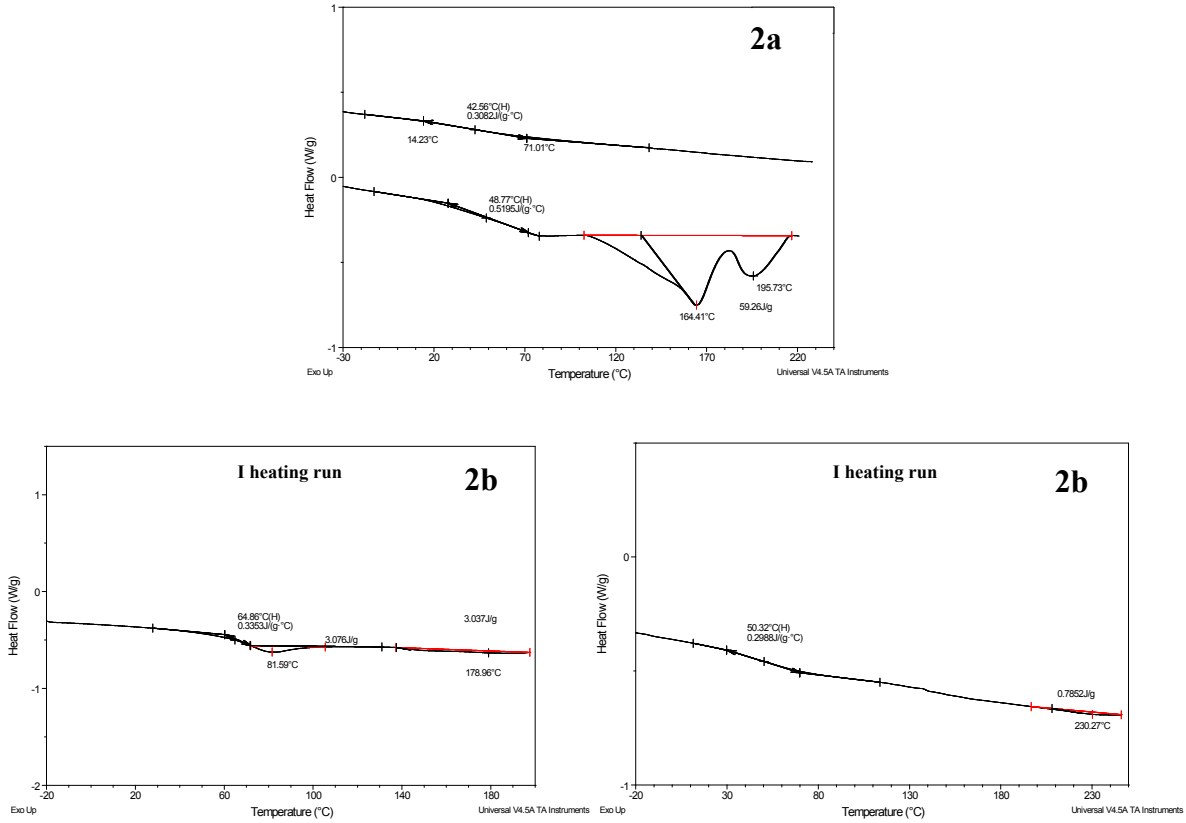


Figure S2. DSC curves of compound **2a** and **2b** registered during the first and second heating scans. Heating rate: 20 °C/min.

DFT calculations

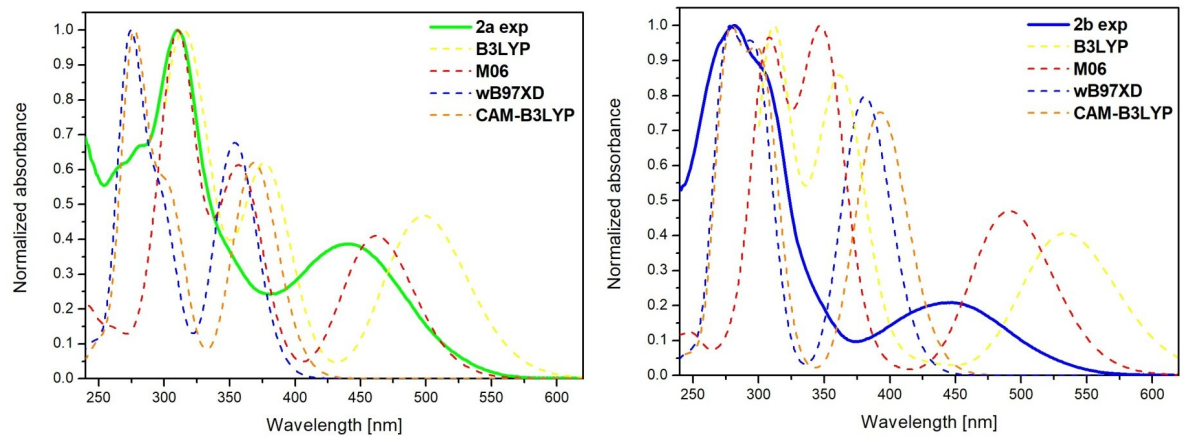


Figure S3. The absorption spectra of **2a** and **2b** in $CHCl_3$: experimental and theoretical TD/DFT method (B3LYP, M06, CAM-B3LYP, wB97XD).

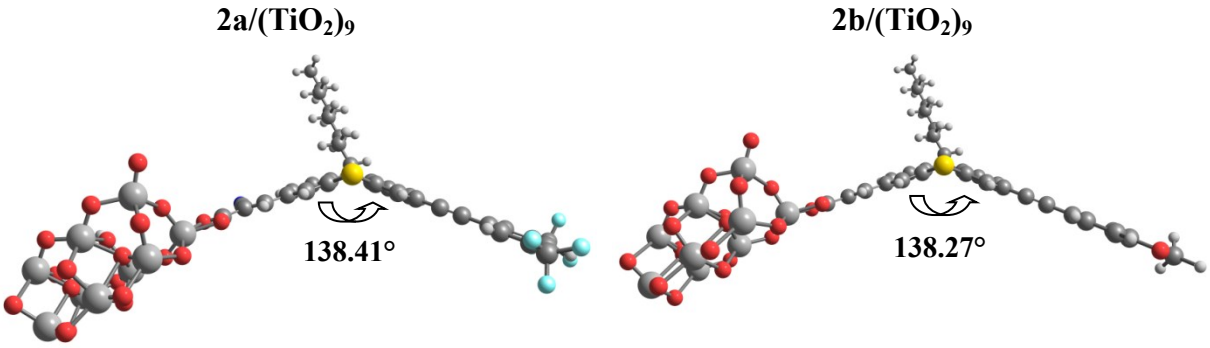


Figure S4. The side view of optimized geometries of **2a/(TiO$_2$)$_9$** and **2b/(TiO$_2$)$_9$** with the values of the angles.

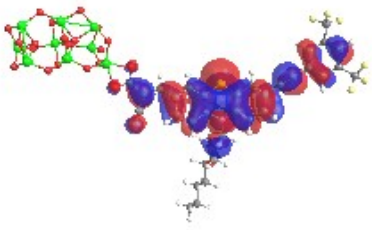
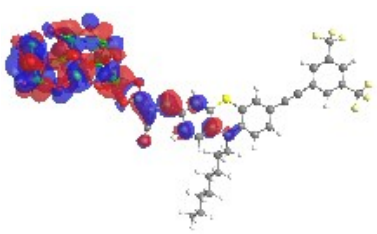
Table S1. Theoretically calculated energy gaps for **2a** and **2b** with various hybrid potentials: B3LYP, M06, CAM-B3LYP, wB97XD.

	B3LYP	**CAM-B3LYP**	**M06**	**wB97XD**
2a	2.93	5.47	3.41	6.64
2b	2.69	5.11	3.14	6.21

Table S2. Calculated TD-DFT bands in absorption spectra for **2a** and **2b** and the analogs containing (TiO$_2$)$_9$ cluster at M06/6-31G** level.

	M06
2a	310, 357, 462
2a/(TiO$_2$)$_9$	308, 364, 504
2b	308, 347, 491
2b/(TiO$_2$)$_9$	312, 353, 518

Table S3. Natural transition orbitals (NTOs) with pairs occupied (holes) and unoccupied (electrons) for **2a/(TiO$_2$)$_9$** presenting the nature of absorption spectra (M06/6-31G(d,p)). For each state, the respective number of the state and the oscillator strength are listed (isovalue 0.01 e bohr^{-3}).

2a/(TiO$_2$)$_9$	**Hole**	**Electron**
S_4 522.20 nm (0.114) 96%		

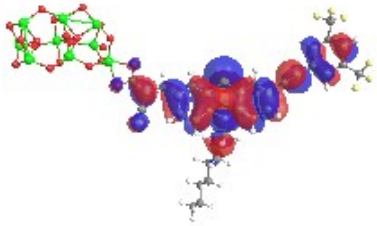
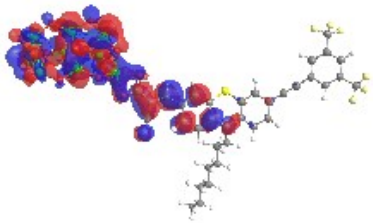
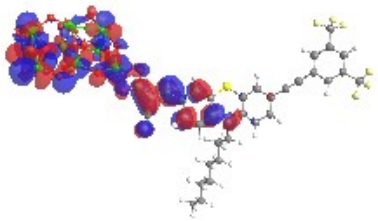
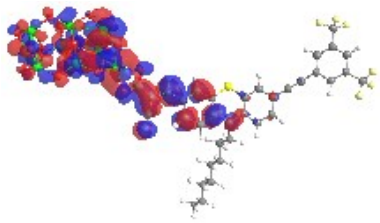
S_5 509.58 nm (0.197) 96%		
S_6 497.51 nm (0.159) 97%		
S_9 468.88 nm (0.131) 95%		

Table S4. Dipole moment [D] for **2a** and **2b** in $CHCl_3$ from DFT with various hybrid potentials: B3LYP, M06, CAM-B3LYP, wB97XD.

	B3LYP	**CAM-B3LYP**	**M06**	**wB97XD**
2a	10.75	9.97	10.59	9.35
2b	10.55	8.98	10.14	8.85

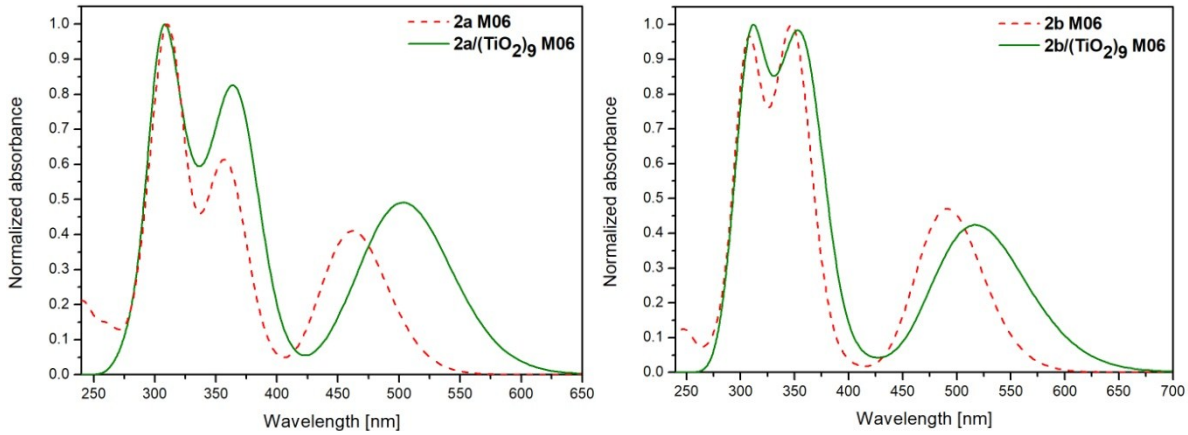


Figure S5. Calculated UV-Vis spectra for **2a** and **2b** at M06/6-31G** level compared with the analogs containing $(TiO_2)_9$ cluster.

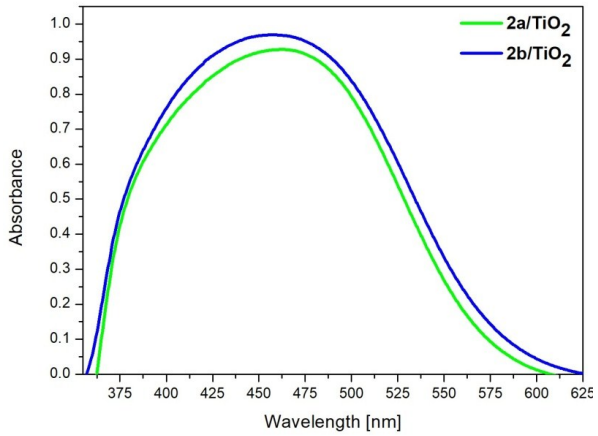


Figure S6. Absorption spectra of **2a** and **2b** adsorbed on TiO_2.

^{1}H NMR and MS spectra of 2a and 2b

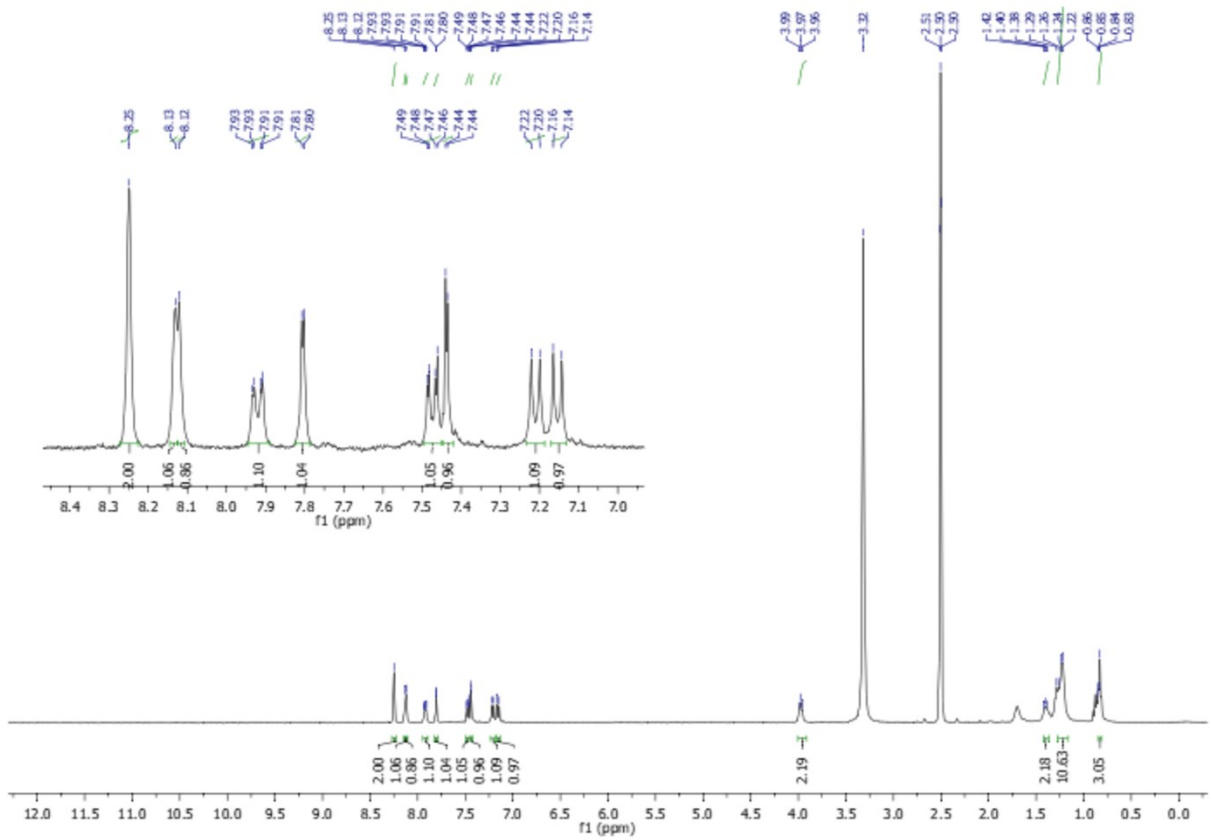


Figure S7. The ^{1}H spectrum of **2a** in DMSO-d_6

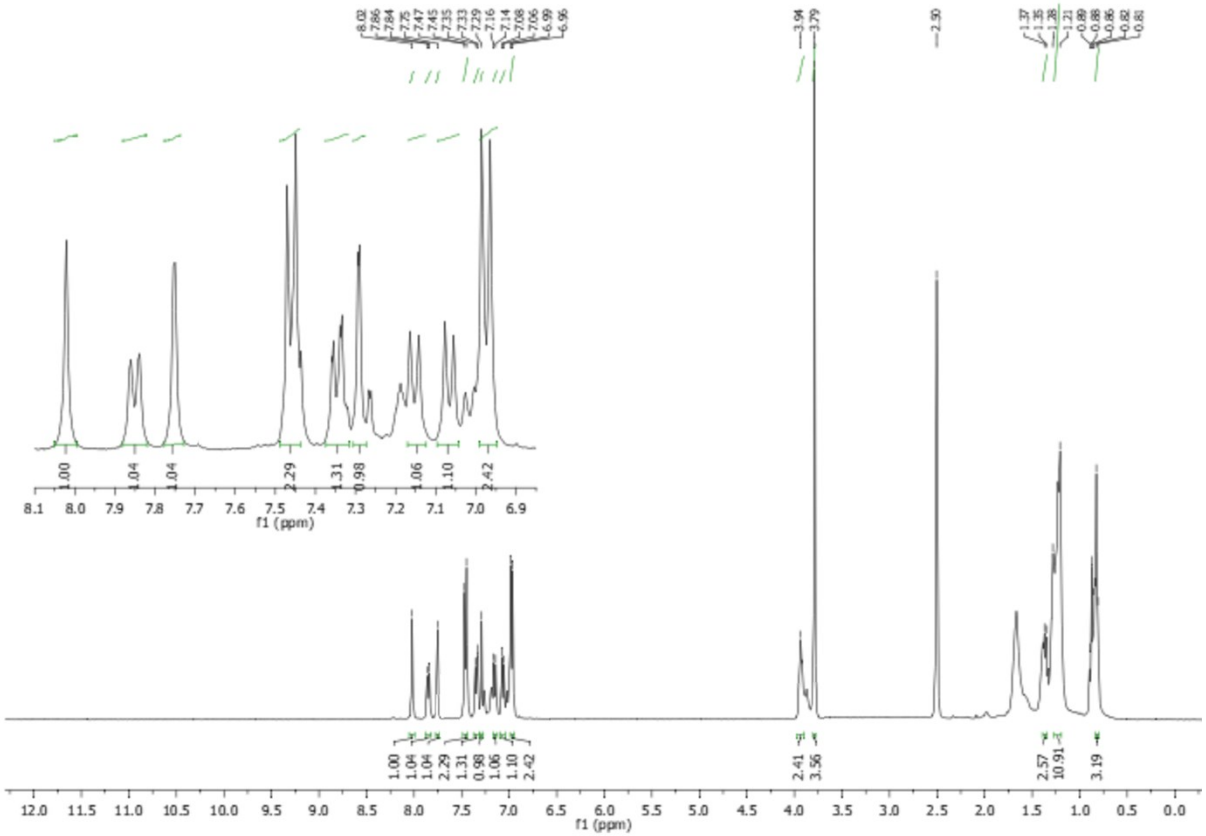
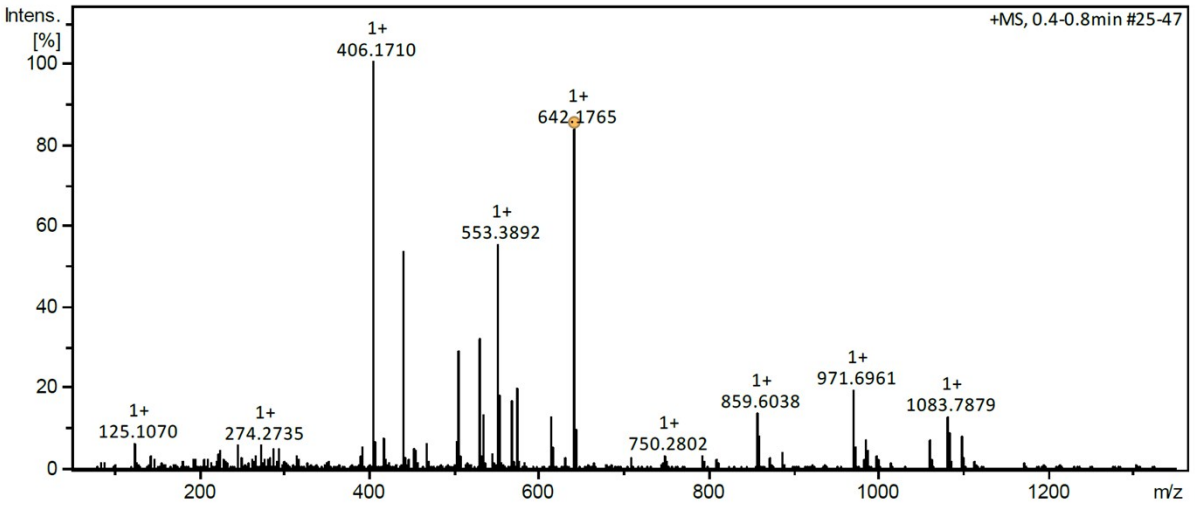


Figure S8. The ^{1}H spectrum of **2b** in DMSO-d_6



The isotopic pattern of peak 642 m/z (experimental at the top, theoretical at the bottom)

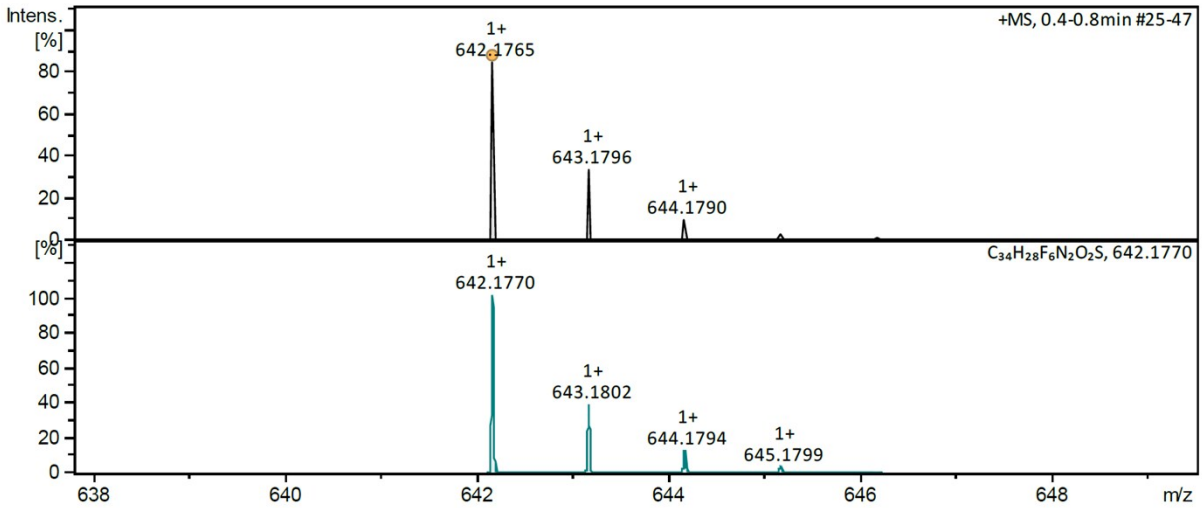
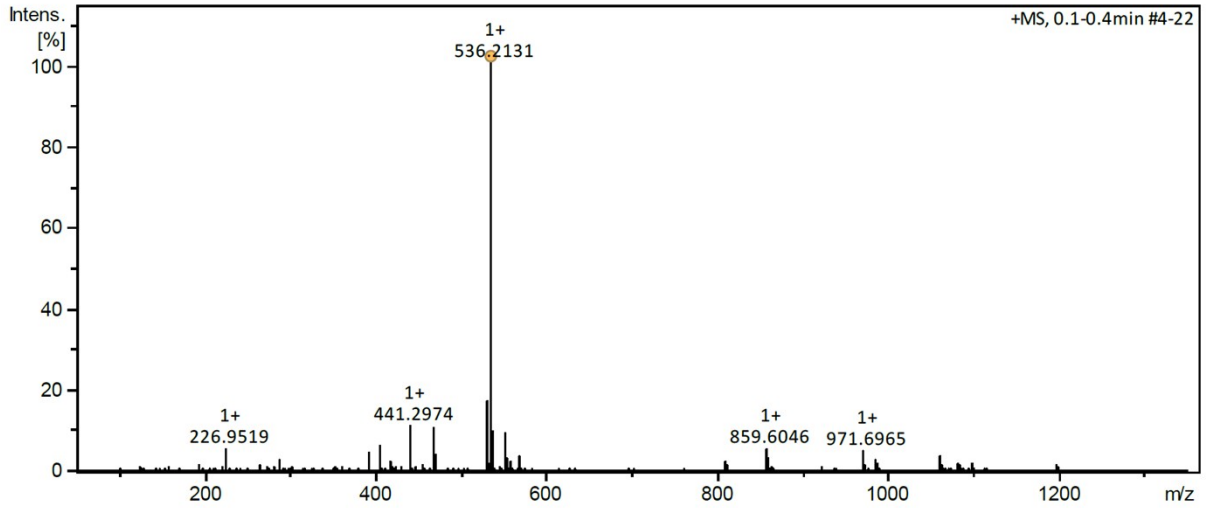


Figure S9. MS spectrum of **2a**.



The isotopic pattern of peak 536 m/z (experimental at the top, theoretical at the bottom)

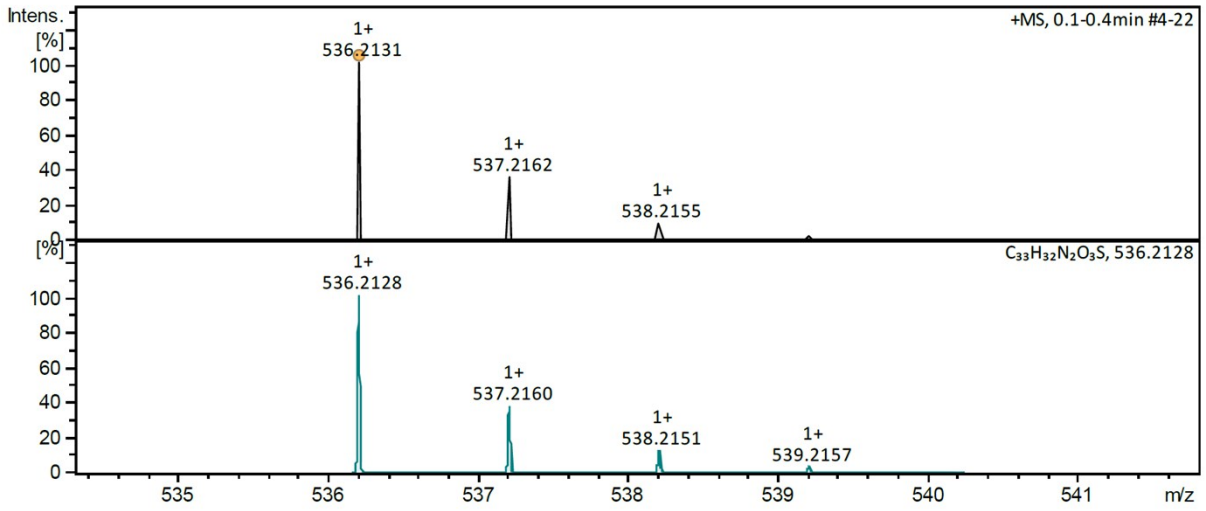


Figure S10. MS spectrum of **2b**.

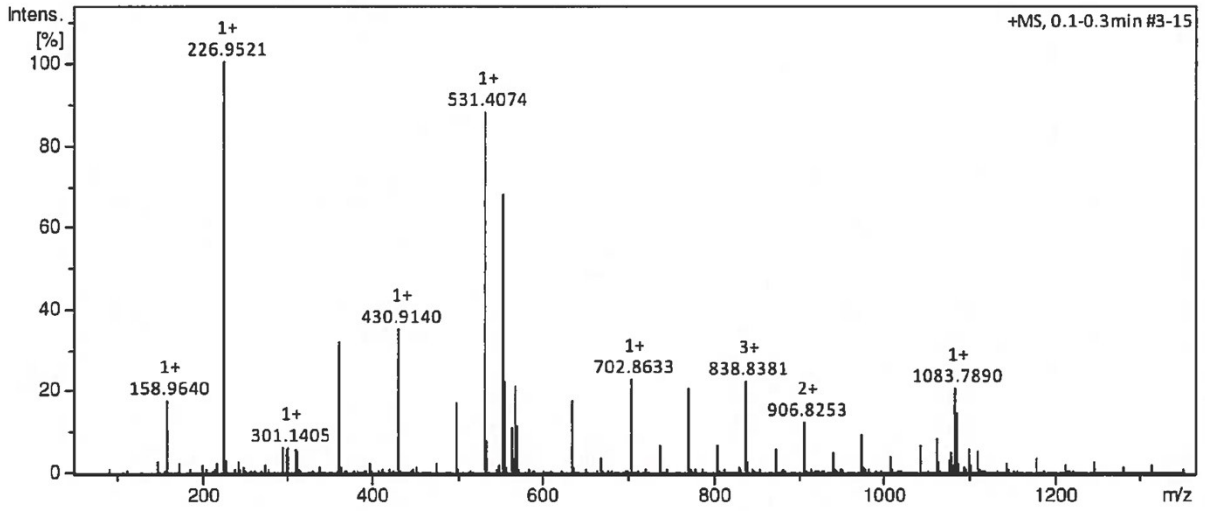


Figure S11. ESI-MS spectrum of a mixture of 10 mM ammonium bicarbonate in acetonitrile with water 90:10 (v / v) in positive ion mode.

Cartesian coordinates of DFT-optimized structure of **2a** by B3LYP /6-31G**/$CHCl_3$:

C	-0.111199000	-1.508429000	0.216769000
C	0.503569000	-0.411153000	-0.418132000
C	-0.295890000	0.442846000	-1.200014000
C	-1.658460000	0.210601000	-1.341613000
C	-2.282184000	-0.862595000	-0.683775000
C	-1.480392000	-1.715667000	0.100759000
S	-2.259042000	-3.031100000	1.018957000
C	-3.509716000	-3.458582000	-0.175153000
C	-4.118544000	-2.431184000	-0.933517000
N	-3.669752000	-1.108871000	-0.813917000
C	-3.932066000	-4.773952000	-0.292522000
C	-5.025817000	-5.124550000	-1.114213000
C	-5.610275000	-4.103539000	-1.891818000
C	-5.154670000	-2.795385000	-1.816228000
C	-5.411311000	-6.527353000	-1.166800000
C	1.899928000	-0.180196000	-0.274875000
C	3.093731000	0.019831000	-0.152974000
C	-4.565781000	0.002488000	-1.182477000
C	-4.568026000	1.135405000	-0.147311000
C	-5.541102000	2.255894000	-0.536846000
C	-5.565132000	3.408956000	0.474273000
C	-6.529884000	4.536749000	0.088055000
C	-6.548087000	5.696565000	1.091009000
C	-7.508717000	6.827587000	0.703527000
C	-7.517265000	7.984428000	1.707317000
H	0.486388000	-2.186955000	0.815717000
H	0.160348000	1.284486000	-1.709366000
H	-2.238997000	0.872636000	-1.971782000
H	-3.432664000	-5.541859000	0.290615000
H	-6.388127000	-4.337399000	-2.608711000
H	-5.591820000	-2.055537000	-2.474888000
H	-5.574578000	-0.406725000	-1.234246000
H	-4.329717000	0.386704000	-2.184117000
H	-3.561686000	1.551121000	-0.030728000
H	-4.847703000	0.714667000	0.826037000
H	-6.554212000	1.842910000	-0.640993000
H	-5.268420000	2.648607000	-1.526518000
H	-4.550732000	3.818645000	0.579478000
H	-5.839394000	3.017938000	1.463972000
H	-7.545247000	4.127488000	-0.012141000
H	-6.258399000	4.921170000	-0.905501000
H	-5.532081000	6.104334000	1.192836000
H	-6.821693000	5.313907000	2.084727000
H	-8.524522000	6.421087000	0.604885000
H	-7.236521000	7.207567000	-0.290630000
H	-7.820044000	7.642030000	2.703492000
H	-8.211275000	8.774506000	1.402343000
H	-6.522117000	8.433946000	1.801840000

C	4.490326000	0.257412000	-0.016258000
C	5.296325000	-0.615010000	0.738178000
C	6.661230000	-0.368366000	0.871907000
C	7.249751000	0.741523000	0.265529000
C	6.451900000	1.609197000	-0.483351000
C	5.087268000	1.376791000	-0.628038000
H	4.846931000	-1.474589000	1.221455000
H	4.475812000	2.060469000	-1.204466000
C	7.514643000	-1.343171000	1.641219000
C	7.089032000	2.781065000	-1.183955000
F	8.641364000	-0.766608000	2.111279000
F	6.851957000	-1.864051000	2.697408000
F	7.897291000	-2.385636000	0.867026000
F	7.570206000	2.430911000	-2.399962000
F	8.129064000	3.279920000	-0.480674000
F	6.211728000	3.788275000	-1.383696000
H	8.308485000	0.934604000	0.385973000
C	-6.602265000	-7.121438000	-1.474090000
C	-6.623725000	-8.550818000	-1.579972000
C	-7.945095000	-6.491766000	-1.718650000
O	-8.789511000	-7.023162000	-2.404398000
O	-8.215538000	-5.323829000	-1.098843000
N	-6.625336000	-9.712390000	-1.654344000
H	-7.478874000	-5.042474000	-0.533035000
H	-4.604242000	-7.217068000	-0.927717000

Cartesian coordinates of DFT-optimized structure of **2b** by B3LYP /6-31G**/$CHCl_3$:

C	-1.187382000	-1.284910000	-0.437604000
C	-1.804311000	-0.265132000	0.314003000
C	-1.001241000	0.491384000	1.188280000
C	0.360813000	0.240480000	1.305754000
C	0.983721000	-0.754390000	0.535160000
C	0.181250000	-1.510020000	-0.340678000
S	0.957082000	-2.726962000	-1.387411000
C	2.197912000	-3.284829000	-0.235456000
C	2.821607000	-2.342484000	0.619622000
N	2.372975000	-1.021039000	0.650044000
C	2.619218000	-4.601599000	-0.259336000
C	3.705600000	-5.057148000	0.532500000
C	4.325745000	-4.110401000	1.380068000
C	3.884622000	-2.799223000	1.428498000
C	4.041850000	-6.450276000	0.379855000
C	-3.200749000	-0.018722000	0.196457000
C	-4.396431000	0.190362000	0.098796000
C	3.267970000	0.052474000	1.120209000
C	3.277193000	1.269055000	0.184778000
C	4.253278000	2.349544000	0.668128000
C	4.313042000	3.564386000	-0.266331000
C	5.289495000	4.648783000	0.205234000
C	5.359835000	5.858738000	-0.734202000
C	6.337979000	6.943293000	-0.266151000
C	6.406051000	8.145623000	-1.212613000
H	-1.784207000	-1.892446000	-1.109219000
H	-1.455077000	1.272329000	1.788525000
H	0.940487000	0.827662000	2.007376000
H	2.114625000	-5.297438000	-0.923277000
H	5.140463000	-4.427191000	2.014382000
H	4.359634000	-2.122840000	2.128092000
H	4.276401000	-0.358841000	1.144921000
H	3.022869000	0.348265000	2.148776000
H	2.272299000	1.695758000	0.099528000
H	3.560109000	0.929727000	-0.819030000
H	5.259223000	1.917706000	0.765232000
H	3.964419000	2.680174000	1.675766000
H	3.307552000	3.997272000	-0.363616000
H	4.599261000	3.230976000	-1.273630000
H	6.292966000	4.212032000	0.309293000
H	4.999737000	4.986163000	1.210653000
H	4.356897000	6.296971000	-0.838853000
H	5.648951000	5.521003000	-1.739782000
H	7.339354000	6.504444000	-0.159262000
H	6.047514000	7.283404000	0.737272000
H	6.727004000	7.842038000	-2.215675000
H	7.112461000	8.900411000	-0.851764000
H	5.426505000	8.627268000	-1.311913000

C	-5.794766000	0.431568000	-0.015676000
C	-6.584879000	-0.301602000	-0.929854000
C	-7.945383000	-0.067409000	-1.039296000
C	-8.564941000	0.907477000	-0.238674000
C	-7.797216000	1.644982000	0.673576000
C	-6.429101000	1.404472000	0.778218000
O	-9.904382000	1.058539000	-0.422620000
H	-6.115386000	-1.056721000	-1.551746000
H	-8.555020000	-0.628343000	-1.739898000
H	-5.839891000	1.977923000	1.486446000
C	-10.592391000	2.029327000	0.362727000
H	-8.251064000	2.401745000	1.301546000
H	-11.636965000	1.976021000	0.055395000
H	-10.210522000	3.039679000	0.176032000
H	-10.517155000	1.804945000	1.432985000
C	4.963271000	-7.331177000	0.907751000
C	4.890011000	-8.671979000	0.409096000
C	6.030530000	-7.094413000	1.924338000
O	6.803521000	-8.158118000	2.240733000
O	6.249864000	-6.035062000	2.478004000
N	4.879747000	-9.779109000	0.040790000
H	3.393566000	-6.935674000	-0.347347000
H	6.551842000	-8.955473000	1.746316000

Cartesian coordinates of DFT-optimized structure of **2a/$(TiO_2)_9$** by B3LYP/ 6-31G**/LANL2DZ/$CHCl_3$:

Ti	10.424158000	-2.224565000	2.011182000
Ti	9.564549000	0.363272000	2.911230000
Ti	6.701610000	0.014602000	1.541394000
Ti	10.970998000	0.108303000	0.426580000
Ti	3.776077000	0.395847000	0.133293000
Ti	7.688470000	-2.665336000	0.499791000
Ti	5.177479000	-2.216654000	-0.836494000
Ti	8.279647000	-0.267796000	-1.258167000
Ti	5.503787000	0.082309000	-2.854733000
O	10.205820000	-1.236733000	3.563844000
O	9.216769000	-3.380859000	1.434765000
O	7.852499000	0.821447000	2.841840000
O	10.068062000	0.414403000	-1.065760000
O	10.784113000	1.263486000	1.855578000
O	11.714554000	-1.516745000	0.899671000
O	3.788645000	-1.458849000	0.026828000
O	7.007597000	-1.712985000	1.984461000
O	6.293201000	-3.581593000	-0.164358000
O	6.549207000	-1.003722000	-0.293575000
O	5.113807000	-1.763942000	-2.536619000
O	5.008493000	0.539132000	1.554872000
O	7.647669000	1.062079000	0.112796000
O	4.526855000	0.884068000	-1.361379000
O	8.656485000	-2.027791000	-0.965046000
O	4.956748000	0.593574000	-4.308138000
O	7.436958000	0.123883000	-2.742338000
O	9.442153000	-0.704026000	1.299002000
O	1.730315000	0.433340000	-0.159693000
O	2.758123000	2.069200000	0.843190000
C	-2.140604000	2.147404000	0.135477000
C	-0.768649000	1.718340000	0.101539000
C	0.383854000	2.291224000	0.582719000
C	0.464472000	3.546411000	1.257621000
C	1.655286000	1.581427000	0.413406000
N	0.539047000	4.569410000	1.809220000
H	8.148430000	1.869566000	0.316918000
C	-2.613220000	3.331484000	0.747269000
C	-3.097114000	1.305886000	-0.483712000
C	-4.441065000	1.636459000	-0.516260000
C	-4.910662000	2.812620000	0.117815000
C	-3.960314000	3.647300000	0.746387000
S	-5.578727000	0.656580000	-1.474698000
C	-7.003497000	0.836905000	-0.420697000
C	-7.217979000	2.063885000	0.240184000
N	-6.273994000	3.114956000	0.122160000
C	-7.912956000	-0.208707000	-0.306386000
C	-9.090766000	-0.056658000	0.451719000

C	-9.297646000	1.161098000	1.126012000
C	-8.369034000	2.191425000	1.036898000
C	-6.707343000	4.508557000	0.344402000
C	-6.224075000	5.469545000	-0.751280000
C	-6.705309000	6.903741000	-0.490003000
C	-6.253913000	7.897835000	-1.568417000
C	-6.727357000	9.333193000	-1.302866000
C	-6.275434000	10.335809000	-2.372682000
C	-6.747643000	11.770942000	-2.103653000
C	-6.292202000	12.768112000	-3.174521000
C	-10.037805000	-1.113980000	0.545278000
C	-10.853467000	-2.012551000	0.631092000
C	-11.812322000	-3.059292000	0.733199000
C	-11.576519000	-4.310194000	0.128495000
C	-12.520940000	-5.327299000	0.233703000
C	-13.713558000	-5.126696000	0.934111000
C	-13.949498000	-3.889799000	1.534397000
C	-13.012555000	-2.861808000	1.440813000
C	-12.243805000	-6.682787000	-0.363165000
C	-15.254424000	-3.635179000	2.243318000
F	-13.359550000	-7.229464000	-0.894936000
F	-11.312475000	-6.628979000	-1.338171000
F	-11.791310000	-7.551408000	0.571037000
F	-15.814407000	-4.776829000	2.696679000
F	-15.096666000	-2.810044000	3.301486000
F	-16.158176000	-3.050206000	1.422935000
H	-0.600124000	0.762127000	-0.388814000
H	-1.927520000	4.003235000	1.247444000
H	-2.766461000	0.390804000	-0.967143000
H	-4.282715000	4.548266000	1.253183000
H	-7.720393000	-1.145879000	-0.818271000
H	-10.183422000	1.289921000	1.739075000
H	-8.541386000	3.096173000	1.607560000
H	-6.401938000	4.858813000	1.339582000
H	-7.796977000	4.507465000	0.333068000
H	-6.603701000	5.113550000	-1.717390000
H	-5.130417000	5.458768000	-0.820928000
H	-6.334251000	7.239881000	0.489343000
H	-7.803039000	6.915086000	-0.422186000
H	-6.627227000	7.565692000	-2.548019000
H	-5.156452000	7.883618000	-1.638279000
H	-6.356834000	9.660563000	-0.320046000
H	-7.825385000	9.345912000	-1.234172000
H	-6.646360000	10.010855000	-3.356226000
H	-5.177454000	10.323197000	-2.442260000
H	-6.376923000	12.094912000	-1.120630000
H	-7.844844000	11.783475000	-2.034510000
H	-5.197710000	12.803504000	-3.242357000
H	-6.645429000	13.782079000	-2.953566000
H	-6.675770000	12.489296000	-4.163906000

H	-10.656630000	-4.473026000	-0.420637000
H	-14.445788000	-5.921815000	1.011310000
H	-13.201221000	-1.905615000	1.915658000

Cartesian coordinates of DFT-optimized structure of **2b/(TiO$_2$)$_9$** by B3LYP/ 6-31G**/LANL2DZ/CHCl$_3$:

Ti	-9.600723000	-2.064546000	-0.772031000
Ti	-8.414958000	-0.298960000	-2.704911000
Ti	-5.574021000	-0.447012000	-1.245963000
Ti	-9.724858000	0.778206000	-0.386213000
Ti	-2.561393000	0.043632000	-0.078744000
Ti	-6.903660000	-2.205680000	0.848108000
Ti	-4.289571000	-1.618647000	1.905143000
Ti	-7.039359000	0.781198000	1.347888000
Ti	-4.174246000	1.338492000	2.710000000
O	-9.317765000	-1.899942000	-2.599462000
O	-8.553326000	-3.024316000	0.279329000
O	-6.649352000	-0.124519000	-2.793739000
O	-8.704196000	1.586837000	0.809857000
O	-9.436062000	1.145069000	-2.171105000
O	-10.712701000	-0.763485000	-0.091887000
O	-2.839448000	-1.548746000	0.834857000
O	-6.157522000	-2.122791000	-0.883024000
O	-5.630291000	-2.941331000	1.884939000
O	-5.487528000	-0.565872000	0.856378000
O	-4.081560000	-0.497551000	3.248500000
O	-3.825116000	-0.253618000	-1.450444000
O	-6.271583000	1.255613000	-0.447963000
O	-3.163702000	1.233206000	1.043161000
O	-7.700182000	-0.843114000	1.848316000
O	-3.487078000	2.349404000	3.795344000
O	-6.075525000	1.648909000	2.523871000
O	-8.374250000	-0.557115000	-0.782803000
O	-0.520656000	-0.092092000	0.193729000
O	-1.364176000	1.144031000	-1.387587000
C	3.503311000	1.081648000	-0.502054000
C	2.103552000	0.769404000	-0.411391000
C	1.012869000	1.251029000	-1.096226000
C	1.057802000	2.217633000	-2.145630000
C	-0.321843000	0.751848000	-0.757402000
N	1.085482000	3.003033000	-3.005191000
H	-6.663319000	1.953264000	-0.999735000
C	4.059155000	2.109979000	-1.298425000
C	4.395381000	0.303230000	0.276649000
C	5.759262000	0.540351000	0.271756000
C	6.310449000	1.563360000	-0.540126000
C	5.422663000	2.340621000	-1.317134000
S	6.825280000	-0.335235000	1.399694000
C	8.269103000	-0.421460000	0.357566000
C	8.565785000	0.664205000	-0.489321000
N	7.687706000	1.777826000	-0.562030000
C	9.107622000	-1.529450000	0.427401000
C	10.295378000	-1.582947000	-0.329490000

C	10.582862000	-0.504171000	-1.187551000
C	9.725222000	0.586277000	-1.278573000
C	8.213547000	3.092895000	-0.975928000
C	7.778825000	4.228214000	-0.037851000
C	8.344913000	5.583410000	-0.484109000
C	7.946064000	6.735129000	0.448611000
C	8.497327000	8.096518000	0.004237000
C	8.099140000	9.249931000	0.934508000
C	8.645739000	10.612996000	0.489320000
C	8.243043000	11.759514000	1.423144000
C	11.168788000	-2.702919000	-0.244743000
C	11.924502000	-3.656132000	-0.187516000
C	12.812025000	-4.767600000	-0.129547000
C	12.574454000	-5.845796000	0.753294000
C	13.440396000	-6.926284000	0.803346000
C	14.574045000	-6.968318000	-0.027350000
C	14.826039000	-5.907044000	-0.908852000
C	13.951435000	-4.823225000	-0.953799000
H	1.848576000	0.011153000	0.325692000
H	3.422840000	2.732445000	-1.914212000
H	3.997960000	-0.486744000	0.907968000
H	5.808975000	3.126353000	-1.954388000
H	8.849761000	-2.356751000	1.080634000
H	11.477244000	-0.534262000	-1.801142000
H	9.959953000	1.374661000	-1.984308000
H	7.942886000	3.314055000	-2.017183000
H	9.300624000	3.024048000	-0.942554000
H	8.125557000	3.990550000	0.975877000
H	6.685510000	4.288807000	0.011582000
H	7.998585000	5.806232000	-1.503980000
H	9.441784000	5.523290000	-0.538817000
H	8.297208000	6.514760000	1.467186000
H	6.849247000	6.789306000	0.508584000
H	8.145664000	8.314683000	-1.015119000
H	9.594492000	8.041590000	-0.056924000
H	8.452435000	9.033781000	1.953826000
H	7.002024000	9.303474000	0.997943000
H	8.292257000	10.829002000	-0.529048000
H	9.742123000	10.559941000	0.426369000
H	7.151938000	11.860386000	1.478282000
H	8.649419000	12.717809000	1.079226000
H	8.610824000	11.587670000	2.442449000
H	11.701145000	-5.823062000	1.397811000
H	14.151375000	-4.004725000	-1.638564000
O	15.358074000	-8.072728000	0.097238000
C	16.516080000	-8.179611000	-0.725731000
H	15.692727000	-5.914489000	-1.559301000
H	13.260730000	-7.756438000	1.479349000
H	16.250481000	-8.184797000	-1.789926000
H	17.222378000	-7.363483000	-0.530508000

H 16.980526000 -9.131122000 -0.463320000