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Supplementary information

One Pot Oxygen Mediated Syntheses of Stable Radicals

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Materials

Materials. 8-Hydroxyjulolidine-9-carboxaldehyde, DMPO and CD_3OD were bought from TCI Chemicals, India. Malononitrile, piperidine, 4-aminopiperidine, trimethylamine, triethylamine, and aniline were sourced from Avra Chemicals. Ethanol was bought from CH fine chemicals. Molecular biology grade DMSO was from SRL Chemicals. HPLC grade acetonitrile, analytical grade DMSO, formic acid and diethyl ether were obtained from Rankem. Millipore water was used for aqueous phase solution preparation. Eurisotop DMSO-d_6 and Aldrich D_2O were used for NMR analysis.

Chemical Syntheses

Synthesis of DCP• radical. 651 mg of 8-Hydroxyjulolidine-9-carboxaldehyde was taken in 5 mL of ethanol and allowed to stir until it completely dissolve. 594 mg of malononitrile and 15 µL of piperidine were added to this solution. Color of the solution changed from colorless to red within 15 minutes. The reaction mixture was stirred for 2 h for precipitation at room temperature. The precipitate was filtered, thoroughly washed with ethanol, followed by diethyl ether and dried under vacuum to yield a red solid of DCP• (843 mg, y. 71 %). ^{1}H NMR (DMSO-d_6, 500 MHz) δ 6.96 (s, 2H), 6.74 (s, 1H), 6.63 (s, 2H), 4.68 (d, J = 4.0 Hz, 1H), 4.66 (d, J = 4.0 Hz, 1H), 3.18 – 3.07 (m, 4H), 2.67 (dd, J = 15.7, 6.6 Hz, 4H), 1.91 – 1.84 (m, 4H); ^{13}C NMR (DMSO-d_6, 125 MHz) δ 161.2, 160.8, 157.2, 148.1, 144.1, 126.2, 117.1, 114.2, 113.7, 108.2, 104.5, 85.0, 70.7, 49.6, 49.1, 35.0, 31.1, 27.2, 21.9, 21.2; m/z found: 396.1586; M.W. $[C_{22}H_{18}N_7O]$•: 396.1573 [M]•; FTIR (KBr) /cm^{-1}: 3442, 2924, 2852, 2202, 1625, 1593, 1567, 1492, 1460, 1385, 1310; Elemental Analysis: Calcd. for: C, 66.65; H, 4.58; N, 24.73. Found: C, 66.64; H, 4.52; N, 24.79.

Synthesis of CP• radical. Method I. 78 mg of 8-Hydroxyjulolidine-9-carboxaldehyde was taken in 3 mL of ethanol and allowed to stir until it completely dissolve. 71 mg of malononitrile and 108 µL of piperidine were added to this solution. Color of the solution changed from colorless to red within 15 minutes. The reaction mixture was stirred for 2 h for precipitation at room temperature. The precipitate was filtered, thoroughly washed with ethanol, followed by diethyl ether and dried under vacuum to yield a red solid of CP• (72 mg, y. 60 %)

Method II. Conversion of DCP• radical to CP• radical. 40 mg of DCP• radical was dissolved in 3 mL of DMSO. This solution was injected in Agilent 1260 infinity II Prep HPLC, having C-18 column of dimension 25cm × 21.2 mm. Red colored solution was separated by HPLC with a gradient flow of 10–40 % acetonitrile in water containing 0.1% formic acid and the flow rate was kept at 10.62 mL/min. The collected solution (at λ = 535 nm) was lyophilized to obtain CP• radical using Eyela lyophilizer at –80 °C (16 mg, y. 33 %).

^{1}H NMR (DMSO-d_6, 500 MHz) δ 6.51 (s, 1H), 6.44 (s, 2H), 6.32 (s, 2H), 3.45 (s, 2H), 3.04 (m, 4H), 2.63 (m, 4H), 1.86 (m, 4H); ^{13}C NMR (DMSO-d_6, 125 MHz) δ 159.8, 159.2, 157.4, 146.7, 142.6, 126.2, 117.2, 108.5, 106.2, 86.7, 70.3, 49.8, 49.2, 27.1, 22.5, 22.2, 21.6, 21.2; ^{1}H NMR (D_2O, 500 MHz) δ 8.43 (s), 7.82 (s, 1H), 7.04 (s, 1H), 3.61 (s, 4H), 2.79 (s, 2H), 2.68 (s, 2H), 2.02 (s, 4H); ^{13}C NMR (D_2O, 125 MHz) δ 161.1, 160.5, 155.8, 150.8, 149.8, 128.8, 127.2, 114.1, 106.3, 95.8, 79.3, 70.1, 51.1, 26.9, 23.8, 19.4, 18.4; m/z found: 332.1512; M.W. $[C_{19}H_{18}N_5O]$•: 332.1511 [M]•; FTIR (KBr) /cm^{-1}: 3432, 2928, 2852,

2212, 1625, 1599, 1553, 1484, 1466, 1389, 1315; Elemental Analysis: Calcd. for: C, 68.66; H, 5.46; N, 21.07. Found: C, 68.76; H, 5.39; N, 21.16.

Synthesis of DCPC• radical. Method I. 78 mg of 8-Hydroxyjulolidine-9-carboxaldehyde was taken in 150 mL of ethanol and allowed to stir until it completely dissolve. 71 mg of malononitrile and 54 µL of piperidine were added to this solution. Color of the solution changed from colorless to fluorescent green with 30 minutes. The reaction mixture was stirred for 16 h for precipitation at room temperature. The precipitate was filtered, thoroughly washed with ethanol, followed by diethyl ether and dried under vacuum, to yield a yellow solid of DCP• radical (26 mg, y. 18 %).

Method II. 78 mg of 8-Hydroxyjulolidine-9-carboxaldehyde was dissolved in 4 mL of DMSO. 71 mg of malononitrile and 54 µL of piperidine were added to this solution. After 2h of stirring at room temperature, the reaction mixture was poured into a glass vial. After 6 days, dark yellow crystals of DCPC• radical were obtained directly and were separated by filtration. The yellow solid was washed thoroughly with DMSO, followed by methanol and ether, before finally drying under vacuum (28 mg, y. 19 %).

^{1}H NMR (DMSO-d_6, 500 MHz at 130 °C) δ 8.31 (s, 1H), 6.76 (s, 5H), 3.34 (m, 4H), 2.79–2.73 (m, 4H), 1.98–1.95 (m, 4H); ^{13}C NMR (DMSO-d_6, 125 MHz at 130 °C) δ 162.91, 158.90, 158.16, 149.80, 148.01, 142.58, 122.48, 119.58, 119.11, 116.69, 107.17, 103.60, 76.49, 75.24, 50.00, 49.44, 27.80, 21.43, 20.61; m/z found: 396.1583; M.W. [$C_{22}H_{18}N_7O$]•: 396.1573 [M]•; FTIR (KBr) /cm^{-1}: 3434, 3322, 3205, 2938, 2853, 2192, 1626, 1588, 1556, 1494, 1470, 1457, 1439, 1385, 1311. Elemental Analysis: Calcd. for: C, 66.65; H, 4.58; N, 24.73. Found: C, 66.75; H, 4.41; N, 24.96.

Experimental procedures

Electron paramagnetic resonance (EPR). All the EPR experiments were done on Bruker Biospin, EMXmicro A200-9.5/12/S/W. Solid samples of DCP•**,** CP• and DCPC• radicals were analyzed at different temperatures. Before scanning, the solid samples were allowed to equilibrate for 5 minutes at that desired temperature. The instrument parameters for solid state EPR were set as at 100 kHz modulation frequency, 1×10^3 receiver gain, 3.00 G modulation amplitude, 5.120 ms time constant, 75.00 ms conversion time, 3300 G center field, 100 G sweep width, 25 dB microwave attenuation and 1024 number of data points. The solution state EPR experiments of radicals were performed in water or dry DMSO at 10 mM concentration. The parameters were kept the same as for the solid samples. For confirmation of superoxide radical during the formation of DCPC• radical, all the instrument parameters were kept the same, except the number of scans was increased to 5. In solution state, first the DMPO solution was made in DMSO, and then the radical were mixed into the DMPO solution, and let it rest for 10 minutes. The EPR spectrum was recorded at 100K with 100 kHz modulation frequency, 1×10^4 receiver gain, 3.00 G modulation amplitude, 163 ms time constant, 75.00 ms conversion time, 3350 G center field, 200 G sweep width, 25 dB microwave attenuation and 1024 number of data points, with number of scans as 2.

Nuclear magnetic resonance (NMR). All the NMR experiments were done using Jeol 400 and 500 MHz NMR. In the temperature-dependent NMR experiment, DCP• radical was dissolved in DMSO-d_6, kept at the desired temperature for 5 min to equilibrate and the scans

were taken at the same temperature. An NMR scale reaction in DMSO-d_6 was performed for few days to confirm *in situ* formation of DCPH in NMR solvent and its final conversion to $DCPC^+$. For this experiment, 10 mg of 8-Hydroxyjulolidine-9-carboxaldehyde was taken in 700 μL of DMSO-d_6 to dissolve. 8.25 μL malononitrile and 6.75 μL piperidine were added to this solution. The contents were transferred to NMR tube and its spectra were taken at different time interval. For reaction in dry CD_3OD, all the reactants were taken according to the DCP• synthesis in 600 μL of dry CD_3OD in an inert atmosphere, and were examined via NMR till 4h.

Thermogravimetric analysis (TGA), elemental analysis, X-ray crystallography and high-resolution mass (HRMS). Thermal analysis was performed on SII 6300 EXSTAR. All the samples were heated in presence of air within a temperature range of 30–800 °C at a 10 °C/min rate. Elemental analyses were performed on Elementar vario EL analyzer. Single crystal data were collected on both Bruker SMART APEX four-circle diffractometer equipped with a CMOS photon 100 detector (Bruker Systems Inc.) with a Cu Kα radiation (1.5418 Å), and Bruker SMART APEX Duo diffractometer using Mo Kα radiation (0.71073 Å).

Absorption and emission spectroscopy. Photophysical studies i.e., absorbance and emission spectra in solution state were taken on Cary 3500 UV-Vis spectrophotometer and Cary Eclipse Fluorescence spectrophotometer. 25 mM separate stock solutions of DCP• and DCPC• radicals were prepared in molecular biology grade DMSO. 25 μM sample solution in DMSO and water were used for absorbance and emission. For temperature-dependent absorbance and emission studies, 25 μM concentrated solutions were used. The scans were taken after the desired temperature was reached, and waited for 5 minutes to equilibrate at that temperature. Relative quantum yields of $CP(KC)^+$ and $DCPC^+$ have been calculated by comparing rhodamine-6G in DMSO and fluorescein in 0.1 M NaOH respectively.[1] For acid-base reversible cycle in case of CP(KC)+, 20 μM of solution was used, and 2 μL of 1 M of NaOH and 2 μL of 1M of HCl was added alternatively. For absorbance in the solid state, 20 mg of samples were taken and finely grounded with 2 g of barium sulphate, and then absorbance was measured using a Shimadzu 2450 UV-visible spectrophotometer attached with a diffuse reflectance accessory. Solid-state emission was investigated on Cary Eclipse Fluorescence spectrophotometer with a slit width 10 nm for both excitation and emission wavelength. Absolute quantum yields were recorded (l_{ex} = 440-470 nm) using a Fluoromax-4 spectrofluorometer from Horiba Scientific, USA with an integrating sphere.

Time-correlated single-photon count (TCSPC). Fluorescence lifetime decay measurements were done using a 1 cm quartz cell on a Horiba Jobin Yvon "Fluorocube Fluorescence Lifetime System" equipped with NanoLEDs and LDs as the excitation source and an automated polarization accessory (Model 5000 U-02). A 25 μM solution of DCP in phosphate buffer of different pH were analyzed using NanoLED of 460 nm as an excitation source, and the emission was checked at 560 nm.

Theoretical calculations. Density functional theoretical calculations were carried out with dispersion corrected density functional (B3LYP-GD3) in conjunction with 6-311G(d,p) basis set using the Gaussian 09 suite of programs. The absorption spectra of the optimized geometries are simulated using the time dependent density functional (TDDFT) methods. The negative of the value of isotropic shielding at the geometrical centers of the rings were calculated at

B3LYP/6-311G(d,p) level and reported as the aromaticity index nuclear independent chemical shift (NICS(0)) to assess the aromaticity of various cyclic rings. The negative value of NICS(0) indicates the aromatic nature of the rings. The spin density plots are generated for the isovalue of 0.04 and density 0.02.

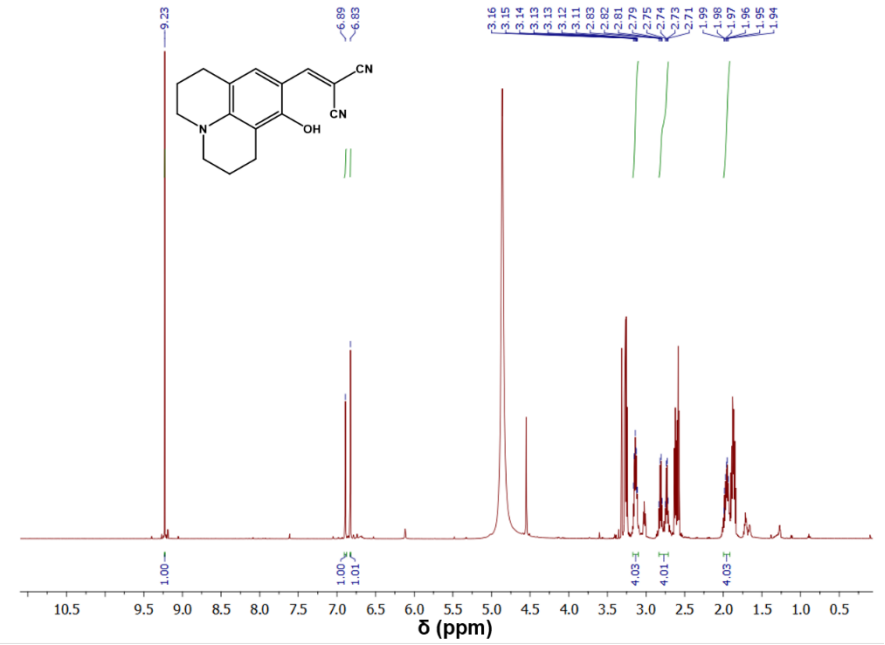


Figure S1. ^{1}H NMR of i*n situ* formation of marked molecule responsible for red color of reaction carried out in absence of oxygen in methanol-d_4.

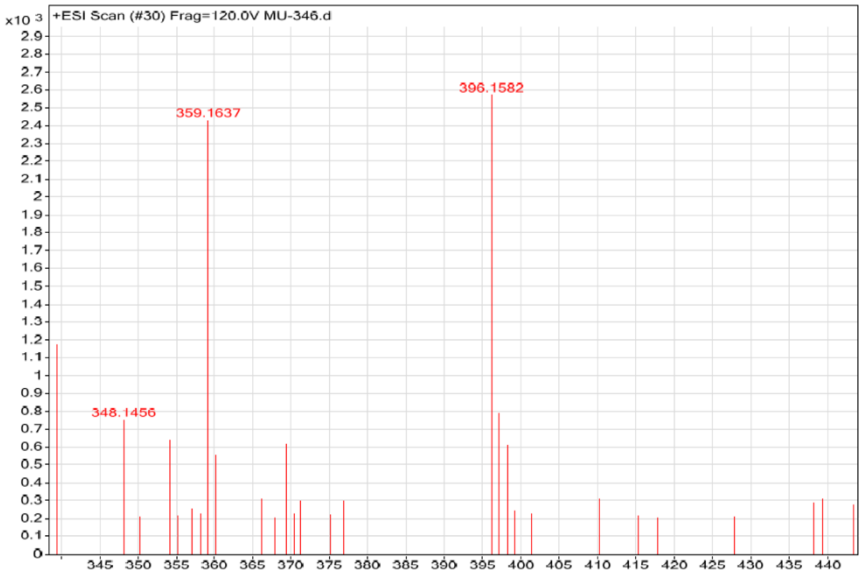


Figure S2. HRMS spectrum of DCP•.

Figure S3. HRMS spectrum of CP•.

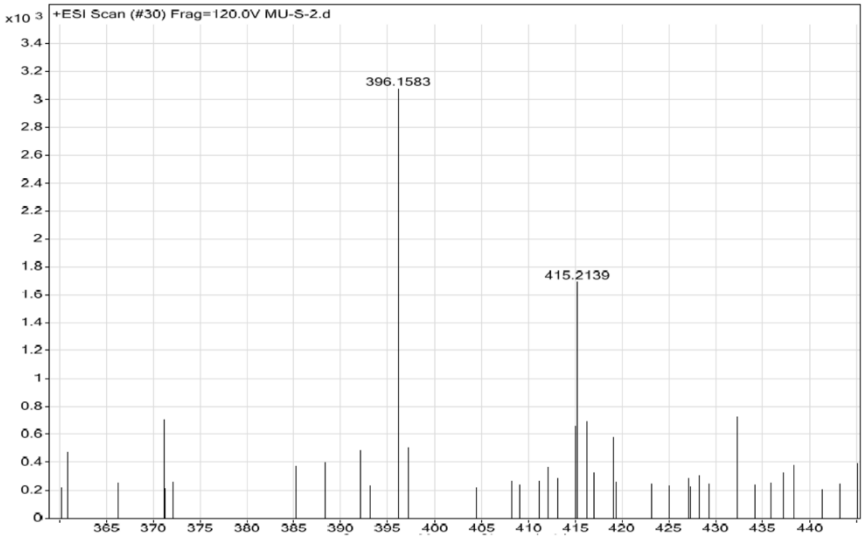


Figure S4. HRMS spectrum of DCPC•.

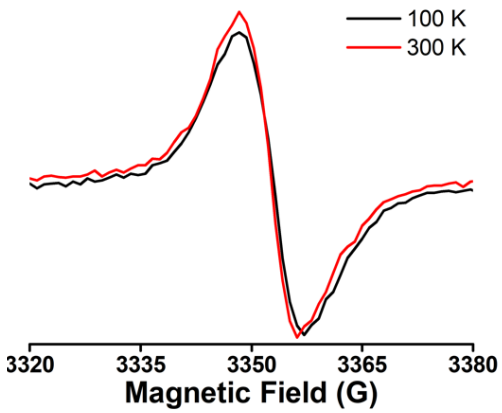


Figure S5. Temperature independent EPR of DCP•.

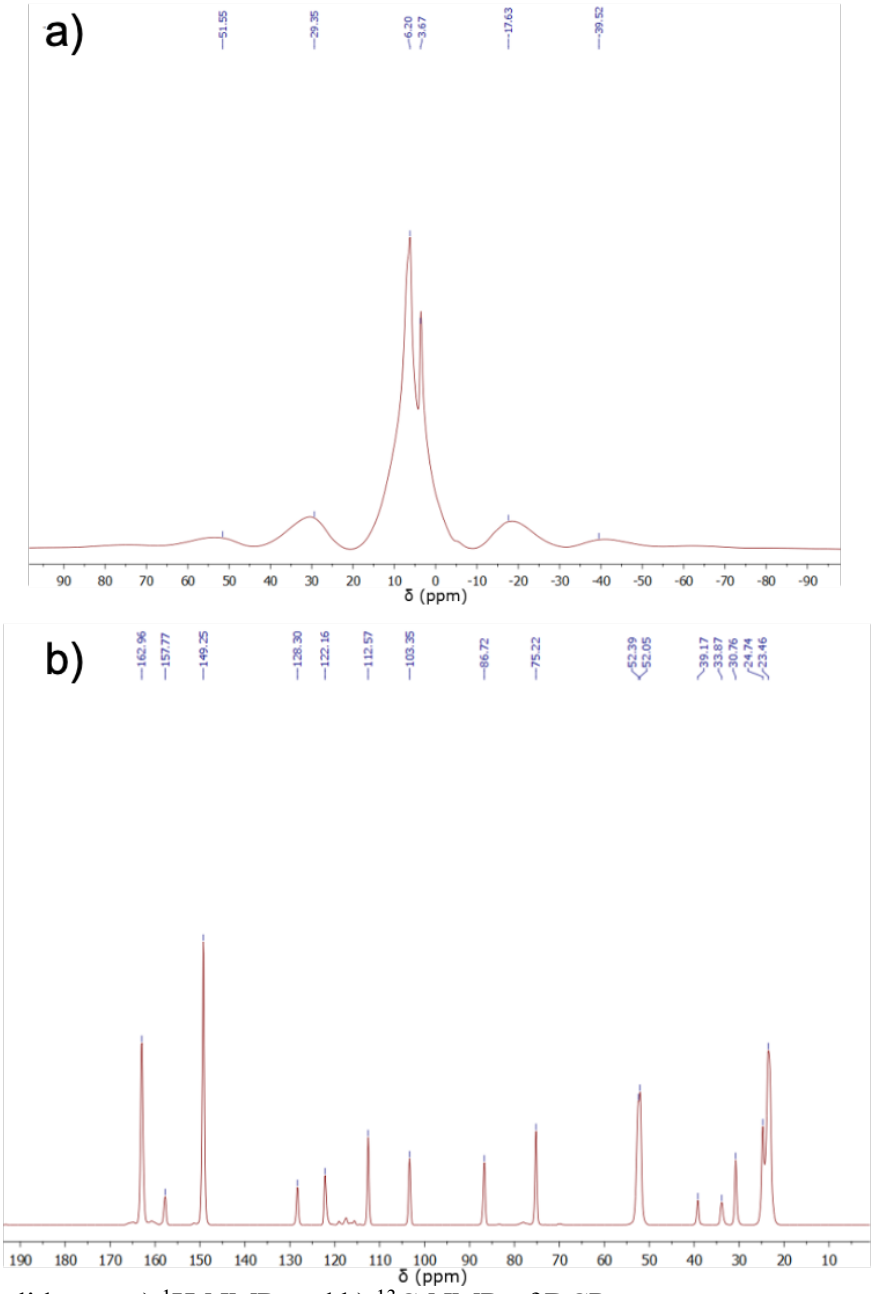


Figure S6. Solid-state a) ^{1}H-NMR and b) ^{13}C-NMR of DCP•.

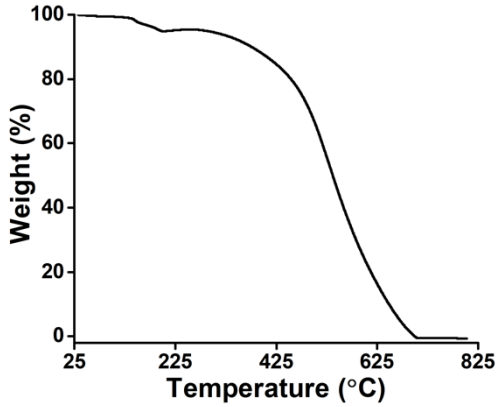


Figure S7. TGA spectrum of DCP• in air.

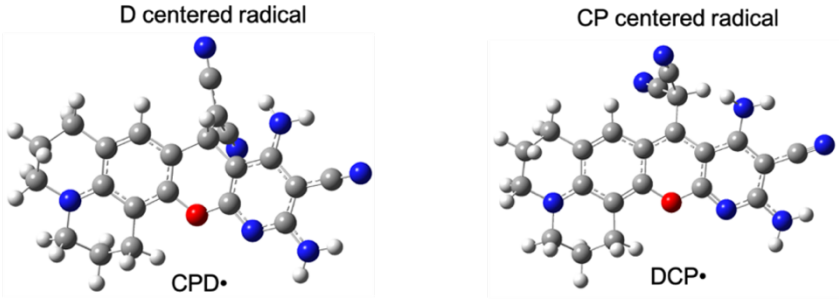


Figure S8. Optimized geometries of CPD• and DCP•.

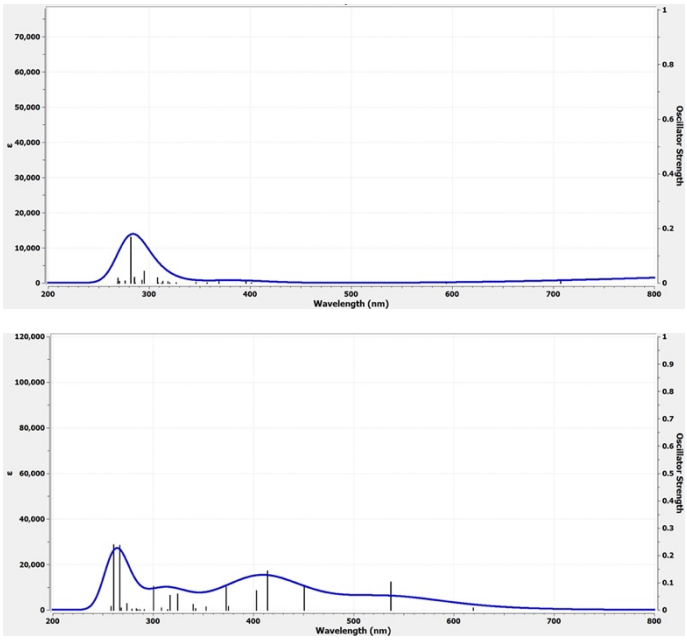


Figure S9. Simulated absorption spectra of (top) CPD• and (bottom) DCP•.

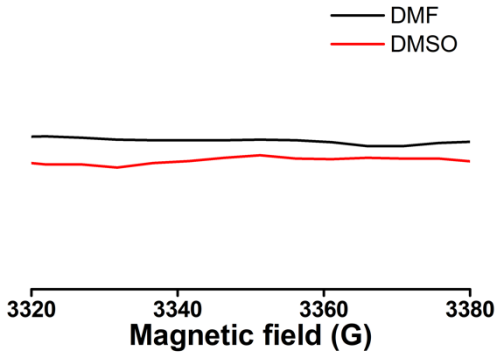


Figure S10. EPR spectrum at 300 K for the DMF (black) and DMSO (red) solution of DCP•. This data was collected after 10 min of the solution preparation. Y axis has been compared with the solid state (for more details, see Figure S12).

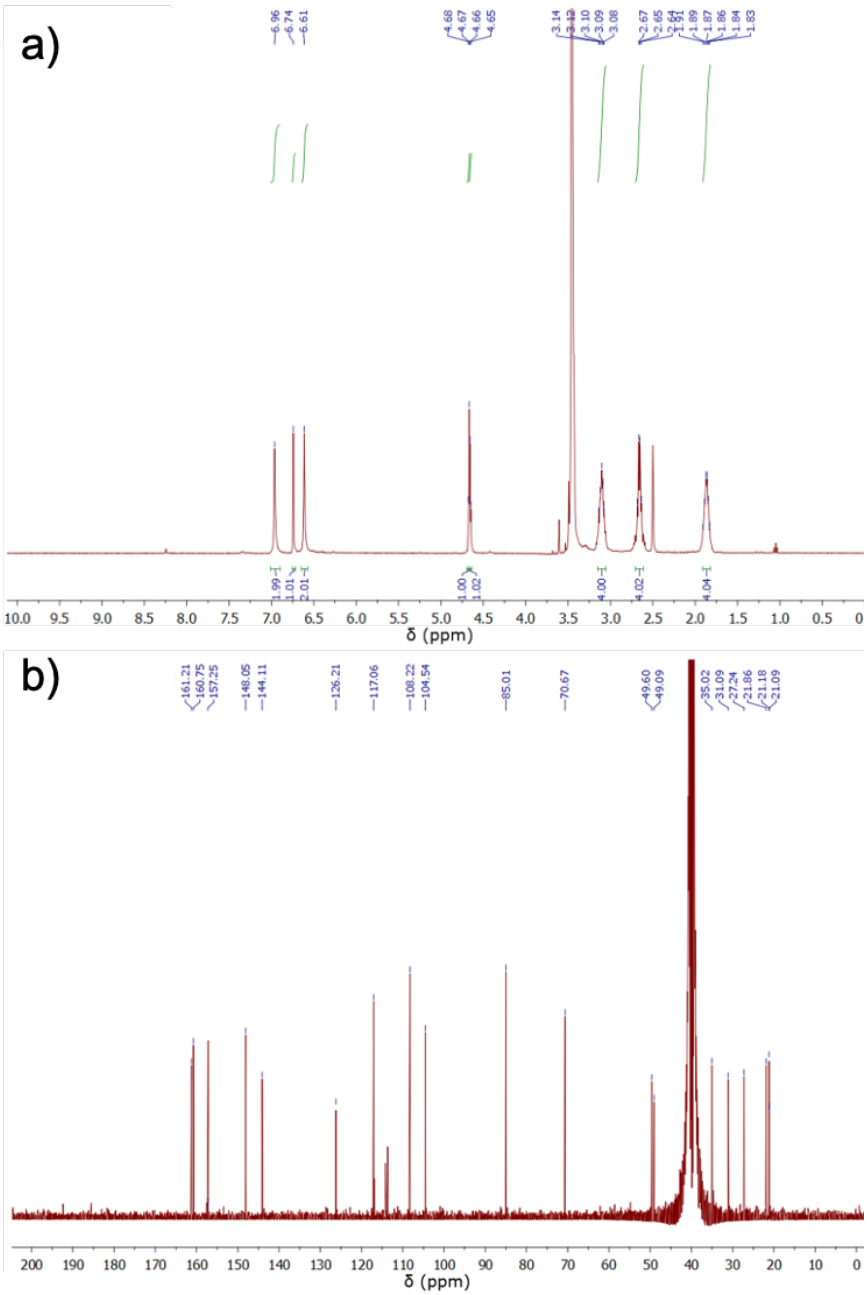


Figure S11. a) ^{1}H-NMR and b) ^{13}C-NMR of DCP• as DCPH in DMSO-d_6.

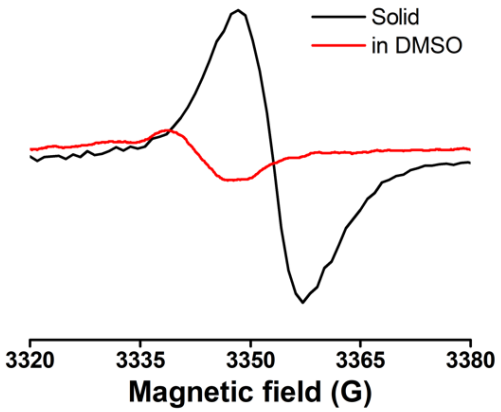


Figure S12. EPR spectrum of DMSO radical at 300 K for the DMSO solution of DCP•. This data was collected immediately after the solution preparation. The poor intensity of the DMSO radical disappears within next 10 min (Figure S10).

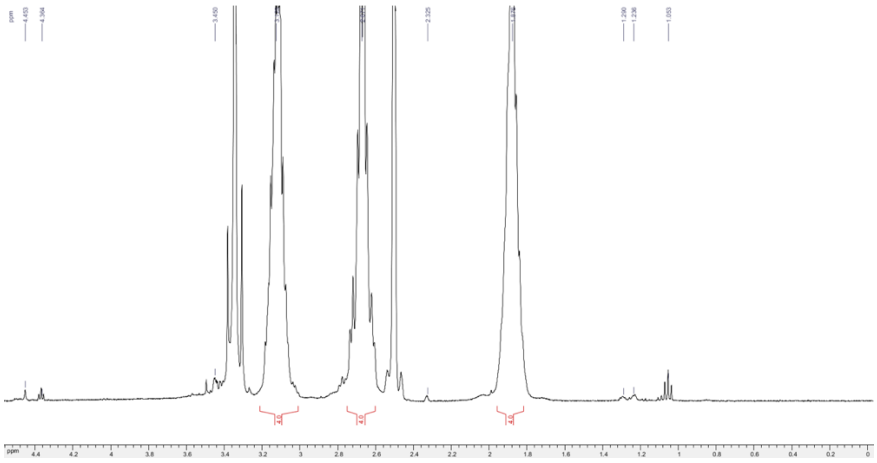


Figure S13. Noise in ^{1}H NMR spectrum due to the by-products of DMSO radical. The major peaks are due to julolidine part of DCPH, water and methyl group in DMSO.

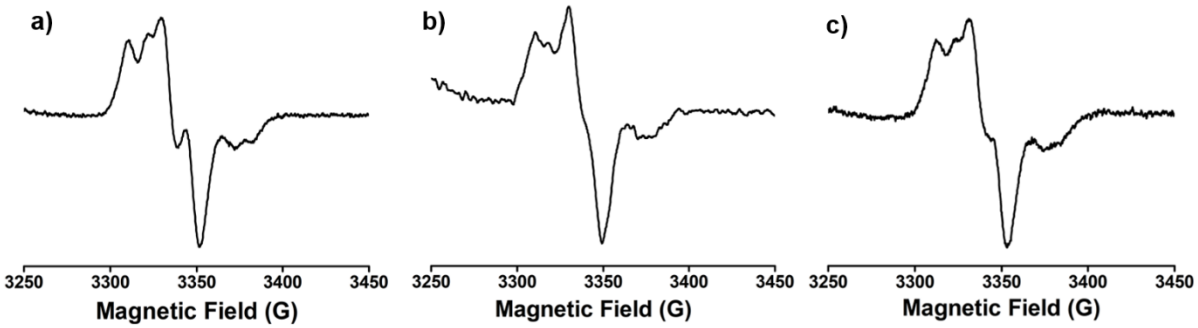


Figure S14. EPR spectra in DMSO solution of (a) DCP•, (b) DCPC• and (c) CP• in presence of radical trapping agent DMPO at 100 K after 10 min of the solution preparation.

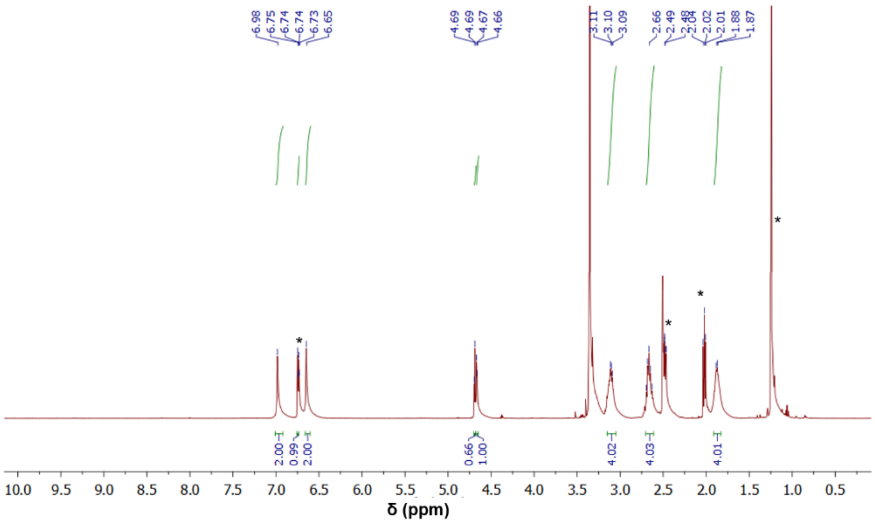


Figure S15. ^{1}H-NMR broad peaks of DCP• as DCPH in DMSO-d_6 in presence of DMPO (marked with *).

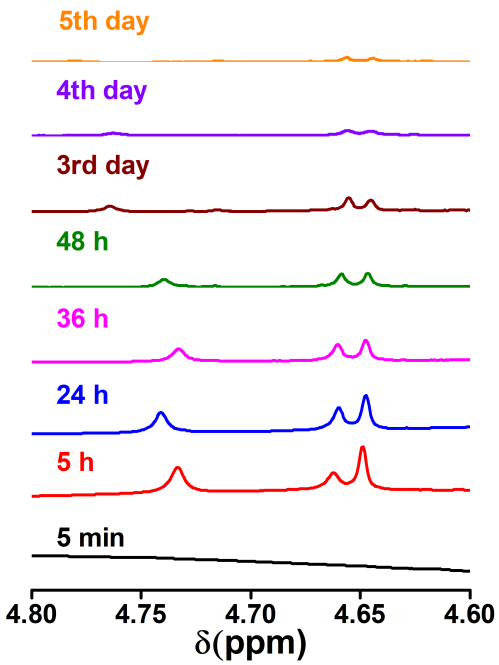


Figure S16. *In situ* formation of characteristics ^{1}H NMR peaks for C(sp^3)–H of DCPH in NMR spectra after 36 h, which is obtained from the NMR scale synthesis of DCPC• in DMSO-d_6.

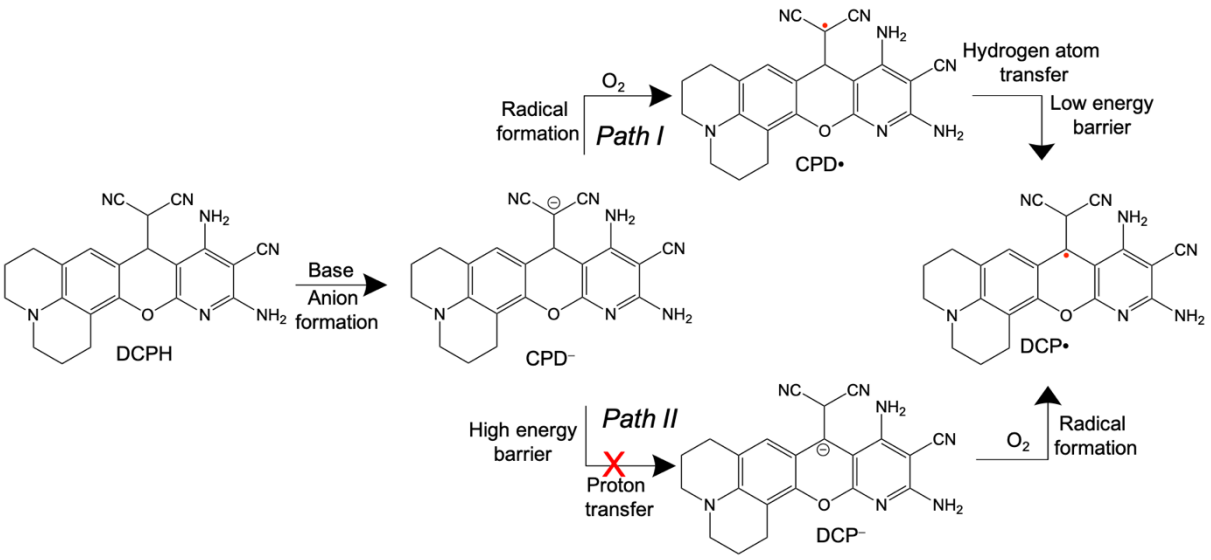


Figure S17. Synthesis of DCP• from *in situ* generated DCPH via two probable pathways.

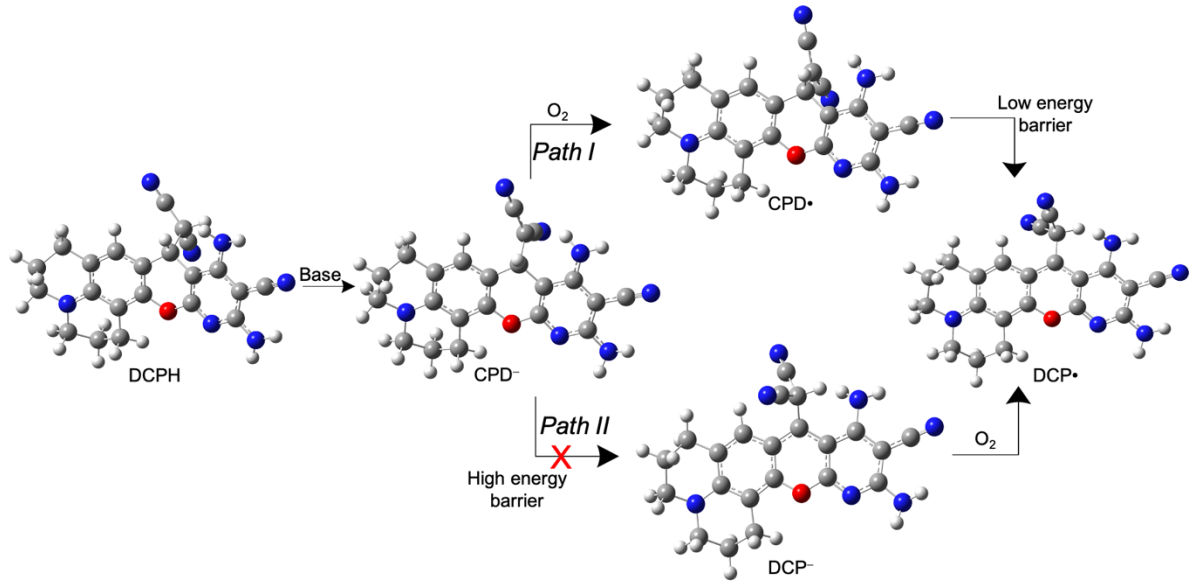


Figure S18. Optimized geometries of the individual molecules as mentioned in Fig. S17.

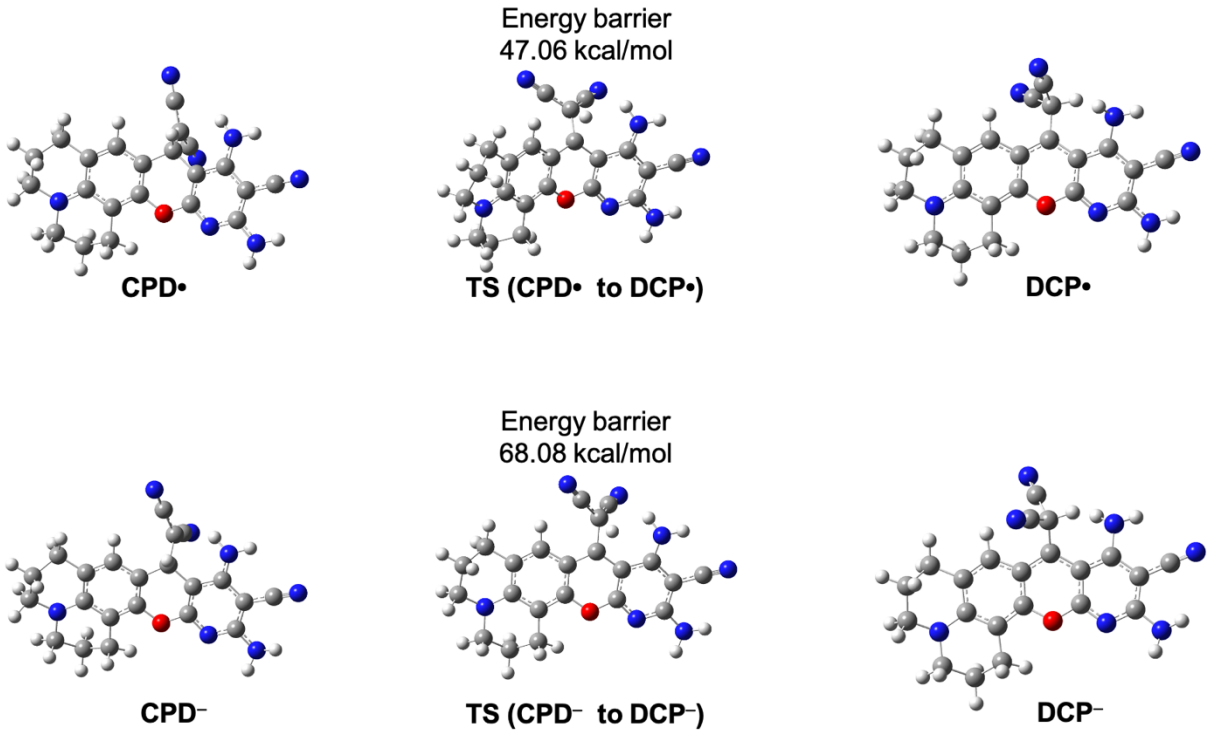


Figure S19. High energy barrier of proton transfer pathway disfavors Path II for DCP• generation from *in situ* generated DCPH.

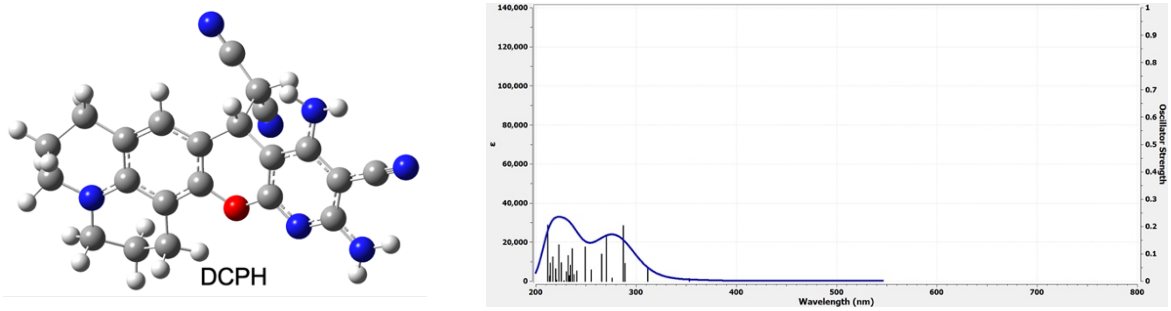


Figure S20. The (left) optimized geometry and (right) simulated absorption spectrum of DCPH.

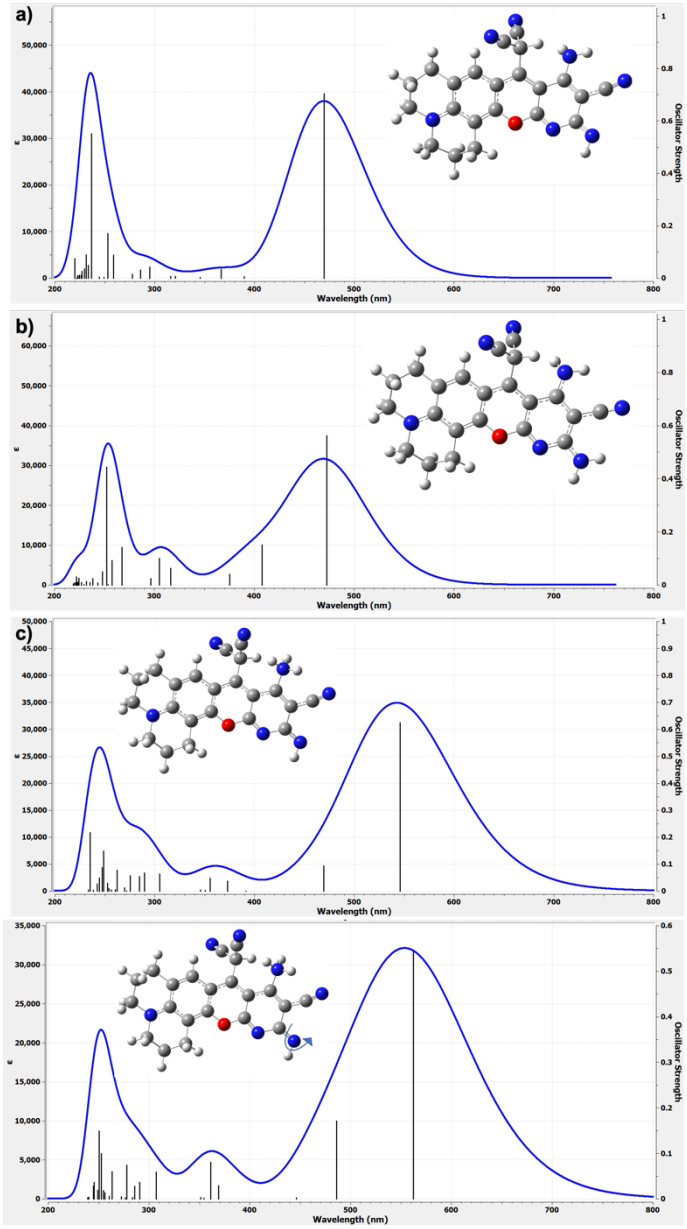


Figure S21. The optimized geometries and simulated absorption spectra of (a) DCP-H, (b) $DCP(TC)^+$, (c) $DCP(KC)^+$ and its imine N–H rotamer.

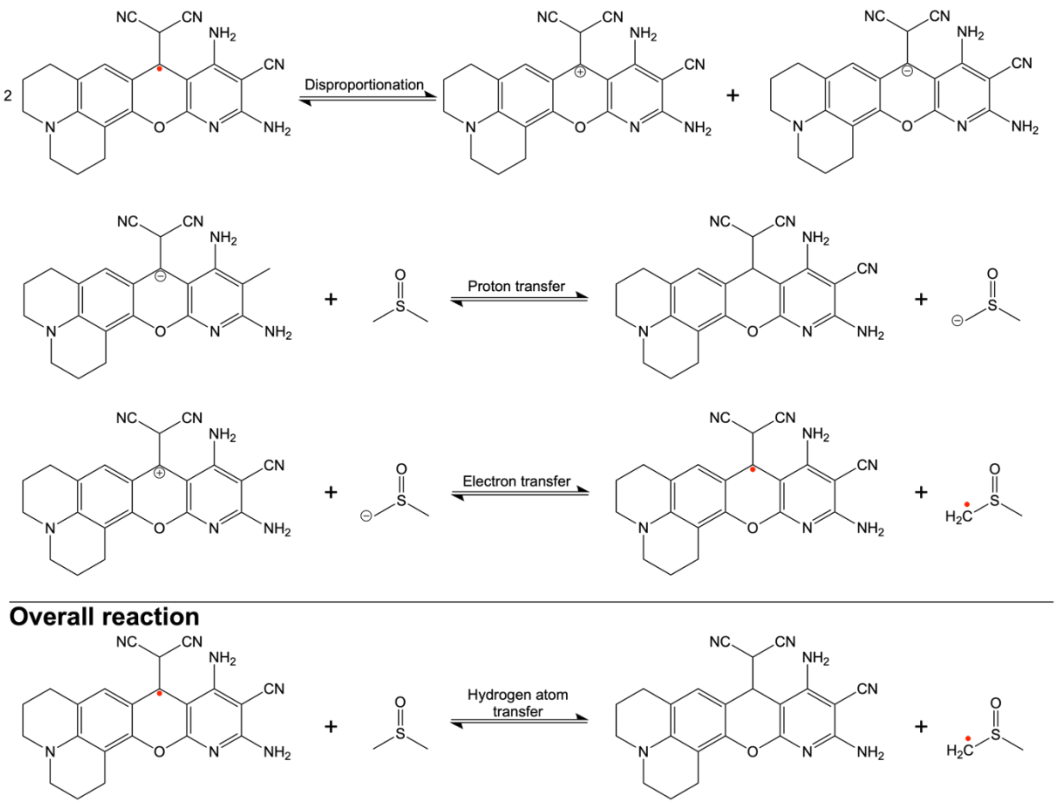


Figure S22. Formation of DCPH from DCP• in DMSO through disproportionation.

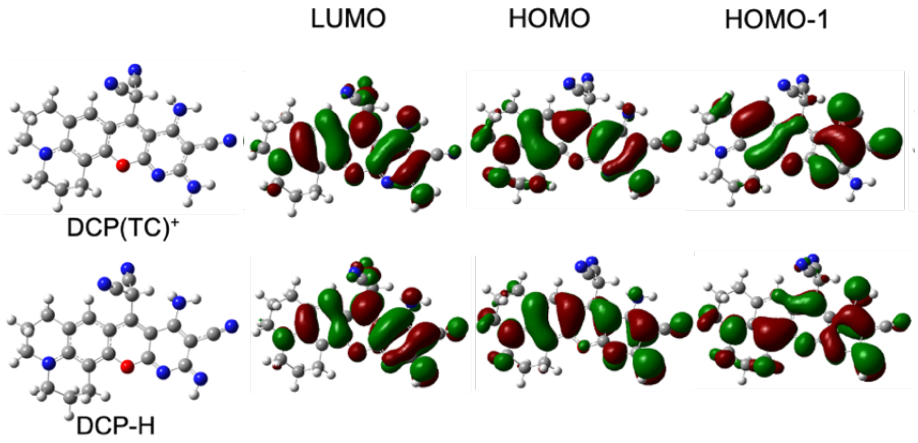


Figure S23. Frontier molecular orbitals, which are involved in electronic transitions for DCP-H and $DCP(TC)^{+}$.

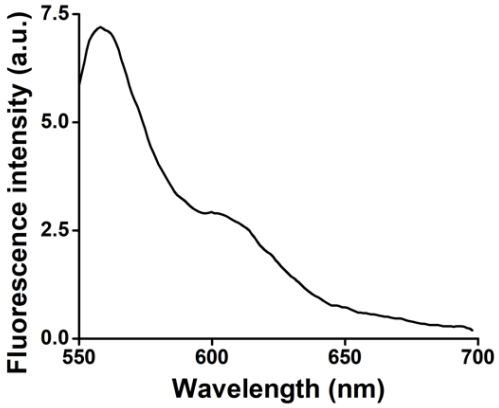


Figure S24. Emission spectra of DCP• as $DCP(KC)^+$ in DMSO solution.

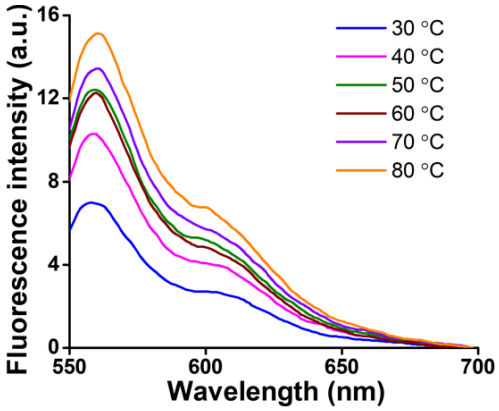


Figure S25. Temperature dependent emission studies of DCP• as $DCP(KC)^+$ in DMSO.

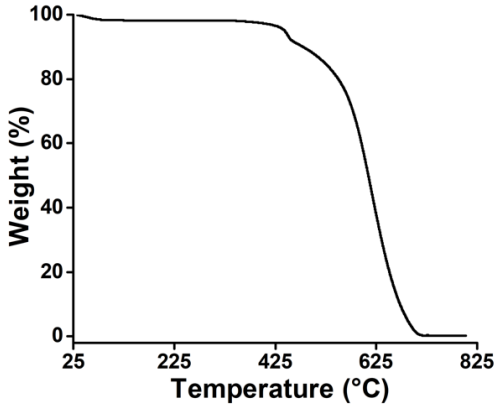


Figure S26. TGA spectrum of DCPC• in air.

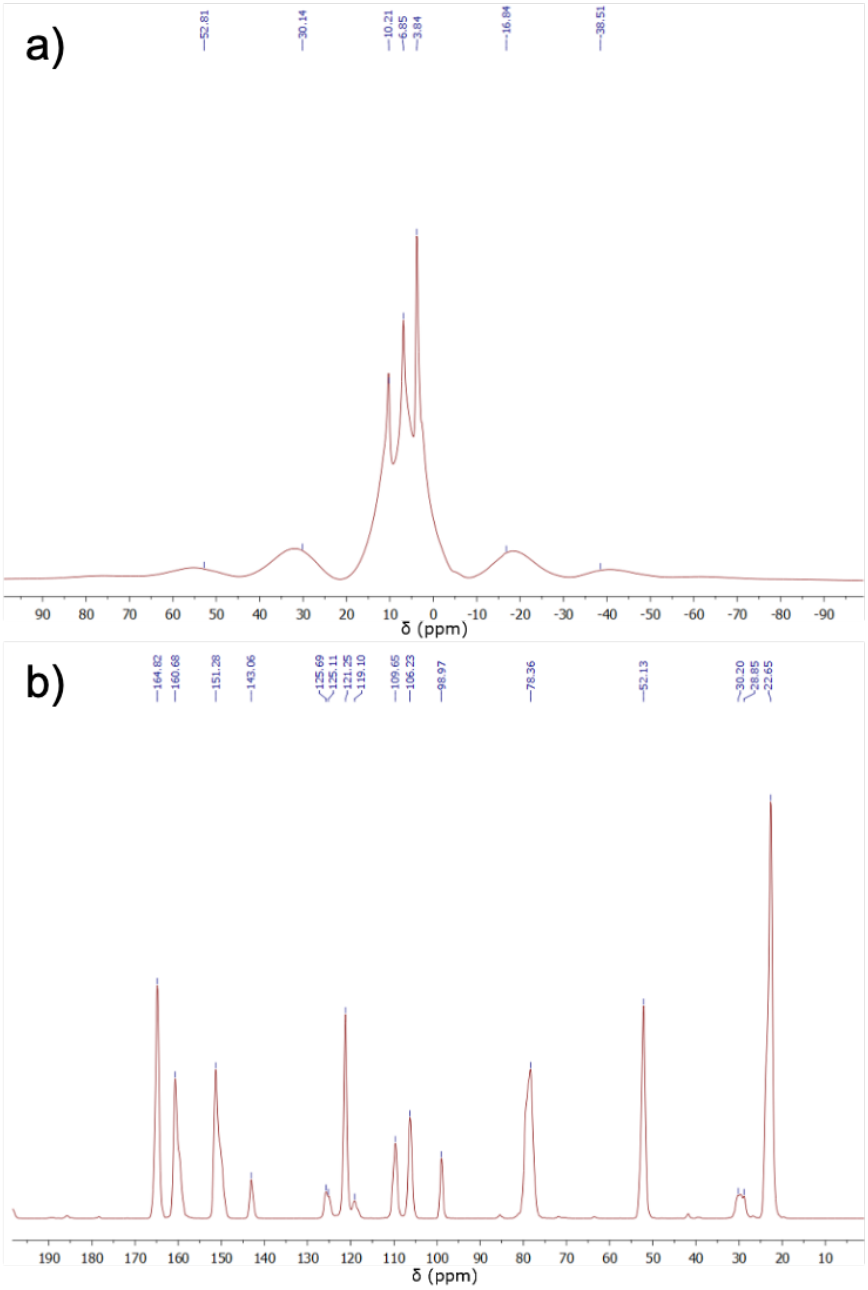


Figure S27. Solid-state a) ^{1}H-NMR and b) ^{13}C-NMR of DCPC•.

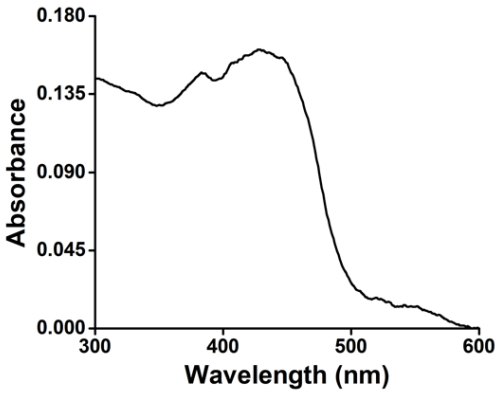


Figure S28. Absorption spectrum of DCPC• in solid state.

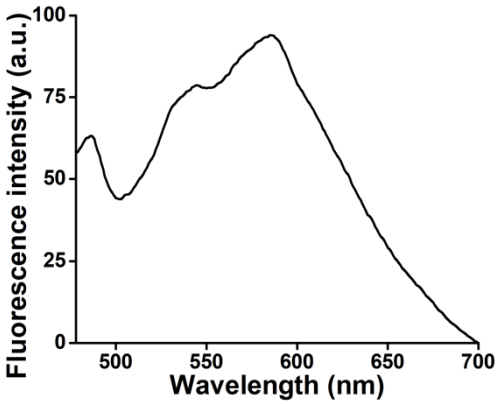


Figure S29. Emission spectrum (λ_{ex} = 435 nm) of DCPC• in solid state.

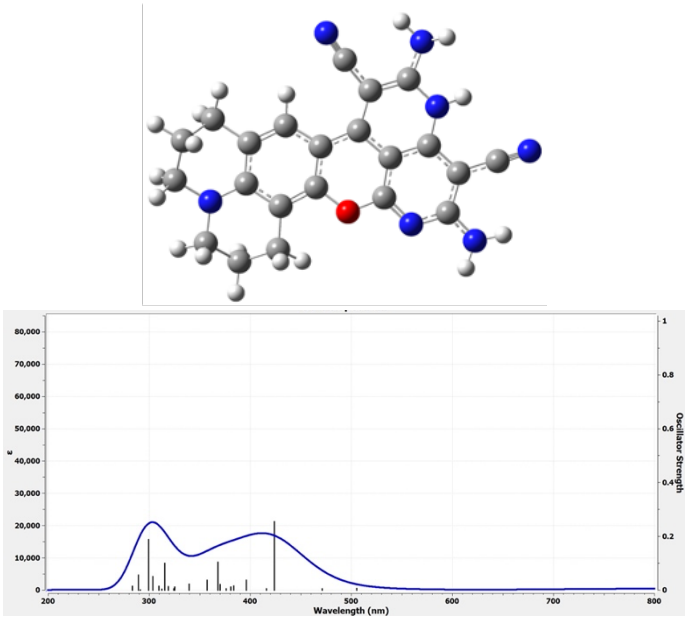


Figure S30. The (top) optimized geometry and (bottom) simulated absorption spectrum of DCPC•.

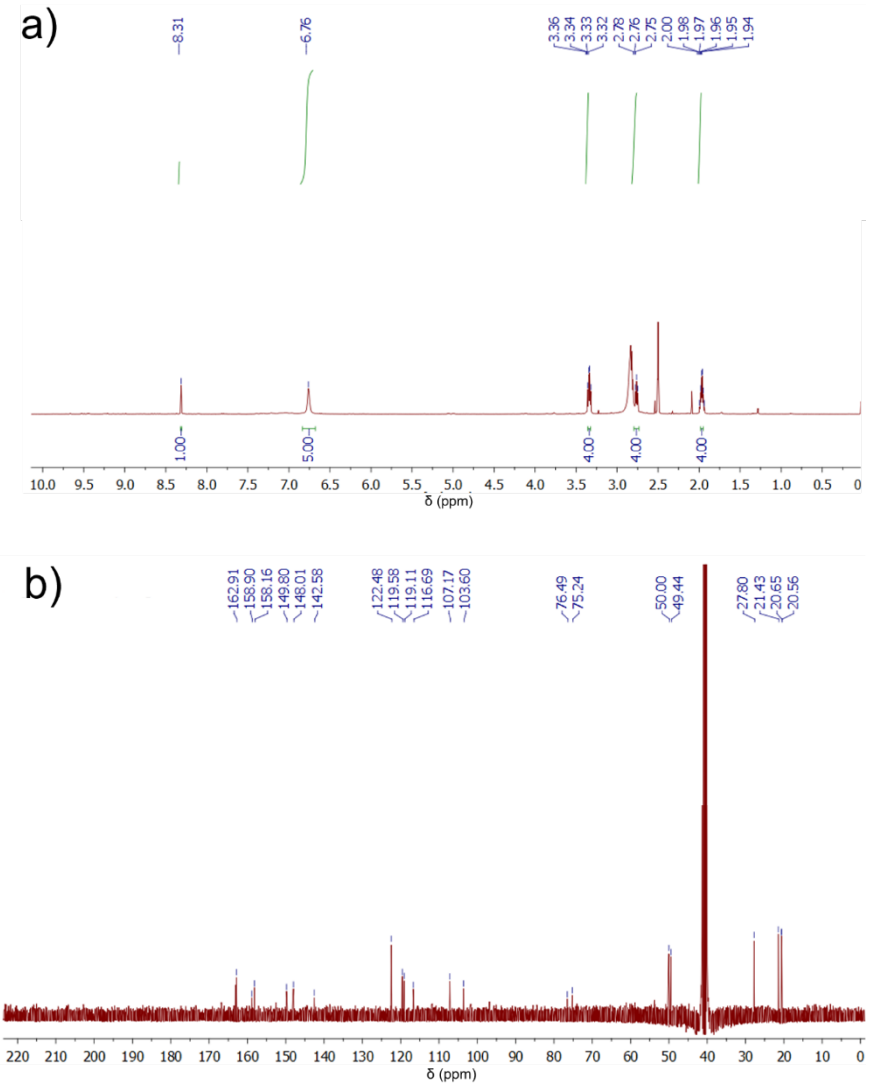


Figure S31. a) ^{1}H-NMR and b) ^{13}C-NMR of DCPC• as DCPC^{+} at 130 °C in DMSO-d_6.

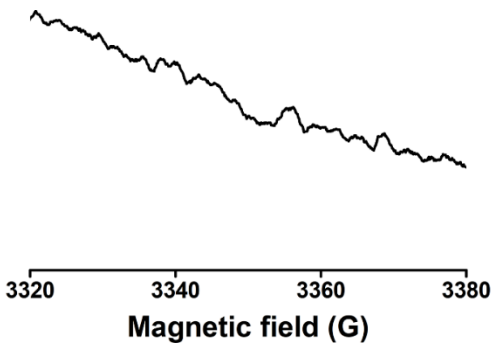


Figure S32. EPR spectra of DCPC• as DCPC^{+} in DMSO only.

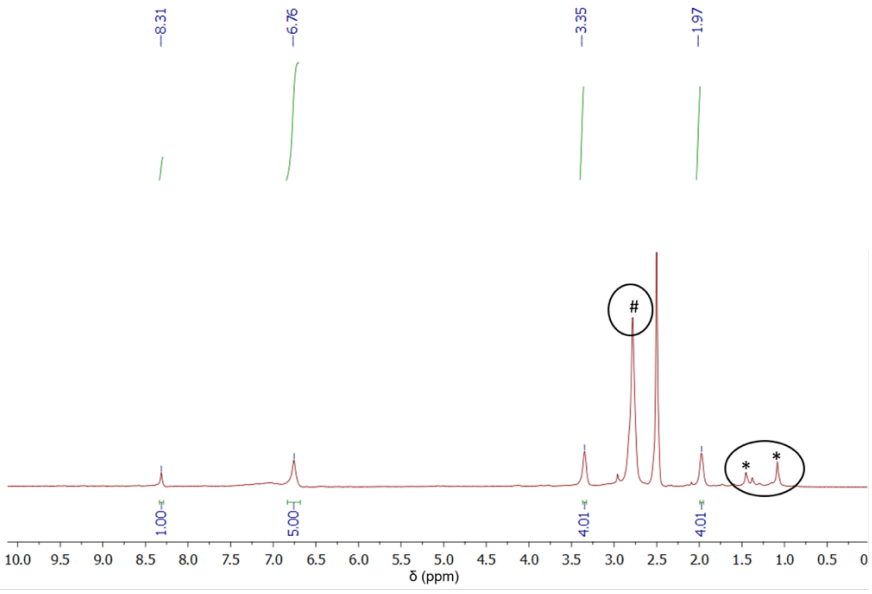


Figure S33. ^{1}H NMR spectrum of DCPC^{+} in presence of TEMPO ($^{\#}$peak contains julolidine peak for 4H; *peaks are due to TEMPO).

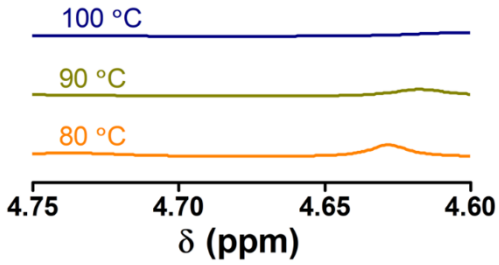


Figure S34. Temperature dependent ^{1}H NMR showing disappearance of characteristics peak of DCPH above 80 °C in DMSO-*d6* solution of DCP•.

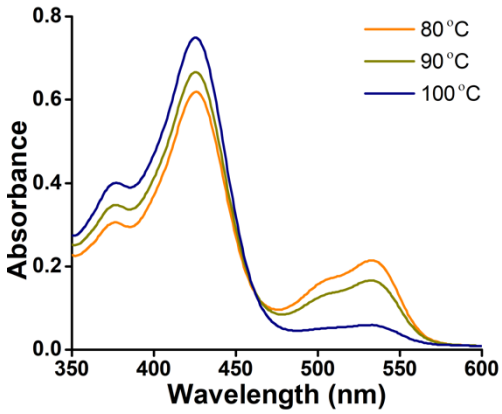


Figure S35. Temperature dependent conversion of DCP(KC)$^{+}$ to DCPC^{+} after 80 °C.

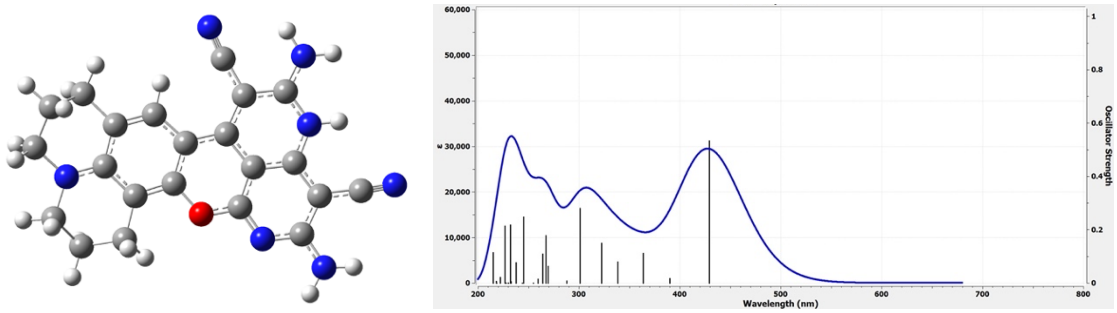


Figure S36. The (top) optimized geometry and (bottom) simulated absorption spectrum of $DCPC^{+}$.

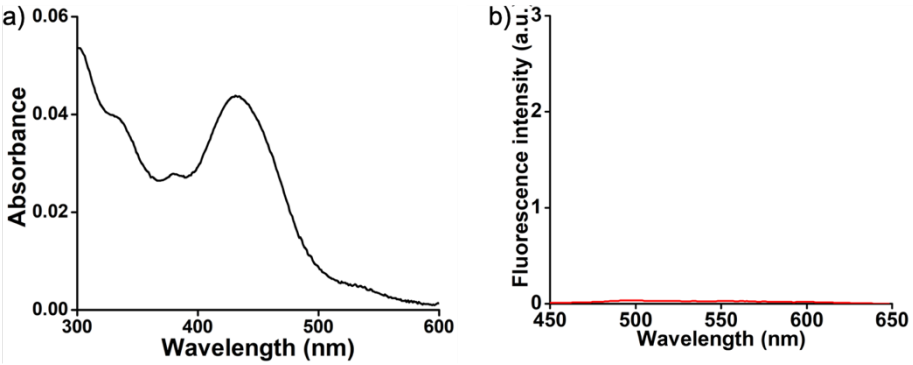


Figure S37. Absorption and emission spectra of $DCPC^{+}$ in water.

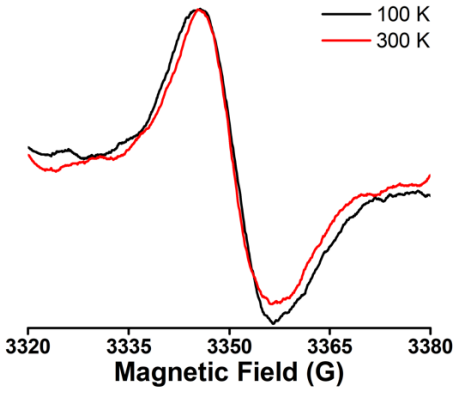


Figure S38. Temperature independent EPR of CP•.

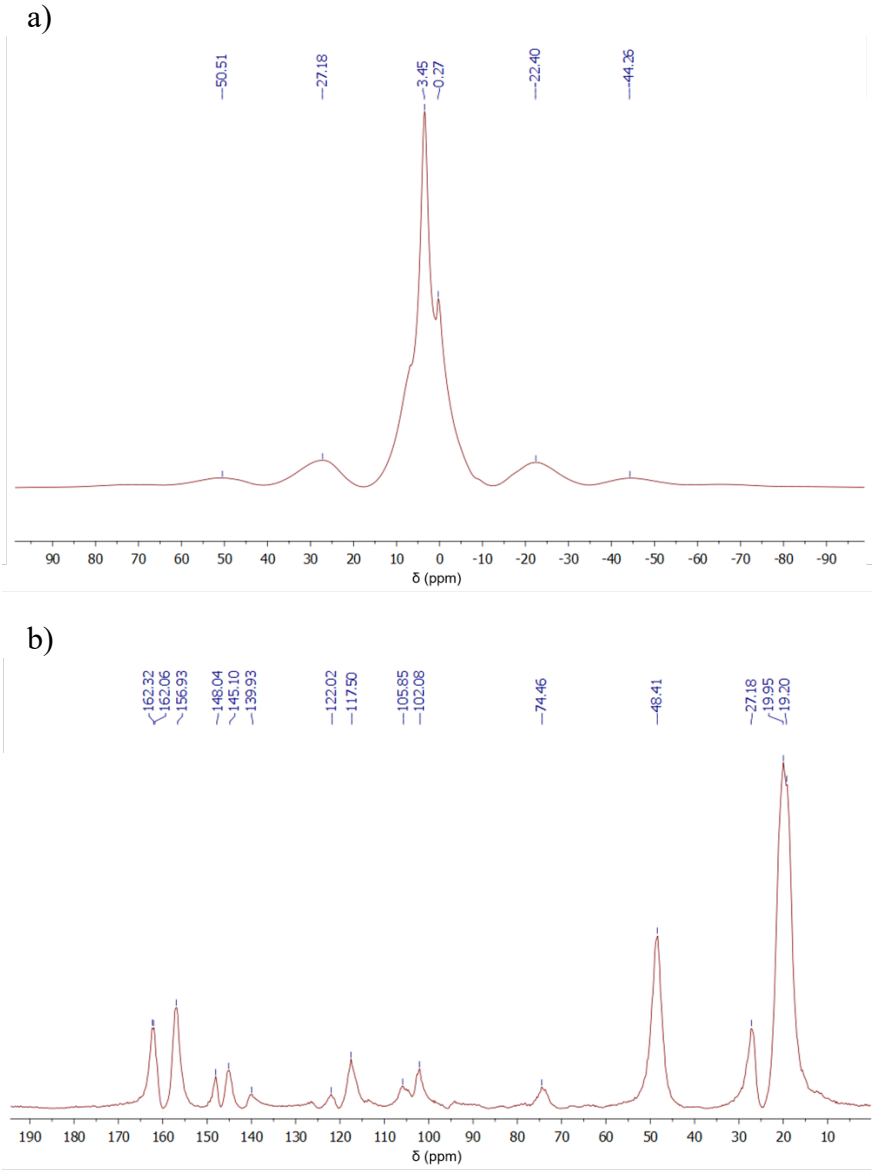


Figure S39. Solid-state a) ^{1}H-NMR and b) ^{13}C-NMR of CP•.

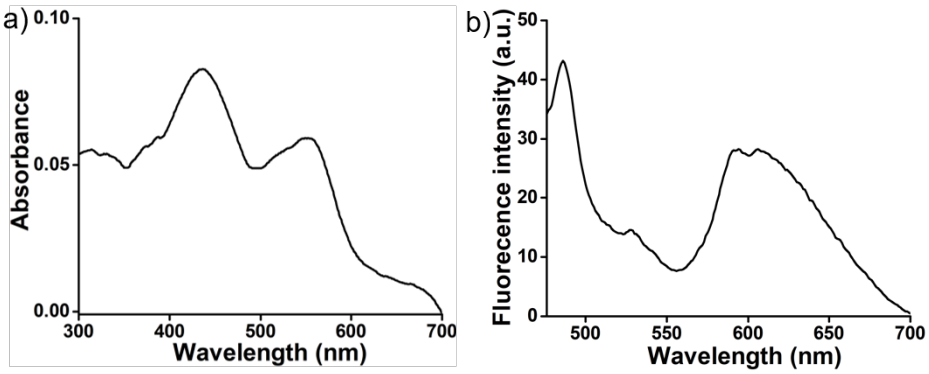


Figure S40. Absorption (left) and emission (right) spectra (λ_{ex} = 435 nm) of CP• in solid state.

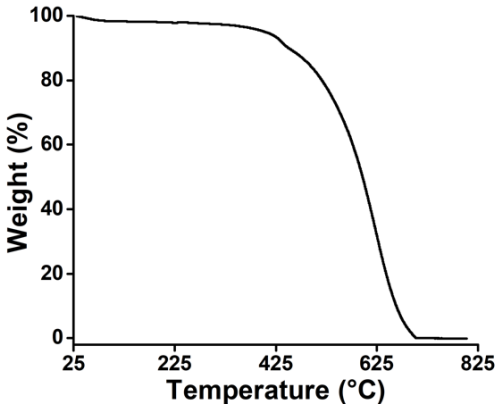


Figure S41. TGA spectrum of CP• in air.

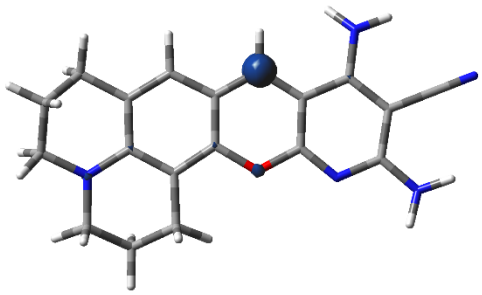


Figure S42. Localized spin density of CP•.

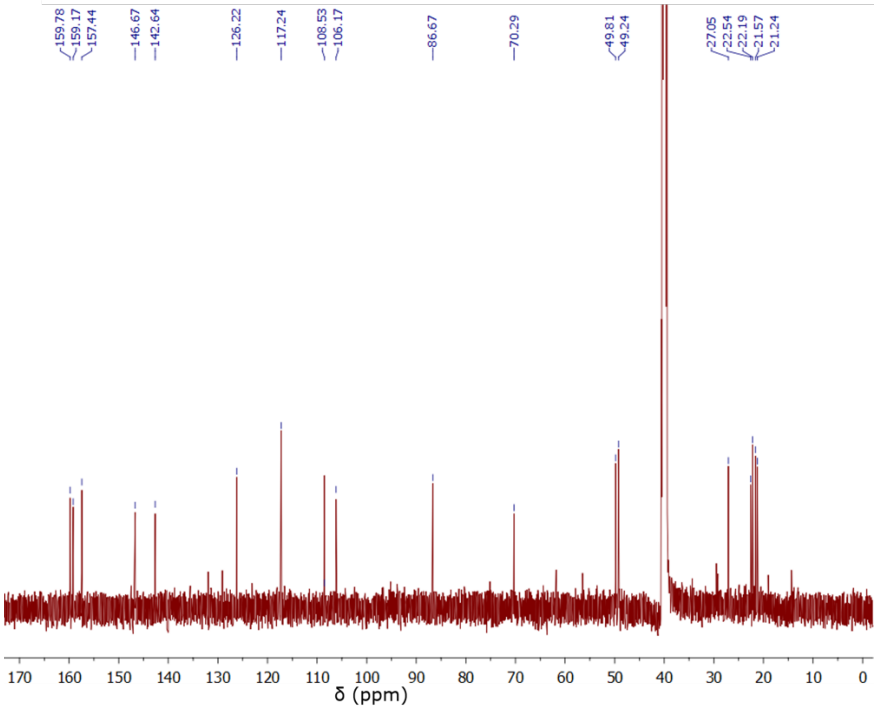


Figure S43. ^{13}C-NMR of CP• as CPH in DMSO-d_6.

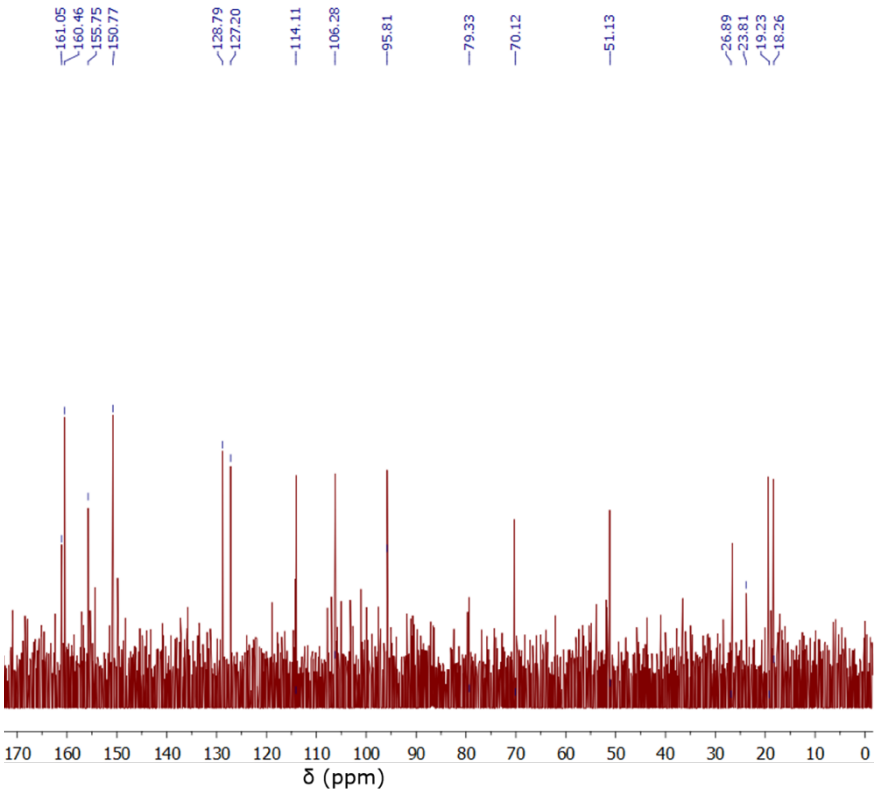


Figure S44. ^{13}C-NMR of CP• as CP(KC)$^{+}$ in D_2O.

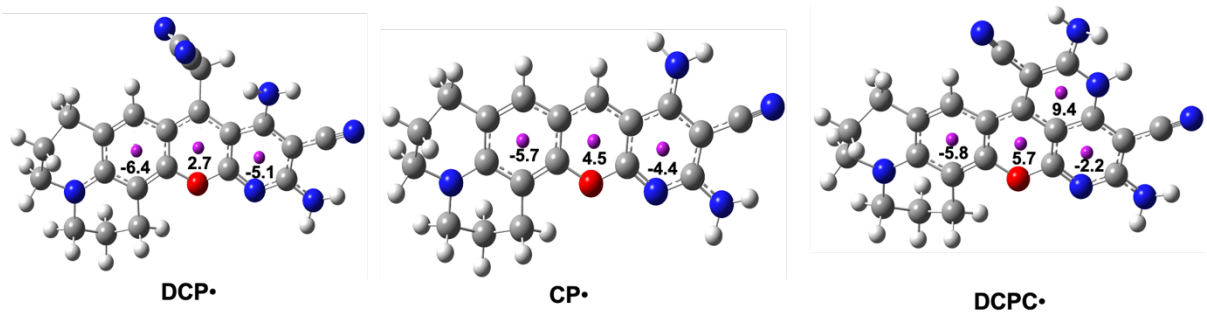


Figure S45. Nucleus independent chemical shift values for rings of DCP•, CP• and DCPC•

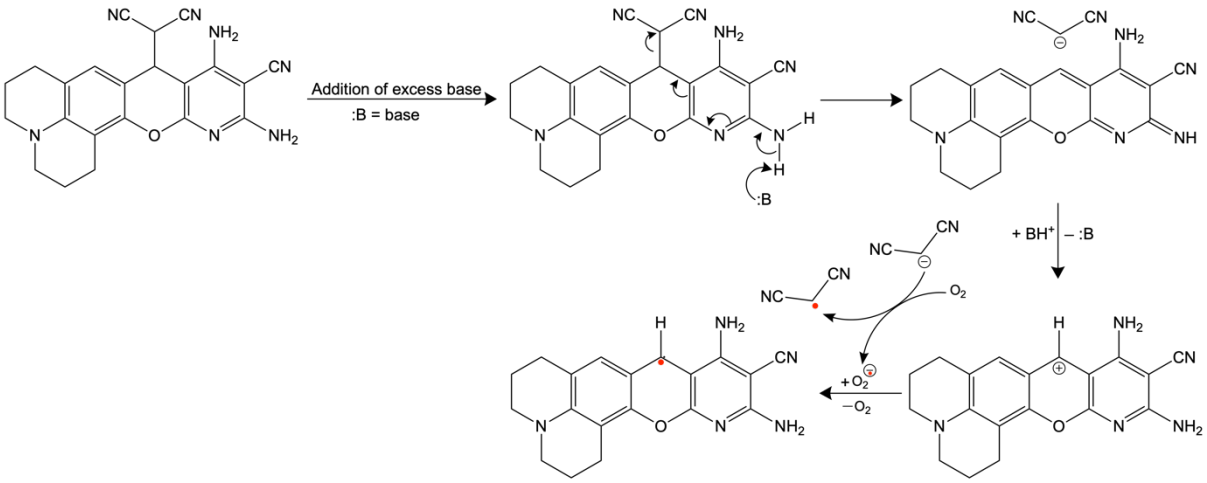


Figure S46. Proposed mechanism for excess base mediated conversion of DCPH to CP• radical.

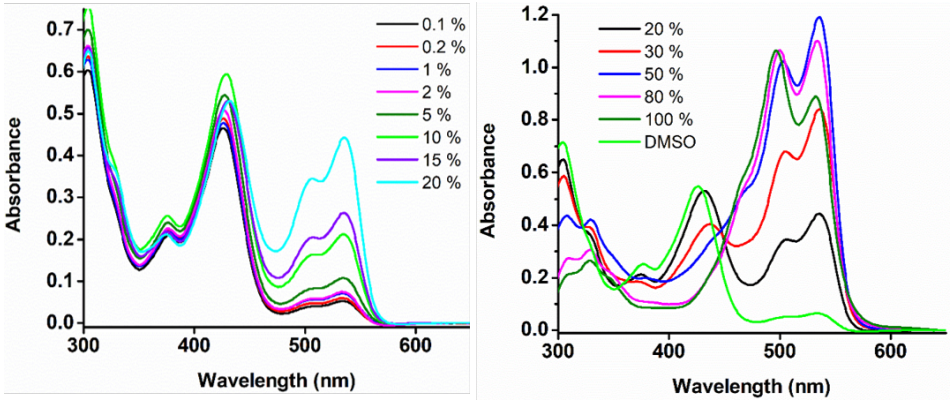


Figure S47. Absorbance spectra after addition of different percentage of water to DCP• (25 μM) in DMSO; the change is due to formation of $DCP(KC)^+$ to $CP(KC)^+$.

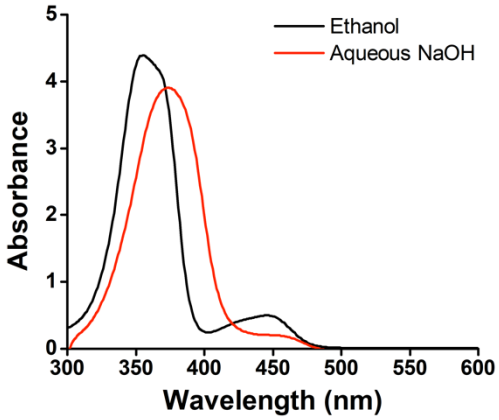


Figure S48. Absorbance spectrum of CP-H intermediate in the reaction of CP• synthesis.

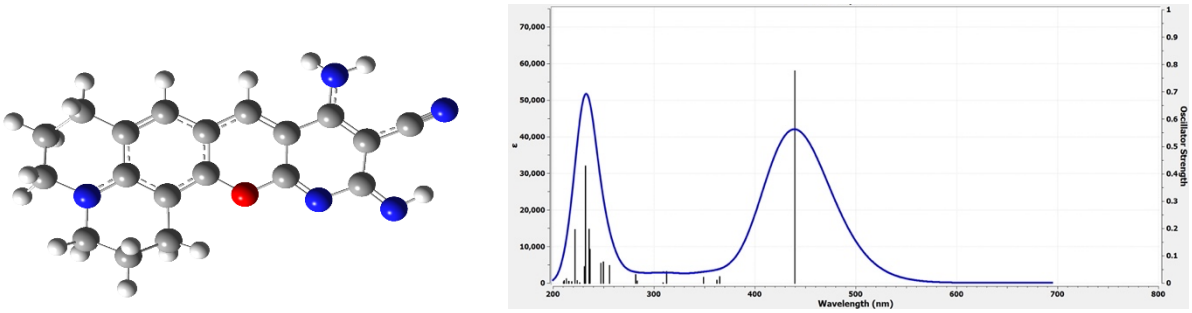


Figure S49. The optimized geometry and simulated absorption spectrum of CP-H.

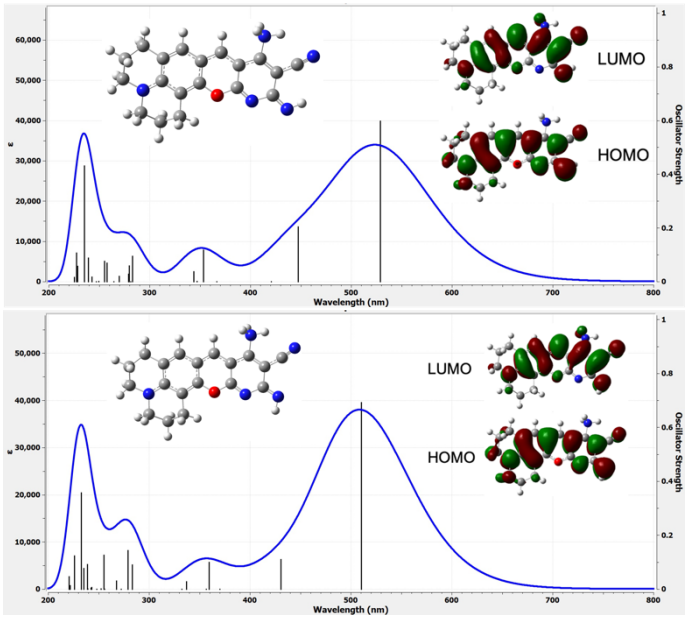


Figure S50. The optimized geometries and simulated absorption spectra and frontier molecular orbitals, which are involved in electronic transitions for (top) $CP(KC)^{+}$ and (bottom) its rotamer.

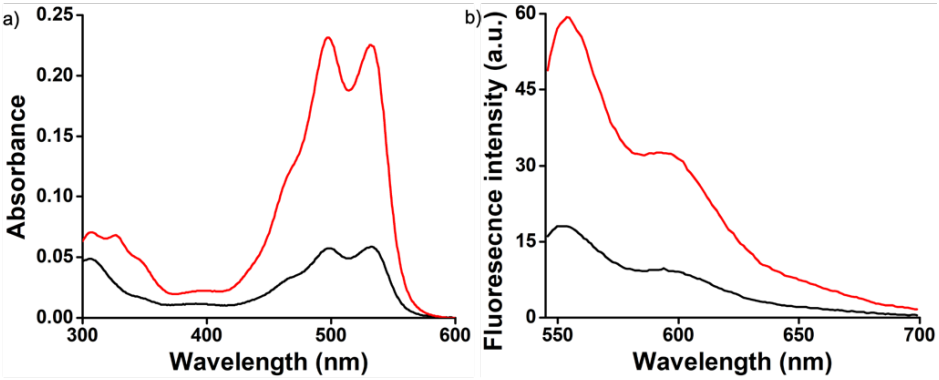


Figure S51. Absorbance and emission spectra after addition of CP• (10 μM) in water containing 0.1 % DMSO (black) and 0.0 % DMSO (red).

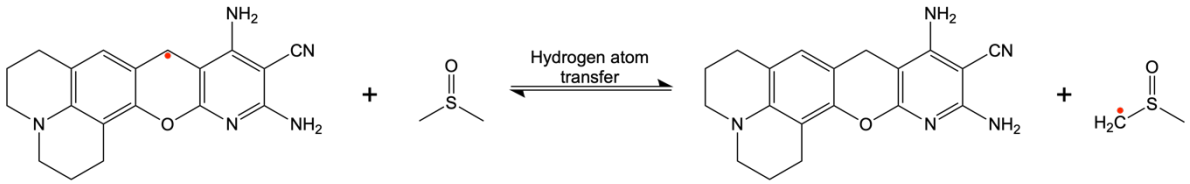


Figure S52. CPH formation in DMSO.

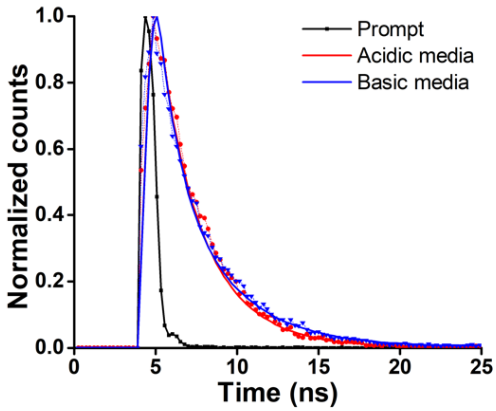


Figure S53. Fluorescence lifetime decay profile for $CP(KC)^+$ and CP-H.

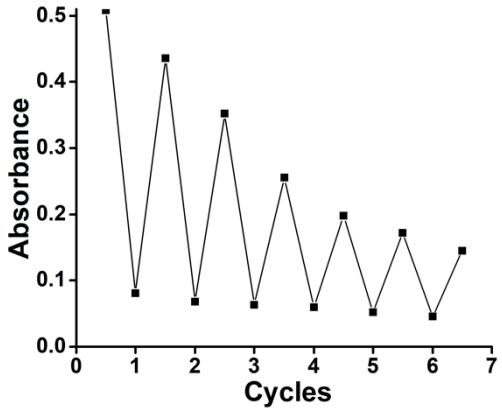


Figure S54. Absorbance profile at 500 nm of acid-base reversible cycle for shifting of equilibrium from $CP(KC)^+$ *vs*. CP-H towards $CP(TC)^+$ *vs*. CP-H.

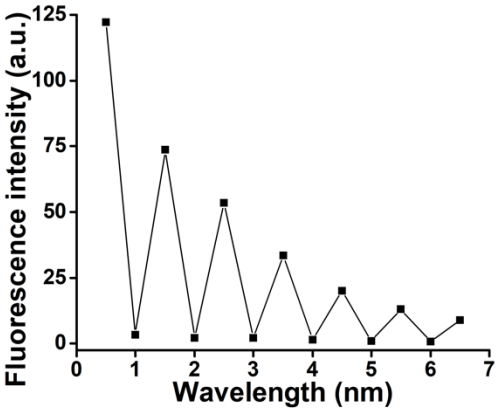


Figure S55. Emission profile at 555 nm of acid-base reversible cycle for shifting of equilibrium from $CP(KC)^+$ *vs*. CP-H towards $CP(TC)^+$ *vs*. CP-H.

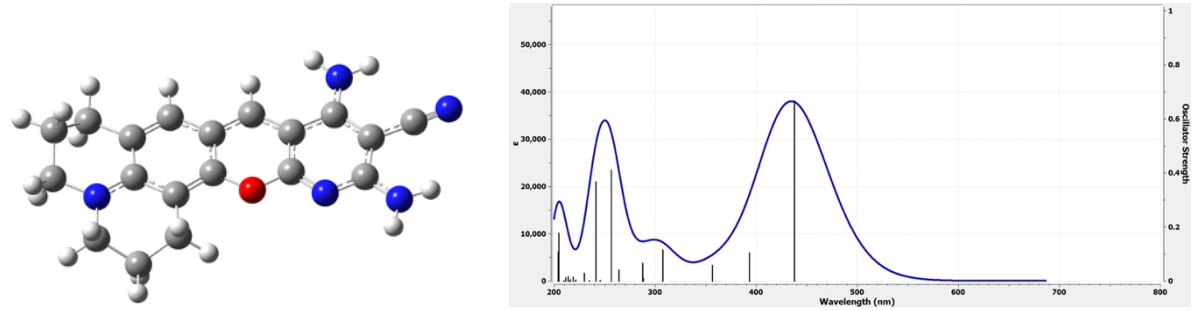


Figure S56. The optimized geometry and simulated absorption spectrum of $CP(TC)^+$.

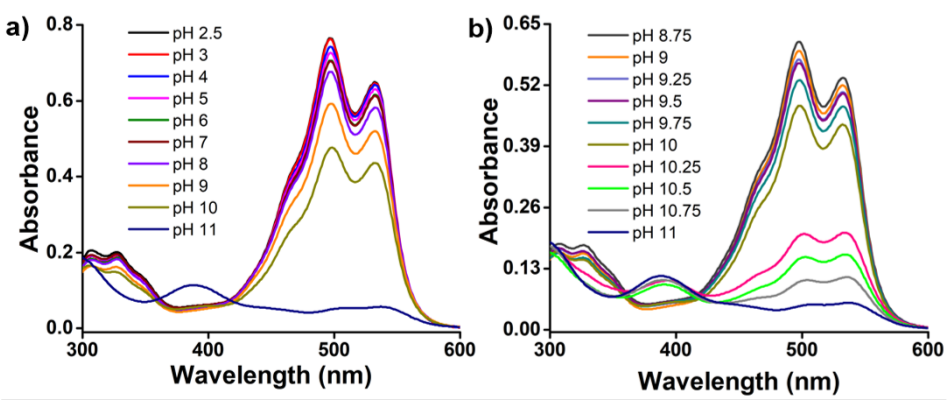


Figure S57. pH dependent change in absorbance of $CP(KC)^+$ to CP-H.

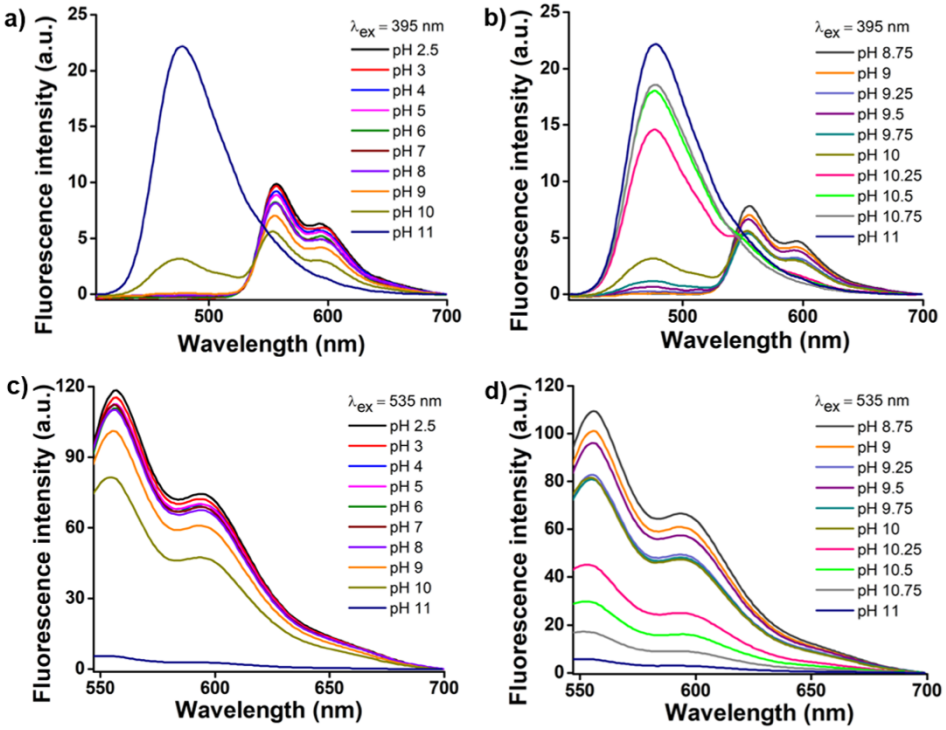


Figure S58. pH and excitation wavelength dependent change in emission of $CP(KC)^+$ to CP-H.

Table S1. Percentage yield of DCP• and CP• at different conditions

Entry	Julolidine (mmol)	Malononitrile (mmol)	Base	Base (mmol)	Ethanol volume (mL)	DCP• (% yield)	CP• (% yield)
1.	3.00	9.00	Piperidine	0.15	5.0	71	-
2.	0.36	1.08	Piperidine	0.18	3.0	< 1	22
3.	0.36	1.08	Piperidine	0.54	3.0	< 1	50
4.	0.36	1.08	Piperidine	1.08	3.0	-	60
5.	0.36	1.08	Piperidine	2.16	3.0	-	63
6.	0.36	1.08	Triethylamine	0.54	3.0	5	-
7.	0.36	1.08	Triethylamine	1.08	3.0	11	1
8.	0.36	1.08	Trimethylamine	0.54	3.0	-	-
9.	0.36	1.08	Trimethylamine	1.08	3.0	< 1	-
10.	3.00	9.00	4-aminopiperidine	0.15	5.0	66	-
11.	0.36	1.08	4-aminopiperidine	1.08	3.0	-	53
12.	3.00	9.00	Aniline	0.15	5.0	-	-
13.	0.36	1.08	Aniline	1.08	3.0	-	-

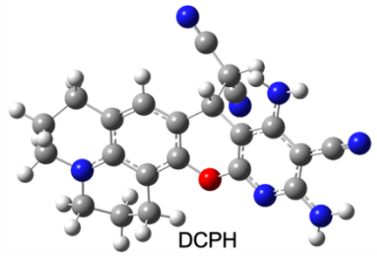
Table S2. Quantum yield, lifetime, radiative and non-radiative decay rate constants of $CP(KC)^+$ and CP-H

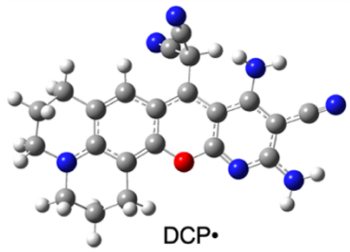
Molecular form	Quantum yield (ϕ)	Lifetime (τ) (ns)					Radiative decay rate constant (k_r) (s^{-1})	Non-radiative decay rate constant (k_{nr}) (s^{-1})
		A_1	τ_1	A_2	τ_2	Avg		
$CP(KC)^+$	0.77	8.33	3.53	91.67	11.29	11.08	70.0×10^6	20.3×10^6
CP-H	0.14	25.74	4.04	74.26	15.19	14.15	9.9×10^6	60.7×10^6

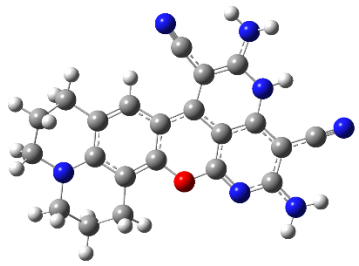
Table S3. Crystallographic data for DCPC•

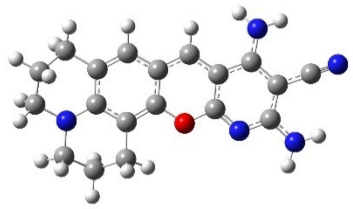
	DCPC•
CCDC Number	2211819
Empirical formula	C_{22} H_{18} N_7 O_1, 2(C_2 H_6 S O)
Formula weight	552.69
Temperature	100 (2)
Wavelength	0.71073
Crystal System	orthorhombic
Space Group	Pbcn
Unit cell dimensions	a = 22.273 (7) Å, b = 15.970 (5), c = 15.234 (5) a = 90º, b = 90º, c = 90º
Volume ($Å^3$)	5419 (3)
Z	8
Density(calculated) (g/cm^3)	1.355
Absorption coefficient (mm^{-1})	0.239
F(000)	2328
Crystal size (mm^3)	0.33 × 0.25 × 0.18
Theta range for data collection	1.569 to 24.999º
Index ranges	$-26 \le h \le 26$, $-18 \le k \le 18$, $-18 \le k \le 17$
Reflections collected	71448
Independent reflections	4776 [R(int) = 0.1775]
Completeness to theta	θ = 24.999 (100%)
Absorption Correction	multi-scan
Max. and min. transmission	0.2085 and 0.1602
Refinement Method	Full-matrix least-squares on F^2
Data / restraints / parameters	4776/ 72/ 402
Goodness-of-fit on F^2	1.306
Final R indices [I>2sigma(I)]	0.1335
R indices (all data)	0.2051
Largest diff. peak and hole ($e.Å^{-3}$)	1.444 and –0.420

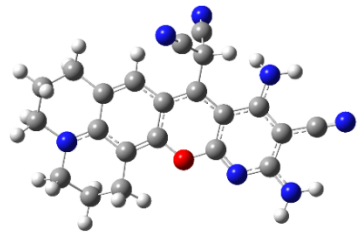
Coordinates of the optimized geometries

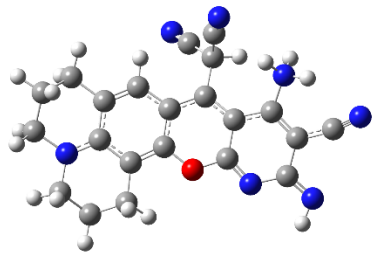
System	Optimized Coordinates
DCPH  -1308.6379479	C,4.006276164,1.9061021313,-0.9371396613 C,2.8316774301,1.0191757678,-0.6020772814 C,3.0625935297,-0.3329290374,-0.2345172195 N,4.3487599578,-0.8345804395,-0.1895469314 C,5.5065637358,-0.0634721989,-0.6326799989 C,5.1212227641,1.0735445838,-1.5722976236 C,4.6447540968,-2.1836286166,0.2828374396 C,3.5362846657,-2.7366032256,1.1697564264 C,2.1856248471,-2.6046929177,0.4646112536 C,1.9608242409,-1.1650574442,0.0706990928 C,1.5335818686,1.4976449416,-0.6473132308 C,0.4299748003,0.7059070009,-0.3187853388 C,0.6806176038,-0.6214772555,0.0217356938 C,-0.9697923377,1.2500518167,-0.2660325572 C,-1.9841077346,0.1393988753,-0.3011899811 C,-1.6299139362,-1.1683201199,0.0531967281 O,-0.3456468707,-1.505301899,0.3130506887 C,-3.3443919883,0.3694507859,-0.5736599021 C,-4.2532473952,-0.7062934854,-0.4619883578 C,-3.7545349244,-1.9770076546,-0.0651710165 N,-2.460653564,-2.1919370493,0.1762242148 C,-1.2285455799,2.145639778,1.0376275792 C,-0.4893125589,3.4082471634,0.9804074347 N,-4.5805603966,-3.0469628668,0.0542889159 C,-5.6273081935,-0.5195290108,-0.738460595 N,-6.7529388377,-0.3629553291,-0.9667003718 N,-3.8007832631,1.6328218648,-0.8729592035 C,-0.9174670503,1.3956912204,2.2554818946 N,-0.6826916868,0.7673896357,3.1911328421 H,1.3735465719,2.5333923517,-0.927582006 H,3.690974626,2.7127051629,-1.6038634343 H,4.3876358623,2.3835844759,-0.0250380951 H,6.0042348697,1.6829258305,-1.781517807 H,4.7712731976,0.6589643496,-2.5234828683 H,6.0437839925,0.3388758087,0.2399637661 H,6.1949280915,-0.7485802591,-1.1407192426 H,5.5874465748,2.1476583602,0.8406651282 H,4.8074334144,-2.8531765393,-0.576157959 H,3.7534238359,-3.7803367241,1.4108927334 H,3.509718663,-2.1786569139,2.111175105 H,1.3741484958,-2.9482872739,1.1062261163 H,2.1694500289,-3.2445997082,-0.4273105049 H,-3.1621458992,2.26342651,-1.3320497658 H,-5.5806182281,-2.9393174182,0.0309161099 H,-4.1875722888,-3.8906403775,0.4369149557 H,-4.7542837109,1.7102472221,-1.1982683315 H,-2.296300935,2.3936026842,1.0572185428

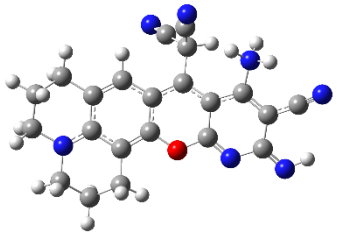
	N,0.0777905666,4.4041543063,0.864067644 H,-1.113626586,1.9405450071,-1.1058396504
DCP•  -1308.0014299	C,3.9858142201,-2.3277928726,-0.0624954884 C,2.763347819,-1.4434307019,-0.0892019568 C,2.9311771228,-0.0333592622,-0.0073677969 N,4.190366886,0.5154533844,0.1025112733 C,5.3883608293,-0.2975241411,0.3049225982 C,5.0623876867,-1.6943467913,0.8199743414 C,4.4160520162,1.9577918122,0.0779332382 C,3.285002901,2.700211796,-0.6217084994 C,1.9411210049,2.3043314993,-0.009383567 C,1.7856159609,0.8027339628,-0.0460359637 C,1.496115291,-1.980993641,-0.1780601407 C,0.3302764169,-1.1847197152,-0.211907474 C,0.539358166,0.2115687989,-0.1496595915 C,-1.004324807,-1.673830573,-0.3107518897 C,-2.0898731537,-0.7482465554,-0.108898088 C,-1.8095625637,0.6413474599,-0.162415735 O,-0.5306840071,1.0830813086,-0.2368165043 C,-3.4439311167,-1.06530512,0.1754406039 C,-4.4064672778,-0.0311435161,0.1635707912 C,-3.9824963721,1.3047788099,-0.0512087191 N,-2.6881452494,1.6218482768,-0.1600523973 C,-1.2690891588,-3.0969422321,-0.7972417624 C,-1.0490462117,-4.1016650478,0.2609937445 N,-4.8702777409,2.3288849733,-0.1450792743 C,-5.7685760899,-0.3121170234,0.4262889855 N,-6.8845752927,-0.5335647921,0.6468297667 N,-3.8304542234,-2.3705268499,0.4348925859 C,-0.5148919539,-3.4341625004,-2.0161340611 N,0.0526802566,-3.6796810907,-2.9876581508 H,1.4075490436,-3.0598610046,-0.2100121474 H,3.7210470529,-3.3251593456,0.2964029458 H,4.3776205835,-2.4517535522,-1.0804971339 H,5.9750279395,-2.2955789769,0.8293615688 H,4.6979729105,-1.6299059931,1.8503585313 H,5.9492836766,-0.3665369724,-0.6391450782 H,6.0331301846,0.224886226,1.0207303352 H,5.3639750578,2.1405788069,-0.4398111858 H,4.534888145,2.3336046248,1.1059964247 H,3.4526578414,3.7768652613,-0.5372271942 H,3.2897380717,2.4479629079,-1.6870631629 H,1.1145730865,2.7790415713,-0.5386612286 H,1.8890359843,2.6586994647,1.0282107444 H,-3.2065183032,-2.9003532776,1.0301529323 H,-5.8401474741,2.1939682693,0.0880894611 H,-4.4946164453,3.2625437722,-0.1310714434 H,-4.7984143366,-2.4901693721,0.7036895883

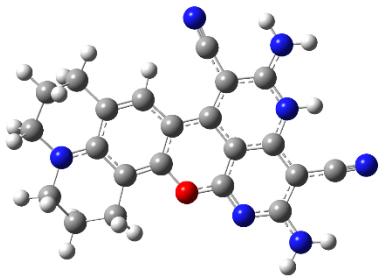
	H,-2.3274329136,-3.1776051523,-1.0658714447 N,-0.9321984639,-4.8345409135,1.1431496185
DCPC•  -1308.0413153	C,0,2.841418,2.421177,-0.08632 N,0,3.675163,1.314491,-0.101457 C,0,3.181739,0.02425,-0.022218 C,0,1.79426,-0.155815,0.030998 C,0,0.866428,0.945995,-0.009279 C,0,1.468209,2.268205,-0.009223 C,0,1.363327,-1.491345,0.112198 N,0,2.142226,-2.55996,0.140484 C,0,3.463012,-2.381002,0.080092 C,0,4.046135,-1.084178,0.001491 C,0,-0.527834,0.609521,-0.03251 C,0,-0.905626,-0.754092,0.061609 O,0,0.043142,-1.770331,0.173336 C,0,-2.217089,-1.198724,0.062615 C,0,-3.262763,-0.246695,-0.042214 C,0,-2.927662,1.123117,-0.166886 C,0,-1.601952,1.51718,-0.151066 N,0,-4.58599,-0.651142,-0.032543 C,0,-5.69345,0.297848,0.034786 C,0,-5.251454,1.67684,0.512374 C,0,-4.038088,2.137653,-0.297939 C,0,-4.96586,-2.057216,0.007147 C,0,-3.869613,-2.956783,-0.549546 C,0,-2.544076,-2.670984,0.157378 N,0,4.236037,-3.503186,0.066056 C,0,5.447699,-0.904159,-0.051613 N,0,6.594395,-0.740651,-0.094006 C,0,0.747728,3.484515,0.118497 N,0,0.249863,4.52627,0.221027 H,0,-1.396452,2.573565,-0.241989 H,0,-3.692499,3.118904,0.035961 H,0,-4.328589,2.245039,-1.351601 H,0,-6.086738,2.375393,0.415139 H,0,-4.981629,1.628507,1.572398 H,0,-6.171196,0.380771,-0.953799 H,0,-6.449003,-0.107968,0.71813 H,0,-5.884018,-2.17714,-0.579218 H,0,-5.206523,-2.355412,1.040587 H,0,-4.161379,-4.003026,-0.425692 H,0,-3.758654,-2.76972,-1.622736 H,0,-1.736826,-3.263032,-0.274449 H,0,-2.615954,-2.970365,1.211187 H,0,5.227314,-3.441131,0.230197 H,0,3.771877,-4.369827,0.283231 N,0,3.509334,3.623484,-0.183113 H,0,2.917935,4.442613,-0.137222

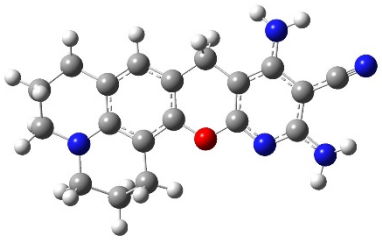
	H,0,4.335581,3.709739,0.396201 H,0,4.637497,1.448767,-0.380372
CP•  -1084.1646706	C,2.751839757,-1.4613396861,-0.1266684801 C,2.951484191,-0.0581132974,-0.0338879484 C,1.8238557619,0.8007613471,0.0435995399 C,0.5600516378,0.2382009501,0.0296659171 C,0.3225184922,-1.153730613,-0.0517906548 C,1.4680795999,-1.9737707523,-0.1198441913 O,-0.4989171346,1.1251552118,0.125603737 C,-1.7907337075,0.6942078506,0.1079951075 C,-2.0804821721,-0.6852015803,0.0013783412 C,-1.0112556236,-1.6233428338,-0.0522677576 C,3.9577366054,-2.3651906553,-0.2159934779 C,5.1129205395,-1.7674544174,0.5893888275 C,5.4232628544,-0.3659064224,0.0750658492 N,4.230901227,0.4700496428,-0.0189962259 C,4.4811385402,1.9067846638,-0.0264789043 C,3.3053220397,2.6900572067,-0.5964913503 C,2.0155825981,2.2958037547,0.1240698214 C,-3.4601214815,-1.0164845978,-0.0346116953 C,-4.4117580598,0.0234934928,0.0752403654 N,-2.6618012342,1.6786878429,0.2103299435 N,-3.8572264738,-2.3263645544,-0.1312052742 C,-5.7962222892,-0.2663425699,0.039800199 N,-6.9302183306,-0.5054155008,0.0111366785 C,-3.9609527191,1.3622286753,0.2013111993 N,4.8402895273,2.4041787937,0.2747074544 H,1.3302936572,-3.0493723884,-0.1752910599 H,-1.1961181272,-2.6896010608,-0.0490800563 H,3.705743802,-3.3654677289,0.1458130342 H,4.26938713,-2.4766569477,-1.2632091915 H,6.012705386,-2.38421507,0.5170600978 H,4.8304400952,-1.7158309545,1.6459895429 H,5.9111465417,-0.429666097,-0.9101371649 H,6.1338465243,0.1285308754,0.7480762408 H,5.3808889784,2.0906987874,-0.6250078762 H,4.7018544966,2.2545366033,0.9954855728 H,3.5013543515,3.7606774774,-0.4950236962 H,3.2073954637,2.4722280317,-1.6651115645 H,1.1529723972,2.8062535421,-0.3054426021 H,2.0690302438,2.6100854224,1.1745925787 H,-4.8332468236,-2.4999089342,-0.3225269561 H,-5.8059528979,2.2317033582,0.5021697397 H,-3.2257520119,-2.9634575272,-0.5903609194 H,4.4482938778,3.2958103694,0.5299731795

DCP(TC)$^{+}$  -1307.8029453	C,-3.9271211144,1.3200874688,0.3309783403 C,-4.3716471784,0.01555472,-0.0455939457 C,-3.4322713081,-0.9939842271,-0.285290651 C,-2.0418567743,-0.6990436438,-0.0441048536 C,-1.755307285,0.6835774165,0.1791977755 N,-2.6222634044,1.6380326215,0.3818119815 C,-0.9614411338,-1.6165443985,0.0392990784 C,0.3533831021,-1.1509673179,0.0205321034 C,0.5823182721,0.259998235,0.0776094118 O,-0.4754524719,1.1057517215,0.235149594 C,1.51877115,-1.9712276319,-0.0778056927 C,2.7751707219,-1.452468939,-0.1332214964 C,2.9655766345,-0.0175991054,-0.0352839768 C,1.8266501979,0.8400757152,0.0582255824 N,4.206954688,0.496412577,-0.0306312917 C,5.427725608,-0.3320989854,-0.0037303942 C,5.1603011499,-1.7479736761,0.4819645743 C,3.9843344507,-2.3362536422,-0.2971565822 C,4.4633951049,1.94862116,-0.0229209967 C,3.2880569789,2.7432137522,-0.5688897473 C,2.0040646813,2.33505581,0.1526405533 N,-3.834923343,-2.223977156,-0.7259722541 C,-5.7525437113,-0.2285352658,-0.2554719183 N,-6.8796813184,-0.4268837695,-0.4241018859 N,-4.795032383,2.2998659012,0.6014177379 H,1.4146172136,-3.0442091388,-0.1576480838 C,-1.2408447281,-3.1215010988,0.2463501392 H,3.7550740887,-3.3497956218,0.0360754216 H,4.2453628465,-2.3999252633,-1.3609798262 H,6.0620181894,-2.3477189379,0.3466582293 H,4.9298135798,-1.7374669819,1.5515498824 H,5.8562228879,-0.3398075691,-1.0132645981 H,6.1424622182,0.1739465322,0.6499695701 H,5.3599983495,2.1191844654,-0.6234975713 H,4.6963632145,2.2493942611,1.0058307766 H,3.4866202704,3.8085513983,-0.439270785 H,3.1861993068,2.5571292875,-1.6423847042 H,1.1377391093,2.8431713342,-0.271089786 H,2.0545241659,2.6330290381,1.206888156 H,-4.8258486464,-2.3460487494,-0.8958062454 H,-5.7929300345,2.1566826216,0.5715387365 H,-3.2578069065,-2.7038944872,-1.4033204922 H,-4.4348101508,3.218086242,0.8117540287 H,-2.2884561908,-3.2372368366,0.5425885516 C,-1.0806924804,-3.8598503464,-1.0131827096 C,-0.4493097349,-3.6985063221,1.3400119967 N,0.1465064801,-4.1441377847,2.2178175796 N,-1.0107823621,-4.3723773828,-2.0422923126

DCP(KC)$^{+}$  -1307.704693	C,-3.9769033826,1.4273136072,-0.1560136506 C,-4.3586449462,0.0342912373,0.1524642405 C,-3.414286771,-0.9531610921,0.1288765558 C,-2.0308436512,-0.6889091613,-0.1364148575 C,-1.7588043747,0.7499262242,-0.1536878066 N,-2.6123683787,1.7019451352,-0.1850354364 C,-0.9597780934,-1.5682502641,-0.3610796801 C,0.3684414246,-1.1132245336,-0.2746049603 C,0.5931153445,0.288587581,-0.1434361716 O,-0.4604659539,1.1552268944,-0.1634405437 C,1.5282908839,-1.9384902087,-0.2594663139 C,2.7906680111,-1.4335243813,-0.1419503845 C,2.9784631479,-0.0060230178,-0.0216021815 C,1.8397931747,0.8570489122,-0.032121114 N,4.2189174776,0.5042187336,0.1081661877 C,5.422318096,-0.3340844054,0.2516200546 C,5.0956058459,-1.7364165447,0.740208015 C,3.9991864912,-2.3354043141,-0.1395787399 C,4.4796011388,1.9538868114,0.1402350211 C,3.3676387824,2.7510797874,-0.5225858646 C,2.01631608,2.352248205,0.0690300316 N,-3.8893975363,-2.2980760515,0.5824909531 C,-5.6869541884,-0.2842381946,0.5381079878 N,-6.7017562155,-0.7179929507,0.8881298744 N,-4.9112922949,2.2799895254,-0.3165172042 H,1.4274832645,-3.0134571657,-0.3165101103 C,-1.2513568238,-3.0305286657,-0.7629598694 H,3.7220271718,-3.3356006182,0.1988915829 H,4.3717948273,-2.4410431537,-1.1661526302 H,6.0012292317,-2.3449866854,0.7110186323 H,4.7594276031,-1.6964127138,1.7809598466 H,5.9368887144,-0.3687500664,-0.7166076832 H,6.0861616069,0.1752639165,0.9546101008 H,5.4322487551,2.1210340331,-0.3683057708 H,4.6093364997,2.2585159767,1.1862843497 H,3.5568314053,3.8163470318,-0.3787818856 H,3.3718489866,2.560216191,-1.6000967181 H,1.1988392244,2.8609117088,-0.4415357062 H,1.9631027369,2.6567978998,1.1214027803 H,-4.767576221,-2.1709557892,1.1129712138 H,-4.1243361711,-2.9309219915,-0.188803465 H,-4.5209020604,3.2071258214,-0.4909261885 H,-2.2397170523,-3.0519509427,-1.2352301757 C,-0.3722844726,-3.5746660359,-1.80531634 C,-1.3217091376,-3.8930419889,0.4256058118 N,-1.5022527706,-4.4616421365,1.4122852044 N,0.2685121201,-4.0133541394,-2.6540703391 H,-3.2127830406,-2.7774596005,1.1920066371

DCP(KC)$^{+}$ rotamer  -1307.6963879	C,-3.7592941433,-2.2096369463,0.3285547391 C,-4.2218537386,-0.8630273737,-0.1124387698 C,-3.3337592469,0.1790645845,-0.1648679106 C,-1.9409812007,0.0158412719,0.0977792741 C,-1.5878099362,-1.4048994079,0.1791982314 N,-2.379266161,-2.3953415856,0.2942042426 C, -0.9190978657,0.966906088,0.2620493868 C,0.4291930095,0.5852300603,0.1662783591 C,0.7319194516,-0.8075485642,0.0723626673 O,-0.2640104608,-1.7332421917,0.1408627967 C,1.5399662538,1.4754928784,0.1059386146 C,2.8263698739,1.0413372869,-0.0225415692 C,3.0938249758,-0.3773670542,-0.1082798585 C,2.0078913927,-1.3043443714,-0.0487909088 N,4.3580478919,-0.8183108052,-0.2505635071 C,5.5084587622,0.0830784632,-0.4415645627 C,5.0926559139,1.4509441857,-0.9588893385 C,3.9809666055,2.009680881,-0.0718520971 C,4.702287414,-2.2514588607,-0.2481533987 C,3.6531480392,-3.0918211305,0.4617581361 C,2.2687668442,-2.7893359846,-0.1097109485 N,-3.8829928912,1.4653584429,-0.7064985371 C,-5.5604450313,-0.6559419326,-0.5276290557 N,-6.6285957994,-0.389313891,-0.8888222962 N,-4.5126551263,-3.1775855603,0.6746499757 H,1.3777383361,2.5439730405,0.136704665 C,-1.293586392,2.4242679833,0.6103886697 H,3.6408603275,2.9836658851,-0.4287776644 H,4.3665049724,2.1621685865,0.9440300556 H,5.9623918073,2.1104066046,-0.9639641771 H,4.7393751438,1.3642469099,-1.991105226 H,6.0387432145,0.172353713,0.5145800885 H,6.1861849855,-0.4072238632,-1.1447634918 H,5.6739850684,-2.3475109365,0.2423065363 H,4.8269967331,-2.5770950113,-1.2883970214 H,3.9011237856,-4.1480744402,0.3433709204 H,3.6691604512,-2.8699910072,1.5331988959 H,1.4929497101,-3.3277009673,0.4342185766 H,2.2100556651,-3.1286561168,-1.1511044204 H,-4.7230694894,1.2567021055,-1.2676733465 H,-4.192194133,2.1155601233,0.0235058742 H,-5.5016180038,-2.928486829,0.6497627188 H,-2.2777581165,2.4046505927,1.0921289025 C,-0.4382335125,3.062423541,1.6182116376 C,-1.4289473678,3.2306503365,-0.6115771137 N,-1.6575985101,3.7412815704,-1.6198748337 N,0.1854504309,3.5725594356,2.4393321216 H,-3.2151285435,1.9627182605,-1.312115753

DCPC^{+}  -1307.8777231	C,-3.9225101204,-2.141772682,0.0021851677 N,-4.1188220176,-0.7933058958,0.0429140576 C,-3.0803131743,0.1107883302,0.0533627352 C,-1.7676806934,-0.3878875792,0.0172817325 C,-1.4786109766,-1.7881693193,-0.0299985172 C,-2.6097391149,-2.6629075067,-0.0338449313 C,-0.746149182,0.5897637854,0.0307309987 N,-0.9273720963,1.8874612572,0.071864437 C,-2.1854901119,2.3575763467,0.1053834564 C,-3.3189422363,1.4874611731,0.0978870605 C,-0.1059763121,-2.1548950471,-0.0685320428 C,0.8850007697,-1.1288109637,-0.0522746934 O,0.5366891215,0.2028441461,0.0013354478 C,2.243431357,-1.3644189795,-0.076537182 C,2.6974998235,-2.7139781132,-0.1174072618 C,1.72948793,-3.7775810372,-0.1620950365 C,0.3955515227,-3.4832039773,-0.1243666868 N,4.0201069024,-2.9965362664,-0.1137845717 C,4.5472633338,-4.3683258921,-0.0276395108 C,3.5249064921,-5.3494428923,0.5257732653 C,2.2135923433,-5.2035730827,-0.2463803191 C,5.0499880523,-1.9483040963,-0.16063357 C,4.5228910567,-0.6596902228,-0.7720520986 C,3.2402987986,-0.2298911647,-0.060290226 N,-2.3306345645,3.6897348047,0.1465270485 C,-4.6471610299,1.9749449944,0.1331516367 N,-5.7501962775,2.3251849501,0.1606653096 C,-2.5519877875,-4.0793123594,-0.0689463521 N,-2.6353747258,-5.2334875615,-0.094519546 H,-0.2934462074,-4.3125323194,-0.1467049612 H,1.4496836089,-5.8832991747,0.1357803241 H,2.3798355498,-5.4709747942,-1.2975204431 H,3.921438324,-6.3632899874,0.4444538004 H,3.3543681036,-5.1465760368,1.5876414351 H,4.8795349462,-4.678761018,-1.0263885828 H,5.4326970816,-4.3352438574,0.6129489173 H,5.8854958309,-2.3386091316,-0.7475623529 H,5.4208804561,-1.7723025817,0.8573496716 H,5.2887344531,0.1144198662,-0.6944899285 H,4.3208527037,-0.8158471242,-1.836252889 H,2.8125431334,0.6547635391,-0.5315515755 H,3.4643981131,0.048169848,0.976811195 H,-3.2350846632,4.1328580539,0.1725015481 H,-1.5011445431,4.2623576859,0.1513572136 N,-5.013006912,-2.920528327,-0.0013188458 H,-4.9166670758,-3.9255022988,-0.0318734863 H,-5.9456877541,-2.5408909304,0.0274128566 H,-5.0636152313,-0.4256515604,0.0667472962

CPH  -1084.7927141	C,2.7697455568,-1.4537223561,-0.1617853408 C,2.9563264971,-0.0535708537,-0.0427086717 C,1.8255805173,0.7876149232,0.0392676018 C,0.5550301994,0.2100148915,0.0098475304 C,0.3460886535,-1.1614621492,-0.0871537213 C,1.4816942587,-1.9669225432,-0.1667437878 O,-0.4934330249,1.1124211796,0.0974168617 C,-1.7820118225,0.6810764771,0.078847353 C,-2.1022202632,-0.6726867813,-0.01370126 C,-1.0452568154,-1.743291061,-0.0957095209 C,3.9806017922,-2.3491223041,-0.259391946 C,5.123145274,1.7603126992,0.5711592111 C,5.4311145017,-0.346447493,0.0884600975 N,4.2350546335,0.4825238437,-0.0135073562 C,4.4713105444,1.919995228,0.0197783457 C,3.2973609087,2.7028768662,-0.5550669274 C,1.9987407043,2.2846364851,0.1357746565 C,-3.4708086048,-0.9917797709,-0.0080548257 C,-4.4192123805,0.0571811253,0.0795534895 N,-2.6450051365,1.687141267,0.1654347328 N,-3.8846778963,-2.2942644364,-0.0444152631 C,-5.8042026461,-0.2237015239,0.0787450532 N,-6.9394177525,-0.4606049638,0.0783010987 C,-3.9436949021,1.3914167914,0.1610123424 N,-4.8093221657,2.445098942,0.204870385 H,1.3525849854,-3.0437651373,-0.2393522349 H,3.7321882551,3.35898703,0.0782571632 H,4.3059671948,-2.4364987662,-1.3049262038 H,6.027697154,-2.370106845,0.4980401514 H,4.826918595,-1.7314088215,1.6249013037 H,5.9405361462,-0.3892883867,-0.8870618639 H,6.12569535,0.1383508798,0.7853555641 H,5.3794535266,2.1284328897,-0.5579257618 H,4.6693464704,2.248281206,1.0531735316 H,3.4805460712,3.7735841187,-0.4318395785 H,3.2197530105,2.5027854513,-1.6288569842 H,1.1393383887,2.7891398316,-0.3067829418 H,2.0259577418,2.5914280961,1.1895909418 H,-4.8616109319,-2.4870354077,-0.2031916828 H,-5.7792740316,2.2925089621,0.42734369 H,-3.2409985707,-3.0029917019,-0.3517214186 H,-4.4069868583,3.3399486027,0.430612712 H,-1.1833605851,-2.340330442,-1.0111517297 H,-1.1611987531,-2.4464765338,0.742325894

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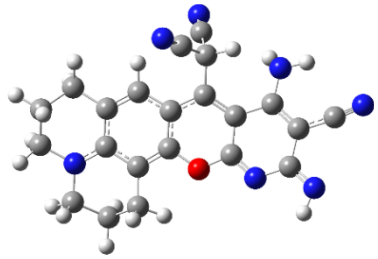

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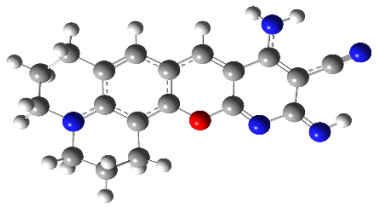

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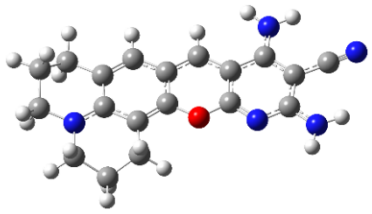
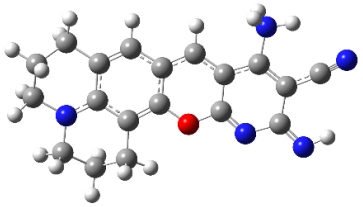
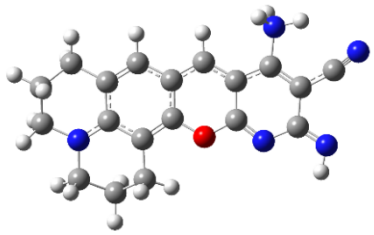
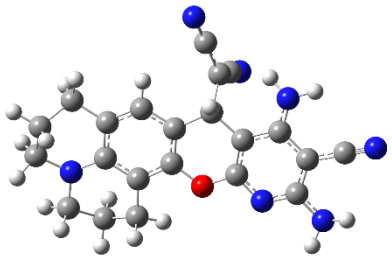
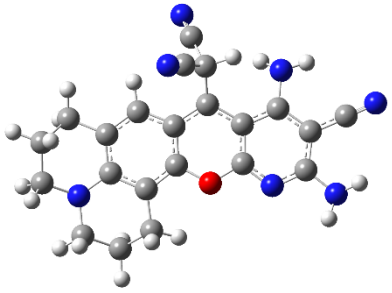
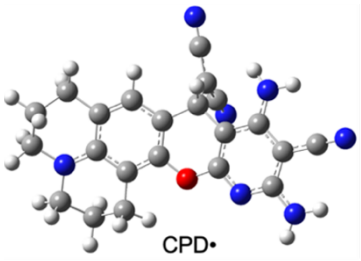
CP(TC)$^+$  -1083.9881269	C,2.7342833577,-1.4676861753,-0.1596949325 C,2.9432021264,-0.0382033418,-0.0290453607 C,1.8211933574,0.8431972847,0.0470595342 C,0.5638932928,0.2876167607,0.0181065803 C,0.3246695583,-1.1140966182,-0.0821708361 C,1.4640843846,-1.9614915134,-0.16858526 O,-0.495166257,1.1458931934,0.0991332808 C,-1.7816555587,0.725053147,0.0856543512 C,-2.0629202361,-0.6703241347,-0.0051097739 C,-0.9878223157,-1.5627195719,-0.0914060221 C,3.9358901221,-2.3695905815,-0.2844114936 C,5.0944187139,-1.8073541661,0.5384953358 C,5.4004800544,-0.3930254101,0.0713309887 N,4.1970553921,0.4558523652,0.019488175 C,4.4785446861,1.9018545979,0.0497257739 C,3.3360476805,2.7219565372,-0.5276852503 C,2.024461102,2.3339991844,0.1535262383 C,-3.4560608311,-1.0365602975,-0.0059510191 C,-4.3987073857,0.0016701421,0.0739587893 N,-2.6506635671,1.69541637,0.1605634113 N,-3.8494028547,-2.3204456753,-0.0837927874 C,-5.7839410149,-0.2951126599,0.0769487572 N,-6.9141001431,-0.5437010974,0.0794896503 C,-3.9549256218,1.3553053458,0.1541587638 N,-4.8284335321,2.3662217492,0.2291563104 H,1.3073325997,-3.0316222514,-0.252112329 H,-1.1573320678,-2.63114772,-0.1713762791 H,3.6790691527,-3.382271304,0.0321824181 H,4.2354876303,-2.4317611443,-1.3381443813 H,5.9905055163,-2.4211879652,0.4305020623 H,4.827481326,-1.7980275949,1.5997776318 H,5.8592868592,-0.4038730123,-0.9250910389 H,6.1073287322,0.0924137617,0.7491955757 H,5.3966255191,2.0630359852,-0.5206888938 H,4.6829436256,2.1937104862,1.0873985495 H,3.5506621054,3.7829331507,-0.3875113956 H,3.262544459,2.5416212113,-1.6045328946 H,1.1793690693,2.8587427494,-0.2926025996 H,2.0503447814,2.6273900806,1.2099917511 H,-4.8309801771,-2.555565217,-0.0773670677 H,-5.8254789082,2.216232363,0.2299489673 H,-3.1975654719,-3.0836403007,-0.1159573331 H,-4.4696388413,3.3065909973,0.2864699727

CP(KC)$^+$  -1083.8845654	C,-6.1980452737,0.9166533412,0.1079128677 C,-6.1430039003,-0.5287802908,0.1295547203 C,-4.8777740972,-1.1953947862,0.1172700314 C,-3.737689773,-0.4262973143,0.1064109061 C,-3.7611808,0.9985918997,0.107523965 C,-5.0332262602,1.6285818741,0.1110059345 O,-2.5479811722,-1.0980903211,0.1049625538 C,-1.3338435523,-0.4658513141,0.0915089112 C,-1.3395397331,0.9924286467,0.0970860292 C,-2.5457215985,1.6839817343,0.1041138534 C,-7.5440705058,1.5957570598,0.0816591538 C,-8.5556437129,0.7712415246,0.8772216882 C,-8.6182670664,-0.635629696,0.3027108912 N,-7.2858557963,-1.2468348771,0.1629213171 C,-7.3022829253,-2.7178388006,0.0845441205 C,-6.0481095432,-3.2723861402,-0.5716403965 C,-4.8085350139,-2.7021338494,0.11560538 C,-0.0353099701,1.5327379806,0.0899803853 C,1.0980314042,0.7696877085,0.0765242232 N,-0.3189051971,-1.2361236757,0.0766503684 N,0.1177344358,3.015452668,0.0960462855 C,2.3597242882,1.4142968017,0.0711570021 N,3.3347604501,2.0404753705,0.0676307729 C,0.9790829544,-0.7213599916,0.0657281255 N,1.9636678622,-1.5325730927,0.0470769653 H,-5.0747439458,2.7130761631,0.1081062314 H,-2.5775136961,2.7710974524,0.1044933015 H,-7.4610776914,2.6096788662,0.4784197253 H,-7.8878932122,1.6874849921,-0.9563761429 H,-9.550661864,1.2184247549,0.8367425464 H,-8.2557781786,0.7285955477,1.9288904708 H,-9.1030071766,-0.6312101196,-0.6816587057 H,-9.2067927227,-1.2902906022,0.9508090212 H,-8.1930787831,-3.0001847333,-0.4823500043 H,-7.4204960844,-3.1180337742,1.0994117661 H,-6.0630975895,-4.3619958173,-0.5090778775 H,-6.04033745,-3.0051219466,-1.6328678573 H,-3.8952696915,-3.0327670171,-0.378945329 H,-4.7510703799,-3.0678687481,1.1480556691 H,1.1199957385,3.2618336923,0.0947500024 H,-0.3109084823,3.4335534693,0.9290209081 H,2.8634448075,-1.052024644,0.040104935 H,-0.3141659711,3.4402479144,-0.731862246

CP(KC)$^+$ rotamer  -1083.893388	C,0,2.715485,-1.471426,-0.125231 C,0,2.935622,-0.046718,-0.022855 C,0,1.819201,0.844876,0.031935 C,0,0.554757,0.303954,0.005383 C,0,0.307521,-1.095159,-0.072712 C,0,1.43651,-1.951418,-0.133903 O,0,-0.490557,1.186737,0.069076 C,0,-1.796841,0.794491,0.052233 C,0,-2.07039,-0.633995,-0.024812 C,0,-1.018021,-1.537283,-0.085412 C,0,3.908048,-2.389495,-0.219733 C,0,5.067445,-1.81809,0.596049 C,0,5.388944,-0.417332,0.097989 N,0,4.195118,0.44093,0.022285 C,0,4.487818,1.883995,0.024348 C,0,3.352254,2.701211,-0.570742 C,0,2.036386,2.335306,0.114251 C,0,-3.45812,-0.92393,-0.03148 C,0,-4.423132,0.036069,0.026911 N,0,-2.654479,1.743362,0.107954 N,0,-3.89452,-2.343152,-0.107897 C,0,-5.787023,-0.356726,0.013959 N,0,-6.824821,-0.869793,-0.007616 C,0,-4.022191,1.459967,0.1011 N,0,-4.954363,2.329544,0.153191 H,0,1.272742,-3.022387,-0.197331 H,0,-1.19392,-2.608655,-0.146439 H,0,3.639382,-3.39086,0.123006 H,0,4.215341,-2.484206,-1.268876 H,0,5.958883,-2.442081,0.508468 H,0,4.793859,-1.78069,1.655064 H,0,5.852932,-0.45657,-0.895626 H,0,6.098823,0.07523,0.767776 H,0,5.408044,2.027645,-0.547728 H,0,4.692887,2.196556,1.056133 H,0,3.573602,3.76324,-0.449995 H,0,3.279757,2.501336,-1.644281 H,0,1.196074,2.860344,-0.339956 H,0,2.063617,2.644934,1.166137 H,0,-4.928252,-2.380941,-0.100157 H,0,-3.549567,-2.888371,0.689513 H,0,-3.565878,-2.793464,-0.968922 H,0,-4.558059,3.269017,0.201502

CPD^{-}  -1308.1050544	C,4.0917663864,1.8482773686,0.5738050002 C,2.8951247787,0.9448571548,-0.4117414889 C,3.1135416631,-0.4328835975,-0.1783023699 N,4.4181155213,-0.9274023515,-0.0824439555 C,5.5771875734,-0.1647665205,-0.528241358 C,5.1990049814,1.0907261546,-1.3110878286 C,4.6764599789,-2.3279189163,0.197166551 C,3.5457013963,-2.9622909399,0.9994194957 C,2.2102688776,-2.7537415385,0.2833897961 C,2.008502109,-1.2861382227,-0.0139636707 C,1.5978654672,1.4271786547,0.488903816 C,0.4785354843,0.6071078426,-0.3303616107 C,0.7219741826,-0.7399367976,-0.0974395131 C,-0.9303350331,1.1807640484,-0.3778887716 C,-1.9537346582,0.0699635377,-0.2131878422 C,-1.599275322,-1.259498354,-0.0178103537 O,-0.3008069573,-1.6599567881,0.0549542598 C,-3.3396433032,0.3398353522,-0.2752706423 C,-4.2518875488,-0.7433810062,-0.1625159926 C,-3.7335946551,-2.0469545161,0.0319223507 N,-2.4331318023,-2.2967895927,0.1003750595 C,-1.1484814696,2.3445345586,0.6056526009 C,-0.8054700281,3.6340341552,0.1830922124 N,-4.5760585765,-3.1252431751,0.2018253092 C,-5.6469575022,-0.5321976584,-0.2360924663 N,-6.795587107,-0.3806538102,-0.3072191195 N,-3.7724864466,1.613840797,-0.4839368747 C,-1.2837843764,2.0605742131,1.9729653278 N,-1.4334038066,1.785801555,3.0963363873 H,1.4403727273,2.4883162942,-0.6524071628 H,3.8093560681,2.7566535615,1.1117551093 H,4.4668930799,2.1658679403,0.4090920731 H,6.0921700221,1.7083362864,1.4482483874 H,4.8358930908,0.8080539873,2.3050263717 H,6.1928272696,0.1157051578,0.3418959202 H,6.2044236928,-0.8130313339,-1.1576984919 H,5.6185109448,-2.3969111926,0.7565373204 H,4.8262945506,-2.8920569877,-0.7420281184 H,3.7545846897,-4.0269456731,1.1433274826 H,3.5035410656,-2.4955348216,1.9891170525 H,1.3814404433,-3.1254118165,0.8874456339 H,2.1950770058,-3.3373634061,-0.6474562727 H,-5.5145652949,-3.0506514939,-0.1587124393 H,-4.123812556,-4.0185539694,0.0863179592 H,-4.7501256006,1.7985384559,-0.3112263839 N,-0.5272496857,4.6909671332,-0.2319706396 H,-1.0813165689,1.6123248944,-1.3777836331 H,-3.1151631815,2.323567487,-0.1437433376

DCP^-  -1308.056497	C,4.0628602899,1.8282450042,0.3526302682 C,2.8534729992,0.941557067,0.2131385247 C,3.0752048024,-0.4335768249,0.0763004196 N,4.3968450939,-0.9418732477,0.1522270628 C,5.5246806008,-0.1188119454,-0.2923941872 C,5.1420021678,1.3292064376,-0.6149240167 C,4.6163948302,-2.3598257866,-0.0595867303 C,3.4696555826,-3.1966281728,0.4957404099 C,2.1557048452,-2.7887994136,-0.1741563875 C,1.9614460918,-1.2936466566,-0.0629599796 C,1.5565314318,1.4548117424,0.1863091068 C,0.4179951654,0.6392993672,0.0476071867 C,0.6911019023,-0.737988874,-0.0882388959 C,-0.9500448962,1.0910975111,0.0091296153 C,-1.9844976338,0.0834805113,0.0309718146 C,-1.6472750799,-1.2765402711,-0.1764023664 O,-0.3437110483,-1.6487961807,-0.324950528 C,-3.3460193954,0.2806841255,0.3524141592 C,-4.2693757006,-0.7973334361,0.2426802866 C,-3.7840922838,-2.074009195,-0.0959888062 N,-2.4805171602,-2.3005254933,-0.2631215601 C,-1.2589129385,2.4985071459,-0.4495425192 C,-0.6217956157,2.8544554721,-1.7413149769 N,-4.6259960652,-3.1810013627,-0.2101567936 C,-5.645938585,-0.6014641708,0.5013480072 N,-6.7771422837,-0.4427586726,0.7107295857 N,-3.7824783095,1.5524558513,0.7554456362 C,-0.9685028353,3.5467575475,0.5607164691 N,-0.7841625529,4.320348274,1.3981446976 H,1.4344357837,2.5273416266,0.2873875051 H,3.8019809631,2.8692677087,0.1442618166 H,4.4534635627,1.7906669138,1.38002237 H,6.0427775923,1.9513445061,-0.5811527156 H,4.7405553896,1.3874227038,-1.6312044489 H,6.2946522628,-0.1346313794,0.4929514782 H,5.9844230126,-0.5728820568,-1.1870333756 H,5.5631277594,-2.6353956537,0.4236047512 H,4.7372121872,-2.5862994153,-1.1386604192 H,3.6802948345,-4.2588231053,0.333424264 H,3.3986790364,-3.0333364811,1.5766678334 H,1.3063367235,-3.3065798397,0.2752902133 H,2.1714011792,-3.0930719737,-1.2296233958 H,-5.5654802919,-2.9812641893,-0.5239297399 H,-4.1829925131,-3.9315063826,-0.7211918941 H,-4.7119996375,1.554613074,1.157257915 H,-2.3378419968,2.5724594505,-0.6252207792 N,-0.1370329595,3.0715479213,-2.7662296848 H,-3.1141440077,1.9895671087,1.386585094

CPD•  -1308.0008373	C,4.0407122952,2.0402972148,-0.8440608636 C,2.8784415913,1.1193513149,-0.5638459006 C,3.1304032384,-0.2384428399,-0.2145338579 N,4.4214765279,-0.708197863,-0.1450752107 C,5.5746980368,0.0988695525,-0.5416913188 C,5.1908125188,1.2474368659,-1.4664923399 C,4.7407442965,-2.0635963053,0.3009959196 C,3.6273612401,-2.6678271755,1.1459506118 C,2.2910215834,-2.5491063697,0.4129503429 C,2.0405075832,-1.107122485,0.0480446035 C,1.5729325249,1.560649268,-0.6393041044 C,0.4802788575,0.7248448014,-0.3774506553 C,0.7481730801,-0.6012359207,-0.0332533874 C,-0.9354399665,1.2492324489,-0.363188815 C,-1.9366255047,0.1254288932,-0.3410428333 C,-1.5583977121,-1.1831254735,-0.0443236782 O,-0.2589626193,-1.5107459438,0.2064199671 C,-3.3096115652,0.3536073342,-0.5624782619 C,-4.1917685436,-0.7509132374,-0.5058557273 C,-3.6609445111,-2.0320027437,-0.2000691548 N,-2.3615940434,-2.232036201,0.030535097 C,-1.0425669237,2.1484003004,0.8787448208 C,-0.9027630932,3.5321732765,0.7450163221 N,-4.4616593264,-3.1286552898,-0.1484095055 C,-5.5790602196,-0.57509215,-0.7157192238 N,-6.717011624,-0.4298779231,-0.8815417328 N,-3.7797433485,1.6005090253,-0.8580633514 C,-1.1750517992,1.5722227609,2.1485227204 N,-1.300271143,1.0571429332,3.1823607955 H,1.3845525217,2.5982176894,-0.8975732171 H,3.7251720716,2.8546529798,-1.5006361271 H,4.3857321101,2.5035221582,0.0896342593 H,6.0659149525,1.8796297576,-1.6359652948 H,4.8774990233,0.847713897,-2.4364165773 H,6.0749109826,0.4897244191,0.3567810468 H,6.2899673986,-0.5629930748,-1.0418775855 H,5.6702989511,-2.0157039772,0.8783663888 H,4.939242383,-2.6998327289,-0.5745848841 H,3.8655607953,-3.7121379431,1.3622338399 H,3.5670051814,-2.1386800281,2.1023266537 H,1.4717460837,-2.9262012953,1.0249235339 H,2.3086625723,-3.1657726473,-0.4951052359 H,-3.2375463447,2.4065979754,-0.5949267293 H,-5.4636743764,-3.034170802,-0.136671084 H,-4.0519905197,-3.973085033,0.2151056537 H,-4.7785221118,1.7429265083,-0.8722148393 N,-0.8029795789,4.6757919411,0.5508893912 H,-1.1016195263,1.8837191355,-1.2404964715