**Electronic Supplementary Information**

# Circularly Polarized Luminescence of Natural Products Lycorine and Narciclasine: Role of Excited-State Intramolecular Proton-Transfer and Test of pH Sensitivity

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# NMR data for compounds 1-4

### $^{1}$H and $^{13}$C NMR and EI MS data of Lycorine

$^{1}$H NMR (400 MHz, $CDCl_3$-$CD_3COOD$, 3:1 v/v): δ 6.98 (s, H-12), 6.80 (s, H-8), 5.95 (s, $H_2$-11), 5.77 (br s, H-3), 4.58 (br s, H-1), 4.48 and 4.19 (1H each, d, J=14.0 Hz, $H_2$-7), 4.26 (m, H-2), 3.95 (d, J=11.8 Hz, H-12c), 3.75 and 3.49 (1H each, m, $H_2$-5), 2.99 (d, J=11.8 Hz, H-12b), 2.88 (m, $H_2$-4). $^{13}$C NMR (100 MHz, $CDCl_3$-$CD_3COOD$, 3:1 v/v): δ 149.6 (C-9), 148.1 (C-10), 137.9 (C-3a), 130.7 (C-7a), 125.7 (C-12a), 122.9 (C-3), 108.8 (C-8), 106.4 (C-12), 102.8 (C-11), 71.9 (C-2), 70.1 (C-1), 61.8 (C-12c), 55.1 (C-5), 54.2 (C-7), 38.2 (C-12b), 30.3 (C4).. EI MS, *m/z*: 287 $[M]^+$, 286, 268, 252, 250, 227, 226.

### $^{1}$H and $^{13}$C NMR and EI MS data of Narciclasine

1H NMR (400 MHz, $CD_3SOCD_3$): δ 13.24 (s, HO-7), 7.88 (s, HN-5), 6.83 (s, H-10), 6.15 (ddd, J=4.9, 1.0 ad 2.4 Hz, H-1), 6.09 (d, J=1.2 Hz, H-11A), 6.08 (d, J=1.2 Hz, H-11B), 4.18 (ddd, J=(8.5, 2.4 and 1.2 Hz, H-4a), 4.01 (ddd, J=4.9, 2.4 and 1.2 Hz, H-2), 3.78 (dd, J=8.5 and 2.4 hz, H-4), 3.69 (ddd, J=2.4, 2.4 and 1.2 Hz, H-3); $^{13}$C NMR (100 MHz, $CD_3SOCD_3$): δ 172 (C-6), 169.8 (C-7), 152.3 (C-8), 144.8 (C-9), 133.3 (C-10b) 132.1 (C-10a), 129.2 (C-6a), 124.7 (C-1) 102.0 (c-11), 95.7 (C-10), 72.3 (C-3), 69.1 (C-2), 68.8 (C-4), 52.8 (C-4a); EI MS, m/z: 307 $[M]^+$, 289, 271.

**Table S1** $^{1}H$ and $^{13}C$ NMR data of Tri- and Tetra-acetylnarciclasine (**3** and **4**) recorded in $CDCl_3$ at 400 and 100 MHz, respectively. The chemical shifts are in δ values (ppm) from TMS[a]

| Carbon number | **3** | | **4** | |
|---|---|---|---|---|
| | δH (J in Hz) | δC | δH (J in Hz) | δC |
| 1 | 6.18 m | 118.2 d | 6.18 m | 118.2 d |
| 2 | 5.49 br t (4.0) | 68.5 d | 5.46 br t (4.0) | 68. 3 d |
| 3 | 5.37 m | 71.4 d | 5.37 m | 71.4 d |
| 4 | 5.25 dd (12.0 and 4.0) | 67.9 | 5.24 dd (12.0 and 4.0) | 68.1d |
| 4a | 4.65 br d (12.0) | 50.3 d | 4.61 d (12.0) | 50.2 d |
| 6 | | 170.3 s[b] | | 170.5 s[d] |
| 6a | | 130. 5 s | | 131.7 s |
| 7 | | 170. 3 s[b] | | 162.3 s |
| 8 | | 153.1 s | | 152.5 s |
| 9 | | 145.9 s | | 141.6 |
| 10 | 6.68 s | 96.6 d | 6.95 s | 102.0 d |
| 10a | | 133.2 s | | 133.8 s |
| 10b | | 135.3 s | | 134.2 s |
| 11A | 6.11 br s | 102.6 t | 6.14 br s | 103.1 t |
| 11B | 6.10 br s | | 6.11 br s | |
| $\underline{CH_3}CO$ | 2.16 s | 20.9 q[c] | 2.40 s | 20.9 q[e] |
| $\underline{CH_3}CO$ | 2.15 s | 20.9 q[c] | 2.15 s | 20.9 q[e] |
| $\underline{CH_3}CO$ | 2.13 s | 20.8 q | 2.13 s | 20.8 q |
| $\underline{CH_3}CO$ | | | 2.11 s | 20.7 q |
| $CH_3\underline{CO}$ | | 169.7 s | | 170.5 s[d] |
| $CH_3\underline{CO}$ | | 169.5 s | | 169.7 s |
| $CH_3\underline{CO}$ | | 168.9 s | | 169.5 s |
| $CH_3\underline{CO}$ | | | | 169.1 s |
| HN-5 | 6.01 br s | | 5.96 br s | |
| HO-7 | 12.46 s | | | |

[a]The assignments were made in accordance with the value previously reported for narciclasine[37]
[b,c,d,e]These signals are overlapped

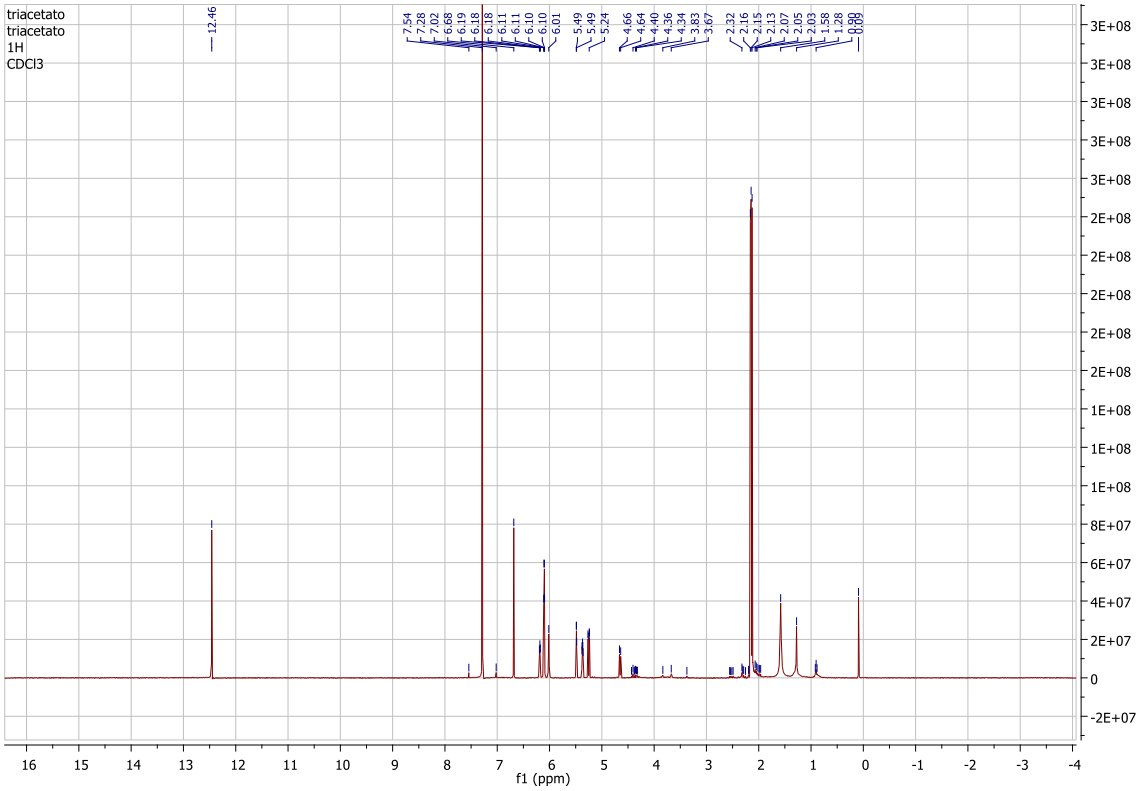



**Fig. S1**. $^{1}$H NMR spectra of triacetylnarciclasine **3**

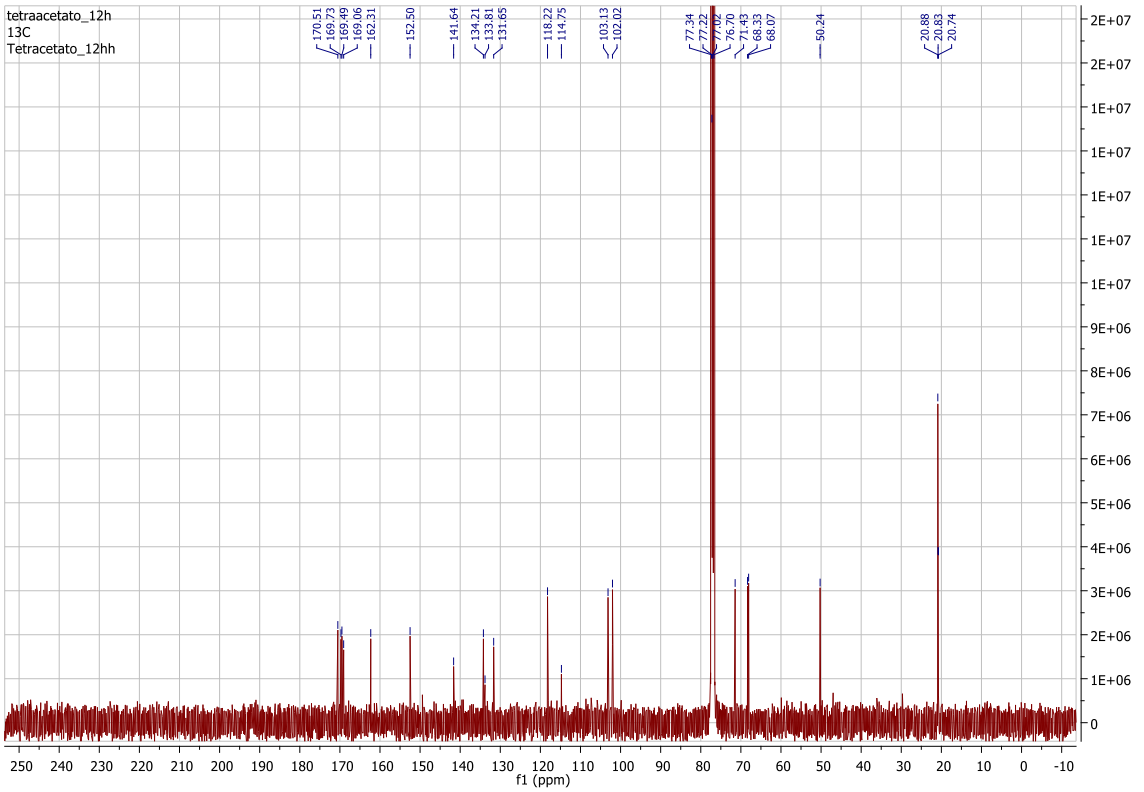



**Fig. S2**. $^{13}$C NMR spectra of triacetylnarciclasine **3**

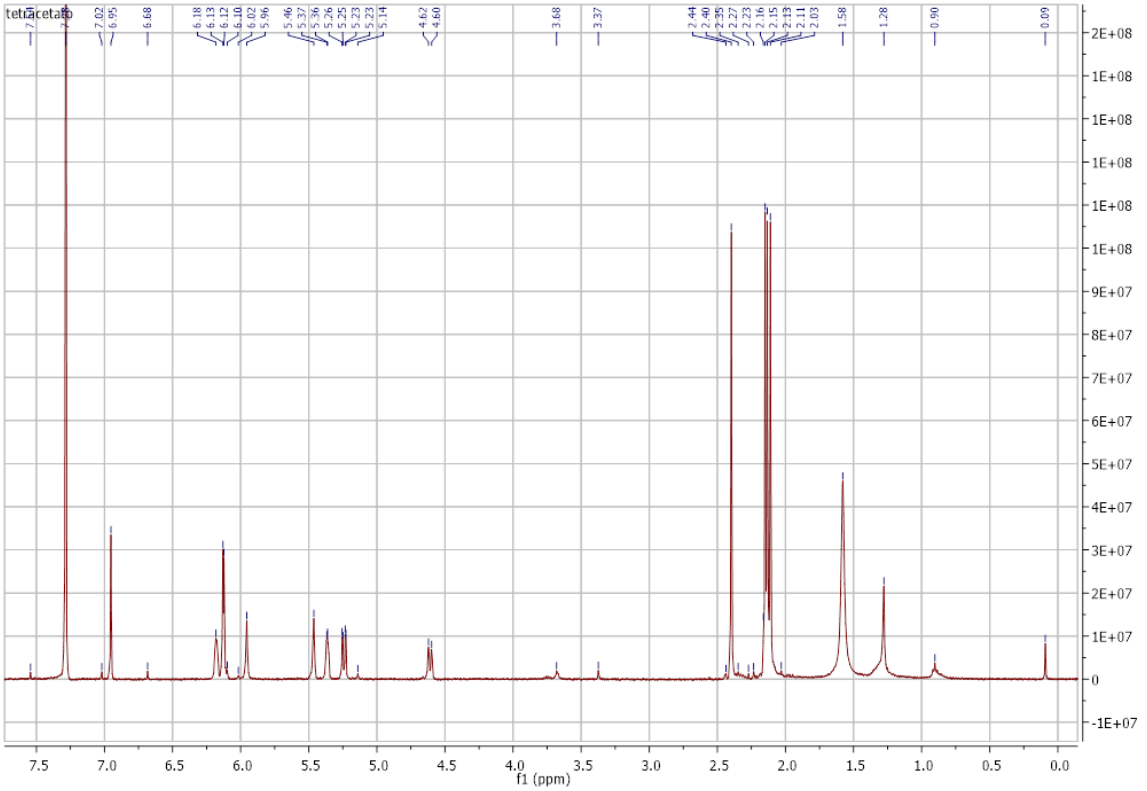



**Fig. S3**. $^{1}$H NMR spectra of tetracetylnarciclasine **4**

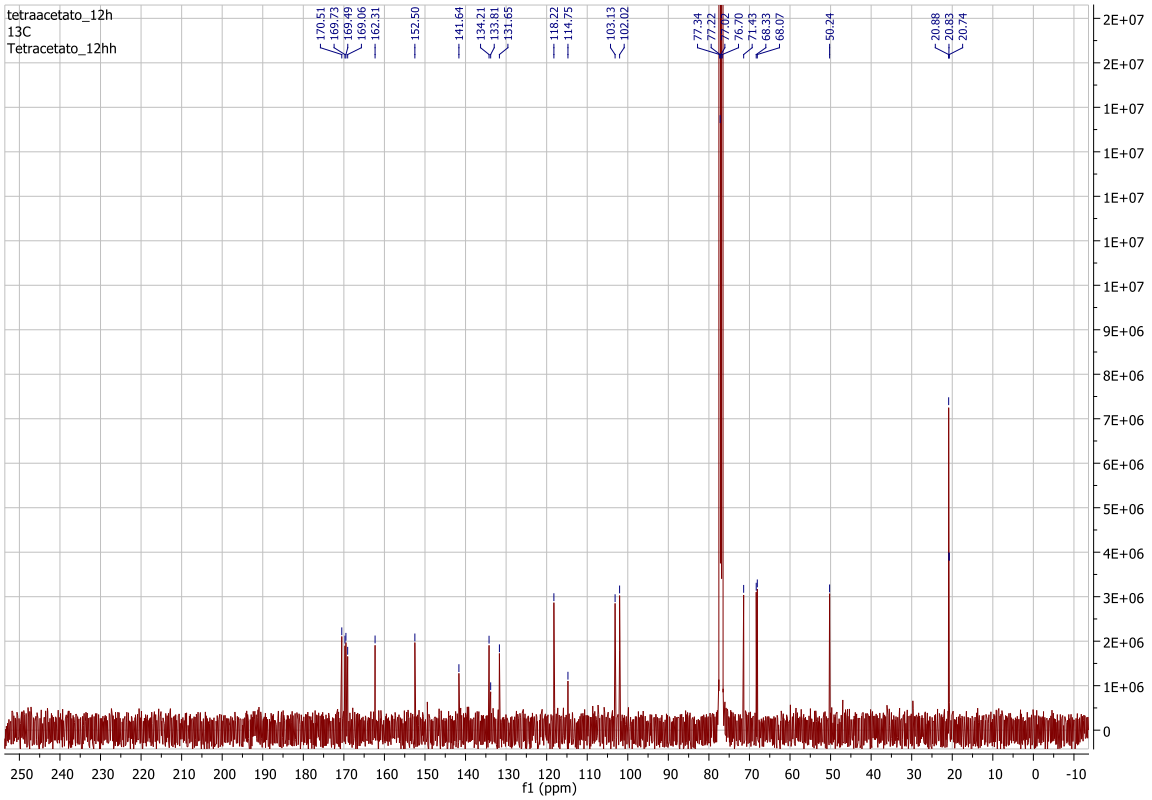



**Fig. S4**. $^{13}$C NMR spectra of tetracetylnarciclasine **4**

# Additional Spectra of Narciclasine Derivatives

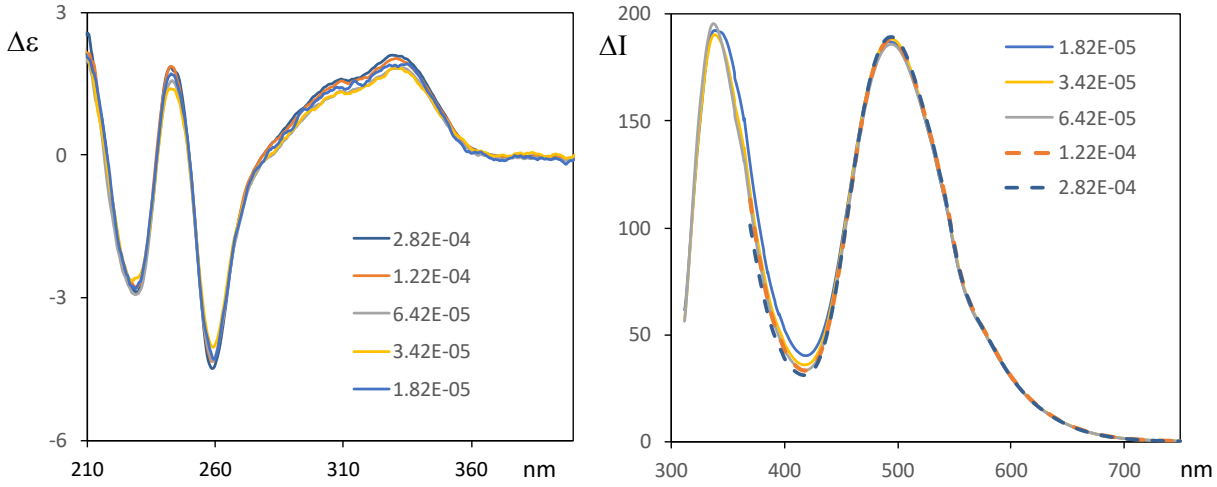



**Fig. S5**. CD (left), fluorescence (right) experimental spectra of narciclasine **2** at different concentrations. Fluorescence spectra were corrected for autoabsorption, i.e. dividing by transmittance (see ref. 56 in the text). Since, when considering highly concentrated solutions, transmittance is nearly zero, for the two most concentrated solutions data were not corrected and are reported only down to 370 nm.

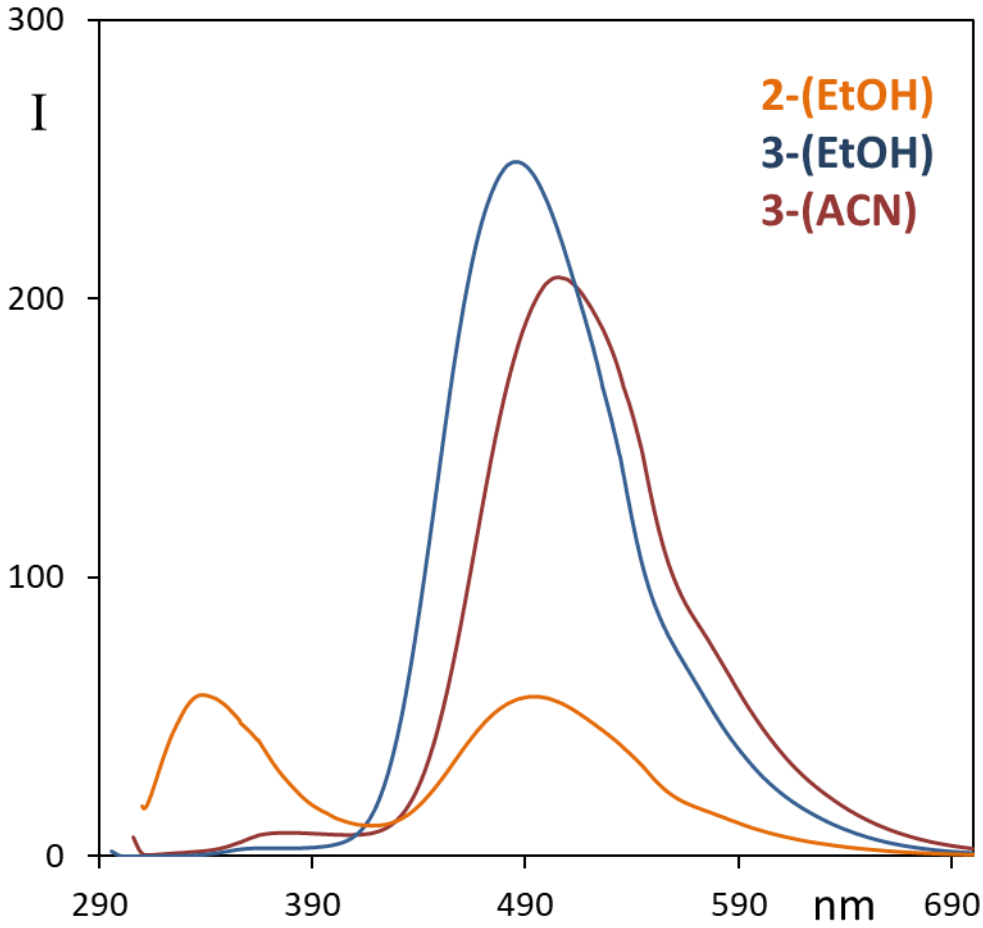



**Fig. S6**. Comparison of experimental fluorescence spectra of narciclasine **2** in ethanol solution (orange line) and of triacetylnarciclasine **3** in acetonitrile (dark red line) and in ethanol (blue line) solutions. Excitation wavelengths: 300 nm.

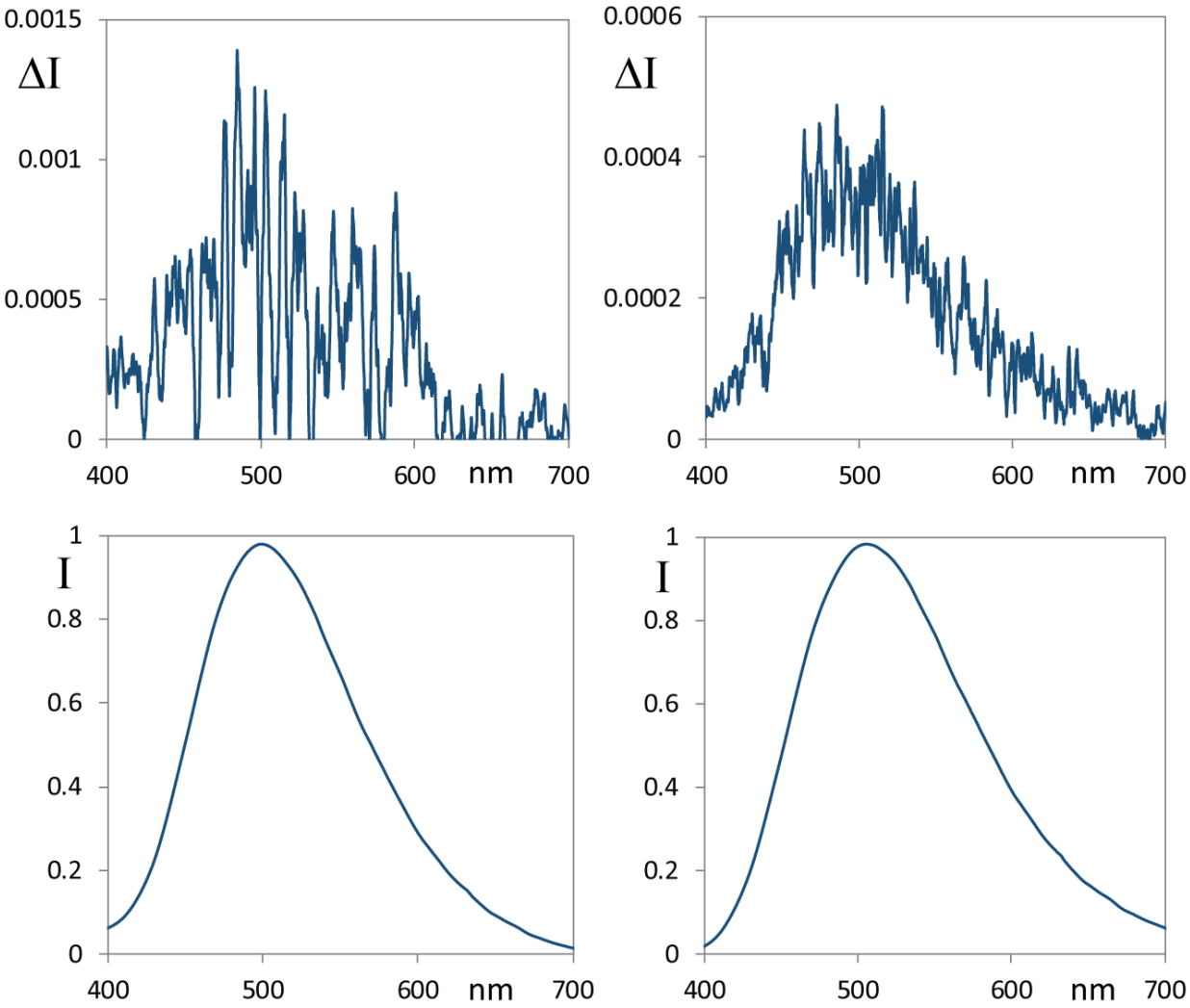



**Fig. S7**. CPL (top) and fluorescence (bottom) spectra in DMSO solution of narciclasine **2** (ca. $10^{-5}$ M, left) and triacetylnarciclasine **3** (ca. $10^{-4}$ M, right). Excitation wavelength: 300 nm.

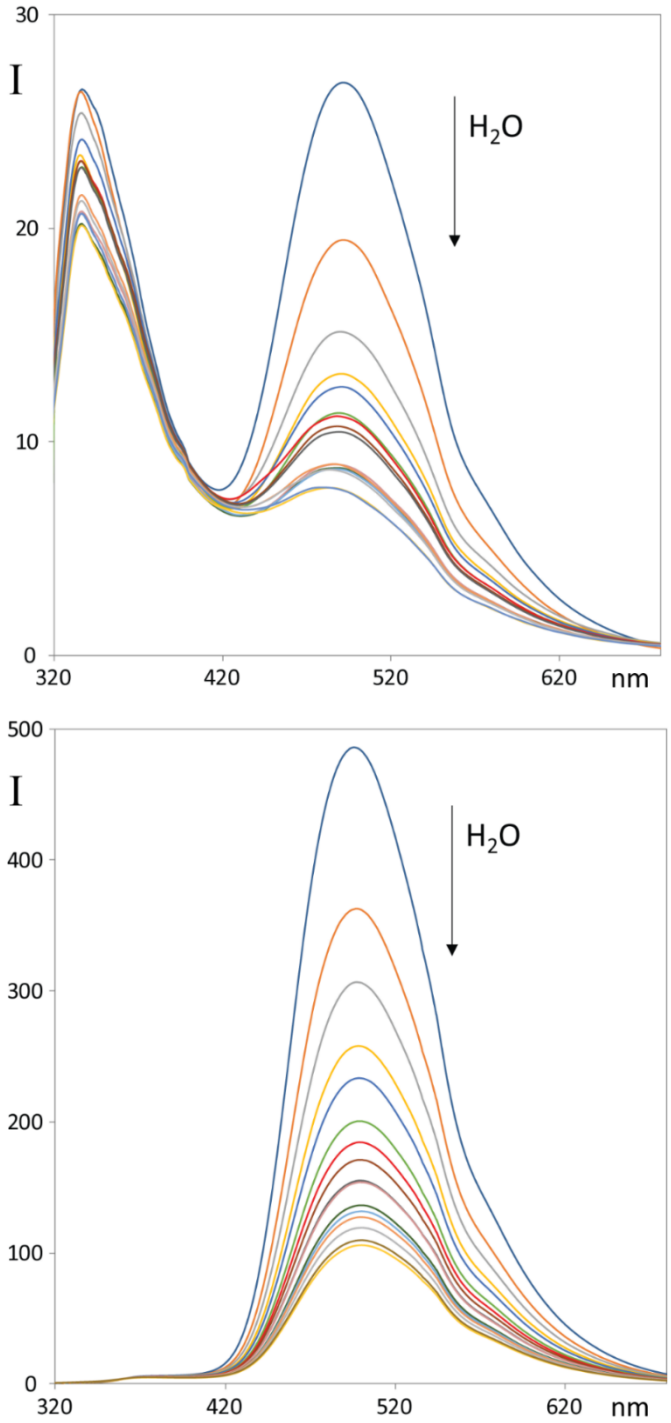



**Fig. S8**. Fluorescence experimental in mixed EtOH/$H_2O$ solution, from 15:1 to a 1:1 ratio v/v for narciclasine **2** (top) and triacetylnarciclasine **3** (bottom). Correction for auto-absorption has been applied. Excitation wavelength: 300 nm.

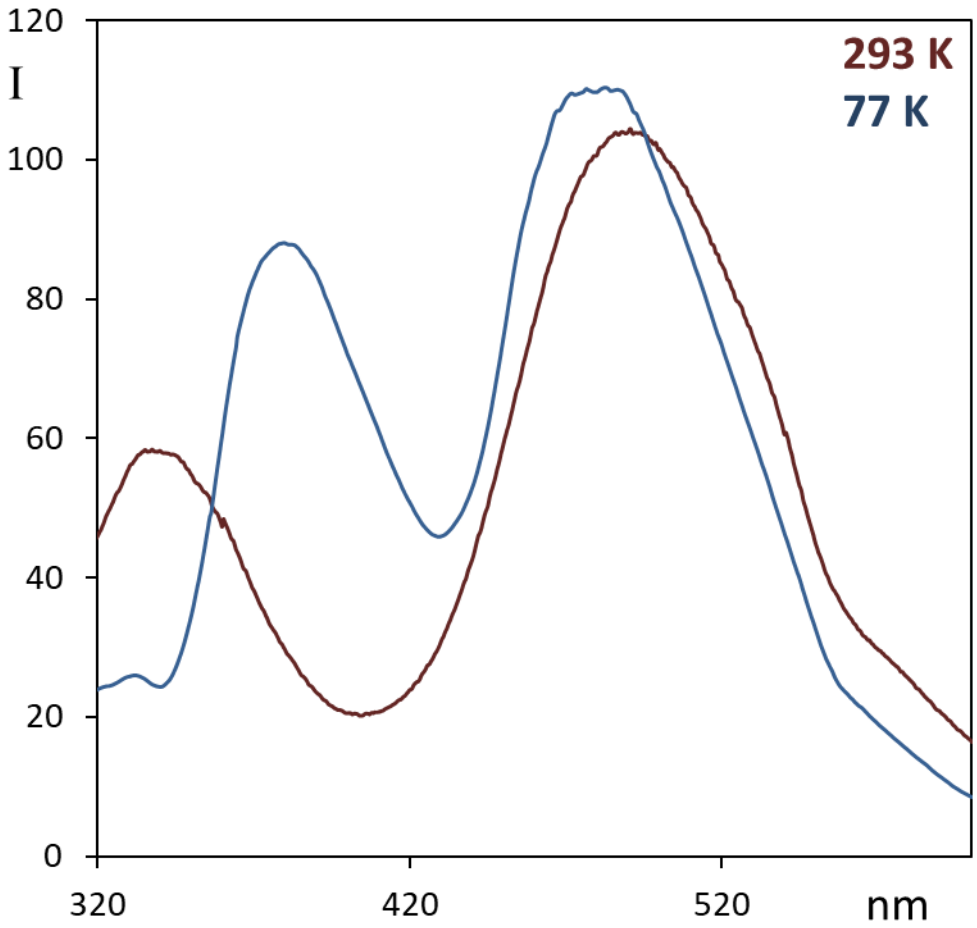



**Fig. S9.** Room temperature (red) and liquid-$N_2$ temperature (blue) fluorescence spectra of narciclasine **2** in solution. Solvent used: EPA (ether, isopentane, ethanol, 5:5:2, by volume). Excitation wavelength: 300 nm. Concentration is ca. $5 \cdot 10^{-5}$ M.

# Narciclasine Derivatives under different pH conditions

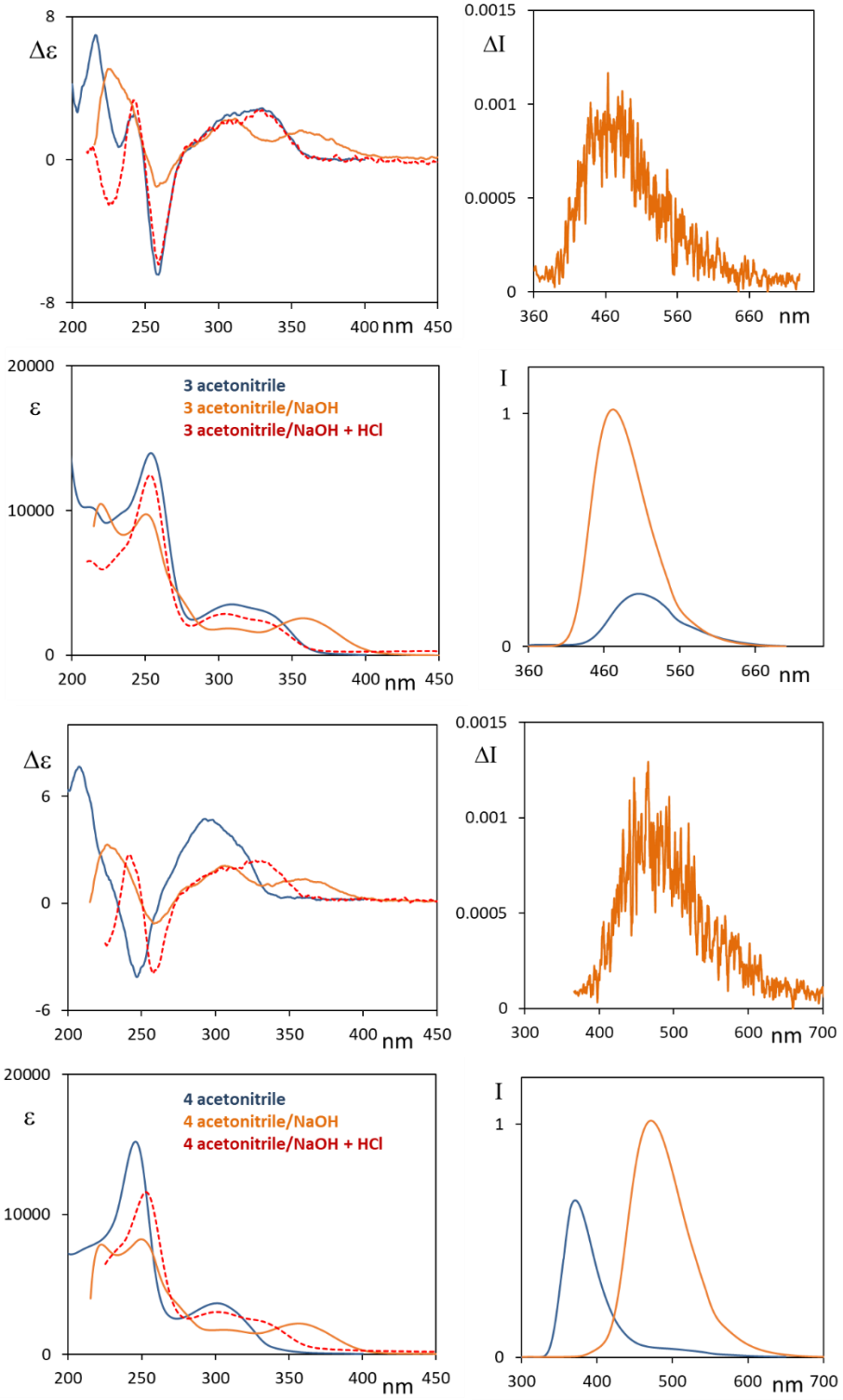
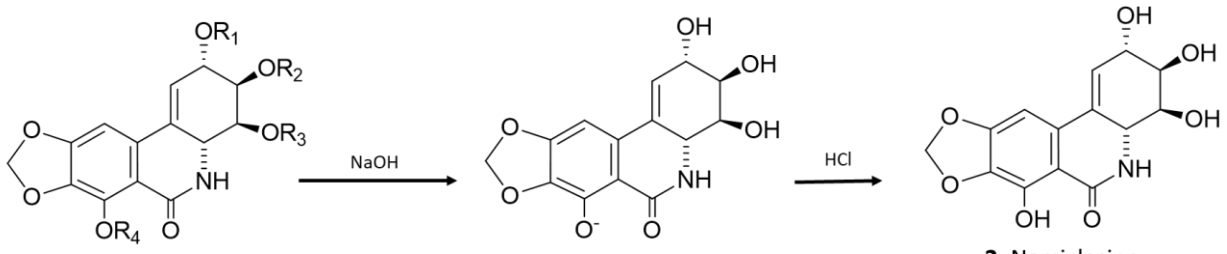



**Fig. S10**. Panels in the top two lines: triacetylnarciclasine **3**. Panels in the bottom two lines: tetraacetylnarciclasine **4**. In the left panels are reported the CD (top) and UV (bottom) spectra in different conditions: acetonitrile solution (solid blue line), NaOH-water solution (acetonitrile:water 1:10, 10mM NaOH) (solid orange line) and same solution with addition of one drop of HCl 1N. Right panels: CPL spectra in NaOH-water solution and fluorescence spectra in acetonitrile (blue) and NaOH-water solution (orange trace). Excitation wavelength for emission spectra: 290 nm for **3** and 280 nm for **4.**

## Narciclasine Derivatives Deprotonation Scheme




**2**, Narciclasine, $R_1=R_2=R_3=R_4=H$
**3**, Triacetylnarciclasine, $R_1=R_2=R_3=Ac$, $R_4=H$
**4**, Tetraacetylnarciclasine, $R_1=R_2=R_3=R_4=Ac$

**2**, Narciclasine

**Scheme S1**. Proposed deprotonation scheme of narciclasine **2**, triacetylnarciclasine **3** and tetraacetylnarciclasine **4** with addition of NaOH and (re)protonation scheme with addition of HCl.

# Lycorine DFT Parameters

**Table S2.** Relevant geometrical parameters and first electronic transition of lycorine **1** ground state conformers (see Fig. S11 for the rings numbering used in Cremer-Pople (CP) parameter definitions). Reported data: ΔE energy differences from the lowest lying conformer in kJ/mol; first transition energies (eV) and wavelengths (nm); oscillator strengths (dimensionless) and rotational strength ($10^{-40}$ $esu^2cm^2$); angle between EDTM and MDTM (°). With the exception of dioxolane ring *φ1*, the polycyclic backbone is quite rigid with the following CP parameters shared among all the conformers: q1 ≈ 0.22, Q3 ≈ 0.53, θ3 ≈ 132, ϕ3 ≈ -140, Q4 ≈ 0.55, θ4 ≈ 130, ϕ4 ≈ -68, q5 ≈ 0.40, *φ5 ≈ 0*.

| | *ΔE (kJ/mol)* | *eV* | *nm* | *f* | *R* | *E_M* | *φ1* | *τ1* | *τ2* |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.00 | 4.93 | 252 | 0.14 | -10.8 | 98 | 36 | -45 | 175 |
| 2 | 0.08 | 4.93 | 252 | 0.14 | -10.8 | 98 | -144 | -45 | 175 |
| 3 | 1.63 | 4.93 | 252 | 0.14 | -11.4 | 98 | 36 | 164 | 174 |
| 4 | 1.74 | 4.93 | 252 | 0.14 | -11.4 | 98 | -144 | 164 | 174 |
| 5 | 1.78 | 4.95 | 251 | 0.14 | -6.3 | 94 | 36 | -44 | -67 |
| 6 | 1.83 | 4.95 | 251 | 0.14 | -6.3 | 94 | -144 | -44 | -67 |

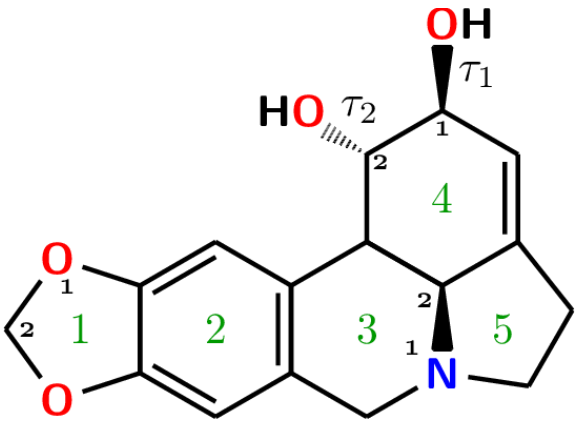



**Fig. S11.** Numbering of cycle moieties and atoms for lycorine **1** employed in Table S1.

# Narciclasine DFT Parameters

**Table S3**. Relevant geometrical parameters and first electronic transition for most populated conformers 1-8 of neutral narciclasine **2** in its ground state S0, structures marked x have too high energy values and are reported just for sake of completeness. Excited state S1 has been optimized starting from the lowest energy conformers. Reported data are: ΔE energy differences from the lowest lying conformer in kJ/mol; first transition energies (eV) and wavelengths (nm); oscillator strengths (dimensionless) and rotational strength ($10^{-40}$ $esu^2cm^2$); angle between EDTM and MDTM (°); geometrical parameters *φ1* (dioxolane envelope); *ϑ4* and *φ4* (Cremer-Pople parameters defining cyclohexene ring); *τ2, τ3* and *τ4* defining the hydroxyl orientations stemming from cyclohexene (see Fig. S12 for the rings numbering used in CP definitions).

| *S0* | *ΔE (kJ/mol)* | *eV* | *nm* | *f* | *R* | *E_M* | *φ1* | *ϑ4* | *φ4* | *τ2* | *τ3* | *τ4* |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.00 | 4.33 | 286 | 0.22 | 31.9 | 81 | -143 | 131 | -79 | -75 | 163 | 83 |
| 2 | 0.00 | 4.35 | 285 | 0.21 | 31.8 | 82 | -143 | 130 | -79 | -74 | 164 | -74 |
| 3 | 0.11 | 4.33 | 287 | 0.23 | 53.6 | 75 | 38 | 131 | -79 | -75 | 163 | 83 |
| 4 | 0.13 | 4.34 | 286 | 0.22 | 53.3 | 76 | 38 | 130 | -79 | -74 | 164 | -75 |
| 5 | 0.66 | 4.34 | 285 | 0.21 | 31.0 | 82 | -143 | 130 | -80 | 161 | 52 | -75 |
| 6 | 0.79 | 4.34 | 286 | 0.21 | 52.3 | 76 | 38 | 130 | -79 | 161 | 52 | -75 |
| 7 | 1.94 | 4.34 | 286 | 0.21 | 32.8 | 81 | -143 | 130 | -81 | 161 | 52 | 175 |
| 8 | 2.04 | 4.33 | 286 | 0.22 | 54.0 | 75 | 38 | 130 | -81 | 162 | 52 | 175 |
| x | 6.26 | 4.38 | 283 | 0.17 | 53.3 | 75 | 38 | 55 | 61 | -170 | -168 | -159 |
| x | 6.30 | 4.38 | 283 | 0.17 | 32.5 | 81 | -143 | 55 | 61 | -170 | -168 | -159 |
| *S1* | | | | | *Excited state* | | | | | | | |
| T | 0.00 | 2.72 | 456 | 0.32 | 11.6 | 87 | -152 | 132 | -77 | -76 | 163 | 86 |
| T | 0.09 | 2.72 | 455 | 0.32 | 24.5 | 84 | 35 | 132 | -77 | -76 | 163 | 86 |
| N | 19.15 | 3.33 | 372 | 0.46 | 33.9 | 82 | 37 | 132 | -72 | -76 | 162 | 86 |
| N | 19.18 | 3.33 | 372 | 0.45 | 23.9 | 84 | -155 | 132 | -72 | -76 | 161 | 86 |

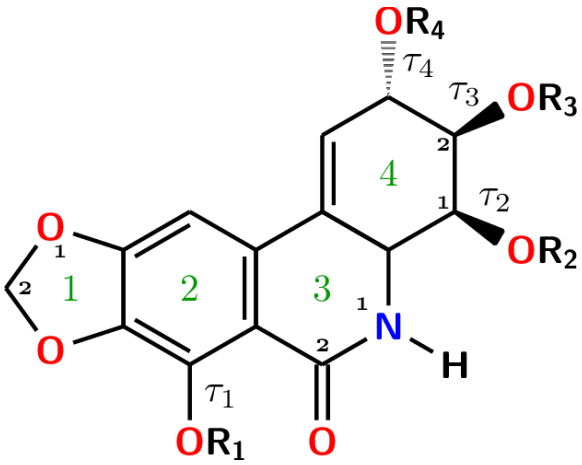



**Fig. S12.** Numbering of cycle moieties and atoms for narciclasine **2** employed in Table S2 and throughout the work.

# Simulated ECD Spectra of Narciclasine Most Populated Conformers

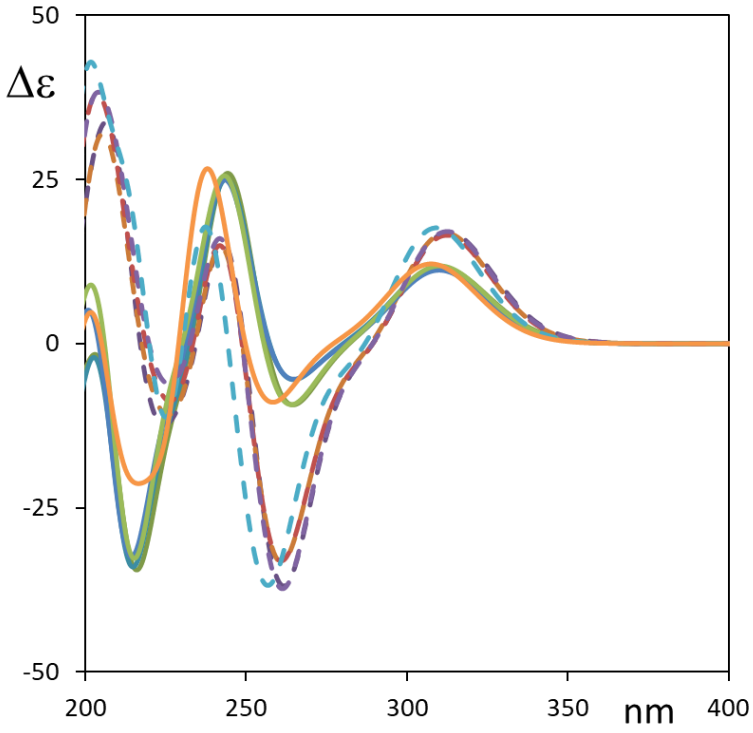



**Fig. S13.** Calculated CD spectra for the most populated conformers of narciclasine **2** in neutral form. Solid lines relative to $\varphi$1=-143°, dashed line $\varphi$1 = 38°. Populated conformers correspond to θ4 ≈130° $\varphi$4≈ -80° half chair, two spectra have been reported also for the opposite half chair (orange line and dashed light blue) for sake of comparison. All spectra have been red shifted by 25 nm for better comparison with experimental data.

# Narciclasine Derivatives' Parameters

**Table S4.** Relevant geometrical parameters and first electronic transition for most populated conformers of neutral triacetylnarciclasine **3**. Reported data are: ΔE energy differences from the lowest lying conformer in kJ/mol; first transition energies (eV) and wavelengths (nm); oscillator strengths (dimensionless) and rotational strength ($10^{-40}$ $esu^2cm^2$); angle between EDTM and MDTM (°); geometrical parameters *φ1* (dioxolane envelope); *ϑ4* and *φ4* (Cremer-Pople parameters defining cyclohexene ring); *τ2, τ3* and *τ4* defining the hydroxyl orientations stemming from cyclohexene (see Fig. S12 for the rings numbering used in CP definitions).

| | *ΔE (kJ/mol)* | *eV* | *nm* | *f* | *R* | *E_M* | *φ1* | *ϑ4* | *φ4* | *τ2* | *τ3* | *τ4* |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.00 | 4.32 | 287 | 0.24 | 33.5 | 84 | -143 | 129 | -79 | 166 | 93 | -80 |
| 2 | 0.14 | 4.32 | 287 | 0.24 | 56.6 | 80 | 38 | 129 | -79 | 166 | 93 | -80 |
| 3 | 1.18 | 4.31 | 288 | 0.23 | 37.8 | 83 | -143 | 130 | -82 | 166 | 93 | -161 |
| 4 | 1.30 | 4.31 | 288 | 0.24 | 59.8 | 78 | 38 | 130 | -82 | 166 | 93 | -161 |

**Table S5.** Relevant geometrical parameters and first electronic transition for most populated conformers of neutral tetraacetylmarciclasine **4**. Reported data are: ΔE energy differences from the lowest lying conformer in kJ/mol; first transition energies (eV) and wavelengths (nm); oscillator strengths (dimensionless) and rotational strength ($10^{-40}$ $esu^2cm^2$); angle between EDTM and MDTM (°); geometrical parameters *φ1* (dioxolane envelope); *ϑ4* and *φ4* (Cremer-Pople parameters defining cyclohexene ring); *τ2, τ3* and *τ4* defining the hydroxyl orientations stemming from cyclohexene (see Fig. S12 for the rings numbering used in CP definitions).

| | *ΔE (kJ/mol)* | *eV* | *nm* | *f* | *R* | *E_M* | *φ1* | *ϑ4* | *φ4* | *T1* | *τ2* | *τ3* | *τ4* |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.00 | 4.5 | 275 | 0.23 | 47.4 | 83 | -144 | 128 | -81 | 101 | 166 | 93 | -80 |
| 2 | 0.43 | 4.49 | 276 | 0.23 | 59.9 | 81 | 37 | 128 | -80 | 103 | 166 | 93 | -80 |
| 3 | 0.52 | 4.47 | 277 | 0.22 | 53.2 | 82 | -144 | 128 | -80 | -117 | 166 | 93 | -81 |
| 4 | 1.03 | 4.47 | 278 | 0.22 | 68 | 81 | 37 | 128 | -80 | -116 | 166 | 93 | -80 |
| 5 | 1.61 | 4.47 | 277 | 0.22 | 63.4 | 80 | -144 | 129 | -83 | -117 | 165 | 93 | -161 |
| 6 | 2.13 | 4.47 | 278 | 0.23 | 77.6 | 78 | 37 | 129 | -83 | -116 | 166 | 93 | -161 |

## Narciclasine Frontier Orbitals

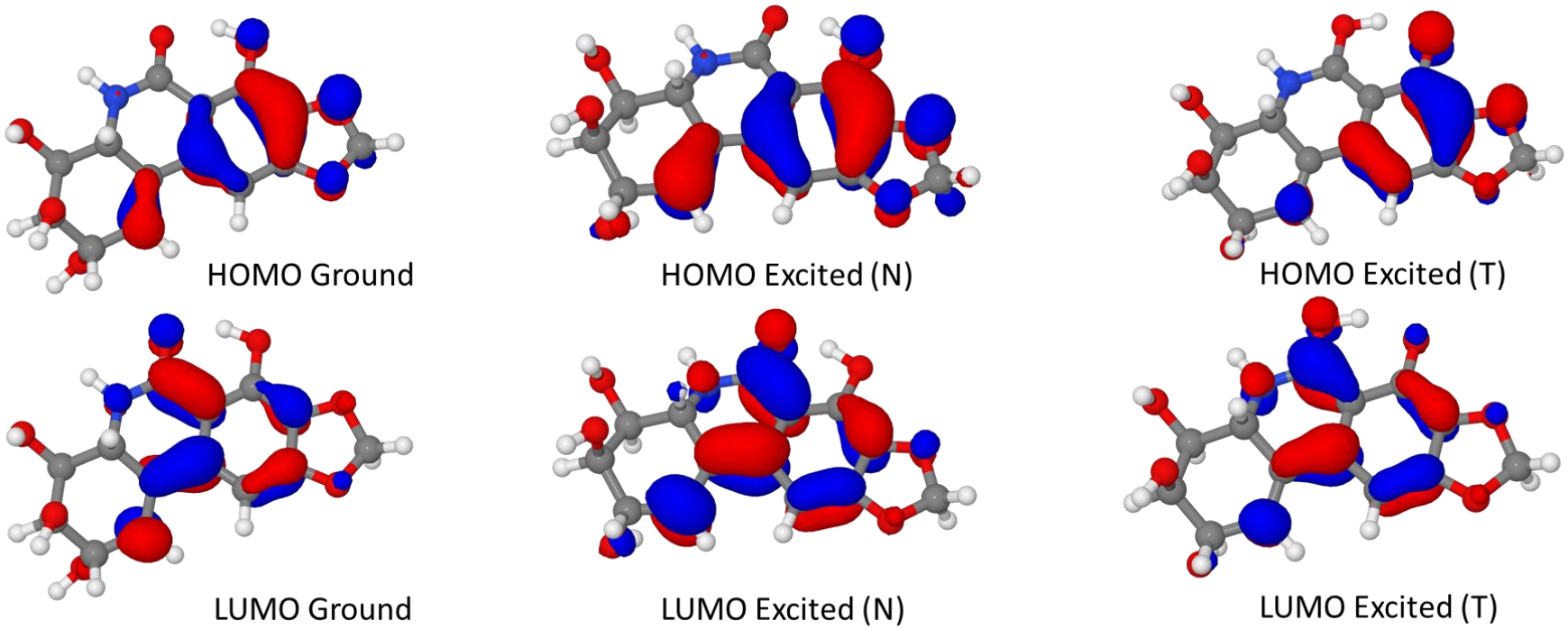



**Fig. S14**. Molecular orbitals representation for narciclasine **2** for ground (left), N form excited (middle) and T form (right) excited states.

# Experimental and Simulated Spectra of Lycorine

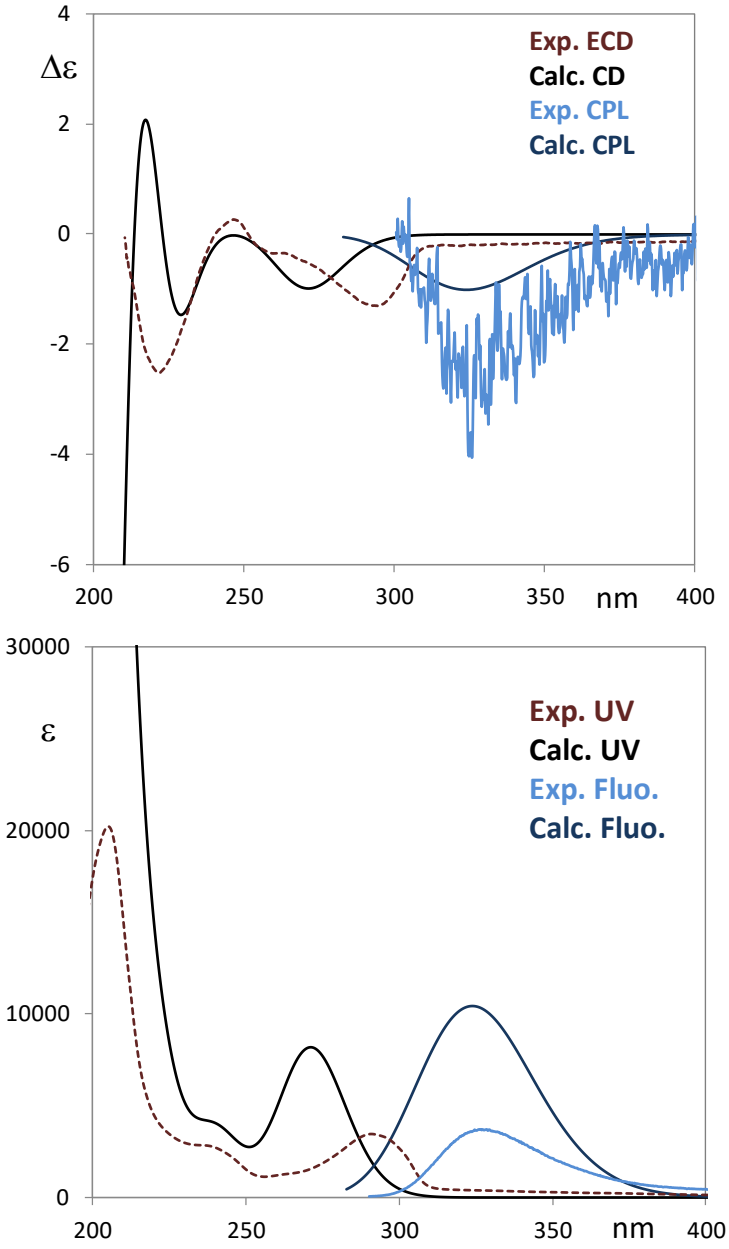



**Fig. S15.** Comparison of experimental and calculated CD and CPL (upper panel) and absorption and fluorescence (lower panel) spectra for lycorine **1**. Calculated spectra were red shifted by 25 nm. For better comparison, calculated CD spectrum has been divided by 4.

# Template DFT Parameters

**Table S6.** Relevant geometrical parameters and first electronic transition for the model compound of Figure 7 (see text). In the ground state S0: neutral condition presents only form N, for charged species three stable tautomeric forms are possible. Only *φ1* (dioxolane envelope) is necessary to distinguish two possible conformations. Analogously first excited state S1 is reported in all possible forms. Reported data are: ΔE energy differences from the lowest lying form in kJ/mol; first transition energy (eV) and wavelengths (nm); oscillator strengths (dimensionless) and rotational strength ($10^{-40}$ $esu^2cm^2$); sign is reported for *φ1* coordinate (dioxolane envelope).

| S0 | *φ1* | nm | *ΔE (KJ/mol)* | *f* | *R* |
|---|---|---|---|---|---|
| N | - | 281 | 0.00 | 0.16 | 31.8 |
| N | + | 281 | 0.04 | 0.16 | 51.0 |
| N(-1) | - | 277 | 7.66 | 0.04 | 7.3 |
| N(-1) | + | 280 | 7.58 | 0.08 | 22.8 |
| T(-1) | - | 299 | 1.55 | 0.17 | -15.9 |
| T(-1) | + | 304 | 1.38 | 0.29 | -5.0 |
| NH(-1) | - | 327 | 0.00 | 0.2 | 6.3 |
| NH(-1) | + | 333 | 1.34 | 0.3 | 22.1 |
| | **Excited state** | | | | |
| S1 | *φ1* | nm | *ΔE (KJ/mol)* | *f* | *R* |
| N | + | 370 | 20.80 | 0.39 | 27.1 |
| N | - | 371 | 20.72 | 0.39 | 19.9 |
| T | + | 451 | 0.21 | 0.27 | 26.7 |
| T | - | 452 | 0.00 | 0.27 | 14.2 |
| T(-1) | + | 376 | 35.12 | 0.35 | 23.2 |
| T(-1) | - | 377 | 35.37 | 0.35 | 7.8 |
| NH(-1) | - | 414 | 0.00 | 0.31 | 25.1 |
| NH(-1) | + | 419 | 0.08 | 0.31 | 38.9 |
| N(-1) | + | 576 | 27.00 | 0.02 | -41.5 |
| N(-1) | - | 579 | 26.54 | 0.02 | -40.5 |

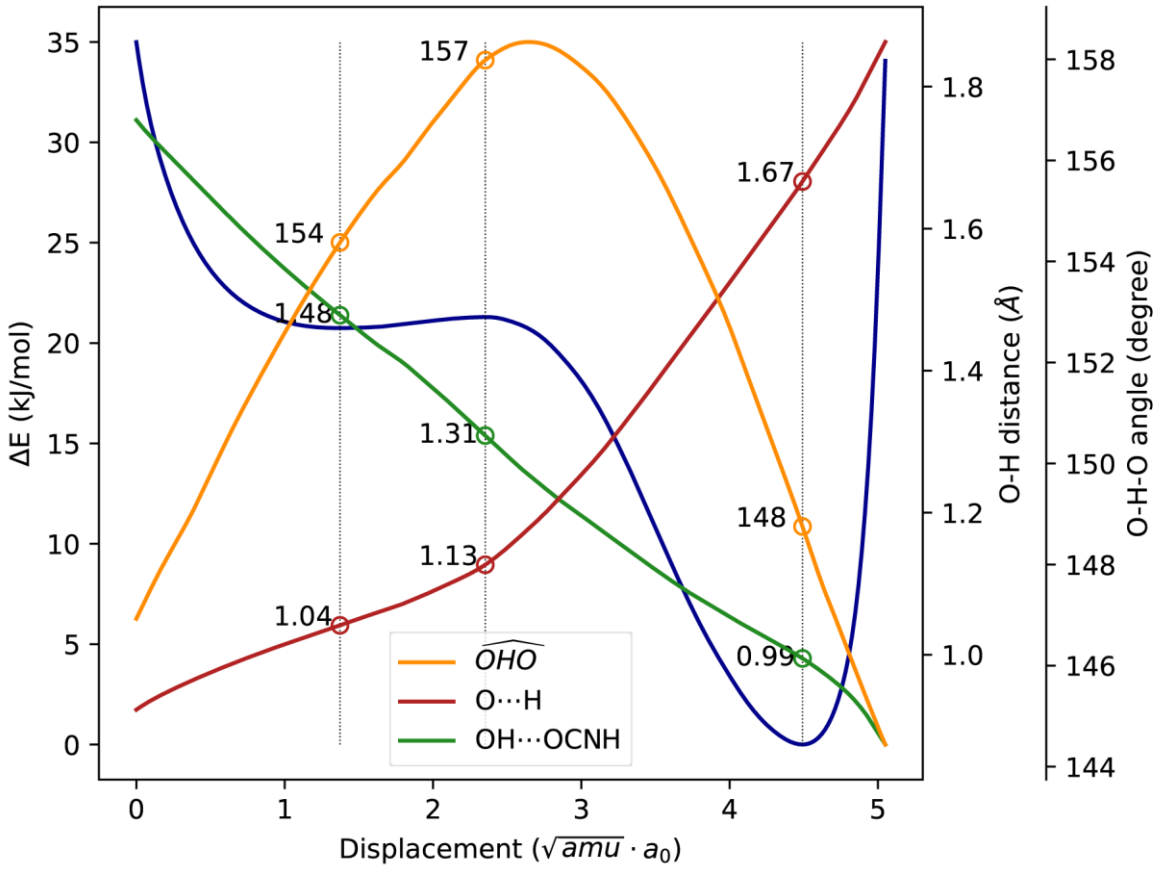



**Fig. S16.** Calculated plots of energy (kJ/mol), C=O····H hydrogen bond distance (Å), OH····OCNH distance (Å), and of OHO angle (degree) as function of the IRC coordinate for the template molecule of Figure 7 (see text)

# Anionic Narciclasine DFT Parameters

**Table S7**. Relevant geometrical parameters and first electronic transition for anionic narciclasine **2** in the ground state S0 in T(-1), NH(-1) and N(-1) forms (see text). Reported data are: ΔE energy differences from the lowest lying form in kJ/mol; first transition energies (eV) and wavelengths (nm); oscillator strengths (dimensionless) and rotational strength ($10^{-40}$ $esu^2cm^2$); angle between EDTM and MDTM (°); geometrical parameters *φ1* (dioxolane envelope); *ϑ4* and *φ4* (Cremer-Pople parameters defining cyclohexene ring); *τ2, τ3* and *τ4* defining the hydroxyl orientations stemming from cyclohexene (see Fig. S12 for the rings numbering used in CP definitions).

| Anion S0 | *ΔE (kJ/mol)* | *eV* | *nm* | *f* | *R* | *E_M* | *φ1* | *ϑ4* | *φ4* | *τ2* | *τ3* | *τ4* |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| T(-1) | 0.00 | 4.15 | 299 | 0.20 | -4.9 | 97 | 39 | 52 | 67 | -170 | -168 | -162 |
| T(-1) | 0.35 | 4.15 | 299 | 0.20 | -19.1 | 108 | -143 | 52 | 67 | -170 | -168 | -162 |
| NH(-1) | 1.19 | 3.68 | 337 | 0.23 | 2.7 | 88 | -141 | 129 | -85 | -73 | 164 | -111 |
| NH(-1) | 2.33 | 3.68 | 337 | 0.23 | 17.1 | 74 | 38 | 129 | -86 | -73 | 164 | -111 |
| NH(-1) | 3.50 | 3.78 | 328 | 0.24 | 9.2 | 85 | -141 | 53 | 62 | -169 | -167 | -162 |
| T(-1) | 3.95 | 4.07 | 305 | 0.19 | -6.8 | 110 | -143 | 130 | -91 | -73 | 164 | 84 |
| T(-1) | 4.07 | 4.07 | 305 | 0.19 | -19.7 | 128 | -143 | 130 | -91 | -73 | 164 | 84 |
| NH(-1) | 4.38 | 3.80 | 326 | 0.24 | 21.9 | 77 | 39 | 53 | 63 | -169 | -167 | -162 |
| N(-1) | 4.50 | 4.52 | 274 | 0.03 | -7.9 | 96 | 39 | 52 | 68 | -171 | -168 | -162 |
| N(-1) | 4.71 | 4.53 | 274 | 0.03 | -8.1 | 96 | -144 | 52 | 68 | -171 | -168 | -162 |
| N(-1) | 9.60 | 4.35 | 285 | 0.03 | 28.9 | 72 | 38 | 130 | -93 | -73 | 164 | 84 |
| N(-1) | 9.65 | 4.36 | 284 | 0.03 | 32.6 | 70 | -144 | 130 | -93 | -73 | 164 | 84 |

**Table S8.** Relevant geometrical parameters and first electronic transition for anionic narciclasine **2** in the excited state S1 in T(-1), NH(-1) and N(-1) forms (see text). Reported data are: ΔE energy differences from the lowest lying form in kJ/mol; transition energies (eV) and wavelengths (nm); oscillator strengths (dimensionless) and rotational strength ($10^{-40}$ $esu^2cm^2$); angle between EDTM and MDTM (°); geometrical parameters *φ1* (dioxolane envelope); *ϑ4* and *φ4* (Cremer-Pople parameters defining cyclohexene ring); *τ2, τ3* and *τ4* defining the hydroxyl orientations stemming from cyclohexene.

| Anion S1 | *ΔE (kJ/mol)* | *eV* | *nm* | *f* | *R* | *E_M* | *φ1* | *ϑ4* | *φ4* | *τ2* | *τ3* | *τ4* |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| NH(-1) | 0.00 | 2.91 | 427 | 0.34 | 19.9 | 73 | -138 | 133 | -83 | -73 | 166 | 98 |
| NH(-1) | 0.39 | 2.88 | 430 | 0.35 | 30.0 | 69 | 30 | 133 | -82 | -73 | 166 | 98 |
| NH(-1) | 12.21 | 2.98 | 416 | 0.34 | 35.1 | 71 | -138 | 58 | 60 | -168 | -165 | -164 |
| NH(-1) | 12.40 | 2.95 | 420 | 0.34 | 49.8 | 60 | 29 | 58 | 60 | -168 | -165 | -164 |
| | | | | | | | | | | | | |
| N(-1) | 29.24 | 2.15 | 577 | 0.01 | -32.6 | 110 | -143 | 126 | -90 | -74 | 167 | 98 |
| N(-1) | 29.57 | 2.16 | 574 | 0.01 | -32.5 | 110 | 39 | 126 | -90 | -74 | 167 | 98 |
| N(-1) | 37.02 | 2.23 | 556 | 0.03 | -57.0 | 115 | -143 | 53 | 60 | -169 | -165 | -166 |
| N(-1) | 37.50 | 2.25 | 552 | 0.03 | -58.7 | 115 | 39 | 53 | 60 | -169 | -165 | -166 |
| | | | | | | | | | | | | |
| T(-1) | 37.73 | 3.21 | 386 | 0.39 | 15.7 | 47 | 36 | 133 | -90 | -72 | 166 | 95 |
| T(-1) | 38.02 | 3.21 | 386 | 0.38 | 1.9 | 87 | -145 | 133 | -89 | -72 | 166 | 95 |
| T(-1) | 41.84 | 3.30 | 376 | 0.38 | 23.8 | 60 | 35 | 56 | 64 | -169 | -166 | -164 |
| T(-1) | 42.21 | 3.30 | 376 | 0.38 | 4.4 | 87 | -146 | 57 | 64 | -169 | -166 | -164 |

# Simulated Spectra of Anionic Narciclasine

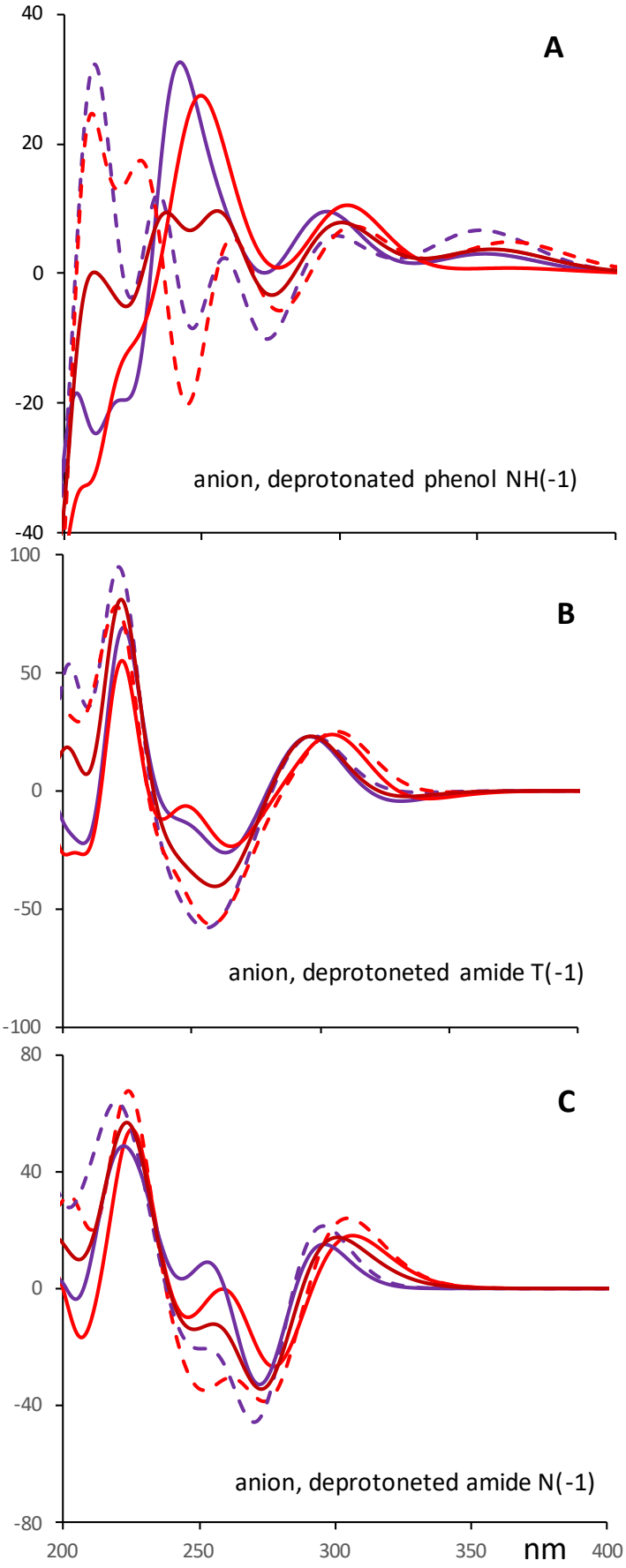



**Fig. S17**. Calculated CD spectra for narciclasine **2** in various charged states and different backbone conformational states. Full lines are relative to $\varphi 1 \approx -143°$, dashed lines to $\varphi 1 \approx 40°$ (dioxolane envelopes). Red lines: $\theta 4 \approx 130°$, $\varphi 4 \approx -85°$, purple lines: $\theta 4 \approx 52°$, $\varphi 4 \approx 67°$ referred to cyclohexene half chair conformation. Brown line represents the arithmetic average of the spectra generated in the four possible polycyclic backbone conformers. All spectra have been red shifted by 25 nm for better comparison with experimental data. Top panel (A): anion, deprotonated phenol NH(-1). Middle panel (B): anion, deprotonated amide tautomer T(-1). Bottom panel (C): anion, deprotonated amide normal N(-1).

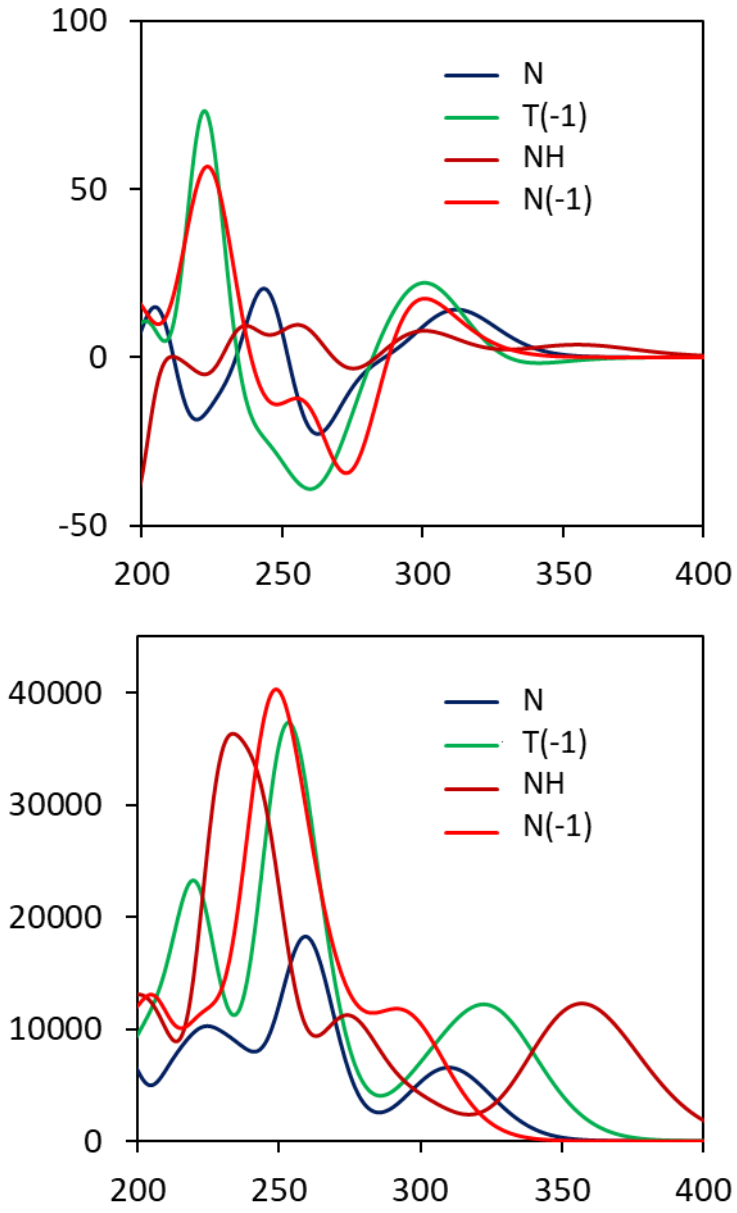



**Fig. S18.** Calculated average CD (Top) and UV (Bottom) spectra for narciclasine **2** in various charged states. (See text for discussion).

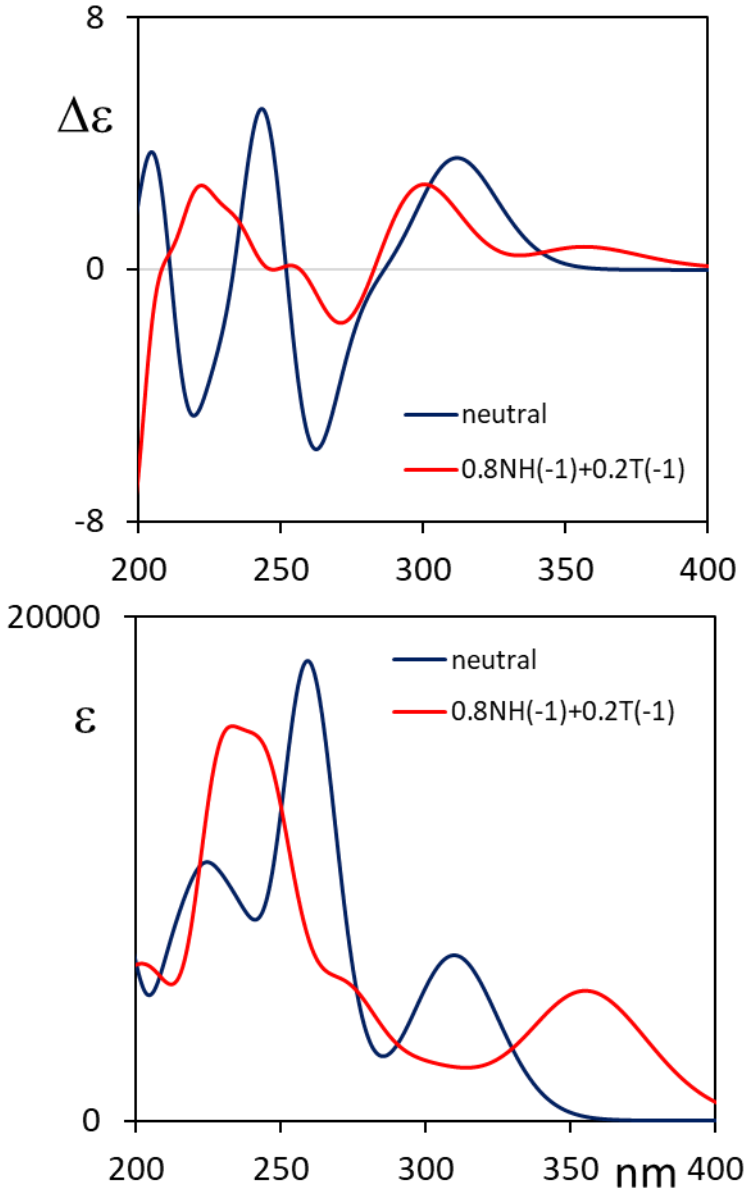



**Fig. S19.** Calculated CD (Top) and absorption (Lower) spectra for narciclasine **2** in the neutral form (blue line) and in anionic form with contributions from both the deprotonated phenol species and from the deprotonated amide in tautomeric form. For sake of comparison with experimental data both calculated ECD spectra have been divided by four and calculated absorption spectra by two. All calculated spectra have been red shifted by 25 nm. The percentage of contribution of the two species is chosen ad hoc to reproduce the experimental data of Figure 5 in the text.

# Geometries in XYZ format

## Lycorine

### Ground State

```
38
Energy:   -975.49504555
H                 -1.387255      -2.161054      -0.293301
C                 -1.637227      -1.112385      -0.197499
C                 -2.337934       1.616406       0.039965
C                 -0.641510      -0.118328      -0.167996
C                 -2.943017      -0.709602      -0.107884
C                 -3.286708       0.629831       0.008004
C                 -0.988537       1.233769      -0.052172
H                 -2.616221       2.658588       0.135597
O                 -4.080727      -1.472693      -0.066349
O                 -4.647711       0.737695       0.125252
C                 -5.142894      -0.541243      -0.271500
H                 -5.396381      -0.514086      -1.334974
H                 -5.991059      -0.812382       0.348378
C                  0.048893       2.346409       0.026402
H                 -0.265166       3.183789      -0.599824
H                  0.079440       2.711817       1.068872
N                  1.362935       1.887062      -0.384723
C                  0.820951      -0.490996      -0.307309
H                  1.062167      -0.559545      -1.375485
C                  1.649072       0.624577       0.271575
H                  1.440457       0.705499       1.355579
C                  3.114184       0.432001       0.072674
C                  3.639044      -0.784834       0.007843
H                  4.699661      -0.943296      -0.160812
C                  2.787595      -2.033870       0.059059
H                  3.144067      -2.704664       0.843543
C                  1.288093      -1.794611       0.340511
H                  0.759788      -2.654482      -0.081161
O                  2.949237      -2.765379      -1.157735
H                  2.906127      -2.141555      -1.891904
O                  1.127662      -1.770051       1.753762
H                  0.210985      -1.543205       1.953250
C                  2.489952       2.743136      -0.002631
H                  2.552597       3.620926      -0.644632
H                  2.378090       3.081839       1.039409
C                  3.714390       1.809473      -0.121440
H                  4.167897       1.881709      -1.110959
H                  4.480496       2.045691       0.616448
```

38
Energy:  -975.49501309
H -1.388208 -2.157429 -0.293430
C -1.635984 -1.110654 -0.174138
C -2.333984 1.617063 0.082242
C -0.639882 -0.117049 -0.148609
C -2.940121 -0.709237 -0.056225
C -3.282394 0.629718 0.068808
C -0.985562 1.234576 -0.023146
H -2.612028 2.660079 0.169230
O -4.082456 -1.465278 -0.096038
O -4.647265 0.744311 0.111296
C -5.109969 -0.583804 0.356760
H -6.019426 -0.763582 -0.206944
H -5.253199 -0.721072 1.432249
C 0.053039 2.345894 0.056440
H -0.265863 3.188170 -0.560858
H 0.092496 2.703453 1.101303
N 1.363440 1.888668 -0.368455
C 0.821550 -0.489740 -0.299431
H 1.054637 -0.553458 -1.369738
C 1.654435 0.622611 0.278759
H 1.454104 0.697890 1.364763
C 3.117885 0.430671 0.067586
C 3.641796 -0.786020 -0.006781
H 4.701030 -0.944059 -0.184323
C 2.790421 -2.035024 0.045523
H 3.152297 -2.708880 0.824900
C 1.292896 -1.796655 0.338541
H 0.761317 -2.654158 -0.083812
O 2.943538 -2.762042 -1.175069
H 2.893611 -2.135895 -1.906841
O 1.141770 -1.779302 1.752970
H 0.226394 -1.553296 1.959298
C 2.493851 2.742298 0.008943
H 2.551689 3.623406 -0.628936
H 2.390615 3.075575 1.053623
C 3.716967 1.808873 -0.124600
H 4.162448 1.885990 -1.117388
H 4.489150 2.041114 0.608204

38
Energy:  -975.49442505
H  -1.382167  -2.157585  -0.296396
C  -1.633206  -1.109360  -0.198707
C  -2.339094  1.617285  0.042890
C  -0.638663  -0.114023  -0.167425
C  -2.939814  -0.709260  -0.108966
C  -3.286174  0.629159  0.009200
C  -0.988954  1.237249  -0.049421
H  -2.619196  2.658877  0.139760
O  -4.076219  -1.474751  -0.069127
O  -4.647643  0.734097  0.126291
C  -5.139761  -0.544829  -0.273991
H  -5.391548  -0.515900  -1.337852
H  -5.988456  -0.818913  0.343869
C  0.046343  2.351815  0.029364
H  -0.271040  3.189956  -0.594238
H  0.079061  2.715151  1.072621
N  1.359324  1.895135  -0.386513
C  0.824403  -0.484224  -0.306924
H  1.072826  -0.563678  -1.371576
C  1.651098  0.633579  0.269561
H  1.446967  0.716143  1.354416
C  3.114699  0.443256  0.058520
C  3.637155  -0.771954  -0.025268
H  4.693523  -0.931467  -0.215199
C  2.792692  -2.021431  0.056968
H  3.164539  -2.665167  0.861565
C  1.293360  -1.784452  0.343772
H  0.755699  -2.642213  -0.074432
O  2.954057  -2.684735  -1.198050
H  2.651246  -3.595034  -1.104513
O  1.135482  -1.762689  1.756963
H  0.222664  -1.522228  1.958437
C  2.486638  2.753511  -0.011347
H  2.543774  3.631120  -0.654220
H  2.379808  3.092855  1.031140
C  3.712444  1.822036  -0.136335
H  4.162426  1.897012  -1.127216
H  4.480200  2.059609  0.599476

38
Energy: -975.49438109

| | | | |
|---|---|---|---|
| H | -1.379008 | -2.160694 | -0.275682 |
| C | -1.628906 | -1.114642 | -0.154651 |
| C | -2.335244 | 1.610072 | 0.105788 |
| C | -0.635517 | -0.118045 | -0.134433 |
| C | -2.933869 | -0.717974 | -0.029844 |
| C | -3.280371 | 0.619546 | 0.097348 |
| C | -0.986050 | 1.232324 | -0.006729 |
| H | -2.616365 | 2.652167 | 0.194048 |
| O | -4.073783 | -1.478303 | -0.063871 |
| O | -4.645605 | 0.729205 | 0.146901 |
| C | -5.102054 | -0.600610 | 0.394480 |
| H | -6.013856 | -0.783619 | -0.164400 |
| H | -5.239094 | -0.738598 | 1.470714 |
| C | 0.048887 | 2.347469 | 0.065875 |
| H | -0.278100 | 3.189051 | -0.548208 |
| H | 0.095545 | 2.704520 | 1.110744 |
| N | 1.356624 | 1.894616 | -0.370165 |
| C | 0.826312 | -0.485959 | -0.293098 |
| H | 1.060870 | -0.561528 | -1.361225 |
| C | 1.658952 | 0.630831 | 0.276750 |
| H | 1.468911 | 0.708742 | 1.364536 |
| C | 3.119900 | 0.443524 | 0.045705 |
| C | 3.642916 | -0.770625 | -0.049089 |
| H | 4.696914 | -0.927943 | -0.253434 |
| C | 2.801362 | -2.021596 | 0.039871 |
| H | 3.184511 | -2.667348 | 0.837523 |
| C | 1.305402 | -1.787893 | 0.346637 |
| H | 0.763641 | -2.644798 | -0.068020 |
| O | 2.947704 | -2.680506 | -1.219316 |
| H | 2.646770 | -3.591353 | -1.125182 |
| O | 1.164976 | -1.771938 | 1.761793 |
| H | 0.254135 | -1.534176 | 1.975100 |
| C | 2.487742 | 2.753054 | -0.006893 |
| H | 2.535048 | 3.633230 | -0.647030 |
| H | 2.394577 | 3.088175 | 1.038268 |
| C | 3.713054 | 1.823840 | -0.151993 |
| H | 4.149645 | 1.903288 | -1.148493 |
| H | 4.490292 | 2.059654 | 0.574377 |

38
Energy:  -975.49436721
H  -1.382526  -2.158989  -0.348200
C  -1.634651  -1.108960  -0.283296
C  -2.337192  1.622856  -0.097211
C  -0.638533  -0.118695  -0.219555
C  -2.941216  -0.701839  -0.254326
C  -3.286689  0.639253  -0.163479
C  -0.985972  1.234536  -0.129562
H  -2.615263  2.666621  -0.019610
O  -4.083270  -1.462227  -0.253364
O  -4.652348  0.750484  -0.104450
C  -5.130835  -0.529750  -0.516164
H  -5.332107  -0.508824  -1.591119
H  -6.009363  -0.794366  0.062969
C  0.050730  2.343893  -0.010865
H  -0.238440  3.184890  -0.644300
H  0.047599  2.705666  1.033394
N  1.376413  1.882507  -0.379288
C  0.826227  -0.493673  -0.308613
H  1.097939  -0.559251  -1.369554
C  1.644052  0.621151  0.288376
H  1.412030  0.703228  1.366748
C  3.113338  0.428554  0.115113
C  3.640624  -0.786328  0.032069
H  4.703649  -0.938877  -0.127026
C  2.786795  -2.034197  0.043273
H  3.154725  -2.733410  0.799291
C  1.285854  -1.793447  0.341792
H  0.749643  -2.652350  -0.071393
O  2.936312  -2.728312  -1.197024
H  2.907197  -2.079921  -1.910247
O  1.051611  -1.687686  1.739371
H  1.217354  -2.544830  2.146133
C  2.490894  2.740084  0.033606
H  2.571063  3.616910  -0.607849
H  2.348683  3.080689  1.071343
C  3.719355  1.807470  -0.048466
H  4.209670  1.886658  -1.019620
H  4.457468  2.038264  0.719223

38
Energy:  -975.49434781
H  -1.390505  -2.156396  -0.331581
C  -1.641583  -1.107967  -0.241538
C  -2.342262  1.622630  -0.032158
C  -0.645004  -0.117837  -0.185757
C  -2.947531  -0.702468  -0.177917
C  -3.291938  0.638036  -0.075994
C  -0.991496  1.234905  -0.084859
H  -2.619757  2.667070  0.038180
O  -4.090886  -1.456966  -0.254135
O  -4.658559  0.754896  -0.086202
C  -5.130055  -0.570010  0.157861
H  -6.022301  -0.754304  -0.431420
H  -5.306521  -0.696337  1.229937
C  0.046455  2.343475  0.028567
H  -0.252108  3.189037  -0.594501
H  0.058571  2.697601  1.075310
N  1.366803  1.884758  -0.362024
C  0.818752  -0.492338  -0.293736
H  1.076351  -0.554899  -1.358421
C  1.644257  0.620440  0.296130
H  1.427120  0.697994  1.377930
C  3.111006  0.429047  0.101999
C  3.637459  -0.785400  0.007892
H  4.698293  -0.937116  -0.165938
C  2.784279  -2.033661  0.027616
H  3.162328  -2.734125  0.777485
C  1.287234  -1.794034  0.346596
H  0.745505  -2.651677  -0.061941
O  2.917847  -2.725542  -1.215650
H  2.877374  -2.076328  -1.927573
O  1.071683  -1.692834  1.747548
H  1.241947  -2.551646  2.148913
C  2.486929  2.740677  0.039107
H  2.557844  3.620553  -0.599244
H  2.359392  3.076294  1.080359
C  3.714238  1.808796  -0.064798
H  4.190182  1.892140  -1.042735
H  4.463545  2.036663  0.692856

# Neutral narciclasine

## Ground State

```
35
Energy:  -1122.61724232
C                -3.263132      -0.048792      -0.061188
C                -2.488179       1.081187       0.091738
C                -1.085279       0.888391       0.075940
C                -0.523604      -0.393516      -0.068661
C                -1.338881      -1.514911      -0.240902
C                -2.698075      -1.298870      -0.224267
C                -0.226355       2.079099       0.239319
C                 0.947294      -0.527013      -0.011097
C                 1.733709       0.700358      -0.395744
N                 1.094162       1.909675       0.103151
C                 3.161873       0.662516       0.142953
H                 3.129297       0.761759       1.230281
C                 3.815107      -0.654189      -0.226089
C                 3.052974      -1.831814       0.390662
C                 1.562474      -1.662166       0.326035
O                -0.707546       3.196039       0.495038
O                -4.625747      -0.136425      -0.151786
O                -3.073634       2.277101       0.236121
H                -0.933192      -2.502938      -0.399375
O                -3.692192      -2.211318      -0.411036
H                 1.660806       2.749419       0.115829
H                 0.982784      -2.531574       0.615141
O                 3.475814      -2.063068       1.731901
H                 4.839192      -0.667890       0.155149
H                -2.337549       2.925202       0.380197
C                -4.891982      -1.532385      -0.024133
H                -5.109754      -1.766151       1.021096
H                -5.699895      -1.813465      -0.690933
O                 3.803411      -0.703826      -1.646428
H                 4.426396      -1.372839      -1.949238
O                 3.895361       1.769904      -0.340204
H                 4.111075       1.585423      -1.265066
H                 1.785254       0.748426      -1.490809
H                 3.337272      -2.733340      -0.158060
H                 2.997780      -1.464368       2.317490
```

35
Energy:  -1122.61724314
C                 -3.265778      -0.054512      -0.059796
C                 -2.493329       1.077052       0.093209
C                 -1.089991       0.887285       0.078236
C                 -0.525599      -0.393564      -0.064259
C                 -1.338242      -1.516937      -0.235871
C                 -2.697944      -1.303678      -0.220469
C                 -0.233100       2.079249       0.244640
C                  0.945501      -0.522572      -0.005490
C                  1.727426       0.705060      -0.396583
N                  1.087570       1.912329       0.108381
C                  3.157235       0.666065       0.135773
H                  3.131860       0.747591       1.223628
C                  3.807656      -0.648353      -0.242789
C                  3.053706      -1.818825       0.397231
C                  1.563854      -1.649257       0.347838
O                 -0.716828       3.194829       0.502890
O                 -4.628603      -0.145308      -0.152081
O                 -3.080926       2.272302       0.236646
H                 -0.929209      -2.504069      -0.391760
O                 -3.690265      -2.218544      -0.407083
H                  1.653642       2.752299       0.125825
H                  0.988278      -2.515717       0.652461
O                  3.410611      -1.952521       1.769967
H                  4.839950      -0.650404       0.119939
H                 -2.345757       2.920891       0.383541
C                 -4.891434      -1.541443      -0.021256
H                 -5.108273      -1.773584       1.024574
H                 -5.698968      -1.825963      -0.687091
O                  3.777230      -0.707953      -1.661757
H                  4.387023      -1.387247      -1.968540
O                  3.888170       1.777256      -0.345137
H                  4.086811       1.606780      -1.276286
H                  1.771543       0.756177      -1.491894
H                  3.321124      -2.732111      -0.146966
H                  4.294108      -2.334852       1.823867

35
Energy:  -1122.61720181
C                 -3.262427      -0.044753      -0.108536
C                 -2.488362       1.081608       0.072235
C                 -1.085309       0.888090       0.065237
C                 -0.523189      -0.393820      -0.076827
C                 -1.337859      -1.514093      -0.258853
C                 -2.696824      -1.294903      -0.267344
C                 -0.227218       2.078082       0.237804
C                  0.948114      -0.526585      -0.017571
C                  1.734441       0.702239      -0.397873
N                  1.093534       1.909709       0.103722
C                  3.161708       0.664015       0.143330
H                  3.126846       0.760823       1.230847
C                  3.816641      -0.651466      -0.227038
C                  3.053912      -1.831008       0.385356
C                  1.563373      -1.661986       0.318222
O                 -0.709210       3.193074       0.500913
O                 -4.627244      -0.145310      -0.110473
O                 -3.074307       2.273051       0.246662
H                 -0.932606      -2.503656      -0.408001
O                 -3.691351      -2.216654      -0.395483
H                  1.660852       2.748784       0.125493
H                  0.983741      -2.532939       0.602755
O                  3.474656      -2.066190       1.726485
H                  4.839775      -0.665183       0.156790
H                 -2.337703       2.918687       0.400314
C                 -4.878086      -1.450574      -0.629804
H                 -5.711160      -1.900924      -0.100989
H                 -5.051115      -1.385381      -1.706929
O                  3.808507      -0.698114      -1.647450
H                  4.431697      -1.367109      -1.949956
O                  3.895418       1.772923      -0.335820
H                  4.113378       1.590698      -1.260607
H                  1.787770       0.753219      -1.492709
H                  3.339490      -2.730789      -0.165578
H                  2.998592      -1.466594       2.312766

35
Energy:  -1122.61719371
C                 -3.264882      -0.049513      -0.110210
C                 -2.493279       1.078397       0.070961
C                 -1.089782       0.887752       0.064975
C                 -0.525067      -0.393086      -0.075598
C                 -1.337153      -1.515196      -0.257627
C                 -2.696613      -1.298702      -0.267267
C                 -0.233550       2.078803       0.241041
C                  0.946392      -0.521642      -0.014292
C                  1.729127       0.707457      -0.399252
N                  1.087339       1.912885       0.107520
C                  3.157141       0.667555       0.138134
H                  3.127621       0.746014       1.226147
C                  3.809839      -0.645467      -0.241427
C                  3.053854      -1.818250       0.391794
C                  1.564086      -1.649147       0.337195
O                 -0.718029       3.192507       0.506573
O                 -4.629956      -0.153205      -0.112863
O                 -3.081343       2.269045       0.244945
H                 -0.928680      -2.503780      -0.404957
O                 -3.689447      -2.222640      -0.395576
H                  1.654150       2.752071       0.134852
H                  0.987938      -2.517289       0.635917
O                  3.405449      -1.956662       1.765324
H                  4.840616      -0.647823       0.125766
H                 -2.345509       2.915101       0.401539
C                 -4.876907      -1.458666      -0.632918
H                 -5.710654      -1.910672      -0.106558
H                 -5.047062      -1.393814      -1.710588
O                  3.785741      -0.701102      -1.660648
H                  4.395213      -1.381194      -1.966380
O                  3.889241       1.780444      -0.336914
H                  4.091683       1.612646      -1.267740
H                  1.777048       0.761799      -1.494226
H                  3.323631      -2.729416      -0.154780
H                  4.288017      -2.340754       1.821416

35
Energy:  -1122.61699345
C                 -3.264735      -0.050109      -0.055893
C                 -2.490527       1.080174       0.097245
C                 -1.087405       0.888565       0.079098
C                 -0.524884      -0.392637      -0.067372
C                 -1.339354      -1.514506      -0.239865
C                 -2.698751      -1.299596      -0.220678
C                 -0.228627       2.078752       0.244876
C                  0.945906      -0.524970      -0.010206
C                  1.728804       0.702273      -0.400557
N                  1.092322       1.909834       0.109046
C                  3.152997       0.652335       0.125661
H                  3.133325       0.742148       1.215904
C                  3.804824      -0.666701      -0.252945
C                  3.050022      -1.831253       0.386079
C                  1.560994      -1.653614       0.342207
O                 -0.709807       3.195547       0.501971
O                 -4.627837      -0.139048      -0.145306
O                 -3.076364       2.275901       0.243889
H                 -0.931986      -2.501685      -0.399625
O                 -3.692468      -2.212806      -0.407117
H                  1.657297       2.750496       0.115704
H                  0.982628      -2.518281       0.646468
O                  3.409656      -1.973706       1.757277
H                  4.835799      -0.675186       0.119976
H                 -2.340285       2.923798       0.388312
C                 -4.892159      -1.535213      -0.017637
H                 -5.107635      -1.769780       1.027927
H                 -5.701102      -1.817038      -0.682911
O                  3.786843      -0.853933      -1.656396
H                  4.158831      -0.059693      -2.061256
O                  3.830412       1.752922      -0.466316
H                  4.627346       1.946805       0.039903
H                  1.772974       0.758216      -1.495200
H                  3.313528      -2.738062      -0.168301
H                  4.286909      -2.370591       1.805682

35
Energy:  -1122.61694330
C                 -3.263962      -0.046237      -0.102909
C                 -2.490608       1.080771       0.075820
C                 -1.087258       0.888648       0.065459
C                 -0.524180      -0.392561      -0.078050
C                 -1.338095      -1.513593      -0.258466
C                 -2.697355      -1.295834      -0.262784
C                 -0.229419       2.078275       0.239736
C                  0.947054      -0.524149      -0.019659
C                  1.730498       0.704826      -0.403987
N                  1.091813       1.910483       0.107119
C                  3.152635       0.653753       0.127893
H                  3.127943       0.738447       1.218488
C                  3.806926      -0.663158      -0.253732
C                  3.050938      -1.830532       0.378647
C                  1.561919      -1.653568       0.330396
O                 -0.711615       3.193321       0.503150
O                 -4.629113      -0.148701      -0.100516
O                 -3.076907       2.271993       0.251973
H                 -0.931255      -2.502376      -0.408735
O                 -3.691332      -2.218810      -0.387914
H                  1.657499       2.750513       0.123486
H                  0.983349      -2.519983       0.629241
O                  3.405972      -1.977454       1.750502
H                  4.836737      -0.672039       0.122396
H                 -2.340111       2.917655       0.404619
C                 -4.879333      -1.453961      -0.619633
H                 -5.710879      -1.905487      -0.089379
H                 -5.054527      -1.388867      -1.696461
O                  3.793607      -0.845194      -1.657912
H                  4.167376      -0.049725      -2.058693
O                  3.832269       1.757451      -0.455626
H                  4.627467       1.948507       0.054557
H                  1.778671       0.763871      -1.498277
H                  3.316867      -2.735215      -0.178031
H                  4.282174      -2.376367       1.800711

35
Energy:  -1122.61650390
C                 -3.262468      -0.044071      -0.057182
C                 -2.485206       1.084029       0.097136
C                 -1.082618       0.888598       0.079328
C                 -0.523725      -0.394111      -0.068544
C                 -1.341201      -1.513598      -0.242290
C                 -2.700002      -1.294929      -0.223558
C                 -0.220692       2.076666       0.245566
C                  0.946631      -0.530028      -0.009290
C                  1.731760       0.695142      -0.402266
N                  1.099745       1.904473       0.108732
C                  3.158490       0.642898       0.116717
H                  3.145602       0.741766       1.206103
C                  3.805808      -0.681391      -0.254739
C                  3.054855      -1.833845       0.397133
C                  1.561431      -1.659596       0.341930
O                 -0.699088       3.194288       0.503866
O                 -4.625628      -0.128942      -0.147025
O                 -3.067979       2.281001       0.244948
H                 -0.936921      -2.501741      -0.403992
O                 -3.696116      -2.205075      -0.411480
H                  1.666681       2.743838       0.114483
H                  0.975136      -2.525696       0.631591
O                  3.518077      -1.895768       1.745504
H                  4.835638      -0.694759       0.117439
H                 -2.330346       2.927018       0.389896
C                 -4.894272      -1.524577      -0.022153
H                 -5.111652      -1.760321       1.022739
H                 -5.703275      -1.802788      -0.688863
O                  3.778497      -0.879991      -1.656144
H                  4.154606      -0.091277      -2.067658
O                  3.837230       1.735626      -0.488043
H                  4.639151       1.928094       0.010883
H                  1.770497       0.749388      -1.497292
H                  3.328899      -2.751829      -0.132933
H                  3.015079      -2.569231       2.216739

35
Energy:  -1122.61646666
C                 -3.261439      -0.037535      -0.110687
C                 -2.484831       1.086752       0.071565
C                 -1.082087       0.890250       0.063243
C                 -0.522964      -0.392504      -0.082460
C                 -1.340036      -1.510615      -0.266574
C                 -2.698578      -1.288506      -0.273019
C                 -0.220813       2.077206       0.240243
C                  0.947681      -0.528313      -0.020181
C                  1.734327       0.698578      -0.405181
N                  1.100020       1.905729       0.107944
C                  3.158435       0.644077       0.120993
H                  3.139403       0.737081       1.210824
C                  3.807951      -0.678180      -0.253678
C                  3.054422      -1.833759       0.389574
C                  1.561291      -1.659153       0.328724
O                 -0.700072       3.192963       0.505558
O                 -4.626749      -0.135542      -0.111006
O                 -3.067837       2.279242       0.249469
H                 -0.936447      -2.500333      -0.419519
O                 -3.695154      -2.207950      -0.402350
H                  1.667965       2.744242       0.124808
H                  0.973997      -2.526626       0.612017
O                  3.511627      -1.902076       1.739598
H                  4.836036      -0.692754       0.123198
H                 -2.329521       2.922570       0.404562
C                 -4.880648      -1.438912      -0.633278
H                 -5.714041      -1.888991      -0.104671
H                 -5.054893      -1.370849      -1.710046
O                  3.787190      -0.870304      -1.656088
H                  4.165671      -0.079959      -2.062278
O                  3.840681       1.739993      -0.473893
H                  4.640923       1.928381       0.029443
H                  1.778299       0.757037      -1.499771
H                  3.330750      -2.749231      -0.143659
H                  3.005268      -2.576641       2.205590

35
Energy:  -1122.61485940
C                  3.310726      -0.066248      -0.062229
C                  2.550304       1.074666      -0.207278
C                  1.149629       0.915331      -0.074147
C                  0.577507      -0.352286       0.141259
C                  1.372313      -1.491110       0.268032
C                  2.733357      -1.301559       0.163644
C                  0.295306       2.109637      -0.234047
C                 -0.895906      -0.424873       0.186336
C                 -1.545842       0.813765       0.753637
N                 -1.018848       1.970364       0.029023
C                 -3.074933       0.798797       0.714304
H                 -3.442706       1.824933       0.603136
C                 -3.608126      -0.032592      -0.438418
C                 -3.093716      -1.459356      -0.341812
C                 -1.593976      -1.452800      -0.290427
O                  0.762174       3.198677      -0.600558
O                  4.669211      -0.200212      -0.175346
O                  3.144485       2.246795      -0.466897
H                  0.948949      -2.466897       0.456991
O                  3.714824      -2.243093       0.224314
H                 -1.087012      -2.318795      -0.703881
O                 -3.587974      -2.131139      -1.494837
H                 -3.260849       0.396174      -1.385922
C                  4.932972      -1.500168       0.348537
H                  5.711496      -1.979459      -0.235138
H                  5.191919      -1.420195       1.407394
O                 -5.020046       0.003724      -0.354368
H                 -5.361226      -0.672600      -0.953827
O                 -3.514118       0.261732       1.949286
H                 -4.462967       0.098014       1.863706
H                 -1.265833       0.897641       1.810755
H                 -3.509338      -1.919285       0.561097
H                 -3.582413      -3.081242      -1.338072
H                  2.415877       2.902448      -0.597861
H                 -1.543912       2.835604       0.055559

35
Energy:  -1122.61484516
C                  3.310234      -0.061408      -0.017666
C                  2.551074       1.077310      -0.185437
C                  1.149328       0.919656      -0.062268
C                  0.576734      -0.341968       0.184863
C                  1.371459      -1.475736       0.351751
C                  2.732233      -1.290316       0.239829
C                  0.295002       2.107437      -0.265594
C                 -0.896707      -0.417469       0.209178
C                 -1.558131       0.835003       0.730654
N                 -1.022897       1.972127      -0.018456
C                 -3.086454       0.814643       0.669092
H                 -3.454860       1.836032       0.522069
C                 -3.600786      -0.052234      -0.465981
C                 -3.083920      -1.473912      -0.319677
C                 -1.585109      -1.461089      -0.247322
O                  0.765354       3.188362      -0.650792
O                  4.674851      -0.177038      -0.011559
O                  3.148502       2.248515      -0.442117
H                  0.947241      -2.444789       0.571345
O                  3.717613      -2.215604       0.403256
H                 -1.069935      -2.336892      -0.628607
O                 -3.559763      -2.181307      -1.459006
H                 -3.241233       0.349384      -1.420773
C                  4.904096      -1.582546      -0.089412
H                  5.050302      -1.870139      -1.133699
H                  5.746772      -1.851622       0.538280
O                 -5.013864      -0.017819      -0.403139
H                 -5.344788      -0.712569      -0.987061
O                 -3.542511       0.313415       1.912991
H                 -4.489507       0.144131       1.818275
H                 -1.294465       0.949812       1.789066
H                 -3.511163      -1.908072       0.590548
H                 -3.552781      -3.126231      -1.273799
H                  2.421879       2.900965      -0.595919
H                 -1.547802       2.837911      -0.017331

## Excited state S1

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35
Energy TD-DFT:  -1122.48525389
C                  3.276443      -0.040959       0.078685
C                  2.518286       1.147129      -0.013706
C                  1.067037       0.935949      -0.015087
C                  0.515863      -0.373661       0.009723
C                  1.366869      -1.540350       0.112262
C                  2.700598      -1.337161       0.138361
C                  0.236306       2.041768      -0.224344
C                 -0.919830      -0.527157      -0.017486
C                 -1.725851       0.723836       0.273313
N                 -1.101746       1.884928      -0.342755
C                 -3.159877       0.626444      -0.232541
H                 -3.148550       0.621594      -1.324938
C                 -3.802091      -0.649741       0.273565
C                 -3.041335      -1.880752      -0.228163
C                 -1.553479      -1.709254      -0.207069
O                  0.684997       3.284747      -0.395321
O                  4.607828      -0.133594       0.142801
O                  3.030922       2.296899      -0.095274
H                  0.952594      -2.532816       0.196079
O                  3.710682      -2.237599       0.291340
H                 -1.652258       2.734629      -0.312263
H                 -0.988098      -2.609733      -0.414124
O                 -3.490751      -2.247762      -1.535223
H                 -4.829029      -0.706228      -0.096039
H                  1.676975       3.225825      -0.327234
C                  4.921421      -1.532033       0.052591
H                  5.281774      -1.739076      -0.955940
H                  5.650999      -1.783518       0.815883
O                 -3.783019      -0.557335       1.692273
H                 -4.401613      -1.195880       2.062570
O                 -3.893273       1.771893       0.157688
H                 -4.093338       1.670398       1.098773
H                 -1.759186       0.854824       1.365271
H                 -3.320173      -2.724015       0.410313
H                 -2.999142      -1.732836      -2.185961
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35
Energy TD-DFT:  -1122.48521966

| | | | |
|---|---|---|---|
| C | 3.276163 | -0.037603 | 0.110168 |
| C | 2.518044 | 1.148858 | -0.003321 |
| C | 1.067140 | 0.936502 | -0.012829 |
| C | 0.516087 | -0.373288 | 0.018288 |
| C | 1.367922 | -1.539163 | 0.124707 |
| C | 2.701265 | -1.334425 | 0.160064 |
| C | 0.236767 | 2.040995 | -0.229311 |
| C | -0.919232 | -0.527122 | -0.011305 |
| C | -1.725926 | 0.724888 | 0.273499 |
| N | -1.101222 | 1.884083 | -0.345406 |
| C | -3.159055 | 0.625441 | -0.234448 |
| H | -3.145747 | 0.615331 | -1.326783 |
| C | -3.802369 | -0.648156 | 0.276669 |
| C | -3.040999 | -1.881513 | -0.218351 |
| C | -1.553190 | -1.710056 | -0.196943 |
| O | 0.685448 | 3.283230 | -0.405439 |
| O | 4.608528 | -0.131535 | 0.145538 |
| O | 3.030734 | 2.297980 | -0.090877 |
| H | 0.955383 | -2.534081 | 0.183196 |
| O | 3.714366 | -2.241423 | 0.224427 |
| H | -1.651897 | 2.733797 | -0.319086 |
| H | -0.988251 | -2.611601 | -0.400167 |
| O | -3.489414 | -2.254486 | -1.524177 |
| H | -4.828690 | -0.706214 | -0.094382 |
| H | 1.677249 | 3.225149 | -0.335046 |
| C | 4.910630 | -1.503941 | 0.439854 |
| H | 5.684859 | -1.850737 | -0.237461 |
| H | 5.208173 | -1.573864 | 1.486855 |
| O | -3.785638 | -0.549006 | 1.694971 |
| H | -4.406320 | -1.184353 | 2.067265 |
| O | -3.892845 | 1.772880 | 0.149164 |
| H | -4.094308 | 1.675895 | 1.090433 |
| H | -1.761428 | 0.859958 | 1.364907 |
| H | -3.320602 | -2.721874 | 0.423616 |
| H | -2.997220 | -1.742289 | -2.176622 |

35
Energy TD-DFT:  -1122.47796646

| | | | |
|---|---|---|---|
| C | -3.257957 | -0.046187 | -0.107367 |
| C | -2.479254 | 1.106649 | -0.003779 |
| C | -1.076383 | 0.927700 | 0.004594 |
| C | -0.496983 | -0.406391 | -0.020354 |
| C | -1.354134 | -1.568053 | -0.096160 |
| C | -2.682657 | -1.354641 | -0.139293 |
| C | -0.275018 | 2.084258 | 0.226330 |
| C | 0.912945 | -0.531520 | -0.014001 |
| C | 1.712439 | 0.733883 | -0.253062 |
| N | 1.066526 | 1.892076 | 0.339761 |
| C | 3.130638 | 0.635982 | 0.300473 |
| H | 3.083974 | 0.572985 | 1.390219 |
| C | 3.817790 | -0.597732 | -0.255114 |
| C | 3.067830 | -1.873566 | 0.141114 |
| C | 1.583228 | -1.727579 | 0.126138 |
| O | -0.776129 | 3.244214 | 0.372985 |
| O | -4.584375 | -0.132506 | -0.130812 |
| O | -3.032140 | 2.299619 | 0.086392 |
| H | -0.950842 | -2.567976 | -0.133363 |
| O | -3.703087 | -2.249001 | -0.188949 |
| H | 1.629058 | 2.733781 | 0.364833 |
| H | 1.034225 | -2.640405 | 0.322965 |
| O | 3.517805 | -2.336533 | 1.422097 |
| H | 4.830140 | -0.657049 | 0.151955 |
| H | -2.222241 | 2.936495 | 0.220443 |
| C | -4.904561 | -1.513710 | -0.367445 |
| H | -5.645802 | -1.832580 | 0.359277 |
| H | -5.254598 | -1.611991 | -1.395116 |
| O | 3.855543 | -0.418528 | -1.665410 |
| H | 4.517528 | -1.006706 | -2.043675 |
| O | 3.855593 | 1.811745 | -0.006609 |
| H | 4.091773 | 1.758384 | -0.943408 |
| H | 1.794622 | 0.867619 | -1.342647 |
| H | 3.370273 | -2.663379 | -0.554980 |
| H | 3.010481 | -1.882185 | 2.105830 |

35
Energy TD-DFT:  -1122.47795413

| | | | |
|---|---|---|---|
| C | -3.260610 | -0.043762 | -0.069477 |
| C | -2.478494 | 1.111325 | -0.052330 |
| C | -1.075141 | 0.929702 | -0.052498 |
| C | -0.499230 | -0.404348 | 0.002995 |
| C | -1.359336 | -1.566462 | 0.004693 |
| C | -2.687884 | -1.353116 | -0.035975 |
| C | -0.270426 | 2.095171 | 0.094229 |
| C | 0.910946 | -0.532873 | 0.007925 |
| C | 1.713068 | 0.714075 | -0.307079 |
| N | 1.071124 | 1.907550 | 0.215911 |
| C | 3.131330 | 0.645550 | 0.251143 |
| H | 3.084421 | 0.645325 | 1.342731 |
| C | 3.816521 | -0.619089 | -0.232872 |
| C | 3.063088 | -1.869287 | 0.232650 |
| C | 1.578648 | -1.720730 | 0.210970 |
| O | -0.768719 | 3.263666 | 0.172198 |
| O | -4.586926 | -0.127696 | -0.094786 |
| O | -3.026755 | 2.309058 | -0.027025 |
| H | -0.958153 | -2.567895 | 0.007507 |
| O | -3.708734 | -2.246804 | -0.097573 |
| H | 1.635346 | 2.747974 | 0.186881 |
| H | 1.028258 | -2.620720 | 0.456854 |
| O | 3.511822 | -2.262633 | 1.537089 |
| H | 4.827932 | -0.657805 | 0.178930 |
| H | -2.211245 | 2.950592 | 0.056990 |
| C | -4.918500 | -1.518982 | 0.051724 |
| H | -5.325501 | -1.668839 | 1.051810 |
| H | -5.617868 | -1.798774 | -0.730512 |
| O | 3.857614 | -0.519135 | -1.650932 |
| H | 4.522731 | -1.125011 | -1.994159 |
| O | 3.858383 | 1.800325 | -0.122997 |
| H | 4.095342 | 1.692001 | -1.054857 |
| H | 1.795048 | 0.781902 | -1.402756 |
| H | 3.362822 | -2.696876 | -0.419212 |
| H | 3.006118 | -1.769734 | 2.194833 |

# Charged narciclasine

## Ground State

```
34
Energy:  -1122.13154364
C                  3.295892      -0.081341      -0.101256
C                  2.530022       1.068146      -0.341504
C                  1.124859       0.859044      -0.143612
C                  0.579120      -0.401812       0.151342
C                  1.385959      -1.522881       0.339325
C                  2.746073      -1.303763       0.208693
C                  0.194198       1.980574      -0.386605
C                 -0.894977      -0.460696       0.188519
C                 -1.518727       0.825816       0.675533
N                 -1.048072       1.985302      -0.081482
C                 -3.045532       0.791333       0.700829
H                 -3.409561       1.816383       0.590040
C                 -3.605698      -0.056788      -0.424466
C                 -3.102557      -1.485623      -0.311632
C                 -1.603267      -1.500164      -0.251182
O                  0.725462       3.055872      -0.976547
O                  4.666655      -0.217465      -0.244237
O                  3.024088       2.198962      -0.724172
H                  0.981337      -2.494174       0.584901
O                  3.750839      -2.235186       0.308134
H                 -1.106773      -2.394300      -0.617063
O                 -3.604934      -2.169104      -1.459797
H                 -3.267464       0.353488      -1.383408
H                  1.748918       2.893415      -0.981649
C                  4.942020      -1.450544       0.401096
H                  5.754948      -1.961344      -0.104916
H                  5.160574      -1.268437       1.459067
O                 -5.021047      -0.013814      -0.330951
H                 -5.365552      -0.700729      -0.915833
O                 -3.455744       0.259482       1.956296
H                 -4.406806       0.101782       1.896045
H                 -1.210249       0.960094       1.723066
H                 -3.532531      -1.931980       0.591817
H                 -3.561730      -3.118598      -1.305857
```

34
Energy:  -1122.13141008
C                  3.299958      -0.064554       0.014753
C                  2.543767       1.100021      -0.178930
C                  1.134339       0.888275      -0.018450
C                  0.580136      -0.377424       0.237792
C                  1.380704      -1.505450       0.411838
C                  2.742313      -1.290627       0.294136
C                  0.211632       2.018597      -0.251780
C                 -0.894167      -0.436597       0.233040
C                 -1.532049       0.838712       0.731425
N                 -1.038021       2.017348       0.020618
C                 -3.059216       0.805985       0.710128
H                 -3.418530       1.833431       0.606756
C                 -3.587303      -0.021247      -0.445765
C                 -3.087132      -1.451941      -0.344628
C                 -1.589937      -1.467328      -0.245825
O                  0.760233       3.110444      -0.793682
O                  4.679785      -0.175561       0.013161
O                  3.050360       2.249440      -0.482389
H                  0.968811      -2.480431       0.629426
O                  3.747837      -2.211084       0.467069
H                 -1.083483      -2.353490      -0.617186
O                 -3.559444      -2.115433      -1.516979
H                 -3.222606       0.405948      -1.387465
H                  1.783717       2.950641      -0.762732
C                  4.898832      -1.573471      -0.091368
H                  4.976652      -1.852975      -1.147761
H                  5.781239      -1.854449       0.474563
O                 -5.004709       0.020360      -0.391038
H                 -5.332375      -0.657728      -0.995590
O                 -3.507436       0.252836       1.943134
H                 -4.456225       0.096663       1.851109
H                 -1.255852       0.946287       1.790978
H                 -3.540289      -1.913628       0.539574
H                 -3.519193      -3.067426      -1.378402

34
Energy:  -1122.13109197
C                 -3.252315      -0.063055      -0.107817
C                 -2.540401       1.162857       0.024514
C                 -1.103424       0.941880       0.139341
C                 -0.528557      -0.351483       0.010878
C                 -1.302622      -1.492500      -0.184267
C                 -2.673603      -1.291727      -0.228447
C                 -0.222897       2.096599       0.413092
C                  0.943697      -0.501320       0.075427
C                  1.719742       0.718341      -0.345366
N                  1.121072       1.888986       0.262737
C                  3.185820       0.656606       0.073810
H                  3.243216       0.787325       1.156861
C                  3.784873      -0.684370      -0.294763
C                  3.048962      -1.817200       0.426552
C                  1.560118      -1.632362       0.428387
O                 -0.605848       3.201824       0.793203
O                 -4.621341      -0.180329      -0.309418
O                 -3.138331       2.269113       0.016734
H                 -0.870059      -2.469408      -0.337275
O                 -3.643998      -2.236132      -0.476850
H                  1.689906       2.724094       0.305382
H                  0.981702      -2.487226       0.760436
O                  3.550691      -1.971384       1.755066
H                  4.835258      -0.705196       0.007972
C                 -4.857325      -1.565370      -0.128489
H                 -5.075416      -1.764083       0.927428
H                 -5.658129      -1.897001      -0.782111
O                  3.667578      -0.791436      -1.707884
H                  4.241424      -1.497668      -2.022642
O                  3.912224       1.731246      -0.494470
H                  4.015962       1.533013      -1.435146
H                  1.680835       0.789297      -1.441890
H                  3.297981      -2.752017      -0.083309
H                  3.067795      -1.371474       2.335153

34
Energy:  -1122.13065538
C                 -3.262823      -0.022090      -0.154528
C                 -2.548525       1.197909       0.018320
C                 -1.111880       0.969601       0.126773
C                 -0.546527      -0.331464       0.030358
C                 -1.326949      -1.470383      -0.148904
C                 -2.695124      -1.258345      -0.225814
C                 -0.220150       2.120497       0.381483
C                  0.925931      -0.489179       0.082899
C                  1.702575       0.715635      -0.376996
N                  1.120955       1.900563       0.219859
C                  3.175994       0.653694       0.015500
H                  3.255493       0.813475       1.093167
C                  3.757955      -0.701704      -0.326565
C                  3.027540      -1.807329       0.441069
C                  1.539718      -1.614588       0.456943
O                 -0.589221       3.233660       0.751919
O                 -4.643945      -0.145421      -0.225226
O                 -3.147763       2.303026       0.055629
H                 -0.900798      -2.454026      -0.273312
O                 -3.678826      -2.211415      -0.367680
H                  1.695779       2.732316       0.242192
H                  0.960124      -2.458063       0.815256
O                  3.547675      -1.920737       1.766595
H                  4.813924      -0.722253      -0.043796
C                 -4.830104      -1.451366      -0.742988
H                 -5.719524      -1.900636      -0.311902
H                 -4.878311      -1.407564      -1.837316
O                  3.612191      -0.847991      -1.733559
H                  4.176375      -1.565608      -2.039774
O                  3.899254       1.706645      -0.595817
H                  3.984317       1.481564      -1.532299
H                  1.642591       0.765042      -1.473820
H                  3.264901      -2.759284      -0.041946
H                  3.072985      -1.302820       2.334451

34
Energy:  -1122.13021232
C                  3.311375      -0.077950       0.021982
C                  2.616535       1.160272      -0.098685
C                  1.171037       0.967074      -0.098814
C                  0.587557      -0.310340       0.122893
C                  1.344294      -1.463045       0.292957
C                  2.720369      -1.290021       0.224459
C                  0.287837       2.116184      -0.383803
C                 -0.887017      -0.403997       0.151047
C                 -1.542692       0.842195       0.689129
N                 -1.057642       1.939542      -0.133032
C                 -3.070054       0.801470       0.698709
H                 -3.457580       1.820039       0.581124
C                 -3.622258      -0.057349      -0.424062
C                 -3.081986      -1.473023      -0.322589
C                 -1.581636      -1.444234      -0.306157
O                  0.653841       3.190616      -0.852974
O                  4.690692      -0.220170       0.119525
O                  3.232508       2.253420      -0.172781
H                  0.895797      -2.423669       0.498836
O                  3.688441      -2.247640       0.424029
H                 -1.071802      -2.307704      -0.721523
O                 -3.597764      -2.166219      -1.457188
H                 -3.308723       0.362680      -1.386771
C                  4.883215      -1.613854      -0.039914
H                  5.010400      -1.846580      -1.103790
H                  5.727314      -1.945974       0.556452
O                 -5.034591      -0.043819      -0.304143
H                 -5.375895      -0.741867      -0.877858
O                 -3.472041       0.278980       1.954992
H                 -4.418272       0.093252       1.890520
H                 -1.227352       0.977747       1.732526
H                 -3.474981      -1.930815       0.591934
H                 -3.531795      -3.114673      -1.304766
H                 -1.577531       2.807203      -0.116146

34
Energy:  -1122.13004206
C                 -3.243981      -0.045732      -0.023788
C                 -2.483215       1.120094       0.133708
C                 -1.068863       0.880618       0.090617
C                 -0.516506      -0.405771      -0.002712
C                 -1.326855      -1.536165      -0.131733
C                 -2.688028      -1.298567      -0.140126
C                 -0.147716       2.026869       0.227364
C                  0.956902      -0.505637       0.059826
C                  1.691213       0.729598      -0.419760
N                  1.112582       1.988472       0.036416
C                  3.172838       0.706885      -0.037348
H                  3.258761       0.965234       1.020460
C                  3.781690      -0.664695      -0.266353
C                  3.073185      -1.738592       0.558267
C                  1.582385      -1.602195       0.496346
O                 -0.715655       3.186301       0.579251
O                 -4.622932      -0.155517       0.008310
O                 -2.994124       2.293603       0.313634
H                 -0.924660      -2.532678      -0.239174
O                 -3.694750      -2.230391      -0.218294
H                  1.008941      -2.449936       0.856544
O                  3.542046      -1.726417       1.908667
H                  4.835300      -0.638806       0.025821
H                 -1.737887       3.022626       0.538265
C                 -4.861243      -1.456748      -0.506358
H                 -5.721792      -1.898666      -0.014419
H                 -4.987202      -1.401592      -1.593149
O                  3.660078      -0.917708      -1.663000
H                  4.244164      -1.643527      -1.905769
O                  3.908420       1.686391      -0.747954
H                  3.982309       1.365863      -1.656635
H                  1.645663       0.717648      -1.519736
H                  3.370159      -2.714566       0.164496
H                  3.042657      -1.060771       2.395773

34
Energy:  -1122.12999401
C                 -3.242967      -0.033370      -0.084989
C                 -2.480755       1.129961       0.083259
C                 -1.066955       0.886343       0.059106
C                 -0.516670      -0.397922      -0.069906
C                 -1.328346      -1.521778      -0.241989
C                 -2.688951      -1.282504      -0.242942
C                 -0.145131       2.025503       0.243944
C                  0.954167      -0.506445       0.023292
C                  1.705151       0.740325      -0.397671
N                  1.118611       1.987867       0.078432
C                  3.175734       0.699186       0.024568
H                  3.233374       0.919748       1.092833
C                  3.786855      -0.665765      -0.236340
C                  3.053438      -1.765683       0.529974
C                  1.565185      -1.620164       0.436714
O                 -0.717245       3.177762       0.612381
O                 -4.619227      -0.122634      -0.190418
O                 -2.990475       2.306381       0.248844
H                 -0.926562      -2.514693      -0.380541
O                 -3.695589      -2.196935      -0.441351
H                  0.980532      -2.476306       0.756544
O                  3.488015      -1.804759       1.891383
H                  4.832022      -0.654160       0.085372
H                 -1.738708       3.022693       0.530231
C                 -4.875027      -1.508502      -0.020126
H                 -5.045503      -1.720263       1.041085
H                 -5.713661      -1.809973      -0.639504
O                  3.703111      -0.867850      -1.643901
H                  4.293297      -1.585087      -1.897060
O                  3.933764       1.699855      -0.630739
H                  4.032030       1.410569      -1.547573
H                  1.690745       0.762019      -1.498289
H                  3.356576      -2.728092       0.108513
H                  2.982391      -1.151201       2.388408

34
Energy:  -1122.12987548
C                  3.311991      -0.081624      -0.035036
C                  2.616893       1.152162      -0.201056
C                  1.171242       0.966382      -0.140658
C                  0.590579      -0.316804       0.059463
C                  1.346726      -1.473124       0.200256
C                  2.723430      -1.297627       0.139300
C                  0.282987       2.127570      -0.349861
C                 -0.883303      -0.409343       0.118671
C                 -1.523780       0.814610       0.720313
N                 -1.057248       1.942736      -0.070310
C                 -3.050395       0.772933       0.764444
H                 -3.440139       1.795481       0.701551
C                 -3.629112      -0.035167      -0.382342
C                 -3.089747      -1.454491      -0.355567
C                 -1.589245      -1.428717      -0.366710
O                  0.638147       3.225289      -0.770737
O                  4.690465      -0.245060      -0.104874
O                  3.236891       2.232382      -0.369029
H                  0.898143      -2.437625       0.386520
O                  3.691356      -2.273094       0.218826
H                 -1.089152      -2.275609      -0.825966
O                 -3.628689      -2.094957      -1.510309
H                 -3.336202       0.427018      -1.332114
C                  4.893142      -1.532749       0.448673
H                  5.724823      -2.025479      -0.045403
H                  5.047378      -1.446350       1.530741
O                 -5.038509      -0.025471      -0.230576
H                 -5.394340      -0.693888      -0.830129
O                 -3.422551       0.194496       2.005491
H                 -4.370424       0.012763       1.956075
H                 -1.183500       0.909120       1.760513
H                 -3.466247      -1.952750       0.544617
H                 -3.560083      -3.049476      -1.403507
H                 -1.566888       2.813078       0.009989

34
Energy:  -1122.12983046
C                  3.308043      -0.070979      -0.036750
C                  2.528683       1.059823      -0.201043
C                  1.132145       0.873781      -0.059990
C                  0.584989      -0.396085       0.153562
C                  1.393318      -1.530720       0.286346
C                  2.750500      -1.315377       0.193825
C                  0.226988       2.054468      -0.260216
C                 -0.888039      -0.446150       0.182641
C                 -1.494675       0.817749       0.745858
N                 -1.029456       2.016012       0.050382
C                 -3.021675       0.785314       0.779659
H                 -3.381791       1.816828       0.739655
C                 -3.592201       0.016785      -0.396317
C                 -3.102059      -1.420843      -0.378432
C                 -1.602893      -1.452358      -0.319206
O                  0.792262       3.105689      -0.765510
O                  4.675656      -0.192500      -0.156523
O                  3.045189       2.250721      -0.501337
H                  0.980885      -2.513135       0.468137
O                  3.756897      -2.245491       0.253602
H                 -1.113874      -2.326848      -0.739414
O                 -3.610281      -2.023074      -1.569338
H                 -3.252071       0.485919      -1.327038
C                  4.947457      -1.470803       0.406238
H                  5.761789      -1.944307      -0.132203
H                  5.163219      -1.359086       1.473523
O                 -5.007745       0.065053      -0.297709
H                 -5.358279      -0.578100      -0.926993
O                 -3.430345       0.171925       1.999296
H                 -4.382828       0.026183       1.933166
H                 -1.182174       0.879171       1.799925
H                 -3.536653      -1.922428       0.493279
H                 -3.574593      -2.980895      -1.478128
H                  2.163355       2.822998      -0.682031

34
Energy:  -1122.12974949
C                  3.307445      -0.060979       0.027468
C                  2.529769       1.067012      -0.161764
C                  1.131815       0.882720      -0.033790
C                  0.583905      -0.380611       0.214574
C                  1.392186      -1.509249       0.392709
C                  2.749263      -1.297580       0.295102
C                  0.227788       2.055224      -0.283028
C                 -0.888954      -0.435898       0.215427
C                 -1.511954       0.843081       0.724437
N                 -1.033923       2.022072       0.005550
C                 -3.039546       0.807312       0.724124
H                 -3.400359       1.835653       0.637244
C                 -3.582177      -0.006158      -0.434684
C                 -3.087648      -1.440029      -0.353360
C                 -1.589801      -1.462395      -0.264839
O                  0.800206       3.094833      -0.803737
O                  4.681510      -0.161515       0.034878
O                  3.050209       2.256323      -0.463230
H                  0.978540      -2.484714       0.606758
O                  3.760213      -2.207788       0.474278
H                 -1.089185      -2.348218      -0.645644
O                 -3.570916      -2.088890      -1.530056
H                 -3.223995       0.429646      -1.374803
C                  4.916458      -1.561830      -0.061045
H                  5.022159      -1.840607      -1.114293
H                  5.788463      -1.829748       0.526425
O                 -4.999635       0.039754      -0.367843
H                 -5.334318      -0.629264      -0.978536
O                 -3.475151       0.239076       1.956137
H                 -4.425534       0.088037       1.873486
H                 -1.224658       0.937432       1.783245
H                 -3.537070      -1.910140       0.528290
H                 -3.532263      -3.042455      -1.402415
H                  2.172186       2.821615      -0.675338

34
Energy:  -1122.12788961
C                 -3.238346      -0.049727      -0.022880
C                 -2.458592       1.083320       0.122196
C                 -1.056588       0.873477       0.104686
C                 -0.508601      -0.408645       0.015689
C                 -1.324815      -1.540928      -0.115845
C                 -2.680889      -1.309902      -0.135784
C                 -0.157941       2.062026       0.256185
C                  0.963477      -0.502421       0.075795
C                  1.682797       0.738639      -0.413441
N                  1.114540       1.996589       0.057719
C                  3.171475       0.713504      -0.058067
H                  3.274877       0.985597       0.994747
C                  3.779694      -0.660083      -0.278384
C                  3.084399      -1.725724       0.567679
C                  1.592862      -1.595615       0.514842
O                 -0.754630       3.165395       0.598456
O                 -4.611980      -0.151371      -0.007101
O                 -2.978346       2.296515       0.288332
H                 -0.919929      -2.537246      -0.219032
O                 -3.691743      -2.233796      -0.219554
H                  1.023726      -2.443537       0.882182
O                  3.564813      -1.692166       1.913916
H                  4.836899      -0.628640       0.000498
H                 -2.086939       2.881152       0.467381
C                 -4.856316      -1.459684      -0.511125
H                 -5.716347      -1.892312      -0.010594
H                 -4.987504      -1.411251      -1.596722
O                  3.642868      -0.932695      -1.670322
H                  4.228113      -1.658759      -1.909465
O                  3.899913       1.682352      -0.792375
H                  3.950928       1.353294      -1.699434
H                  1.620783       0.717840      -1.513578
H                  3.382548      -2.705997       0.185651
H                  3.068215      -1.019540       2.394229

34
Energy:  -1122.12786964
C                 -3.246825      -0.055141      -0.109697
C                 -2.468595       1.065621       0.116179
C                 -1.066890       0.854369       0.112370
C                 -0.518229      -0.418374      -0.065034
C                 -1.332616      -1.535623      -0.298263
C                 -2.688340      -1.303613      -0.312125
C                 -0.170662       2.025849       0.373432
C                  0.950951      -0.522806       0.029451
C                  1.687396       0.749228      -0.340770
N                  1.106372       1.970764       0.203778
C                  3.163760       0.690520       0.060087
H                  3.233259       0.876204       1.134290
C                  3.776854      -0.663265      -0.250872
C                  3.054195      -1.790392       0.485312
C                  1.565163      -1.649893       0.399337
O                 -0.774680       3.104290       0.776554
O                 -4.616056      -0.134518      -0.232553
O                 -2.990250       2.270222       0.333702
H                 -0.925517      -2.520509      -0.476244
O                 -3.695306      -2.201306      -0.563926
H                  0.984025      -2.520891       0.684595
O                  3.493846      -1.866628       1.843791
H                  4.824841      -0.658250       0.062251
H                 -2.104526       2.837863       0.577807
C                 -4.881942      -1.529655      -0.138249
H                 -5.082096      -1.790676       0.905729
H                 -5.705010      -1.792527      -0.794547
O                  3.683278      -0.822361      -1.663744
H                  4.275158      -1.528596      -1.942539
O                  3.917315       1.712364      -0.569448
H                  3.996436       1.457927      -1.498244
H                  1.662215       0.811823      -1.440746
H                  3.361839      -2.738279       0.035154
H                  2.986866      -1.229520       2.360377

## Excited state S1

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34
Energy TD-DFT:  -1122.01192818
C                     3.276222      -0.046361       0.130469
C                     2.504764       1.154939       0.211826
C                     1.055181       0.966167      -0.017883
C                     0.492858      -0.340445      -0.032543
C                     1.359584      -1.515557      -0.028574
C                     2.699476      -1.317106       0.043892
C                     0.241968       2.109512      -0.385245
C                    -0.924564      -0.523535      -0.056776
C                    -1.715055       0.735357       0.206584
N                    -1.109488       1.840111      -0.513998
C                    -3.173254       0.619298      -0.215210
H                    -3.223971       0.591214      -1.305918
C                    -3.786642      -0.649829       0.339811
C                    -3.052272      -1.881436      -0.195418
C                    -1.568650      -1.728581      -0.194438
O                     0.656981       3.243336      -0.676458
O                     4.605198      -0.170271       0.395545
O                     3.035443       2.240287       0.503983
H                     0.950203      -2.513878      -0.029304
O                     3.693348      -2.254925       0.186934
H                    -1.679171       2.674698      -0.576648
H                    -1.009573      -2.640956      -0.357255
O                    -3.560556      -2.179190      -1.514504
H                    -4.832327      -0.707384       0.024423
C                     4.908388      -1.523699       0.057204
H                     5.247497      -1.559996      -0.982008
H                     5.648267      -1.914541       0.748036
O                    -3.705113      -0.544280       1.757547
H                    -4.268296      -1.216482       2.155076
O                    -3.902989       1.767939       0.189313
H                    -4.015528       1.699865       1.147223
H                    -1.697373       0.930334       1.292709
H                    -3.350362      -2.739917       0.415581
H                    -2.940213      -1.801110      -2.148718
```

34
Energy TD-DFT:  -1122.01177832

| | | | |
|---|---|---|---|
| C | 3.281785 | -0.000495 | 0.171829 |
| C | 2.509268 | 1.202672 | 0.181252 |
| C | 1.060668 | 0.999427 | -0.040854 |
| C | 0.508212 | -0.311946 | -0.023732 |
| C | 1.381419 | -1.483447 | -0.002808 |
| C | 2.717361 | -1.275840 | 0.089509 |
| C | 0.232892 | 2.131919 | -0.409586 |
| C | -0.908250 | -0.508108 | -0.036715 |
| C | -1.710487 | 0.747823 | 0.202691 |
| N | -1.116388 | 1.844522 | -0.539407 |
| C | -3.167483 | 0.608435 | -0.216078 |
| H | -3.217588 | 0.552012 | -1.305752 |
| C | -3.769271 | -0.651338 | 0.371859 |
| C | -3.024149 | -1.889799 | -0.131887 |
| C | -1.542071 | -1.721268 | -0.146365 |
| O | 0.629226 | 3.273845 | -0.694072 |
| O | 4.627170 | -0.103611 | 0.329428 |
| O | 3.042904 | 2.305109 | 0.395895 |
| H | 0.978581 | -2.483898 | -0.026496 |
| O | 3.733088 | -2.201203 | 0.142562 |
| H | -1.692415 | 2.674748 | -0.603837 |
| H | -0.976812 | -2.632218 | -0.294564 |
| O | -3.536457 | -2.233242 | -1.437832 |
| H | -4.814545 | -0.726738 | 0.059014 |
| C | 4.853728 | -1.479821 | 0.643783 |
| H | 5.759625 | -1.820209 | 0.152858 |
| H | 4.902553 | -1.588709 | 1.730968 |
| O | -3.687995 | -0.508427 | 1.786433 |
| H | -4.246626 | -1.173777 | 2.201504 |
| O | -3.907406 | 1.760461 | 0.159213 |
| H | -4.020416 | 1.715198 | 1.118408 |
| H | -1.695069 | 0.963985 | 1.284787 |
| H | -3.308355 | -2.732944 | 0.506631 |
| H | -2.926043 | -1.865072 | -2.087345 |

34
Energy TD-DFT:  -1122.00728172

| | | | |
|---|---|---|---|
| C | 3.353274 | -0.073104 | 0.040986 |
| C | 2.637042 | 1.151898 | 0.182071 |
| C | 1.164944 | 1.014616 | 0.056098 |
| C | 0.567569 | -0.276472 | 0.103832 |
| C | 1.383134 | -1.479844 | 0.018547 |
| C | 2.729942 | -1.329525 | -0.020759 |
| C | 0.367203 | 2.168728 | -0.283207 |
| C | -0.859615 | -0.394580 | 0.166496 |
| C | -1.533526 | 0.898054 | 0.579248 |
| N | -1.013869 | 1.946195 | -0.287719 |
| C | -3.062235 | 0.870779 | 0.548502 |
| H | -3.433740 | 1.863854 | 0.269215 |
| C | -3.597511 | -0.138488 | -0.448361 |
| C | -3.073522 | -1.527907 | -0.130067 |
| C | -1.578682 | -1.519868 | -0.107377 |
| O | 0.786317 | 3.285937 | -0.635371 |
| O | 4.693618 | -0.246604 | 0.206311 |
| O | 3.218647 | 2.220334 | 0.445030 |
| H | 0.932045 | -2.460655 | 0.048739 |
| O | 3.703888 | -2.298344 | 0.037538 |
| H | -1.092070 | -2.446578 | -0.387594 |
| O | -3.603525 | -2.375752 | -1.156287 |
| H | -3.259045 | 0.134505 | -1.454527 |
| C | 4.925800 | -1.601437 | -0.178403 |
| H | 5.179266 | -1.627240 | -1.242093 |
| H | 5.706572 | -2.027434 | 0.443232 |
| O | -5.014017 | -0.098875 | -0.367325 |
| H | -5.342601 | -0.888120 | -0.817177 |
| O | -3.516305 | 0.546867 | 1.855527 |
| H | -4.459258 | 0.349226 | 1.779383 |
| H | -1.253600 | 1.103582 | 1.624829 |
| H | -3.502972 | -1.840914 | 0.831067 |
| H | -3.516899 | -3.293279 | -0.877683 |
| H | -1.527250 | 2.818829 | -0.275595 |

34
Energy TD-DFT:  -1122.00720960

| | | | |
|---|---|---|---|
| C | 3.355632 | -0.046042 | 0.006766 |
| C | 2.639342 | 1.177862 | 0.157397 |
| C | 1.165955 | 1.037817 | 0.053336 |
| C | 0.575953 | -0.257631 | 0.073901 |
| C | 1.392801 | -1.456935 | -0.055563 |
| C | 2.737804 | -1.302009 | -0.093330 |
| C | 0.355253 | 2.198598 | -0.229788 |
| C | -0.850785 | -0.385712 | 0.147534 |
| C | -1.527236 | 0.886613 | 0.614408 |
| N | -1.025490 | 1.967276 | -0.222580 |
| C | -3.056113 | 0.850657 | 0.601565 |
| H | -3.436509 | 1.851142 | 0.363830 |
| C | -3.598042 | -0.123954 | -0.425684 |
| C | -3.061323 | -1.520849 | -0.167103 |
| C | -1.566400 | -1.503121 | -0.162740 |
| O | 0.759126 | 3.333749 | -0.539153 |
| O | 4.704554 | -0.207051 | 0.051974 |
| O | 3.225967 | 2.249678 | 0.396524 |
| H | 0.941183 | -2.437522 | -0.078363 |
| O | 3.722133 | -2.259492 | -0.180035 |
| H | -1.078273 | -2.413927 | -0.488562 |
| O | -3.598007 | -2.332034 | -1.218967 |
| H | -3.274488 | 0.188975 | -1.425111 |
| C | 4.901730 | -1.605559 | 0.274048 |
| H | 5.756067 | -1.947590 | -0.300987 |
| H | 5.026424 | -1.776798 | 1.347044 |
| O | -5.013621 | -0.097230 | -0.325173 |
| H | -5.342944 | -0.870451 | -0.801555 |
| O | -3.492184 | 0.475775 | 1.901054 |
| H | -4.434835 | 0.275159 | 1.828819 |
| H | -1.235567 | 1.057579 | 1.662936 |
| H | -3.476528 | -1.873863 | 0.786382 |
| H | -3.501105 | -3.259057 | -0.977755 |
| H | -1.540860 | 2.837036 | -0.166044 |

34
Energy TD-DFT:  -1122.00079966

| | | | |
|---|---|---|---|
| C | 2.736086 | 0.343705 | 0.122944 |
| C | 1.958903 | 1.446368 | -0.025543 |
| C | 0.553918 | 1.228494 | -0.235780 |
| C | -0.016596 | -0.096639 | -0.217862 |
| C | 0.856450 | -1.215783 | -0.056426 |
| C | 2.179061 | -0.955471 | 0.102333 |
| C | -0.284999 | 2.338310 | -0.506356 |
| C | -1.436166 | -0.245240 | -0.259153 |
| C | -2.202866 | 1.099758 | -0.025698 |
| N | -1.576339 | 2.004040 | -0.910575 |
| C | -3.693042 | 0.985628 | -0.314089 |
| H | -3.832422 | 0.968903 | -1.396515 |
| C | -4.270864 | -0.281022 | 0.283158 |
| C | -3.619125 | -1.520404 | -0.330574 |
| C | -2.138719 | -1.397940 | -0.444181 |
| O | 0.065597 | 3.552732 | -0.454012 |
| O | 4.091440 | 0.249209 | 0.374013 |
| O | 2.462925 | 2.696222 | 0.001203 |
| H | 0.481176 | -2.228458 | -0.020719 |
| O | 3.195472 | -1.849684 | 0.327268 |
| H | -1.604413 | -2.306479 | -0.703055 |
| O | -4.238987 | -1.779245 | -1.607389 |
| H | -5.343440 | -0.313867 | 0.070896 |
| H | 1.685373 | 3.300521 | -0.145049 |
| C | 4.391040 | -1.108676 | 0.086571 |
| H | 4.664051 | -1.207712 | -0.968738 |
| H | 5.174867 | -1.460522 | 0.749361 |
| O | -4.050090 | -0.190306 | 1.687602 |
| H | -4.575813 | -0.862657 | 2.133042 |
| O | -4.383353 | 2.128808 | 0.164938 |
| H | -4.421490 | 2.045022 | 1.127065 |
| H | -2.048682 | 1.361850 | 1.035619 |
| H | -3.890211 | -2.382970 | 0.287712 |
| H | -3.664263 | -1.398710 | -2.281564 |

34
Energy TD-DFT:  -1122.00067280

| | | | |
|---|---|---|---|
| C | 3.247991 | -0.020602 | 0.164192 |
| C | 2.480976 | 1.091761 | 0.033142 |
| C | 1.069583 | 0.891638 | -0.147747 |
| C | 0.484642 | -0.427431 | -0.132872 |
| C | 1.347997 | -1.557648 | 0.007900 |
| C | 2.675717 | -1.312850 | 0.145823 |
| C | 0.238138 | 2.012571 | -0.396944 |
| C | -0.936496 | -0.560006 | -0.143494 |
| C | -1.683588 | 0.791184 | 0.113700 |
| N | -1.065089 | 1.695937 | -0.776043 |
| C | -3.180124 | 0.695755 | -0.147417 |
| H | -3.339825 | 0.686430 | -1.227131 |
| C | -3.761719 | -0.567101 | 0.454047 |
| C | -3.135158 | -1.811084 | -0.176658 |
| C | -1.656193 | -1.704246 | -0.319813 |
| O | 0.604736 | 3.221965 | -0.351035 |
| O | 4.621195 | -0.137103 | 0.264201 |
| O | 3.004800 | 2.333475 | 0.025251 |
| H | 0.961712 | -2.565984 | 0.045968 |
| O | 3.693532 | -2.223772 | 0.275962 |
| H | -1.137661 | -2.617141 | -0.594981 |
| O | -3.783200 | -2.058622 | -1.441887 |
| H | -4.838142 | -0.586770 | 0.260381 |
| H | 2.231307 | 2.947557 | -0.099551 |
| C | 4.811121 | -1.462800 | 0.734453 |
| H | 5.724761 | -1.872772 | 0.316289 |
| H | 4.817331 | -1.466968 | 1.828897 |
| O | -3.515851 | -0.485226 | 1.854905 |
| H | -4.042482 | -1.152864 | 2.306331 |
| O | -3.847827 | 1.844438 | 0.350221 |
| H | -3.869349 | 1.755762 | 1.312423 |
| H | -1.506756 | 1.044076 | 1.173844 |
| H | -3.403549 | -2.672999 | 0.443766 |
| H | -3.217143 | -1.682555 | -2.125861 |

34
Energy TD-DFT:  -1121.99783556

| | | | |
|---|---|---|---|
| C | 3.332587 | -0.045647 | 0.099763 |
| C | 2.588508 | 1.086702 | 0.027608 |
| C | 1.163155 | 0.922278 | -0.074652 |
| C | 0.554183 | -0.381948 | -0.007349 |
| C | 1.388566 | -1.534336 | 0.061528 |
| C | 2.730174 | -1.325215 | 0.110807 |
| C | 0.341432 | 2.058065 | -0.265476 |
| C | -0.875752 | -0.461364 | 0.042265 |
| C | -1.528860 | 0.903553 | 0.466532 |
| N | -1.012033 | 1.781457 | -0.511599 |
| C | -3.054196 | 0.883264 | 0.524735 |
| H | -3.418506 | 1.887866 | 0.287863 |
| C | -3.663542 | -0.098427 | -0.455437 |
| C | -3.150821 | -1.503141 | -0.198342 |
| C | -1.656388 | -1.523456 | -0.269885 |
| O | 0.730782 | 3.263824 | -0.232562 |
| O | 4.700442 | -0.191966 | 0.237204 |
| O | 3.136037 | 2.319653 | 0.026374 |
| H | 0.973827 | -2.531228 | 0.118353 |
| O | 3.730651 | -2.257765 | 0.243707 |
| H | -1.199980 | -2.437161 | -0.638512 |
| O | -3.756753 | -2.313417 | -1.213438 |
| H | -3.380785 | 0.189207 | -1.474549 |
| C | 4.924970 | -1.554809 | -0.092815 |
| H | 5.100359 | -1.645705 | -1.169615 |
| H | 5.751629 | -1.943411 | 0.493003 |
| O | -5.072772 | -0.034306 | -0.289230 |
| H | -5.441132 | -0.808924 | -0.733578 |
| O | -3.424129 | 0.537110 | 1.853383 |
| H | -4.374347 | 0.362474 | 1.838545 |
| H | -1.157946 | 1.125599 | 1.480059 |
| H | -3.531906 | -1.833832 | 0.776467 |
| H | -3.652299 | -3.239838 | -0.973358 |
| H | 2.371025 | 2.950411 | -0.054524 |

34
Energy TD-DFT:  -1121.99765597

| | | | |
|---|---|---|---|
| C | 3.338076 | -0.029480 | -0.002981 |
| C | 2.590352 | 1.102896 | -0.023950 |
| C | 1.163797 | 0.938878 | -0.100973 |
| C | 0.558763 | -0.368956 | -0.075648 |
| C | 1.397284 | -1.521326 | -0.062405 |
| C | 2.738676 | -1.309995 | -0.026847 |
| C | 0.335643 | 2.078674 | -0.233614 |
| C | -0.868681 | -0.454778 | 0.004384 |
| C | -1.514923 | 0.890271 | 0.496594 |
| N | -1.022785 | 1.807951 | -0.457058 |
| C | -3.038559 | 0.864082 | 0.588804 |
| H | -3.409618 | 1.875946 | 0.397866 |
| C | -3.668303 | -0.081941 | -0.413257 |
| C | -3.146794 | -1.493784 | -0.220875 |
| C | -1.654658 | -1.507175 | -0.329140 |
| O | 0.724195 | 3.283002 | -0.172758 |
| O | 4.712598 | -0.176443 | -0.016152 |
| O | 3.138194 | 2.335623 | -0.022817 |
| H | 0.985549 | -2.520572 | -0.033859 |
| O | 3.745738 | -2.244837 | -0.019527 |
| H | -1.205160 | -2.404962 | -0.742629 |
| O | -3.775740 | -2.267757 | -1.250344 |
| H | -3.409501 | 0.244741 | -1.426948 |
| C | 4.908099 | -1.523693 | 0.386027 |
| H | 5.781093 | -1.931997 | -0.112839 |
| H | 4.993005 | -1.572382 | 1.476387 |
| O | -5.073502 | -0.028257 | -0.212687 |
| H | -5.450149 | -0.786662 | -0.677626 |
| O | -3.377796 | 0.467985 | 1.911693 |
| H | -4.327716 | 0.291146 | 1.911636 |
| H | -1.121198 | 1.073059 | 1.509443 |
| H | -3.504001 | -1.861327 | 0.749791 |
| H | -3.665752 | -3.202002 | -1.045758 |
| H | 2.371406 | 2.967734 | -0.063059 |

34
Energy TD-DFT:  -1121.99756684

| | | | |
|---|---|---|---|
| C | 3.264390 | -0.033998 | 0.162680 |
| C | 2.494065 | 1.158799 | 0.047823 |
| C | 1.039318 | 0.966730 | 0.042246 |
| C | 0.483576 | -0.339502 | 0.054398 |
| C | 1.347156 | -1.509657 | 0.151137 |
| C | 2.688419 | -1.307943 | 0.205427 |
| C | 0.148042 | 2.056706 | -0.274254 |
| C | -0.932288 | -0.493640 | -0.035365 |
| C | -1.711251 | 0.769008 | 0.289571 |
| N | -1.135694 | 1.973633 | -0.288704 |
| C | -3.179553 | 0.668828 | -0.119994 |
| H | -3.245487 | 0.773879 | -1.205378 |
| C | -3.778470 | -0.666362 | 0.286206 |
| C | -3.041936 | -1.834684 | -0.366843 |
| C | -1.562043 | -1.684225 | -0.303190 |
| O | 0.681339 | 3.249929 | -0.660922 |
| O | 4.615198 | -0.136681 | 0.200652 |
| O | 3.034501 | 2.288584 | -0.057064 |
| H | 0.930234 | -2.504932 | 0.198694 |
| O | 3.702770 | -2.233605 | 0.276870 |
| H | -0.986291 | -2.571294 | -0.540455 |
| O | -3.513337 | -1.979997 | -1.725301 |
| H | -4.824426 | -0.693889 | -0.033567 |
| H | 1.651811 | 3.186500 | -0.535452 |
| C | 4.859202 | -1.482088 | 0.627423 |
| H | 5.726037 | -1.874751 | 0.106554 |
| H | 4.985687 | -1.485830 | 1.713428 |
| O | -3.702131 | -0.718351 | 1.709377 |
| H | -4.262576 | -1.433726 | 2.027175 |
| O | -3.949740 | 1.725784 | 0.431786 |
| H | -4.029423 | 1.535774 | 1.375810 |
| H | -1.703377 | 0.877090 | 1.390347 |
| H | -3.359970 | -2.756796 | 0.131519 |
| H | -2.895606 | -1.500530 | -2.289729 |

34
Energy TD-DFT:  -1121.99745677

| | | | |
|---|---|---|---|
| C | 3.273000 | -0.052399 | 0.117178 |
| C | 2.503812 | 1.140531 | -0.002144 |
| C | 1.048168 | 0.953243 | 0.016721 |
| C | 0.490773 | -0.351663 | 0.065413 |
| C | 1.351263 | -1.518503 | 0.212173 |
| C | 2.693926 | -1.320353 | 0.235015 |
| C | 0.157787 | 2.035140 | -0.327411 |
| C | -0.925186 | -0.507781 | -0.021432 |
| C | -1.706581 | 0.764059 | 0.260557 |
| N | -1.126147 | 1.952713 | -0.343845 |
| C | -3.171203 | 0.650671 | -0.159523 |
| H | -3.226374 | 0.718616 | -1.248485 |
| C | -3.775188 | -0.669929 | 0.285792 |
| C | -3.032527 | -1.860571 | -0.318354 |
| C | -1.553175 | -1.707226 | -0.247793 |
| O | 0.692098 | 3.217874 | -0.744467 |
| O | 4.619356 | -0.146488 | 0.244641 |
| O | 3.045459 | 2.268081 | -0.123803 |
| H | 0.930572 | -2.504775 | 0.343420 |
| O | 3.700945 | -2.231252 | 0.453165 |
| H | -0.974417 | -2.601784 | -0.447452 |
| O | -3.491880 | -2.054883 | -1.674717 |
| H | -4.817272 | -0.708059 | -0.045296 |
| H | 1.662108 | 3.158310 | -0.614453 |
| C | 4.895339 | -1.543981 | 0.099347 |
| H | 5.139193 | -1.744052 | -0.947633 |
| H | 5.696572 | -1.826403 | 0.774022 |
| O | -3.715903 | -0.673205 | 1.710758 |
| H | -4.280431 | -1.377373 | 2.045943 |
| O | -3.946864 | 1.725619 | 0.347951 |
| H | -4.034599 | 1.568945 | 1.297363 |
| H | -1.709067 | 0.901206 | 1.358213 |
| H | -3.354585 | -2.764281 | 0.210117 |
| H | -2.869757 | -1.595275 | -2.250696 |

34
Energy TD-DFT:  -1121.99600430

| | | | |
|---|---|---|---|
| C | 3.332901 | -0.076942 | 0.002084 |
| C | 2.594746 | 1.136313 | -0.021725 |
| C | 1.132707 | 0.986338 | 0.090358 |
| C | 0.554699 | -0.313025 | 0.143464 |
| C | 1.381129 | -1.503820 | 0.118934 |
| C | 2.729096 | -1.341835 | 0.061425 |
| C | 0.250676 | 2.090116 | -0.171674 |
| C | -0.874531 | -0.408010 | 0.161657 |
| C | -1.527259 | 0.870857 | 0.655577 |
| N | -1.040148 | 2.038629 | -0.064457 |
| C | -3.055550 | 0.834098 | 0.648043 |
| H | -3.417087 | 1.852641 | 0.480084 |
| C | -3.598367 | -0.067254 | -0.442640 |
| C | -3.089989 | -1.487574 | -0.263678 |
| C | -1.595581 | -1.499245 | -0.219675 |
| O | 0.771425 | 3.263867 | -0.632929 |
| O | 4.680731 | -0.217288 | -0.074319 |
| O | 3.148958 | 2.257697 | -0.150227 |
| H | 0.932163 | -2.486185 | 0.166934 |
| O | 3.723758 | -2.292563 | 0.016884 |
| H | -1.107256 | -2.402852 | -0.569690 |
| O | -3.615071 | -2.223753 | -1.376284 |
| H | -3.253579 | 0.301262 | -1.416028 |
| H | 1.746373 | 3.184080 | -0.578734 |
| C | 4.919048 | -1.577474 | 0.304710 |
| H | 5.738657 | -1.977990 | -0.282444 |
| H | 5.118824 | -1.610191 | 1.379365 |
| O | -5.017047 | -0.028541 | -0.367475 |
| H | -5.344938 | -0.764398 | -0.900398 |
| O | -3.501236 | 0.366192 | 1.919234 |
| H | -4.447163 | 0.190683 | 1.832218 |
| H | -1.246328 | 0.979577 | 1.718492 |
| H | -3.534443 | -1.892008 | 0.655777 |
| H | -3.534667 | -3.165024 | -1.191159 |

34
Energy TD-DFT:  -1121.99586191

| | | | |
|---|---|---|---|
| C | 3.330968 | -0.089038 | 0.052701 |
| C | 2.596576 | 1.125339 | 0.002601 |
| C | 1.132772 | 0.982118 | 0.105372 |
| C | 0.551368 | -0.314986 | 0.176191 |
| C | 1.375196 | -1.506711 | 0.208566 |
| C | 2.724055 | -1.349730 | 0.156834 |
| C | 0.257341 | 2.082275 | -0.188763 |
| C | -0.878404 | -0.408072 | 0.178554 |
| C | -1.537379 | 0.883181 | 0.631660 |
| N | -1.035812 | 2.034278 | -0.103869 |
| C | -3.065780 | 0.848733 | 0.598475 |
| H | -3.421630 | 1.862250 | 0.392460 |
| C | -3.591911 | -0.084631 | -0.473387 |
| C | -3.088016 | -1.499468 | -0.245173 |
| C | -1.594439 | -1.510237 | -0.177848 |
| O | 0.787075 | 3.246164 | -0.665340 |
| O | 4.681070 | -0.228203 | 0.079023 |
| O | 3.154875 | 2.244189 | -0.131944 |
| H | 0.924693 | -2.483858 | 0.314931 |
| O | 3.719191 | -2.294118 | 0.273517 |
| H | -1.100677 | -2.424428 | -0.491307 |
| O | -3.596100 | -2.267289 | -1.344216 |
| H | -3.231222 | 0.254978 | -1.451507 |
| H | 1.760816 | 3.166716 | -0.592968 |
| C | 4.900709 | -1.624594 | -0.148124 |
| H | 5.052691 | -1.783722 | -1.219355 |
| H | 5.745033 | -1.959253 | 0.445229 |
| O | -5.011551 | -0.042804 | -0.422422 |
| H | -5.331606 | -0.794185 | -0.938179 |
| O | -3.535211 | 0.421565 | 1.875427 |
| H | -4.479778 | 0.244779 | 1.776841 |
| H | -1.274717 | 1.013006 | 1.697069 |
| H | -3.546754 | -1.877260 | 0.678560 |
| H | -3.521093 | -3.202839 | -1.130079 |

# Triacetyl-narciclasine

## Ground State

```
50
Energy:  -1580.58203455
C                -4.764749       0.014762       0.136885
C                -4.013327      -1.025339      -0.368165
C                -2.607562      -0.859919      -0.331836
C                -2.022231       0.313986       0.176126
C                -2.811965       1.340630       0.697799
C                -4.175086       1.152891       0.652513
C                -1.771414      -1.953871      -0.863288
C                -0.552021       0.445154       0.120332
C                 0.219872      -0.851807       0.116854
N                -0.441594      -1.843180      -0.719691
C                 1.632352      -0.644811      -0.401493
H                 1.608702      -0.401734      -1.466114
C                 2.312433       0.490836       0.341123
C                 1.555318       1.791088       0.086491
C                 0.067705       1.624935       0.090792
O                -2.271719      -2.941522      -1.423303
O                -6.122471       0.083819       0.285423
O                -4.623750      -2.116262      -0.848398
H                -2.385067       2.230853       1.135141
O                -5.148078       1.976170       1.130631
H                 0.098541      -2.660325      -0.977602
H                -0.504292       2.544391       0.064305
H                 3.347412       0.592411       0.022458
H                -3.906043      -2.702119      -1.196921
C                -6.369187       1.455513       0.593232
H                -6.610640       1.995885      -0.325378
H                -7.154224       1.528038       1.338090
O                 2.265637       0.249601       1.749686
O                 2.310863      -1.884876      -0.199912
H                 0.281227      -1.228771       1.145039
C                 3.322813      -0.376769       2.311571
O                 4.281904      -0.735235       1.680074
C                 3.487158      -2.049746      -0.847750
O                 3.908934      -1.240604      -1.631043
C                 3.123625      -0.547984       3.784637
H                 4.002400      -1.013324       4.219338
H                 2.940417       0.422369       4.244553
H                 2.245487      -1.170682       3.956824
C                 4.154049      -3.324809      -0.444808
H                 4.977101      -3.536559      -1.120286
H                 4.532996      -3.195934       0.570270
H                 3.437126      -4.143777      -0.440087
H                 1.861349       2.517379       0.840709
O                 1.914716       2.292837      -1.213941
C                 3.083316       2.963021      -1.306517
O                 3.803474       3.144038      -0.359574
C                 3.341927       3.413255      -2.710308
H                 2.475463       3.948999      -3.094653
H                 3.499861       2.535736      -3.338388
H                 4.223561       4.045978      -2.732477
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50
Energy:  -1580.58198184
C                  -4.605722       1.426273       0.322222
C                  -4.144145       0.397979      -0.471947
C                  -2.750730       0.148820      -0.429804
C                  -1.889758       0.938443       0.353593
C                  -2.390469       1.972194       1.147668
C                  -3.750651       2.181096       1.101601
C                  -2.224179      -0.957044      -1.253120
C                  -0.440206       0.656776       0.303408
C                  -0.061629      -0.758374      -0.060437
N                  -0.926052      -1.268086      -1.115432
C                   1.378731      -0.832632      -0.536369
H                   1.482052      -0.324265      -1.497589
C                   2.306885      -0.170365       0.465330
C                   1.957647       1.310665       0.580631
C                   0.484740       1.577521       0.574210
O                  -2.947593      -1.578299      -2.047109
O                  -5.885106       1.894231       0.444272
O                  -5.002897      -0.295971      -1.229578
H                  -1.756197       2.567740       1.787038
O                  -4.471678       3.133898       1.753280
H                  -0.619658      -2.104832      -1.597021
H                   0.194418       2.594952       0.806332
H                   3.345000      -0.287138       0.162495
H                  -4.456581      -0.944070      -1.741362
O                   2.117471      -0.745900       1.760470
O                   1.672553      -2.221896      -0.686126
H                  -0.164420      -1.391276       0.829434
C                   2.925622      -1.769721       2.113157
O                   3.779418      -2.208596       1.388217
C                   2.789607      -2.538151      -1.380899
O                   3.462036      -1.706478      -1.930730
C                   2.606561      -2.254044       3.492482
H                   3.296437      -3.044712       3.769398
H                   2.675130      -1.425636       4.196555
H                   1.582016      -2.626107       3.512754
C                   3.051925      -4.008809      -1.345836
H                   3.818114      -4.261206      -2.072309
H                   3.397124      -4.261465      -0.342035
H                   2.135899      -4.563196      -1.541388
H                   2.412801       1.698487       1.493018
O                   2.512479       2.010155      -0.548454
C                   3.825059       2.321181      -0.487296
O                   4.515299       2.036472       0.456421
C                   4.273923       3.030437      -1.726525
H                   3.614433       3.871890      -1.932833
H                   4.212214       2.341093      -2.569384
H                   5.297591       3.368756      -1.601050
C                  -5.838795       2.738198       1.594773
H                  -6.147347       2.168921       2.474973
H                  -6.454118       3.616018       1.429658

50
Energy:  -1580.58158409
C                 -4.588943       0.270499      -0.214277
C                 -3.801087       1.223030       0.396645
C                 -2.403753       0.996021       0.366078
C                 -1.862685      -0.152542      -0.239857
C                 -2.688096      -1.088988      -0.865671
C                 -4.041752      -0.841954      -0.824215
C                 -1.529679       1.994317       1.012650
C                 -0.401043      -0.356928      -0.174871
C                  0.424089       0.899856      -0.043498
N                 -0.203458       1.834178       0.880413
C                  1.826135       0.594039       0.453753
H                  1.794340       0.273961       1.497386
C                  2.457352      -0.511346      -0.375154
C                  1.647548      -1.790526      -0.220627
C                  0.164829      -1.561717      -0.250726
O                 -1.995412       2.946864       1.656744
O                 -5.945333       0.278724      -0.387622
O                 -4.370939       2.292214       0.967335
H                 -2.293584      -1.955083      -1.375835
O                 -5.041825      -1.571470      -1.390474
H                  0.367740       2.598194       1.221098
H                 -0.445585      -2.452378      -0.329463
H                  3.484593      -0.685574      -0.062987
H                 -3.635043       2.808516       1.381219
C                 -6.248283      -1.045519      -0.825966
H                 -6.532608      -1.656427       0.034266
H                 -7.020760      -1.011256      -1.586597
O                  2.419638      -0.158805      -1.760332
O                  2.554293       1.817330       0.340271
H                  0.504796       1.368233      -1.032214
C                  3.498154       0.471375      -2.274996
O                  4.474400       0.735844      -1.623706
C                  3.736935       1.888817       0.993507
O                  4.127205       1.009768       1.715007
C                  3.297195       0.778305      -3.725603
H                  3.053404      -0.136411      -4.264355
H                  2.455382       1.463110      -3.831494
H                  4.197396       1.229121      -4.130745
C                  4.453762       3.161960       0.679883
H                  4.836525       3.085554      -0.339109
H                  3.768202       4.006066       0.724786
H                  5.278551       3.297201       1.372723
H                  1.936027      -2.491578      -1.004866
O                  2.048256      -2.334143       1.053860
C                  1.799382      -3.640771       1.261437
O                  1.266256      -4.337648       0.437070
C                  2.263406      -4.076239       2.616670
H                  2.104317      -5.143921       2.729617
H                  1.704372      -3.532441       3.378258
H                  3.318184      -3.833890       2.739552

50
Energy:  -1580.58154117
C                 -4.570941      -0.374723       0.310656
C                 -3.778242      -1.280716      -0.361441
C                 -2.384301      -1.031847      -0.341272
C                 -1.853076       0.102671       0.298779
C                 -2.684621       1.000997       0.970701
C                 -4.033303       0.724599       0.951667
C                 -1.504178      -1.990669      -1.037289
C                 -0.394399       0.328550       0.228528
C                  0.445834      -0.911007       0.040200
N                 -0.179042      -1.817361      -0.912804
C                  1.838079      -0.567089      -0.459810
H                  1.790215      -0.206862      -1.489659
C                  2.464176       0.513434       0.404827
C                  1.635933       1.786547       0.309240
C                  0.156735       1.536759       0.345830
O                 -1.964152      -2.921384      -1.716675
O                 -5.934214      -0.358522       0.419162
O                 -4.341045      -2.320760      -0.989690
H                 -2.298493       1.858855       1.500593
O                 -5.042963       1.453376       1.501247
H                  0.399396      -2.556775      -1.293167
H                 -0.463938       2.415548       0.466709
H                  3.485387       0.713660       0.088550
H                 -3.602042      -2.805987      -1.435149
C                 -6.190541       0.598307       1.446880
H                 -7.067491       1.183045       1.191806
H                 -6.294134       0.082684       2.404754
O                  2.446981       0.106401       1.775399
O                  2.583468      -1.783885      -0.402482
H                  0.543575      -1.415892       1.009195
C                  3.539332      -0.529430       2.252641
O                  4.511418      -0.754552       1.580680
C                  3.759461      -1.813664      -1.070839
O                  4.130019      -0.901722      -1.761228
C                  3.359420      -0.895613       3.692202
H                  3.111263      -0.005841       4.269380
H                  2.527125      -1.594372       3.780655
H                  4.269727      -1.350796       4.068881
C                  4.496096      -3.088615      -0.816028
H                  4.890813      -3.046844       0.200413
H                  3.820703      -3.939222      -0.885498
H                  5.313676      -3.185964      -1.523621
H                  1.923640       2.460131       1.117483
O                  2.015606       2.385145      -0.946895
C                  1.747403       3.695472      -1.100223
O                  1.213767       4.351969      -0.243685
C                  2.191475       4.190179      -2.441720
H                  2.017647       5.259308      -2.510658
H                  1.631304       3.669617      -3.218558
H                  3.247881       3.966661      -2.584686

# Tetraacetyl-narciclasine

## Ground State

```
55
Energy:  -1733.21845319
C                  4.200863      -0.927398       0.554104
C                  3.632713       0.281598       0.256607
C                  2.235347       0.337970       0.086664
C                  1.464367      -0.821956       0.253198
C                  2.061876      -2.049121       0.584123
C                  3.424272      -2.068059       0.712469
C                  1.586971       1.627008      -0.303000
C                 -0.000903      -0.735507       0.089591
C                 -0.593145       0.621284       0.376571
N                  0.239786       1.659966      -0.206714
C                 -1.992227       0.739967      -0.202703
H                 -1.943705       0.763632      -1.293738
C                 -2.849526      -0.440087       0.216421
C                 -2.251911      -1.727592      -0.344036
C                 -0.758456      -1.777003      -0.252385
O                  2.217268       2.596236      -0.707342
O                  5.504253      -1.213206       0.810618
O                  4.435495       1.397792       0.210367
H                  1.473489      -2.937386       0.761630
O                  4.229663      -3.102176       1.071221
H                 -0.185988       2.565022      -0.362689
H                 -0.306901      -2.734226      -0.483390
H                 -3.870565      -0.317338      -0.137754
C                  5.564533      -2.643789       0.834175
H                  5.900625      -3.005318      -0.139503
H                  6.208768      -2.966110       1.644984
O                 -2.847093      -0.564966       1.640842
O                 -2.519829       1.973132       0.287479
H                 -0.655206       0.757787       1.463276
C                 -3.843469       0.040836       2.323017
O                 -4.714478       0.672865       1.785343
C                 -3.630040       2.447605      -0.322181
O                 -4.107974       1.919374      -1.291263
C                 -3.701517      -0.188181       3.794919
H                 -4.535342       0.269973       4.317002
H                 -3.667764      -1.258054       3.997279
H                 -2.761360       0.246320       4.135293
C                 -4.153482       3.662642       0.372713
H                 -3.340824       4.348970       0.603141
H                 -4.901827       4.145223      -0.248288
H                 -4.605524       3.339794       1.311894
H                 -2.694996      -2.569907       0.188965
O                 -2.590277      -1.830508      -1.739103
C                 -3.827215      -2.284691      -2.034299
O                 -4.622807      -2.595946      -1.186832
C                 -4.051702      -2.326698      -3.513478
H                 -5.012354      -2.786638      -3.722423
H                 -3.248308      -2.882313      -3.994764
H                 -4.034934      -1.308154      -3.902636
C                  4.815427       1.834801      -1.028447
O                  4.647593       1.180132      -2.016421
C                  5.449429       3.181665      -0.936360
H                  5.923799       3.430094      -1.880500
H                  6.172514       3.204564      -0.122926
H                  4.660145       3.900710      -0.713230
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55
Energy:  -1733.21829020
C                  4.208543      -0.947342       0.504727
C                  3.642496       0.267749       0.228331
C                  2.243007       0.332314       0.074140
C                  1.471533      -0.831084       0.212826
C                  2.069265      -2.068043       0.505415
C                  3.431036      -2.089706       0.639670
C                  1.592252       1.636753      -0.255898
C                  0.004493      -0.738905       0.064298
C                 -0.586592       0.608075       0.395247
N                  0.245215       1.665451      -0.154238
C                 -1.985932       0.745253      -0.179381
H                 -1.937917       0.798216      -1.269401
C                 -2.844999      -0.444036       0.208631
C                 -2.249810      -1.716999      -0.386682
C                 -0.755920      -1.769281      -0.304020
O                  2.220034       2.624520      -0.617054
O                  5.521876      -1.256649       0.663914
O                  4.454334       1.376893       0.177476
H                  1.482121      -2.962913       0.649907
O                  4.243300      -3.148468       0.895643
H                 -0.179201       2.577439      -0.268103
H                 -0.306897      -2.719772      -0.565615
H                 -3.866155      -0.310473      -0.141208
C                  5.523150      -2.584613       1.200156
H                  6.300829      -3.168340       0.719518
H                  5.644381      -2.534248       2.283728
O                 -2.841995      -0.606933       1.629256
O                 -2.510391       1.966056       0.343841
H                 -0.648303       0.709694       1.485819
C                 -3.836260      -0.016500       2.327773
O                 -4.705386       0.632463       1.807486
C                 -3.620450       2.458377      -0.251902
O                 -4.100799       1.956091      -1.233486
C                 -3.695000      -0.285619       3.792942
H                 -4.526857       0.161758       4.327364
H                 -3.665777      -1.360710       3.966312
H                 -2.753006       0.135624       4.144709
C                 -4.140232       3.656515       0.474320
H                 -3.326114       4.336824       0.717200
H                 -4.890996       4.154119      -0.131729
H                 -4.588142       3.311721       1.407644
H                 -2.690551      -2.572414       0.127145
O                 -2.594588      -1.785528      -1.782296
C                 -3.832789      -2.232603      -2.082835
O                 -4.625340      -2.562157      -1.239424
C                 -4.062627      -2.242526      -3.561753
H                 -5.025781      -2.694332      -3.776845
H                 -3.263141      -2.791402      -4.057140
H                 -4.042900      -1.216321      -3.929969
C                  4.785430       1.846340      -1.063345
O                  4.569670       1.221877      -2.061579
C                  5.437280       3.183822      -0.959931
H                  5.870642       3.456561      -1.916980
H                  6.197280       3.174785      -0.180563
H                  4.667017       3.903040      -0.678731

55
Energy:  -1733.21825591
C                  4.236733      -1.094077       0.146810
C                  3.678569       0.062413      -0.327688
C                  2.271210       0.158173      -0.361113
C                  1.489490      -0.910179       0.103602
C                  2.081322      -2.078923       0.610722
C                  3.447645      -2.142419       0.602718
C                  1.619734       1.372570      -0.939887
C                  0.017481      -0.797076       0.053788
C                 -0.518042       0.611238       0.096798
N                  0.285514       1.473018      -0.753819
C                 -1.957983       0.662353      -0.384054
H                 -2.000676       0.453474      -1.455385
C                 -2.804126      -0.366938       0.342169
C                 -2.285338      -1.766444       0.024363
C                 -0.791213      -1.855021       0.000732
O                  2.235504       2.226050      -1.566806
O                  5.550782      -1.390618       0.327711
O                  4.528359       1.037200      -0.792569
H                  1.489176      -2.885395       1.017433
O                  4.255187      -3.126570       1.078170
H                 -0.126203       2.350914      -1.044922
H                 -0.384496      -2.856863      -0.063483
H                 -3.848125      -0.280896       0.049540
C                  5.569145      -2.791557       0.620702
H                  5.783063      -3.347830      -0.294006
H                  6.289170      -2.987797       1.407610
O                 -2.684834      -0.188512       1.755775
O                 -2.413409       1.991585      -0.129288
H                 -0.484922       0.972553       1.132059
C                 -3.605692       0.587739       2.367896
O                 -4.504482       1.126436       1.776944
C                 -3.559390       2.371697      -0.738793
O                 -4.129680       1.670617      -1.532447
C                 -3.345164       0.669375       3.839102
H                 -2.367014       1.121204       4.004913
H                 -4.117797       1.266048       4.313192
H                 -3.326051      -0.333913       4.263204
C                 -3.993107       3.726905      -0.282384
H                 -4.783211       4.095112      -0.929475
H                 -4.366345       3.630862       0.738423
H                 -3.148578       4.413477      -0.273784
H                 -2.697188      -2.458380       0.760287
O                 -2.747589      -2.149737      -1.283694
C                 -4.013903      -2.610034      -1.372268
O                 -4.737889      -2.704162      -0.415682
C                 -4.367798      -2.958022      -2.784323
H                 -3.620595      -3.633601      -3.197874
H                 -4.365227      -2.047458      -3.384295
H                 -5.351787      -3.415321      -2.810344
C                  4.542068       2.237805      -0.140120
O                  3.999837       2.401075       0.914850
C                  5.313968       3.247591      -0.920462
H                  4.711912       3.520123      -1.788513
H                  6.249736       2.819254      -1.274939
H                  5.498636       4.123390      -0.306463

55
Energy:  -1733.21806035
C                  4.230989      -1.112520       0.105699
C                  3.674221       0.047439      -0.361629
C                  2.267017       0.147426      -0.390214
C                  1.483697      -0.927394       0.056489
C                  2.073990      -2.106912       0.540008
C                  3.440643      -2.167130       0.542946
C                  1.617194       1.377067      -0.938171
C                  0.011535      -0.806140       0.020392
C                 -0.516252       0.603562       0.098476
N                  0.284891       1.479625      -0.739663
C                 -1.959778       0.672900      -0.369155
H                 -2.012382       0.488848      -1.444589
C                 -2.805432      -0.368259       0.340528
C                 -2.296458      -1.762844      -0.012853
C                 -0.803029      -1.858474      -0.049641
O                  2.231764       2.240547      -1.552421
O                  5.545128      -1.444902       0.202560
O                  4.524328       1.018392      -0.834642
H                  1.480905      -2.924997       0.921099
O                  4.245185      -3.189805       0.933136
H                 -0.125113       2.364940      -1.009914
H                 -0.402169      -2.860869      -0.137589
H                 -3.851333      -0.270489       0.058565
C                  5.565186      -2.639642       0.991649
H                  6.271208      -3.343799       0.564455
H                  5.801510      -2.383584       2.025948
O                 -2.673819      -0.222279       1.756764
O                 -2.405928       1.998349      -0.080382
H                 -0.472791       0.941802       1.141121
C                 -3.585658       0.544625       2.393632
O                 -4.486866       1.100341       1.822442
C                 -3.554458       2.398436      -0.671992
O                 -4.134900       1.718643      -1.476719
C                 -3.312213       0.592677       3.863984
H                 -2.331629       1.038739       4.031125
H                 -4.079189       1.180336       4.358092
H                 -3.291587      -0.419786       4.265534
C                 -3.976913       3.745266      -0.181434
H                 -4.770464       4.132196      -0.813185
H                 -4.341930       3.628257       0.840153
H                 -3.128581       4.426980      -0.164678
H                 -2.706398      -2.469092       0.710458
O                 -2.770753      -2.114207      -1.325530
C                 -4.040477      -2.564997      -1.414452
O                 -4.757762      -2.675855      -0.454619
C                 -4.407321      -2.878932      -2.831139
H                 -3.668483      -3.551053      -3.264896
H                 -4.401812      -1.955351      -3.410864
H                 -5.395047      -3.327932      -2.859947
C                  4.564723       2.210024      -0.167361
O                  4.044077       2.365730       0.899634
C                  5.333877       3.220961      -0.948971
H                  4.718151       3.513489      -1.800764
H                  6.256705       2.785957      -1.328332
H                  5.542062       4.085577      -0.326685

55
Energy:  -1733.21784169
C -4.114584 0.917015 0.298457
C -3.541002 -0.178288 -0.289437
C -2.132800 -0.240227 -0.351053
C -1.365369 0.796267 0.201226
C -1.972142 1.900909 0.821639
C -3.339421 1.934997 0.839353
C -1.465838 -1.380991 -1.049762
C 0.107849 0.715647 0.125996
C 0.661877 -0.683910 0.046876
N -0.129063 -1.476578 -0.879712
C 2.106168 -0.684805 -0.423825
H 2.157309 -0.411271 -1.479936
C 2.931913 0.309258 0.373951
C 2.397007 1.715744 0.146500
C 0.898139 1.788386 0.160158
O -2.071650 -2.178142 -1.755413
O -5.431148 1.166201 0.526040
O -4.378489 -1.124468 -0.829935
H -1.389403 2.678309 1.293380
O -4.158692 2.851858 1.418029
H 0.295714 -2.315459 -1.254785
H 0.476900 2.785104 0.196156
H 3.978152 0.261824 0.080284
C -5.473797 2.531641 0.953688
H -5.718106 3.168224 0.101098
H -6.182220 2.634164 1.768485
O 2.802893 0.034750 1.771304
O 2.574931 -2.021870 -0.243152
H 0.625243 -1.132336 1.047590
C 3.726712 -0.771859 2.337729
O 4.642936 -1.250849 1.722595
C 3.729511 -2.356105 -0.863289
O 4.298719 -1.606681 -1.611882
C 3.443012 -0.972253 3.793121
H 3.348479 -0.006478 4.287518
H 2.493161 -1.497159 3.899906
H 4.241234 -1.553918 4.242917
C 4.173794 -3.730084 -0.478324
H 3.334863 -4.422943 -0.504384
H 4.966181 -4.057968 -1.144077
H 4.547852 -3.683791 0.545710
H 2.811169 2.381173 0.905089
O 2.913222 2.107930 -1.141674
C 2.930264 3.426577 -1.412237
O 2.531739 4.252916 -0.632615
C 3.494356 3.697454 -2.772410
H 2.859871 3.228050 -3.524180
H 4.487694 3.257494 -2.851681
H 3.540634 4.768791 -2.939940
C -4.350510 -2.382639 -0.297552
O -3.778805 -2.634862 0.723802
C -5.120870 -3.329658 -1.154392
H -5.268154 -4.266090 -0.625708
H -4.538190 -3.500166 -2.060795
H -6.075825 -2.892226 -1.439932

55
Energy:  -1733.21764260
C -4.108116 0.945452 0.268491
C -3.538390 -0.150644 -0.321369
C -2.130259 -0.219945 -0.378833
C -1.359337 0.819366 0.163349
C -1.962630 1.934017 0.769128
C -3.329897 1.966468 0.798112
C -1.466569 -1.375443 -1.056558
C 0.114201 0.726587 0.100963
C 0.657693 -0.678261 0.046283
N -0.131723 -1.477670 -0.875713
C 2.105933 -0.697621 -0.411582
H 2.168671 -0.439862 -1.471035
C 2.932637 0.301335 0.379048
C 2.411063 1.708544 0.126528
C 0.912751 1.793317 0.126660
O -2.072576 -2.178145 -1.755695
O -5.426351 1.240693 0.418054
O -4.378567 -1.085303 -0.877988
H -1.377725 2.721253 1.221202
O -4.146984 2.928172 1.301451
H 0.290460 -2.323380 -1.238136
H 0.499575 2.793884 0.146807
H 3.980935 0.241364 0.095273
C -5.452881 2.343288 1.331002
H -6.184738 3.071685 0.998606
H -5.656864 1.972010 2.337042
O 2.789311 0.048081 1.779022
O 2.562076 -2.035713 -0.207531
H 0.608727 -1.111999 1.052959
C 3.700801 -0.758847 2.364610
O 4.617568 -1.254997 1.764053
C 3.719841 -2.387916 -0.811534
O 4.302505 -1.653659 -1.564786
C 3.402871 -0.936313 3.820133
H 3.312849 0.037068 4.300251
H 2.447460 -1.451227 3.925955
H 4.191914 -1.518723 4.284902
C 4.148652 -3.760218 -0.403719
H 3.304057 -4.446211 -0.428286
H 4.944394 -4.103891 -1.057404
H 4.513542 -3.703210 0.623066
H 2.824058 2.381656 0.878965
O 2.941663 2.077724 -1.162537
C 2.971769 3.392114 -1.451991
O 2.572139 4.232730 -0.688368
C 3.551854 3.638880 -2.810015
H 2.922801 3.161669 -3.561417
H 4.543413 3.192073 -2.871688
H 3.606352 4.707252 -2.993258
C -4.380291 -2.341606 -0.340676
O -3.831617 -2.598318 0.692147
C -5.149301 -3.279921 -1.208237
H -5.321148 -4.211819 -0.678950
H -4.552642 -3.463137 -2.102974
H -6.091739 -2.828700 -1.513239

# Template Molecule

## Ground State

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25
Energy:   -780.20298310
C                 -3.260375      -0.046766      -0.079939
C                 -2.480859       1.078274       0.084459
C                 -1.078665       0.879266       0.065019
C                 -0.525202      -0.406863      -0.077192
C                 -1.343631      -1.525156      -0.247725
C                 -2.701932      -1.300964      -0.238372
C                 -0.211029       2.060225       0.265809
C                  0.946544      -0.534960      -0.015816
C                  1.696641       0.686275      -0.469047
N                  1.108644       1.886691       0.116544
C                  1.575063      -1.630257       0.399864
O                 -0.686210       3.168752       0.567872
O                 -4.624335      -0.127691      -0.173432
O                 -3.059800       2.276641       0.241085
H                 -0.937144      -2.515160      -0.394127
O                 -3.701379      -2.207939      -0.426421
H                  1.672473       2.723217       0.179046
H                  1.035928      -2.513133       0.718674
H                 -2.321497       2.914409       0.414015
C                 -4.897943      -1.521502      -0.043387
H                 -5.119337      -1.752416       1.001810
H                 -5.706196      -1.799762      -0.711068
H                  1.654705       0.755851      -1.561778
H                  2.739693       0.629272      -0.167991
H                  2.656504      -1.670150       0.435626
```

## Excited State S1 N

```
25
Energy TD-DFT:   -780.061902827
C                  1.762175       0.441522       0.040431
C                  0.611825       1.228359       0.079634
C                 -0.627576       0.544303       0.086994
C                 -0.673489      -0.905393      -0.025752
C                  0.552030      -1.669312      -0.083328
C                  1.710630      -0.984577      -0.046940
C                 -1.805851       1.335828       0.003636
C                 -1.936059      -1.545803      -0.013998
C                 -3.148924      -0.698732       0.305452
N                 -2.990252       0.679830      -0.123135
C                 -2.133848      -2.892982      -0.186210
O                 -1.772769       2.610849      -0.015784
O                  3.029079       0.850033       0.050925
O                  0.680292       2.544703       0.104704
H                  0.543665      -2.746990      -0.136843
O                  2.991698      -1.440777      -0.033656
H                 -3.808828       1.270731      -0.080842
H                 -1.328030      -3.582284      -0.395161
H                 -0.319135       2.841538       0.063116
C                  3.837894      -0.312711      -0.196093
H                  4.202575      -0.262050      -1.222495
H                  4.642270      -0.345351       0.532243
H                 -3.322888      -0.751780       1.389864
H                 -4.027186      -1.113641      -0.186468
H                 -3.133075      -3.306612      -0.134204
```

## Excited State S1 T

```
25
Energy TD-DFT:   -780.069800453
C                 -1.774582       0.429509      -0.059569
C                 -0.639284       1.269921      -0.043618
C                  0.640705       0.552451      -0.049039
C                  0.680519      -0.866850      -0.010899
C                 -0.531991      -1.654737      -0.032770
C                 -1.705903      -0.988870      -0.052550
C                  1.819403       1.291410       0.102826
C                  1.970064      -1.522013       0.008811
C                  3.143232      -0.654326      -0.391066
N                  3.018261       0.667852       0.208440
C                  2.163916      -2.825295       0.292937
O                  1.852005       2.620339       0.225313
O                 -3.053028       0.819182      -0.101616
O                 -0.703865       2.529943      -0.018962
H                 -0.496169      -2.732909      -0.062384
O                 -2.977917      -1.470455      -0.144146
H                  3.823806       1.275147       0.145359
H                  1.353983      -3.493903       0.550984
H                  0.905220       2.920243       0.167521
C                 -3.841410      -0.366145       0.088238
H                 -4.196898      -0.380152       1.119612
H                 -4.652632      -0.374371      -0.632648
H                  3.163302      -0.574800      -1.486687
H                  4.078249      -1.100174      -0.061841
H                  3.161393      -3.246010       0.284236
```

## Excited State S1 N + MeOH

31
Energy:  -895.790595008

| | | | |
|---|---|---|---|
| C | -1.859777 | 0.407962 | 0.031805 |
| C | -0.848927 | 1.310817 | 0.350408 |
| C | 0.478818 | 0.820537 | 0.320093 |
| C | 0.736344 | -0.585520 | 0.035720 |
| C | -0.352236 | -1.478761 | -0.273836 |
| C | -1.596856 | -0.964991 | -0.268879 |
| C | 1.514200 | 1.687603 | 0.754789 |
| C | 2.081238 | -1.033357 | 0.004937 |
| C | 3.169751 | 0.015470 | 0.066915 |
| N | 2.772899 | 1.180894 | 0.834917 |
| C | 2.468114 | -2.337537 | -0.159222 |
| O | 1.283917 | 2.896937 | 1.123106 |
| O | -3.167159 | 0.643015 | -0.029983 |
| O | -1.134879 | 2.561822 | 0.667896 |
| H | -0.178544 | -2.514866 | -0.519613 |
| O | -2.784148 | -1.552675 | -0.570860 |
| H | 3.494776 | 1.859185 | 1.055275 |
| H | 1.764343 | -3.155048 | -0.227670 |
| H | -0.230080 | 2.972694 | 0.915994 |
| C | -3.807904 | -0.627396 | -0.238177 |
| H | -4.291525 | -0.921697 | 0.693384 |
| H | -4.508292 | -0.537805 | -1.063034 |
| H | 3.424587 | 0.299274 | -0.964823 |
| H | 4.065049 | -0.407196 | 0.519448 |
| H | 3.519926 | -2.590272 | -0.204784 |
| H | 2.819658 | 3.840947 | 1.183648 |
| O | 3.757690 | 4.034865 | 0.995099 |
| C | 3.865784 | 4.219989 | -0.406810 |
| H | 3.323769 | 5.108811 | -0.740093 |
| H | 4.919927 | 4.345584 | -0.648299 |
| H | 3.483985 | 3.353584 | -0.958178 |

## Excited State S1 T + MeOH

```
31
Energy:   -895.795519027
C                 -1.845947       0.402202      -0.055974
C                 -0.880017       1.347680       0.353850
C                  0.492004       0.833142       0.376118
C                  0.767336      -0.522722       0.058883
C                 -0.279193      -1.425709      -0.362458
C                 -1.538099      -0.940603      -0.403227
C                  1.501517       1.650545       0.896008
C                  2.139082      -0.979382       0.131085
C                  3.182656       0.115317       0.146888
N                  2.772250       1.197722       1.032962
C                  2.515747      -2.272495       0.126411
O                  1.273350       2.888181       1.362349
O                 -3.155283       0.618507      -0.207262
O                 -1.159018       2.534123       0.685896
H                 -0.055288      -2.437755      -0.663203
O                 -2.687601      -1.538572      -0.824269
H                  3.461162       1.925528       1.203409
H                  1.805455      -3.087167       0.085235
H                  0.297944       3.055158       1.217218
C                 -3.749654      -0.661429      -0.475784
H                 -4.239449      -1.009845       0.434447
H                 -4.437805      -0.566081      -1.309703
H                  3.307614       0.492738      -0.878374
H                  4.139054      -0.272463       0.487899
H                  3.563736      -2.538804       0.180872
H                  2.949616       4.063339       1.233617
O                  3.833772       3.979128       0.851970
C                  3.685321       3.993892      -0.562112
H                  3.321141       4.960383      -0.916521
H                  4.665976       3.807345      -0.995097
H                  2.996681       3.212912      -0.901491
```