Supporting information for:
Solvatochromic Effects on the Absorption Spectrum of 2-Thiocytosine

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Level of Theory

Table S1 presents the dielectric constants at low and infinite frequencies employed in the PCM calculations with MOLCAS for the six considered solvents.

Table S1: Dielectric constants $\epsilon$ and square of refractive index $n^2 = \epsilon_\infty$ employed in the PCM calculations.

| Solvent | $\epsilon$ | $n^2$ |
|---------|------------|-------|
| EtOAc   | 6.02       | 1.882 |
| ACN     | 36.64      | 1.806 |
| DMSO    | 46.70      | 2.179 |
| EtOH    | 24.55      | 1.847 |
| MeOH    | 32.63      | 1.758 |
| $H_2O$  | 78.39      | 1.776 |

For the micro-solvated vertical excitation calculations, it was not possible to use the large ANO-RCC-VQZP basis set like in the vacuum reference calculation, since for the EtOH and EtOAc micro-solvated structures this basis set would imply more than 2300 basis functions, currently too many for MS-CASPT2 computations at our available computational capabilities. Hence, the micro-solvated vertical excitation calculations were conducted with the more economical cc-pVDZ basis set, which leads to only 500 basis functions for the largest systems.

As shown in Reference S1, with such smaller basis sets it is advantageous to set the IPEA shift to zero, because the effect of the small basis set and the effect of the neglected shift cancel out to a large degree.

In order to scrutinize that the combination “cc-pVDZ+zero IPEA shift” still gives satisfactory results compared to the reference setup “ANO-RCC-VQZP+default IPEA shift”, we performed an MS-CASPT2 calculation for the $H_2O$-micro-solvated structure, with ANO-RCC-VQZP for 2tCyt, ANO-RCC-VDZP for water, and the default IPEA shift. This computation should give results very close to the “ANO-RCC-VQZP+default IPEA shift” computation as only the water molecules, which do not participate directly in the excitation, are described with the smaller basis set.

![Graph](image_url)

Figure S1: Comparison of the MS-CASPT2(14,10) vertical excitation energies for micro-solvated (H$_2$O) 2tCyt with “ANO-RCC-VQZP+default IPEA shift” ($E_{QZ+IPEA}$) and with “cc-pVDZ+zero IPEA shift” ($E_{DZ-IPEA}$). Both computations employ the same geometry (optimized with BP86/aug-cc-pVDZ, see below for coordinates).

Figure S1 compares the results of the quadruple-ζ computation ($E_{QZ+IPEA}$) with the double-ζ
the molar absorptivities function using (FWHM), and experimental spectra (Table S2: Fitting parameters and their standard errors for the Gaussian fits of the are given in Table S2.

\[
\sigma(E) = \sum_{i=1}^{N} g_i = \sum_{i=1}^{N} A_i \exp \left(-4 \ln 2 \frac{(E-E_i)^2}{F_{2i}^2}\right),
\]

where \(\sigma(E)\) is the total fitted spectrum, \(A_i\) are the heights of the Gaussians (i.e., the molar absorptivities), \(E_i\) are the central energies of the Gaussians, \(F_i\) are the full widths at half maximum (FWHM), and \(N = 5\) or \(3\) is the number of Gaussians employed. The spectra were fitted to this function using Gnuplot 5.0\textsuperscript{S3} with the Marquardt-Levenberg algorithm, under the constraint that the molar absorptivities \(A_i\) remain larger than zero. The fitted parameters and their standard errors are given in Table S2.

Table S2: Fitting parameters and their standard errors for the Gaussian fits of the experimental spectra (\(E\) and \(F\) in eV, \(A\) in M\(^{-1}\)cm\(^{-1}\)).

| Solvent | \(E_1\) | \(\delta E_1\) | \(E_2\) | \(\delta E_2\) | \(E_3\) | \(\delta E_3\) | \(E_4\) | \(\delta E_4\) | \(E_5\) | \(\delta E_5\) |
|---------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| EtOAc   | 3.78   | ±0.01  | 4.32   | ±0.00  | 4.86   | ±0.01  | —      | —      | —      | —      |
| ACN     | 3.98   | ±0.02  | 4.38   | ±0.00  | 5.05   | ±0.22  | 5.48   | ±0.08  | 6.20   | ±0.03  |
| DMSO    | 4.03   | ±0.02  | 4.34   | ±0.00  | 4.79   | ±0.01  | —      | —      | —      | —      |
| EtOH    | 3.88   | ±0.01  | 4.42   | ±0.00  | 5.12   | ±0.02  | 5.80   | ±0.02  | 6.14   | ±0.09  |
| MeOH    | 3.91   | ±0.02  | 4.45   | ±0.00  | 5.13   | ±0.03  | 5.77   | ±0.01  | 6.22   | ±0.09  |
| H\(_2\)O | 3.96   | ±0.01  | 4.59   | ±0.00  | 5.12   | ±0.00  | 5.46   | ±0.05  | 6.33   | ±0.42  |

| Solvent | \(F_1\) | \(\delta F_1\) | \(F_2\) | \(\delta F_2\) | \(F_3\) | \(\delta F_3\) | \(F_4\) | \(\delta F_4\) | \(F_5\) | \(\delta F_5\) |
|---------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| EtOAc   | 0.29   | ±0.03  | 0.37   | ±0.01  | 0.66   | ±0.08  | —      | —      | —      | —      |
| ACN     | 0.52   | ±0.02  | 0.37   | ±0.01  | 0.79   | ±0.26  | 0.60   | ±0.15  | 0.65   | ±0.23  |
| DMSO    | 0.53   | ±0.02  | 0.36   | ±0.00  | 0.60   | ±0.07  | —      | —      | —      | —      |
| EtOH    | 0.37   | ±0.02  | 0.48   | ±0.01  | 0.74   | ±0.04  | 0.31   | ±0.09  | 0.99   | ±0.25  |
| MeOH    | 0.40   | ±0.03  | 0.48   | ±0.01  | 0.74   | ±0.06  | 0.36   | ±0.10  | 0.99   | ±0.61  |
| H\(_2\)O | 0.28   | ±0.03  | 0.58   | ±0.00  | 0.40   | ±0.02  | 0.75   | ±0.58  | 1.35   | ±0.96  |

| Solvent | \(A_1\) | \(\delta A_1\) | \(A_2\) | \(\delta A_2\) | \(A_3\) | \(\delta A_3\) | \(A_4\) | \(\delta A_4\) | \(A_5\) | \(\delta A_5\) |
|---------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| EtOAc   | 608    | ±52    | 15666  | ±537   | 8670   | ±77    | —      | —      | —      | —      |
| ACN     | 2389   | ±71    | 14851  | ±547   | 8807   | ±3698  | 6770   | ±7210  | 3127   | ±183   |
| DMSO    | 2425   | ±111   | 15291  | ±675   | 8427   | ±76    | —      | —      | —      | —      |
| EtOH    | 1165   | ±48    | 16638  | ±189   | 13633  | ±480   | 1104   | ±662   | 5819   | ±166   |
| MeOH    | 1219   | ±57    | 16445  | ±321   | 14247  | ±948   | 1968   | ±1695  | 6240   | ±211   |
| H\(_2\)O | 435    | ±48    | 17811  | ±904   | 10483  | ±3013  | 9035   | ±21510 | 3596   | ±2713  |

As can be seen in the table, the standard errors for \(g_1\) and \(g_2\) are all relatively small (at most 15\% for \(A_1\) of MeOH). For the remaining Gaussians \(g_3\) to \(g_5\), the central energies also show small relative errors (at most 7\%). Some of the FWHM and absorptivities show larger errors, due to different reasons: Gaussian \(g_4\) for EtOH and MeOH has only a very small intensity; Gaussians \(g_3\)
and $g_4$ for ACN and H$_2$O are noticeably correlated; and $g_5$ is fitted to the absorption at the spectral boundary, making it statistically less meaningful.

The fits show that the EtOAc and DMSO spectra can be well described with three Gaussians. For ACN, at least four Gaussians are required, although the second-lowest absorption bands shape suggests that it is better described with one additional Gaussian, for a total of five. Similarly, the measured spectra of EtOH, MeOH, and H$_2$O could possibly be described with four Gaussians, but the band shape suggests that five Gaussians better describe the spectral features.

Figure S2 presents the residuals from the Gaussian fits. The absolute values of the residuals never exceed 1000 M$^{-1}$cm$^{-1}$, and this value is only reached at the edge of the EtOAc spectrum, where fitting is difficult because the second absorption band is covered by solvent absorption. As can be seen in the figure, the relative errors rarely exceed 5%, with the spectrum in EtOAc showing the largest relative errors. In general, the oscillations in the residuals arise due to the deviation of the actual line shape from the idealized Gaussian line shape we assumed in the fits. These oscillations could be reduced by fitting with more Gaussians, but—since the residuals are already small—these additional Gaussians would hardly be statistically meaningful. We therefore are confident that three or five Gaussians are the proper number to describe the measured spectra.

![Figure S2](image-url)

Figure S2: Residuals from the Gaussian decompositions of the absorptivity spectra of 2tCyt (arranged like in Figure 3 of the main manuscript, but note the different y axis range). The gray area reproduces the experimental spectra divided by 20, therefore showing where the residual exceed a relative error of 5%.
Solvatochromic Analyses

We performed three different solvatochromic analyses with the absorption energies from the six solvents considered here. In these analyses, the solvent-dependent energy shifts of the absorption bands are linearly related to several solvatochromic parameters, as given by Catalán,\textsuperscript{S4} Kamlet-Taft,\textsuperscript{S5} or Reichardt.\textsuperscript{S6} All analyses use the same absorption energy data. We consider the energies of the lowest-energy absorption maximum $E_{\text{max}}$, as well as the energies where the red tail falls below a given absorptivity. The latter energies are denoted as $E_{200}$, $E_{300}$, $E_{400}$, and $E_{500}$ for the energies where the absorptivity is 200 to 500 M\textsuperscript{−1}cm\textsuperscript{−1}, respectively. We focus on these two spectral features, in part because the corresponding transitions play a key role in the photophysics of 2tCyt, but also because in DMSO and EtOAc the high-energy band is overshadowed by the strong absorption of the solvents below 250 nm and thus we cannot determine the energetic position of this band.

The fitting data is presented in Table S3.

Table S3: Energies of the lowest-energy absorption maximum and absorption tail (at 200–500 M\textsuperscript{−1}cm\textsuperscript{−1}) of 2tCyt in different solvents.

| Solvent | $E_{\text{max}}$ (eV) | $E_{200}$ (eV) | $E_{300}$ (eV) | $E_{400}$ (eV) | $E_{500}$ (eV) |
|---------|-----------------|----------------|----------------|----------------|----------------|
| EtOAc   | 4.33            | 3.53           | 3.60           | 3.67           | 3.73           |
| ACN     | 4.38            | 3.47           | 3.51           | 3.55           | 3.58           |
| DMSO    | 4.34            | 3.51           | 3.57           | 3.60           | 3.62           |
| EtOH    | 4.43            | 3.53           | 3.60           | 3.64           | 3.67           |
| MeOH    | 4.46            | 3.55           | 3.62           | 3.66           | 3.69           |
| H$_2$O  | 4.61            | 3.73           | 3.79           | 3.83           | 3.85           |

Catalán Analysis

The Catalán solvent scale employs four parameters, which are the solvent acidity $SA$, solvent basicity $SB$, solvent dipolarity $SdP$, and solvent polarizability $SP$. The parameters for the six solvents are given in Table S4.

Table S4: Catalán parameters$^{S4}$ SA, SB, SdP, and SP for the six solvents.

| Solvent | SA  | SB  | SdP | SP  |
|---------|-----|-----|-----|-----|
| EtOAc   | 0.000 | 0.542 | 0.603 | 0.656 |
| ACN     | 0.044 | 0.286 | 0.974 | 0.645 |
| DMSO    | 0.072 | 0.647 | 1.000 | 0.830 |
| EtOH    | 0.400 | 0.658 | 0.783 | 0.633 |
| MeOH    | 0.605 | 0.545 | 0.904 | 0.608 |
| H$_2$O  | 1.062 | 0.025 | 0.997 | 0.681 |

For $E_{\text{max}}$, a linear regression with the “only SA” model yields:

$$E_{\text{max}} = (4.34 \pm 0.01) + (0.24 \pm 0.02)SA \quad (R^2 = 0.96),$$

whereas the other single-parameter fits did not satisfactorily explain the data ($R^2 = 0.52$ for “only SB”, $R^2 = 0.17$ for “only SdP”, $R^2 = 0.08$ for “only SP”). The “SA+SB” model yielded ($R^2 = 0.99$): $E_{\text{max}} = (4.39 \pm 0.02) + (0.21 \pm 0.02)SA + (-0.09 \pm 0.03)SB \quad (R^2 = 0.99)$,
Both models also have a high statistical significance ($p < 0.001$). Adding the SdP and/or SP parameters to these two models did not lead to statistically significant improvements of the fit.

For the red tail absorption energies, no single-parameter model can describe the energies in Table S3 well. The best results are obtained for the $E_{200}$ set: “only SA” gives $R^2 = 0.81$, “only SB” $R^2 = 0.47$, “only SdP” $R^2 = 0.05$, and “only SP” $R^2 = 0.00$. The best of those, “only SA” model, is given by:

$$E_{200} = (3.48 \pm 0.03) + (0.20 \pm 0.05)\text{SA}.$$

Models with more than one parameter do not significantly improve the fits. Hence, the most important parameter for the position of the red absorption tail seems to be the solvent acidity, although it appears that the Catalán parameters do not describe the tail position as well as the maximum position. This could be due to the low signal-to-noise ratio of the red tail data.

**Kamlet-Taft Analysis**

The Kamlet-Taft solvent scale employs several parameters, of which the solvent polarizability $\pi^*$, hydrogen bond acceptor basicity $\beta$, and hydrogen bond donor acidity $\alpha$ are the most important ones. The relevant data for the Kamlet-Taft analysis is gathered in Table S5.

| Solvent | $\pi^*$ | $\alpha$ | $\beta$ |
|---------|---------|---------|---------|
| EtOAc   | 0.55    | 0.00    | 0.45    |
| ACN     | 0.75    | 0.19    | 0.31    |
| DMSO    | 1.00    | 0.00    | 0.76    |
| EtOH    | 0.54    | 0.83    | 0.77    |
| MeOH    | 0.60    | 0.93    | 0.62    |
| H$_2$O  | 1.09    | 1.17    | 0.18    |

Different linear regression models were found to fit the data:

$$E_{\text{max}} = (4.33 \pm 0.03) + (0.18 \pm 0.04)\alpha$$

$$E_{\text{max}} = (4.41 \pm 0.04) + (0.17 \pm 0.03)\alpha + (-0.14 \pm 0.06)\beta$$

$$E_{\text{max}} = (4.22 \pm 0.05) + (0.18 \pm 0.03)\alpha + (0.15 \pm 0.06)\pi^*$$

$$E_{\text{max}} = (4.31 \pm 0.03) + (0.17 \pm 0.01)\alpha + (-0.10 \pm 0.02)\beta + (0.11 \pm 0.02)\pi^*$$

which all show similar significance ($p < 0.02$). All these models involve $\alpha$, which is apparently the most important parameter to describe the solvatochromic shifts of the absorption maximum, although $\beta$ and $\pi^*$ appear to also play a minor role based on the Kamlet-Taft analysis.

We also carried out the Kamlet-Taft analysis for the red absorption tail energies. No linear regression model involving $\alpha$, $\beta$, and $\pi^*$ was able to describe the tail energies to a significant extent (all models have $p > 0.1$), with $R^2$ never above 0.8. Hence, the Kamlet-Taft scale is not able to describe well the energetic shifts of the red absorption tail.

**Reichardt Analysis**

We also carried out a solvatochromic analysis based on the Reichardt parameter $E_{T}^{N}$, considering also a second, general parameter $f(n^2)$ describing induction and dispersion. The parameters
for the six solvents are given in Table S6. Note that we have chosen to use the dimensionless $E_N^T$ parameter rather than Reichardt’s $E_T(30)$ values, because the parameters of the Catalán and Kamlet-Taft analyses are also dimensionless. Because Reichardt and coworkers\textsuperscript{S11} argue that the $f(n^2)$ parameter should not be applied to protic solvents, we assume a value of zero for these solvents (see Table S6).

**Table S6: Reichardt $E_N^T$ and $f(n^2)$ parameters\textsuperscript{S6,S11} for the six solvents.**

| Solvent | $E_N^T$ | $f(n^2)$ |
|---------|---------|----------|
| EtOAc   | 0.228   | 0.185    |
| ACN     | 0.460   | 0.175    |
| DMSO    | 0.444   | 0.221    |
| EtOH    | 0.654   | 0        |
| MeOH    | 0.762   | 0        |
| H2O     | 1.000   | 0        |

The linear regression for the lowest-energy maximum showed that the $E_N^T$ parameter can describe the absorption energies quite well ($p<0.01$):

$$E_{max} = (3.87 \pm 0.09) + (0.26 \pm 0.04)E_N^T \quad (R^2 = 0.91).$$

The addition of the $f(n^2)$ parameter to the model does not lead to statistically significant improvements of the fit. However, as the $E_N^T$ parameter subsumes both hydrogen bond and electrostatic interactions, this good fit does not allow to draw conclusions regarding the influence of the different solvent effects.

For the red absorption tail data, the $E_N^T$ and $f(n^2)$ parameters do not provide satisfactory fits, with the largest $R^2$ values around 0.6.

**Structural Parameters**

In Table S7, we compile the most relevant bond lengths of 2tCyt in the different solvents, taken from the coordinate data below. Columns printed in bold (the $S=C_2-N_3=C_4-N$ moiety mentioned in the main manuscript) are the ones exhibiting the largest changes when going from vacuum to water.

**Table S7: Bond lengths (Å) of 2tCyt from the above coordinate data.**

| Solvent | $r_{N_1-C_2}$ | $r_{C_2-N_3}$ | $r_{N_3=C_4}$ | $r_{C_4-C_5}$ | $r_{C_5=C_6}$ | $r_{C_6-N_1}$ | $r_{C-S}$ | $r_{C_4-N_{amino}}$ |
|---------|--------------|--------------|--------------|--------------|--------------|--------------|----------|-------------------|
| Vacuum  | 1.416        | 1.364        | 1.339        | 1.442        | 1.374        | 1.360        | 1.685    | 1.364             |
| EtOAc   | 1.396        | 1.352        | 1.357        | 1.440        | 1.372        | 1.364        | 1.718    | 1.348             |
| ACN     | 1.391        | 1.350        | 1.361        | 1.439        | 1.371        | 1.365        | 1.723    | 1.347             |
| DMSO    | 1.391        | 1.349        | 1.365        | 1.440        | 1.372        | 1.364        | 1.728    | 1.345             |
| EtOH    | 1.384        | 1.349        | 1.370        | 1.439        | 1.370        | 1.366        | 1.734    | 1.341             |
| MeOH    | 1.383        | 1.348        | 1.370        | 1.439        | 1.370        | 1.366        | 1.734    | 1.341             |
| H2O     | 1.384        | 1.348        | 1.370        | 1.439        | 1.370        | 1.367        | 1.736    | 1.341             |
Comparison of Gas Phase Calculations

In Figure S3 we compare the gas phase energies, reported in the main manuscript in Tables 3 and 4. In Table 3, the results were computed with MS(9)-CASPT2(14,10)/ANO-RCC-VQZP (default IPEA shift, no level shift). In Table 4, the results were computed with the smaller cc-pVDZ basis set (IPEA shift set to zero, 0.3 a.u. imaginary level shift). The agreement for these two gas-phase calculations is slightly worse than the one above for the micro-solvated geometries. Nevertheless, the standard deviation is only 0.12 eV for the energies and 0.03 for the oscillator strengths, which shows that the cheaper level of theory can reasonably reproduce the results of the more expensive computation. In particular, for the two states involved in the first absorption band, the oscillator strength of $S_4$ is well reproduced with 0.69 vs. 0.66, whereas the oscillator strength of $S_2$ is 0.02 vs. 0.06. These differences are due to slightly different mixing of $S_2$ and $S_4$ at the two levels of theory.

![Figure S3: Comparison of the MS-CASPT2(14,10) vertical excitation energies (a) and oscillator strength (b) for gas-phase 2tCyt with “ANO-RCC-VQZP+default IPEA shift” ($E_{\text{Table 3}}$) and with “cc-pVDZ+zero IPEA shift” ($E_{\text{Table 4}}$). The computations employ different geometries (“Table 3” optimized with RI-MP2/cc-pVQZ, “Table 4” with BP86/aug-cc-pVDZ).](image-url)
Table S8: Vertical excitation energies and oscillator strengths of 2tCyt in various solvents at the MS-CASPT2 level of theory. These calculations only include implicit solvation effects. They are graphically presented in Figure 6 c in the main manuscript.

| State | Char. | EtOAc | ACN | DMSO | EtOH | MeOH | H$_2$O |
|-------|-------|-------|-----|------|------|------|-------|
|       |       |       |     |      |      |      |       |
| $S_1$ | $n_S\pi^*$ | 3.85  | 3.98 | 3.98 | 3.97 | 3.99 | 3.97 |
| $S_2$ | $\pi_S\pi^*$ | 3.79  | 3.95 | 3.95 | 3.92 | 3.93 | 3.93 |
| $S_3$ | $n_S\pi^*$ | 4.11  | 4.38 | 4.34 | 4.30 | 4.32 | 4.34 |
| $S_4$ | $\pi_S\pi^*$ | 4.37  | 4.48 | 4.47 | 4.45 | 4.46 | 4.48 |
| $S_5$ | $n_N\pi^*$ | 5.18  | 5.35 | 5.33 | 5.28 | 5.29 | 5.28 |
| $S_6$ | $\pi\pi^*$ | 5.00  | 4.98 | 4.97 | 4.98 | 4.97 | 4.96 |
| $S_7$ | $n_N\pi^*$ | 5.66  | 5.64 | 5.60 | 5.59 | 5.60 | 5.60 |
| $S_8$ | $\pi\pi^*$ | 5.45  | 5.36 | 5.34 | 5.39 | 5.39 | 5.38 |

|       |       |       |     |      |      |      |       |
|-------|-------|-------|-----|------|------|------|-------|
| $S_1$ | $n_S\pi^*$ | 0.00  | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 |
| $S_2$ | $\pi_S\pi^*$ | 0.02  | 0.02 | 0.02 | 0.02 | 0.02 | 0.04 |
| $S_3$ | $n_S\pi^*$ | 0.00  | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| $S_4$ | $\pi_S\pi^*$ | 0.60  | 0.58 | 0.58 | 0.54 | 0.57 | 0.54 |
| $S_5$ | $n_N\pi^*$ | 0.00  | 0.00 | 0.01 | 0.00 | 0.00 | 0.01 |
| $S_6$ | $\pi\pi^*$ | 0.32  | 0.34 | 0.29 | 0.32 | 0.30 | 0.31 |
| $S_7$ | $n_N\pi^*$ | 0.01  | 0.01 | 0.01 | 0.02 | 0.01 | 0.03 |
| $S_8$ | $\pi\pi^*$ | 0.23  | 0.27 | 0.27 | 0.27 | 0.27 | 0.27 |

*MS-CASPT2(14,10)/cc-pVDZ+PCM // BP86/aug-cc-pvdz+COSMO*
Molecular coordinates

These geometries were optimized with BP86/aug-cc-pVDZ\textsuperscript{SI2-SI4} using Orca 3.0.\textsuperscript{S15} COSMO was used to describe the bulk of the respective solvent, as implemented in Orca (\(\epsilon = 6.02\) and \(n = 1.372\) for ethylacetate).

| Vacuum | Ethylacetate |
|---------|--------------|
| N +3.302660 +3.663440 -2.120494 | N +2.732597 +3.725206 -2.267815 |
| C +1.995258 +3.456048 -2.431695 | C +1.499186 +3.401066 -2.751803 |
| H +1.308120 +3.288435 -1.593526 | H +0.730287 +3.169512 -2.004902 |
| C +1.595640 +3.462509 -3.745989 | C +1.268356 +3.375551 -4.103749 |
| H +0.550866 +3.291267 -4.024061 | H +0.287834 +3.108732 -4.509018 |
| C +2.634212 +3.703735 -4.717089 | C +2.383875 +3.705111 -4.953445 |
| N +3.081308 +3.924676 -3.091066 | N +2.240477 +3.721985 -6.293777 |
| C +1.995258 +3.456048 -2.431695 | H +0.402775 +3.941458 -6.900266 |
| H +0.550866 +3.291267 -4.024061 | H +1.346374 +3.463499 -6.720145 |
| O +5.946143 +3.498188 -6.332029 | O +5.607474 +4.009717 -4.451645 |
| H +5.260745 +2.948838 -0.139764 | C +3.801308 +0.274919 -3.113881 |
| O +4.807869 +2.451074 +0.766877 | O +5.593862 +2.322064 +1.530072 |
| H +4.429151 +1.456400 +0.465818 | O +2.613219 +2.458663 +3.202997 |
| C +2.961798 +4.503144 +4.660248 | H +2.512247 +5.199332 +2.632972 |
| H +1.684350 +3.670883 +3.086127 | H +1.850125 +5.085819 +6.135399 |
| O +2.732597 +3.725206 -2.267815 | H +3.073997 +3.552238 +5.212716 |
| C +1.995258 +3.456048 -2.431695 | H +3.898229 +0.84110 +4.748881 |
| H +1.308120 +3.288435 -1.593526 | C -1.497558 +2.605747 -7.852257 |
| C +1.595640 +3.462509 -3.745989 | O -1.995409 +3.004613 -9.051317 |
| H +0.550866 +3.291267 -4.024061 | C -3.330501 +2.568806 -9.485580 |
| C +2.634212 +3.703735 -4.717089 | C -2.357458 +1.756581 -6.951280 |
| N +3.081308 +3.924676 -3.091066 | H -3.281749 +2.97341 -6.673400 |
| H +0.550866 +3.291267 -4.024061 | H -2.661838 +0.822012 -7.457590 |
| O +5.946143 +3.498188 -6.332029 | H -1.792225 +1.512155 -6.041526 |
| H +4.429151 +1.456400 +0.465818 | C -3.595344 +3.201127 -10.840043 |
| C +2.961798 +4.503144 +4.660248 | H -3.331863 +1.464457 -9.549991 |
| C +1.995258 +3.456048 -2.431695 | H -4.076840 +2.891664 -8.736343 |
| H +1.308120 +3.288435 -1.593526 | H -4.581852 +2.860779 -11.205285 |
| S +0.403476 +3.854808 -5.601961 | C -3.611553 +4.304639 -10.771736 |
| O +6.72594 +5.102903 -6.022716 | H -2.829654 +2.895307 -11.576545 |
| H +2.430986 +4.298727 -8.213509 | H +4.230026 +4.131610 -8.425907 |
| H +4.986651 +4.075060 -7.585805 | C +5.268412 +4.684042 -8.802418 |
| H +4.274709 +5.266128 -8.324380 | C +5.970206 +4.389543 -10.105045 |
| O -0.447937 +3.429550 -6.829744 | O +5.913516 +5.631146 -8.088296 |
| H -0.886659 +4.300455 -6.887083 | C +5.310184 +6.015962 -6.803118 |
| H -0.513659 +3.078897 -7.738671 | C +6.187338 +7.093836 -6.191910 |
| O +7.689020 +5.201705 -4.998800 | H +4.286481 +6.382829 -7.005117 |
| H +8.574973 +4.816972 +4.850081 | H +5.236785 +5.120784 -6.159118 |
| H +7.165047 +4.911145 -4.199988 | H +5.763567 +7.380854 -5.212364 |
| O +4.46792 +3.940908 +0.367315 | H +7.215072 +6.724159 -6.020710 |
| H +4.904284 +3.192069 +0.941130 | H +6.228914 +7.993171 -6.833545 |
| H +5.354542 +3.983120 -0.331167 | H +7.015890 +4.088470 -9.910111 |
| O +5.437549 +3.585448 -10.635214 | H +5.999559 +5.302012 -10.730155 |
acetonitrile
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H +5.211404 +3.826102 +3.507658
H +3.546312 +4.424840 +3.850046
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N +1.730237 +3.105694 -6.603957
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H +5.211404 +3.826102 +3.507658
H +3.546312 +4.424840 +3.850046
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H +5.647926 +4.320936 -10.519503
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