# Supporting Information

# Svetamycins A-G, Unusual Piperazic Acid-Containing Peptides from *Streptomyces* sp.

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**Table S1.** NMR spectroscopic data (500 MHz, $CD_3OD$) for **1**

| | $\delta_C$[a] | $\delta_H$[b] (*J* in Hz) | HMBC[c] | ROESY[d] |
|---|---|---|---|---|
| α-MeSer | | | | |
| 1 | 175.0 | | | |
| 2 | 63.0 | | | |
| 3a | 64.6 | 3.99 d (11.5) | 1, 2, 4 | 4 |
| 3b | | 4.12 d (11.5) | 1, 2, 4 | 4 |
| 4 | 20.1 | 1.54 s | 1, 2, 3 | |
| NH-2 | | | | |
| OH-3 | | | | |
| Pip | | | | |
| 1 | 172.0 | | | |
| 2 | 52.4 | 5.02 br. dd (5.0, 1.6) | 3, 4 | 3ab |
| 3a | 25.2 | 1.87[e] m | 2, 4 | 2, 3b, 4a, 5a |
| 3b | | 2.23 br. d (9.8) | | 2, 3a, 4a |
| 4a | 22.0 | 1.58[e] | | 3b, 4b, 5ab |
| 4b | | 1.90[e] m | 5 | 2, 3b, 4a |
| 5a | 47.9 | 2.83[e] m | 2 | |
| 5b | | 3.12 m | | 4ab |
| NH-5 | | | | |
| γ-ClPip | | | | |
| 1 | 175.2 | | | |
| 2 | 51.6 | 5.85 br. dd (7.0, 2.3) | | 3ab |
| 3a | 36.3 | 2.13 ddd (13.7, 12.0, 7.0) | 1, 3, 4 | 3b, 5a |
| 3b | | 2.52 ddd (13.6, 4.2, 2.0) | 1,4, 5 | 2, 3a, 4 |
| 4 | 52.6 | 4.11[e] | | 3b |
| 5a | 55.2 | 2.86 dd (13.5, 10.4) | 1, 5 | 3a, 5b |

| | | | | |
|---|---|---|---|---|
| 5b | | 3.40 ddd (13.5, 4.6, 1.7) | 3, 4 | 5a |
| NH-5 | | | | |
| Ala | | | | |
| 1 | 176.1 | | | |
| 2 | 46.3 | 5.29 d (7.0)[e] | | |
| 3 | 17.9 | 1.33 d (7.0) | 1, 3, $1_{\beta,\gamma\text{-OHdPip}}$ | |
| NH-2 | | | 1, 2 | |
| β,γ-OHdPip | | | | |
| 1 | 168.5 | | | |
| 2 | 58.4 | 4.89[e] | 1, 3, 4 | |
| 3 | 65.6 | 4.22 t (4.9) | 1, 2, 4, 5 | 5 |
| 4 | 63.7 | 4.09 br. t (3.0) | 2, 3, 5 | 2, 5 |
| 5 | 146.1 | 7.04 br. d (2.7) | 3, 4 | 3, 4 |
| OH-3 | | | | |
| OH-4 | | | | |
| HAAC | | | | |
| 1 | 169.5 | | | |
| 2a | 62.2 | 4.93 d (16.2) | 1, $1_{\alpha\text{-MeSer}}$ | |
| 2b | | 5.31[e] d (16.2) | 1, $1_{\alpha\text{-MeSer}}$ | |

[a]Recorded at 175 MHz; referenced to residual $CD_3OD$ at δ 49.15 ppm.
[b]Recorded at 500 MHz; referenced to residual $CD_3OD$ at δ 3.31 ppm.
[c]Proton showing HMBC correlation to indicated carbon.
[d]Proton showing ROESY correlation to indicated proton.
[e]Signal overlapped

**Table S2.** NMR spectroscopic data (500 MHz, DMSO-*d6*) for **2**

| | $\delta_C$[a] | $\delta_H$[b] (*J* in Hz) | HMBC[c] | ROESY[d] |
|---|---|---|---|---|
| α-MeSer | | | | |
| 1 | 172.0 | | | |
| 2 | 60.5 | | | |
| 3a | 63.9 | 3.71 dd (10.7, 8.0) | 1, 4 | 3b, 4, NH-2, OH-3 |
| 3b | | 3.81 dd (10.8, 5.6) | 1, 4 | 3a, 4, NH-2, OH-3 |
| 4 | 19.1 | 1.43 s | 1, 2, 3 | 3ab, NH-2, OH-3 |
| NH-2 | | 7.55 s | 1, 2, 4,$1_{\delta\text{-MePip}}$ | 3ab, 4, $2_{\delta\text{-MePip}}$, $3b_{\delta\text{-MePip}}$, $NH\text{-}5_{\delta\text{-MePip}}$, OH-3 |
| OH-3 | | 4.44 br. dd (8.0, 5.5) | | 3ab, 4, NH-2 |
| δ-MePip | | | | |
| 1 | 169.0 | | | |
| 2 | 49.7 | 4.88 br. dd (5.5, 1.4) | 1, 3, 4 | 3ab, $NH\text{-}2_{\alpha\text{-MeSer}}$ |
| 3a | 24.3 | 1.76 m | | 2, 3b, |
| 3b | | 2.17 br. d (13.5) | | 2, 3a, 4a, $NH\text{-}2_{\alpha\text{-MeSer}}$ |
| 4a | 28.2 | 1.36 m | | 3ab, 4b, NH-5 |
| 4b | | 1.51 br. dd (12.6, 4.0) | | 4a, 5a, Me-5 |
| 5a | 52.3 | 2.69[e] m | | 3a, 4b, Me-5 |
| Me-5 | 19.3 | 1.00[e] br. d (6.5) | 4, 5 | 4b, 5a, NH-5 |
| NH-5 | | 4.14 d (12.2) | | 4a, Me-5, $2_{\gamma\text{-ClPip}}$, |
| γ-ClPip | | | | |
| 1 | 171.4 | | | |
| 2 | 49.7 | 5.8 d (8.8) | | 3ab, $NH\text{-}5_{\delta\text{-MePip}}$ |
| 3a | 34.7 | 1.93 td (13.0, 6.0) | 1, 2, 4 | 2, 3b |
| 3b | | 2.38 m | | 2, 3a, 4 |
| 4 | 52.6 | 4.36 tt (11.2, 5.4) | | 3b, 5b, NH-5 |
| 5a | 54.1 | 2.67[e] m | | 5b, $3_{Ala}$ |

| | | | | |
|---|---|---|---|---|
| 5b | | 3.39 m | | 4, 5a, NH-5 |
| NH-5 | | 5.27[e] | | 4, 5b, $3_{Ala}$ |
| Ala | | | | |
| 1 | 172.4 | | | |
| 2 | 43.4 | 5.31 q (7.0) | 1 | 3, NH-2, $5a_{\gamma\text{-ClPip}}$ |
| 3 | 18.1 | 1.19 br. d (6.9) | 1, 2 | 2, NH-2 |
| NH-2 | | 7.94 br. d (6.9) | | 2, 3, $2_{\beta,\gamma\text{-OHdPip}}$ |
| β,γ-OHdPip | | | | |
| 1 | 166.3 | | | |
| 2 | 56.9 | 4.67 d (4.8) | 1, 3, 4 | 3, 4, $NH\text{-}2_{Ala}$, OH-3 |
| 3 | 63.7 | 4.05 q (4.3) | 1, 5 | 2, 4, OH-3, OH-4 |
| 4 | 62.4 | 3.94 m | | 2, 3, 5, OH-3, OH-4 |
| 5 | 146.9 | 6.97 br. d (2.0) | 3, 4 | 2, 3, 4, OH-3, OH-4 |
| OH-3 | | 5.27[e] | 1, 2, 3, 4 | 2, 3, 4, 5, OH-4 |
| OH-4 | | 5.85 d (8.7) | 3, 4, 5 | 3, 4, 5, OH-3 |
| HAAC | | | | |
| 1 | 166.4 | | | |
| 2a | 61.9 | 4.71 d (15.9) | 1, $1_{\alpha\text{-MeSer}}$ | 2b |
| 2b | | 5.25[e] d (15.9) | 1, $1_{\alpha\text{-MeSer}}$ | 2a |

[a]Recorded at 175 MHz; referenced to residual DMSO-$d_6$ at δ 39.51 ppm.
[b]Recorded at 500 MHz; referenced to residual DMSO-$d_6$ at δ 2.50 ppm.
[c]Proton showing HMBC correlation to indicated carbon.
[d]Proton showing ROESY correlation to indicated proton.
[e]Signal overlapped

**Table S3.** NMR spectroscopic data (500 MHz, DMSO-*d6*) for **3**

| | $\delta_C$[a] | $\delta_H$[b] (*J* in Hz) | HMBC[c] | ROESY[d] |
|---|---|---|---|---|
| α-MeSer | | | | |
| 1 | 171.9 | | | |
| 2 | 59.8 | | | |
| 3a | 63.4 | 3.61 dd (10.8, 6.4) | 1, 2, 4 | 3b, 4, NH-2, OH-3 |
| 3b | | 3.83 dd (10.8, 5.9) | 1, 2, 4 | 3a, 4, NH-2, OH-3 |
| 4 | 19.9 | 1.37 s | 1, 2, 3 | 3ab, NH-2, OH-3 |
| NH-2 | | 7.78 s | 1, 2, 3, 4, $1_{\delta,\delta\text{-dMePip}}$, $2_{\delta,\delta\text{-dMePip}}$ | 3ab, 4, $2_{\delta,\delta\text{-dMePip}}$, $3b_{\delta,\delta\text{-dMePip}}$, OH-3 |
| OH-3 | | 4.76[e] br. dd (6.2, 5.7) | | 3ab, 4, NH-2 |
| δ,δ-dMePip | | | | |
| 1 | 169.1 | | | |
| 2 | 49.7 | 4.88 br. dd (5.4, 1.6) | 1, 3, 4 | 3ab, 4a, Me-5a, $NH\text{-}2_{\alpha\text{-MeSer}}$ |
| 3a | 21.4 | 1.96 m | 1, 2, 4 | 2, 3b, 4a, Me-5a |
| 3b | | 2.07 dq (13.5, 2.2) | 1, 2, 4 | 2, 3a, 4a, Me-5b, $NH\text{-}2_{\alpha\text{-MeSer}}$ |
| 4a | 31.8 | 1.34 dt (13.3, 3.2) | 3, 5, Me-5ab | 3ab, NH-5 |
| 4b | | 1.42 br. dd (13.3, 4.0) | 3, 5, Me-5ab | 3b, NH-5 |
| 5 | 50.9 | | | |
| Me-5a | 28.3 | 1.00 br, s | 4, 5, Me-5b | 4ab, NH-2 |
| Me-5b | 22.7 | 1.01 br. s | 4, 5, Me-5a | 2, 3a, $2_{\gamma\text{-ClPip}}$, $3b_{\gamma\text{-ClPip}}$ |
| NH-5 | | 4.57[e] s | $1_{\gamma\text{-ClPip}}$ | 4b, Me-5a, $2_{\gamma\text{-ClPip}}$, |
| γ-ClPip | | | | |
| 1 | 171.7 | | | |
| 2 | 48.8 | 5.83 br. s | | 3ab, Me-$5b_{\delta,\delta\text{-dMePip}}$, NH-$5_{\delta,\delta\text{-dMePip}}$ |
| 3a | 34.2 | 1.89 ddd (12.7, 11.2, 6.0) | 1, 2, 4, 5 | 2, 3b, 5a |
| 3b | | 2.40 br. ddd (12.8, 4.5, 1.7) | 2, 4, 5 | 2, 3a, 4, $5a_{\delta,\delta\text{-dMePip}}$ |

| | | | | |
|---|---|---|---|---|
| 4 | 52.3 | 4.46 tt (10.9, 4.6) | 3, 5 | 3b, 5b, NH-5 |
| 5a | 54.0 | 2.69 td (12.7, 11.0) | 3, 4 | 3a, 5b, $3_{Ala}$ |
| 5b | | 3.41 br. ddd (12.8, 4.4, 2.0) | 3, 4 | 4, 5a, NH-5 |
| NH-5 | | 5.21[e] | 2, 4, 5 | 4, 5b |
| Ala | | | | |
| 1 | 172.3 | | | |
| 2 | 43.1 | 5.38 q (7.0) | 1, 3, $1_{\beta,\gamma\text{-OHdPip}}$ | 3, $5a_{\gamma\text{-ClPip}}$, NH-2 |
| 3 | 17.9 | 1.18 d (7.0) | 1, 2 | 2, NH-2, $5a_{\gamma\text{-ClPip}}$ |
| NH-2 | | 7.91 br. d (7.0) | | 2, 3, $2_{\beta,\gamma\text{-OHdPip}}$ |
| β,γ-OHdPip | | | | |
| 1 | 166.4 | | | |
| 2 | 56.9 | 4.56[e] br. d (5.0) | 1, 3, 4 | 3, 4, NH-$2_{Ala}$, OH-3 |
| 3 | 63.7 | 4.06 q (4.0) | 1, 4, 5 | 2, 4, 5, OH-3, OH-4 |
| 4 | 63.0 | 3.95 m | 5 | 2, 3, 5, OH-3, OH-4 |
| 5 | 147.1 | 6.93 br. d (1.1) | 3, 4 | 4, OH-3, OH-4, $2b_{HAAC}$ |
| OH-3 | | 5.22[e] d | 2, 3, 4, 5 | 2, 3, 4, 5 |
| OH-4 | | 5.73 d (8.3) | 3, 4, 5 | 2, 3, 4, 5, $2_{Ala}$, OH-3 |
| HAAC | | | | |
| 1 | 166.1 | | | |
| 2a | 61.3 | 4.73[e] d (16.2) | 1, $1_{\alpha\text{-MeSer}}$ | 2b, NH-$2_{\alpha\text{-MeSer}}$ |
| 2b | | 5.18 d (16.2) | 1, $1_{\alpha\text{-MeSer}}$ | 2a, $5_{\beta,\gamma\text{-OHdPip}}$ |

[a]Recorded at 175 MHz; referenced to residual DMSO-$d_6$ at δ 39.51 ppm.
[b]Recorded at 500 MHz; referenced to residual DMSO-$d_6$ at δ 2.50 ppm.
[c]Proton showing HMBC correlation to indicated carbon.
[d]Proton showing ROESY correlation to indicated proton.
[e]Signal overlapped

**Table S4.** NMR spectroscopic data (500 MHz, DMSO-*d6*) for **5**

| | $\delta_C$[a] | $\delta_H$[b] (*J* in Hz) | HMBC[c] |
|---|---|---|---|
| α-MeSer | | | |
| 1 | 173.5 | | |
| 2 | 60.1 | | |
| 3a | 64.6 | 3.53[e] d (10.8) | 1, 2, 4 |
| 3b | | 3.64 d (10.8) | 1, 2, 4 |
| 4 | 19.6 | 1.35 s | 1, 2, 3 |
| NH-2 | | 7.96 s | 1, 2, 3, 4, $1_{Pip}$ |
| OH-1 | | | |
| OH-3 | | | |
| δ,δ-dMePip | | | |
| 1 | 170.2 | | |
| 2 | 49.5 | 4.88 br. s | |
| 3a | 22.9 | 2.00[e] m | |
| 3b | | 2.00[e] m | |
| 4a | 31.9 | 1.38[e] m | 3, 5 |
| 4b | | 1.38[e] m | |
| 5 | 50.9 | | |
| 5a | 28.4 | 1.03 s | 4, 5, 5b |
| 5b | 22.1 | 1.08 s | 4, 5, 5a |
| NH-5 | | 4.64 s | 5ab |
| γ-ClPip | | | |
| 1 | 172.0 | | |
| 2 | 49.1 | 5.80 br. dd (5.5, 2.3) | 1, 3, 4 |
| 3a | 34.8 | 1.97[e] m | 1, 2, 4, 5 |
| 3b | | 2.65[e] m | |

| | | | |
|---|---|---|---|
| 4 | 52.5 | 4.24 tt (10.9, 4.5) | |
| 5a | 53.6 | 2.68[e] m | 3, 4 |
| 5b | | 3.36[e] | 3, 4 |
| NH-5 | | 5.49 br. dd (12.3, 1.8) | $1_{Ala}$ |
| Ala | | | |
| 1 | 172.8 | | |
| 2 | 45.4 | 5.04 dq (8.5, 6.8) | 1, 3, $1_{\beta,\gamma\text{-OHdPip}}$ |
| 3 | 18.0 | 1.16 d (6.8) | 1, 2 |
| NH-2 | | 7.59 d (8.5) | 1, $1_{\beta,\gamma\text{-OHdPip}}$ |
| β,γ-OHdPip | | | |
| 1 | 165.3 | | |
| 2 | 55.1 | 4.75 br. d (5.2) | 1, 3, 4, $1_{HAAC}$ |
| 3 | 65.2 | 4.00 br. dd (5.2, 3.5) | 1, 2 |
| 4 | 62.3 | 3.96 t (3.3) | |
| 5 | 144.2 | 6.86 d (3.0) | 3, 4 |
| OH-3 | | | |
| OH-4 | | | |
| HAAC | | | |
| 1 | 172.5 | | |
| 2a | 59.9 | 4.30 d (17.3) | 1 |
| 2b | | 4.35 d (17.3) | |
| OH-1 | | | |

[a]Recorded at 175 MHz; referenced to residual DMSO-$d_6$ at δ 39.51 ppm.
[b]Recorded at 500 MHz; referenced to residual DMSO-$d_6$ at δ 2.50 ppm.
[c]Proton showing HMBC correlation to indicated carbon.
[e]Signal overlapped

**Table S5.** NMR spectroscopic data (500 MHz, $CD_3OD$) for **6**

| | $\delta_C$[a] | $\delta_H$[b] (*J* in Hz) | HMBC[c] |
|---|---|---|---|
| α-MeSer | | | |
| 1 | 173.0 | | |
| 2 | 61.8 | | |
| 3a | 63.2 | 4.06[d] d (4.3) | 1, 2, 4 |
| 3b | | 4.06[d] | |
| 4 | 19.5 | 1.57 s | 1, 2, 3 |
| NH-2 | | 7.65 s | 1, 2, 4, $1_{Pip}$ |
| OH-3 | | | |
| Pip | | | |
| 1 | 170.4 | | |
| 2 | 52.2 | 5.04[d] br. dd (5.9, 1.3) | 1, 3, 4, $1_{\gamma\text{-BrPip}}$ |
| 3a | 24.3 | 1.80 m | 1, 2, 4 |
| 3b | | 2.17 dd (13.9, 1.0) | |
| 4a | 21.8 | 1.53 m | |
| 4b | | 2.00 m | 5 |
| 5a | 47.9 | 2.79 td (13.5, 2.7) | 4 |
| 5b | | 3.10 br. ddd (13.5, 4.2, 2.7) | 4 |
| NH-5 | | | |
| γ-BrPip | | | |
| 1 | 173.4 | | |
| 2 | 52.7 | 5.82 br. dd (6.8, 1.6) | 1, 3, 4 |
| 3a | 37.2 | 2.26 td (13.5, 6.9) | 1, 2, 4, 5 |
| 3b | | 2.59 dt (13.5, 2.2) | 2, 4, 5 |
| 4 | 43.9 | 4.22 m | 3, 5 |
| 5a | 55.7 | 2.93 dd (13.4, 11.3) | 3, 4 |

| | | | |
|---|---|---|---|
| 5b | | 3.44 ddd (13.5, 4.5, 2.5) | 3, 4 |
| NH-5 | | | |
| Ala | | | |
| 1 | 173.9 | | |
| 2 | 47.1 | 5.24 dd (13.8, 6.9) | 1, 3, $1_{\beta,\gamma\text{-OHdPip}}$ |
| 3 | 18.5 | 1.33 d (6.9) | 1, 2 |
| NH-2 | | | |
| β,γ-OHdPip | | | |
| 1 | 166.7 | | |
| 2 | 52.8 | 5.02[d] br. d (6.0) | 1, 3, 4, $1_{\text{HAAC}}$ |
| 3 | 65.0 | 4.18 br. dd (5.8, 5.2) | 1, 2, 4, 5 |
| 4 | 62.8 | 4.03 m | 2, 3, 5 |
| 5 | 147.2 | 7.07 d (3.1) | 3, 4 |
| OH-3 | | | |
| OH-4 | | | |
| HAAC | | | |
| 1 | 168.1 | | |
| 2a | 64.2 | 4.82[d] d (16.3) | 1, $1_{\alpha\text{-MeSer}}$ |
| 2b | | 5.41 d (16.3) | 1, $1_{\alpha\text{-MeSer}}$ |

[a]Recorded at 175 MHz; referenced to residual $CD_3OD$ at δ 49.15 ppm.
[b]Recorded at 500 MHz; referenced to residual $CD_3OD$ at δ 3.31 ppm.
[c]Proton showing HMBC correlation to indicated carbon.
[d]Signal overlapped

**Table S6.** NMR spectroscopic data (500 MHz, DMSO-*d6*) for **6**

| | $\delta_C$[a] | $\delta_H$[b] (*J* in Hz) | HMBC[c] |
|---|---|---|---|
| α-MeSer | | | |
| 1 | 171.8 | | |
| 2 | 60.5 | | |
| 3a | 64.3 | 3.69 dd (11.0, 7.7) | 1, 2, 4 |
| 3b | | 3.78 dd (11.0, 5.8) | 1, 2, 4 |
| 4 | 19.3 | 1.43 s | 1, 2, 3 |
| NH-2 | | 7.59 s | 1, 2, 3, 4, $1_{Pip}$ |
| OH-3 | | 4.55 br. dd 7.7, 5.8) | 3 |
| Pip | | | |
| 1 | 169.0 | | |
| 2 | 51.2 | 4.92 m | 1, 3, 4 |
| 3a | 24.2 | 1.72[d] m | 4 |
| 3b | | 2.20 m | 4 |
| 4a | 20.2 | 1.35 m | 3 |
| 4b | | 1.74[d] m | 3 |
| 5a | 46.4 | 2.61 m | |
| 5b | | 2.95 m | |
| NH-5 | | 4.60[d] br. Dd (12.7, 1.6) | |
| γ-BrPip | | | |
| 1 | 171.3 | | |
| 2 | 51.0 | 5.70 br. dd (6.2, 1.3) | 1, 3, 4 |
| 3a | 35.6 | 2.05 td (12.8, 6.2) | 1, 2, 4, 5 |
| 3b | | 2.50[d] | 2, 4, 5 |
| 4 | 45.2 | 4.51 m | 3 |
| 5a | 54.7 | 2.82 q (12.3) | 3, 4 |

| | | | |
|---|---|---|---|
| 5b | | 3.45 m | 3, 4 |
| NH-5 | | 5.28[d] br. dd (12.3, 1.7) | |
| Ala | | | |
| 1 | 172.0 | | |
| 2 | 43.0 | 5.35[d] dq (8.2, 6.9) | 1, 3, $1_{\beta,\gamma\text{-OHdPip}}$ |
| 3 | 18.1 | 1.18 d (6.9) | 1, 2 |
| NH-2 | | 8.13 d (8.2) | $1_{\beta,\gamma\text{-OHdPip}}$ |
| β,γ-OHdPip | | | |
| 1 | 166.3 | | |
| 2 | 56.7 | 4.71 d (5.4) | 1, 3, 4 |
| 3 | 63.8 | 4.05 q (4.6) | 1, 4, 5 |
| 4 | 62.6 | 3.94 ddd (8.6, 4.5, 2.5) | 3, 5 |
| 5 | 146.8 | 6.97 d (2.5) | 3, 4 |
| OH-3 | | 5.26[d] d (4.3) | 2, 3, 4 |
| OH-4 | | 5.81 d (8.6) | 3, 4, 5 |
| HAAC | | | |
| 1 | 166.6 | | |
| 2a | 61.5 | 4.61[d] d (15.8) | 1, $1_{\alpha\text{-MeSer}}$ |
| 2b | | 5.37[d] d (15.8) | 1, $1_{\alpha\text{-MeSer}}$ |

[a]Recorded at 175 MHz; referenced to residual DMSO-$d_6$ at δ 39.51 ppm.
[b]Recorded at 500 MHz; referenced to residual DMSO-$d_6$ at δ 2.50 ppm.
[c]Proton showing HMBC correlation to indicated carbon.
[d]Signal overlapped

**Table S7.** NMR spectroscopic data (500 MHz, $CD_3OD$) for **7**

| | $\delta_C$[a] | $\delta_H$[b] (*J* in Hz) | HMBC[c] |
|---|---|---|---|
| α-MeSer | | | |
| 1 | 172.4 | | |
| 2 | 61.5 | | |
| 3a | 63.0 | 4.06[d] s | 1, 2, 4 |
| 3b | | 4.06[d] | |
| 4 | 17.4 | 1.54 s | 1, 2, 3 |
| NH-2 | | 7.72 s | |
| OH-3 | | | |
| δ,δ-dMePip | | | |
| 1 | 169.9 | | |
| 2 | 49.2 | 5.04 br. dd (5.8, 1.6) | 1, 3, 4, $1_{\gamma\text{-BrPip}}$ |
| 3a | 19.5 | 1.99 m | 1, 2, 4 |
| 3b | | 2.07 m | 2, 4 |
| 4a | 31.4 | 1.46 m | 2, 3, 5, 5b |
| 4b | | 1.76 td (13.3, 3.5) | 3, 5, 5a |
| 5 | 50.5 | | |
| 5a | 27.1 | 1.14 s | 3, 4, 5, 5b |
| 5b | 21.4 | 1.16 s | 4, 5, 5a |
| NH-5 | | | |
| γ-BrPip | | | |
| 1 | 173.8 | | |
| 2 | 50.3 | 5.86 br. dd (6.2, 1.5) | 1, 3, 4 |
| 3a | 35.1 | 2.20 ddd (13.5, 12.4, 6.2) | 1, 2, 4, 5 |
| 3b | | 2.77 ddd (13.5, 4.0, 1.7) | 4 |
| 4 | 41.9 | 4.32 dddd (12.2, 10.5, 4.5, 4.1) | |

| | | | |
|---|---|---|---|
| 5a | 53.9 | 2.94 dd (13.4, 11.0) | 3, 4 |
| 5b | | 3.45 br. dd (13.6, 4.4) | 3, 4 |
| NH-5 | | | |
| Ala | | | |
| 1 | 173.2 | | |
| 2 | 45.1 | 5.27 q (6.9) | 1, 3, $1_{\beta,\gamma\text{-OHdPip}}$ |
| 3 | 16.7 | 1.33 d (6.9) | 1, 2 |
| NH-2 | | | |
| β,γ-OHdPip | | | |
| 1 | 166.6 | | |
| 2 | 55.8 | 4.99 br. d (5.7) | 1, 3, 4 |
| 3 | 62.9 | 4.17 br. dd (5.7, 5.3) | 1, 2, 4, 5 |
| 4 | 60.9 | 4.02 br. dd (5.3, 3.0) | 2, 3, 5 |
| 5 | 145.3 | 7.07 d (3.0) | 3, 4 |
| OH-3 | | | |
| OH-4 | | | |
| HAAC | | | |
| 1 | 166.6 | | |
| 2a | 62.2 | 4.85[d] d (16.3) | 1, $1_{\alpha\text{-MeSer}}$ |
| 2b | | 5.37 d (16.3) | 1, $1_{\alpha\text{-MeSer}}$ |

[a]Recorded at 175 MHz; referenced to residual $CD_3OD$ at δ 49.15 ppm.
[b]Recorded at 500 MHz; referenced to residual $CD_3OD$ at δ 3.31 ppm.
[c]Proton showing HMBC correlation to indicated carbon.
[d]Signal overlapped

**Table S8.** $^{13}C$ experimental and scaled calculated NMR chemical shifts for **1a-h**, with [a]$|\Delta\delta|(^{13}C)$ and [b]CMAE values.

| | $\delta_{exp}$ ($^{13}C$), ppm | $\delta_{scaled}$ ($^{13}C$), ppm | | | | | | | | $\lvert\Delta\delta\rvert$ ($^{13}C$), ppm[a] | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **position** | | **1a** | **1b** | **1c** | **1d** | **1e** | **1f** | **1g** | **1h** | **1a** | **1b** | **1c** | **1d** | **1e** | **1f** | **1g** | **1h** |
| | α-MeSer | | | | | | | | | | | | | | | | |
| 1 | 171.9 | 174.1[c] | 173.9[c] | 172.0[c] | 172.5[c] | 173.1[c] | 174.8[c] | 173.5[c] | 174.3[c] | 2.20 | 1.99 | 0.06 | 0.62 | 1.22 | 2.90 | 1.55 | 2.38 |
| 2 | 60.4 | 61.6 | 61.6 | 60.5 | 63.8 | 64.4 | 65.4 | 64.5 | 65.6 | 1.24 | 1.22 | 0.15 | 3.44 | 3.96 | 5.00 | 4.12 | 5.17 |
| 3 | 63.6 | 60.6 | 60.7 | 65.2 | 65.4 | 61.7 | 64.3 | 62.5 | 64.2 | 2.98 | 2.86 | 1.63 | 1.75 | 1.92 | 0.68 | 1.06 | 0.59 |
| 4 | 19.7 | 18.6 | 18.1 | 19.4 | 18.3 | 19.8 | 17.1 | 19.9 | 18.1 | 1.14 | 1.56 | 0.34 | 1.41 | 0.10 | 2.56 | 0.22 | 1.58 |
| | Pip | | | | | | | | | | | | | | | | |
| 1 | 168.9 | 171.1[c] | 171.1[c] | 172.9[c] | 170.9[c] | 171.3[c] | 170.4[c] | 168.8[c] | 170.1[c] | 2.20 | 2.17 | 4.05 | 1.99 | 2.39 | 1.46 | 0.11 | 1.18 |
| 2 | 50.9 | 48.5 | 48.6 | 48.8 | 47.9 | 49.4 | 50.8 | 50.2 | 51.3 | 2.39 | 2.32 | 2.10 | 2.99 | 1.49 | 0.05 | 0.74 | 0.36 |
| 3 | 24.4 | 21.6 | 21.4 | 21.5 | 21.4 | 22.5 | 22.7 | 22.8 | 23.2 | 2.78 | 2.98 | 2.85 | 2.95 | 1.91 | 1.69 | 1.56 | 1.22 |
| 4 | 20.2 | 17.7 | 17.7 | 18.2 | 18.4 | 18.7 | 19.6 | 18.8 | 19.6 | 2.52 | 2.49 | 2.01 | 1.76 | 1.51 | 0.59 | 1.40 | 0.58 |
| 5 | 46.3 | 43.3 | 43.4 | 43.7 | 44.1 | 43.6 | 43.4 | 43.7 | 43.3 | 2.98 | 2.93 | 2.63 | 2.18 | 2.65 | 2.86 | 2.56 | 3.05 |
| | γ-ClPip | | | | | | | | | | | | | | | | |
| 1 | 171.8 | 175.2[c] | 175.4[c] | 176.6[c] | 176.2[c] | 172.7[c] | 169.0[c] | 171.7[c] | 167.8[c] | 3.36 | 3.59 | 4.78 | 4.36 | 0.86 | 2.82 | 0.08 | 3.97 |
| 2 | 49.8 | 50.4 | 50.0 | 49.6 | 49.9 | 48.2 | 50.1 | 48.8 | 51.0 | 0.59 | 0.24 | 0.25 | 0.06 | 1.64 | 0.26 | 1.00 | 1.22 |
| 3 | 34.5 | 34.3 | 34.4 | 34.5 | 34.1 | 33.5 | 33.0 | 33.8 | 33.2 | 0.18 | 0.05 | 0.05 | 0.36 | 1.04 | 1.48 | 0.66 | 1.34 |
| 4 | 52.5 | 53.7 | 53.6 | 53.9 | 53.8 | 56.0 | 57.8 | 55.4 | 58.1 | 1.16 | 1.07 | 1.36 | 1.33 | 3.46 | 5.27 | 2.93 | 5.59 |
| 5 | 54.0 | 51.1 | 51.1 | 50.9 | 50.8 | 51.2 | 51.4 | 51.3 | 51.4 | 2.88 | 2.88 | 3.07 | 3.21 | 2.84 | 2.61 | 2.72 | 2.63 |
| | Ala | | | | | | | | | | | | | | | | |
| 1 | 172.7 | 176.3[c] | 175.6[c] | 174.9[c] | 173.9[c] | 173.1[c] | 173.4[c] | 172.3[c] | 172.5[c] | 3.58 | 2.94 | 2.17 | 1.22 | 0.44 | 0.71 | 0.44 | 0.22 |
| 2 | 43.1 | 47.5 | 47.5 | 47.3 | 47.4 | 45.7 | 45.2 | 48.0 | 47.6 | 4.43 | 4.41 | 4.16 | 4.31 | 2.64 | 2.07 | 4.90 | 4.47 |
| 3 | 17.9 | 16.2 | 17.0 | 16.9 | 16.5 | 16.8 | 18.3 | 16.1 | 16.8 | 1.70 | 0.93 | 0.95 | 1.45 | 1.10 | 0.36 | 1.82 | 1.08 |
| | β,γ-OHdPip | | | | | | | | | | | | | | | | |
| 1 | 166.6 | 167.1[c] | 166.2[c] | 162.7[c] | 166.6[c] | 168.6[c] | 162.1[c] | 168.2[c] | 169.3[c] | 0.49 | 0.41 | 3.87 | 0.04 | 1.99 | 4.49 | 1.62 | 2.72 |
| 2 | 56.9 | 52.8 | 54.2 | 56.2 | 56.5 | 58.9 | 57.4 | 53.7 | 51.2 | 4.12 | 2.66 | 0.71 | 0.37 | 2.04 | 0.54 | 3.25 | 5.75 |
| 3 | 63.8 | 63.1 | 59.1 | 61.1 | 63.7 | 67.4 | 59.2 | 63.5 | 64.2 | 0.74 | 4.74 | 2.74 | 0.08 | 3.63 | 4.64 | 0.30 | 0.39 |
| 4 | 62.6 | 64.5 | 56.3 | 60.2 | 59.8 | 66.3 | 59.3 | 62.0 | 65.0 | 1.93 | 6.28 | 2.43 | 2.78 | 3.72 | 3.35 | 0.61 | 2.41 |
| 5 | 147.2 | 137.6[d] | 137.8[d] | 140.8[d] | 140.8[d] | 139.9[d] | 141.2[d] | 146.3[d] | 138.1[d] | 9.59 | 9.38 | 6.39 | 6.40 | 7.26 | 6.00 | 0.92 | 9.12 |
| | Haa | | | | | | | | | | | | | | | | |
| 1 | 166.7 | 170.4[c] | 168.8[c] | 168.2[c] | 168.2[c] | 167.0[c] | 168.7[c] | 168.3[c] | 170.6[c] | 3.68 | 2.11 | 1.51 | 1.48 | 0.26 | 2.03 | 1.60 | 3.85 |
| 2 | 61.5 | 61.2 | 60.0 | 61.2 | 60.6 | 60.8 | 60.3 | 61.4 | 61.6 | 0.29 | 1.46 | 0.27 | 0.86 | 0.73 | 1.17 | 0.06 | 0.13 |
| **CMAE[b]** | | | | | | | | | | **2.46** | **2.65** | **2.11** | **1.98** | **2.12** | **2.32** | **1.51** | **2.54** |

[a] **$|\Delta\delta|(^{13}C)$** = $|\delta_{exp} - \delta_{scaled}|$ ($^{13}C$), ppm: absolute differences for experimental versus scaled calculated $^{13}C$ NMR chemical shifts. The $\delta_{scaled}$ values were obtained by the corresponding calculated chemical shift data ($\delta_{calcd}$); the latters were produced using the "multi standard" approach, using: [c] benzene for $sp^2$ $^{13}C$ atoms, (excluding carbonyl carbons), [d] N-Methylformamide for carbonyl carbons, and TMS (all the remaining reported values) for $sp^3$ $^{13}C$ atoms, as reference compounds.

[b] **CMAE** = $(\Sigma[|(\delta_{exp} - \delta_{scaled})|])/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and scaled calculated $^{13}C$ chemical shifts), normalized to the number of the chemical shifts (n).

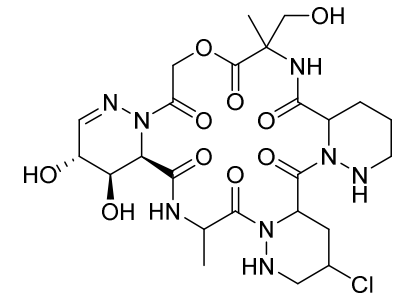
**Table S9.** $^{1}$H experimental and calculated NMR chemical shifts for **1a-h**, with [a]|Δδ|($^{1}$H) and [b]CMAE values.

| $\delta_{exp}$ ($^{1}$H), ppm | | $\delta_{scaled}$ ($^{1}$H), ppm | | | | | | | | |Δδ| ($^{1}$H), ppm[a] | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **position** | | **1a** | **1b** | **1c** | **1d** | **1e** | **1f** | **1g** | **1h** | **1a** | **1b** | **1c** | **1d** | **1e** | **1f** | **1g** | **1h** |
| α-MeSer | | | | | | | | | | | | | | | | | |
| 3a | 3.67 | 4.27 | 4.21 | 4.24 | 4.08 | 3.77 | 3.76 | 3.74 | 3.82 | 0.60 | 0.54 | 0.57 | 0.41 | 0.10 | 0.09 | 0.07 | 0.15 |
| 3b | 3.82 | 4.32 | 4.29 | 4.33 | 4.41 | 4.30 | 3.95 | 4.18 | 3.92 | 0.50 | 0.47 | 0.51 | 0.59 | 0.48 | 0.13 | 0.36 | 0.10 |
| 4 | 1.42 | 1.56 | 1.51 | 1.83 | 1.42 | 1.54 | 1.65 | 1.60 | 1.68 | 0.14 | 0.09 | 0.41 | 0.00 | 0.12 | 0.23 | 0.18 | 0.26 |
| NH-2 | 7.68 | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* |
| OH-3 | 4.57 | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* |
| Pip | | | | | | | | | | | | | | | | | |
| 2 | 4.90 | 5.02 | 5.05 | 5.17 | 5.17 | 4.98 | 5.30 | 5.07 | 5.19 | 0.12 | 0.15 | 0.27 | 0.27 | 0.08 | 0.40 | 0.17 | 0.29 |
| 3a | 1.72 | 1.36 | 1.32 | 1.37 | 1.43 | 1.30 | 1.48 | 1.32 | 1.26 | 0.36 | 0.40 | 0.35 | 0.29 | 0.42 | 0.24 | 0.40 | 0.46 |
| 3b | 2.19 | 1.99 | 1.94 | 2.03 | 2.13 | 2.37 | 2.58 | 2.55 | 2.86 | 0.20 | 0.25 | 0.16 | 0.06 | 0.18 | 0.39 | 0.36 | 0.67 |
| 4a | 1.35 | 1.02 | 1.00 | 1.02 | 1.17 | 1.07 | 1.17 | 1.12 | 1.19 | 0.33 | 0.35 | 0.33 | 0.18 | 0.28 | 0.18 | 0.23 | 0.16 |
| 4b | 1.68 | 2.65 | 2.63 | 2.39 | 2.29 | 2.01 | 1.38 | 1.61 | 1.45 | 0.97 | 0.95 | 0.71 | 0.61 | 0.33 | 0.30 | 0.07 | 0.23 |
| 5a | 2.61 | 2.74 | 2.77 | 2.72 | 2.72 | 2.68 | 2.66 | 2.71 | 2.65 | 0.13 | 0.16 | 0.11 | 0.11 | 0.07 | 0.05 | 0.10 | 0.04 |
| 5b | 2.94 | 3.03 | 3.07 | 2.98 | 3.01 | 2.86 | 2.68 | 2.90 | 2.69 | 0.09 | 0.13 | 0.04 | 0.07 | 0.08 | 0.26 | 0.04 | 0.25 |
| NH-5 | 4.67 | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* |
| γ-ClPip | | | | | | | | | | | | | | | | | |
| 2 | 5.73 | 5.92 | 6.00 | 6.20 | 6.06 | 5.57 | 4.62 | 5.50 | 4.37 | 0.19 | 0.27 | 0.47 | 0.33 | 0.16 | 1.11 | 0.23 | 1.36 |
| 3a | 1.90 | 1.79 | 1.80 | 1.85 | 1.86 | 1.77 | 1.80 | 1.74 | 1.72 | 0.11 | 0.10 | 0.05 | 0.04 | 0.13 | 0.10 | 0.16 | 0.18 |
| 3b | 2.41 | 2.38 | 2.40 | 2.26 | 2.25 | 2.22 | 2.36 | 2.23 | 2.42 | 0.03 | 0.01 | 0.15 | 0.16 | 0.19 | 0.05 | 0.18 | 0.01 |
| 4 | 4.36 | 3.93 | 3.97 | 3.91 | 3.88 | 4.57 | 4.57 | 4.35 | 4.42 | 0.43 | 0.39 | 0.45 | 0.48 | 0.21 | 0.21 | 0.01 | 0.06 |
| 5a | 2.66 | 2.67 | 2.67 | 2.67 | 2.67 | 2.73 | 2.74 | 2.70 | 2.79 | 0.01 | 0.01 | 0.01 | 0.01 | 0.07 | 0.08 | 0.04 | 0.13 |
| 5b | 3.38 | 3.13 | 3.12 | 3.14 | 3.16 | 3.22 | 3.12 | 3.06 | 3.00 | 0.25 | 0.26 | 0.24 | 0.22 | 0.16 | 0.26 | 0.32 | 0.38 |
| NH-5 | 5.23 | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* |
| Ala | | | | | | | | | | | | | | | | | |
| 2 | 5.33 | 5.34 | 5.30 | 5.37 | 5.30 | 5.65 | 5.85 | 5.23 | 5.27 | 0.01 | 0.03 | 0.04 | 0.03 | 0.32 | 0.52 | 0.10 | 0.06 |
| 3 | 1.18 | 1.22 | 1.19 | 1.18 | 1.20 | 1.25 | 1.24 | 1.38 | 1.27 | 0.04 | 0.01 | 0.00 | 0.02 | 0.07 | 0.06 | 0.20 | 0.09 |
| NH-2 | 8.15 | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* |
| β,γ-OHdPip | | | | | | | | | | | | | | | | | |
| 2 | 4.71 | 5.30 | 5.25 | 4.85 | 5.18 | 3.86 | 5.39 | 4.60 | 5.38 | 0.59 | 0.54 | 0.14 | 0.47 | 0.85 | 0.68 | 0.11 | 0.67 |
| 3 | 4.06 | 3.28 | 3.74 | 4.40 | 4.34 | 3.50 | 4.75 | 4.08 | 3.39 | 0.78 | 0.32 | 0.34 | 0.28 | 0.56 | 0.69 | 0.02 | 0.67 |
| 4 | 3.93 | 4.86 | 3.61 | 4.99 | 3.42 | 3.93 | 4.03 | 3.63 | 4.57 | 0.93 | 0.32 | 1.06 | 0.51 | 0.00 | 0.10 | 0.30 | 0.64 |
| 5 | 6.97 | 7.43 [c] | 7.44 [c] | 7.42 [c] | 7.52 [c] | 7.33 [c] | 7.31 [c] | 7.72 [c] | 7.24 [c] | 0.46 | 0.47 | 0.45 | 0.55 | 0.36 | 0.34 | 0.75 | 0.27 |
| OH-3 | 5.27 | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* |
| OH-4 | 5.80 | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* | IGN.* |
| Haa | | | | | | | | | | | | | | | | | |
| 2a | 4.64 | 4.41 | 4.39 | 4.28 | 4.50 | 4.41 | 4.45 | 4.50 | 4.59 | 0.23 | 0.25 | 0.36 | 0.14 | 0.23 | 0.19 | 0.14 | 0.05 |
| 2b | 5.30 | 5.69 | 5.69 | 5.66 | 5.69 | 5.71 | 5.91 | 5.77 | 5.72 | 0.39 | 0.39 | 0.36 | 0.39 | 0.41 | 0.61 | 0.47 | 0.42 |
| **CMAE[b]** | | | | | | | | | | **0.38** | **0.27** | **0.31** | **0.28** | **0.29** | **0.34** | **0.22** | **0.31** |

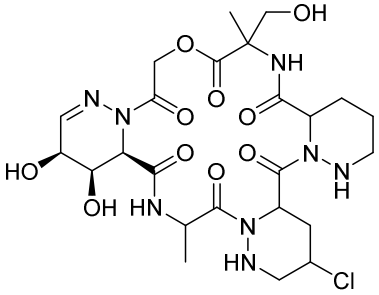
[a] **|Δδ|($^{1}$H)** = $|\delta_{exp} - \delta_{scaled}|$ ($^{1}$H), ppm: absolute differences for experimental versus scaled calculated $^{1}$H NMR chemical shifts. The $\delta_{scaled}$ values were obtained by the corresponding calculated chemical shift data ($\delta_{calcd}$); the latters were produced using the "multi standard" approach, using: [c] benzene for $^{1}$H atoms bound to $sp^{2}$ $^{13}$C atoms, and TMS (all the remaining reported values) for $sp^{3}$ $^{1}$H atoms, as reference compounds.

[b] **CMAE** = $(\Sigma[|(\delta_{exp} - \delta_{scaled})|])/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and calculated $^{1}$H chemical shifts), normalized to the number of the chemical shifts (n).

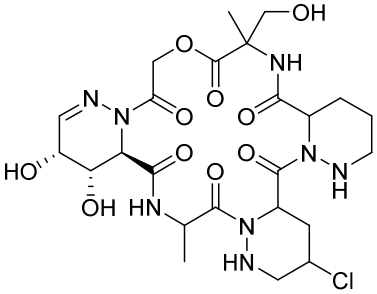
* IGNORED values, related to chemical shift values of hydrogens bound to heteroatoms



**1a**



**1b**



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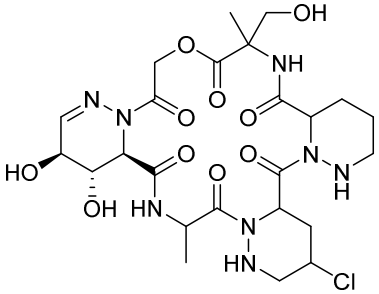

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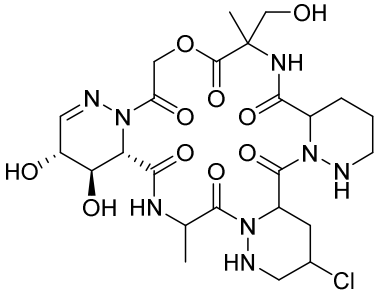

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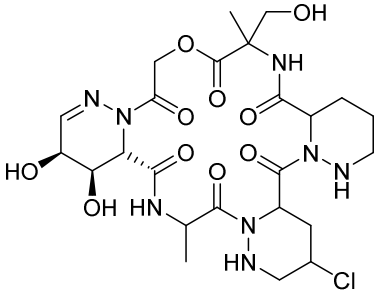

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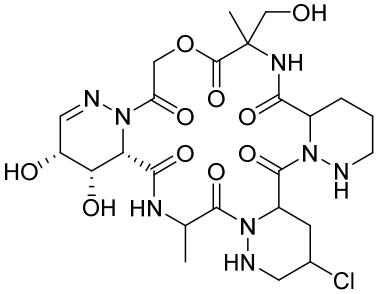
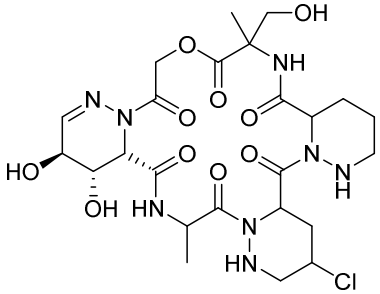


**1g**



**1h**

**Figure S1.** The eight possible stereoisomers of **1** accounted for the prediction of $^{1}H/^{13}C$ chemical shifts (**1a-1h**).

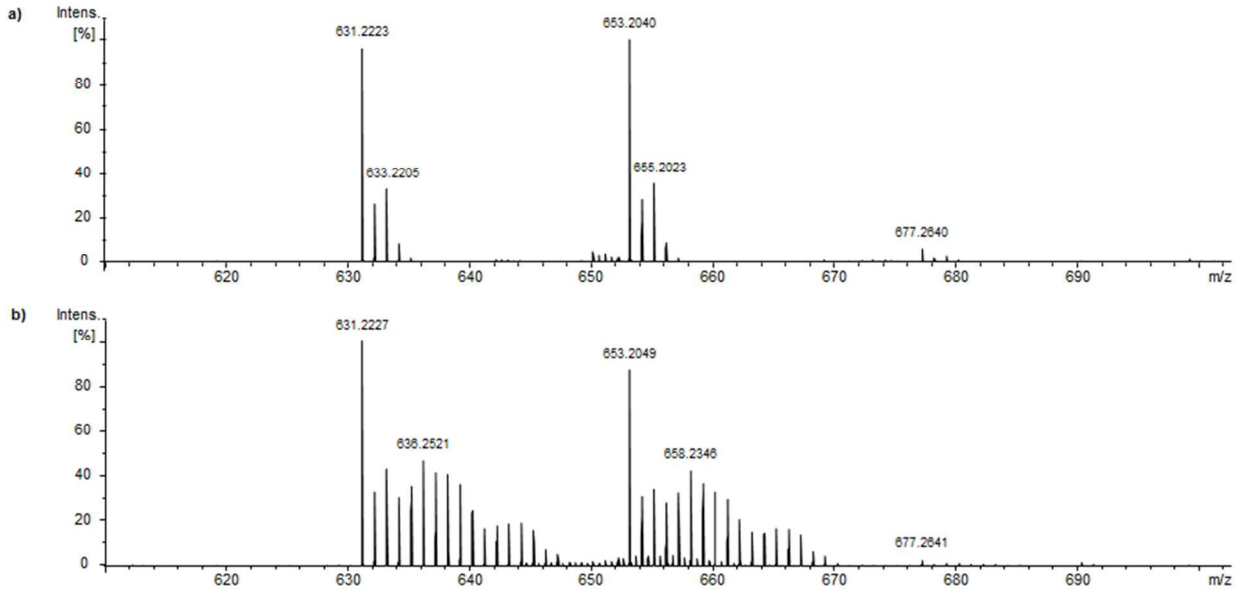



**Figure S2.** ESI-HR-MS spectra of a) non-labeled svetamycin A, and b) svetamycin A obtained from feeding experiments with L-[3,3,4,4,5,5-$^{2}H_6$]-ornithine.

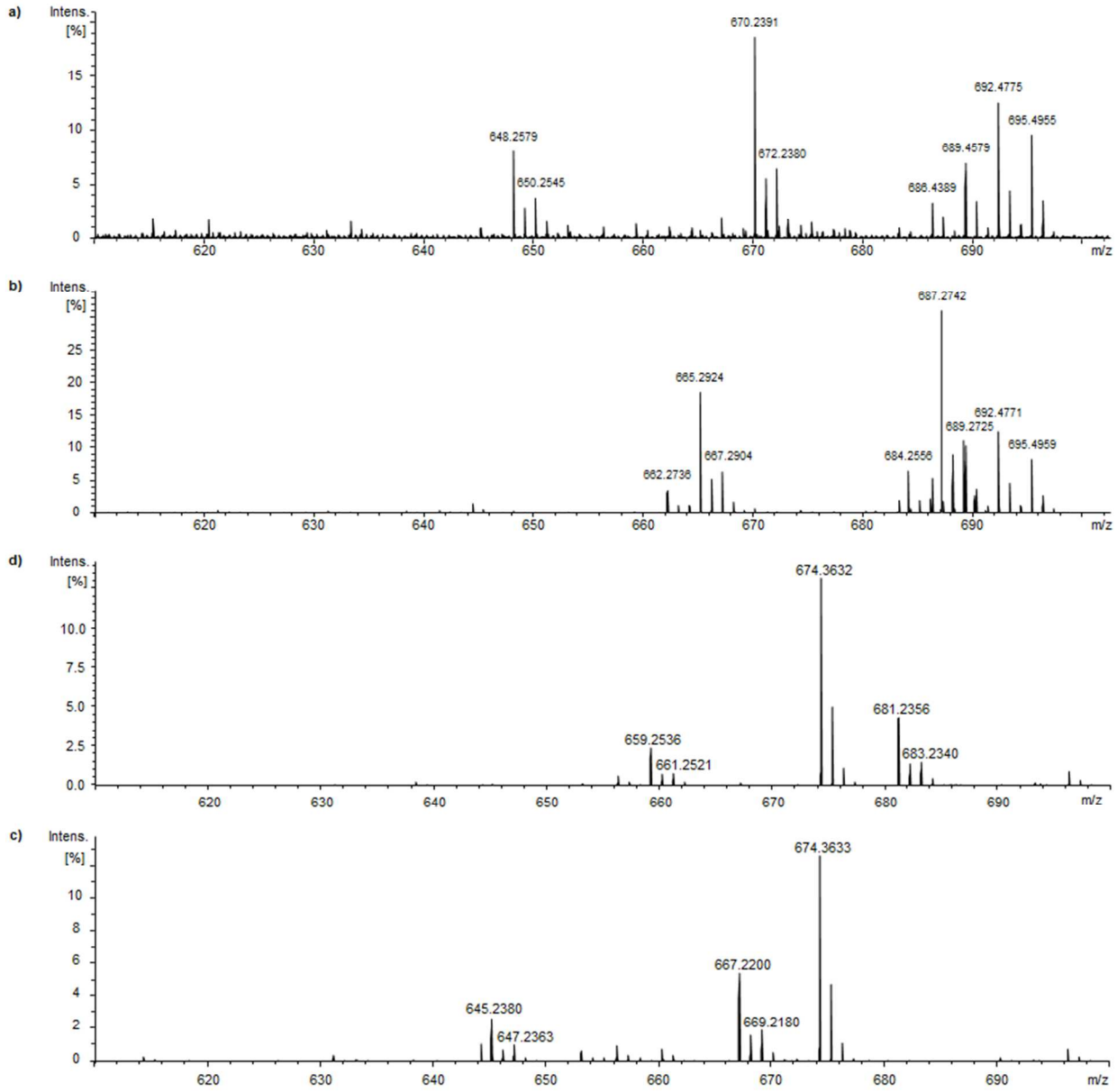



**Figure S3.** ESI-HR-MS spectra of a) svetamycin B, and b) svetamycin C obtained from feeding experiments with L-[methyl-$^{2}H_3$]-methionine; and non-labelled c) svetamycin B and d) svetamycin C.

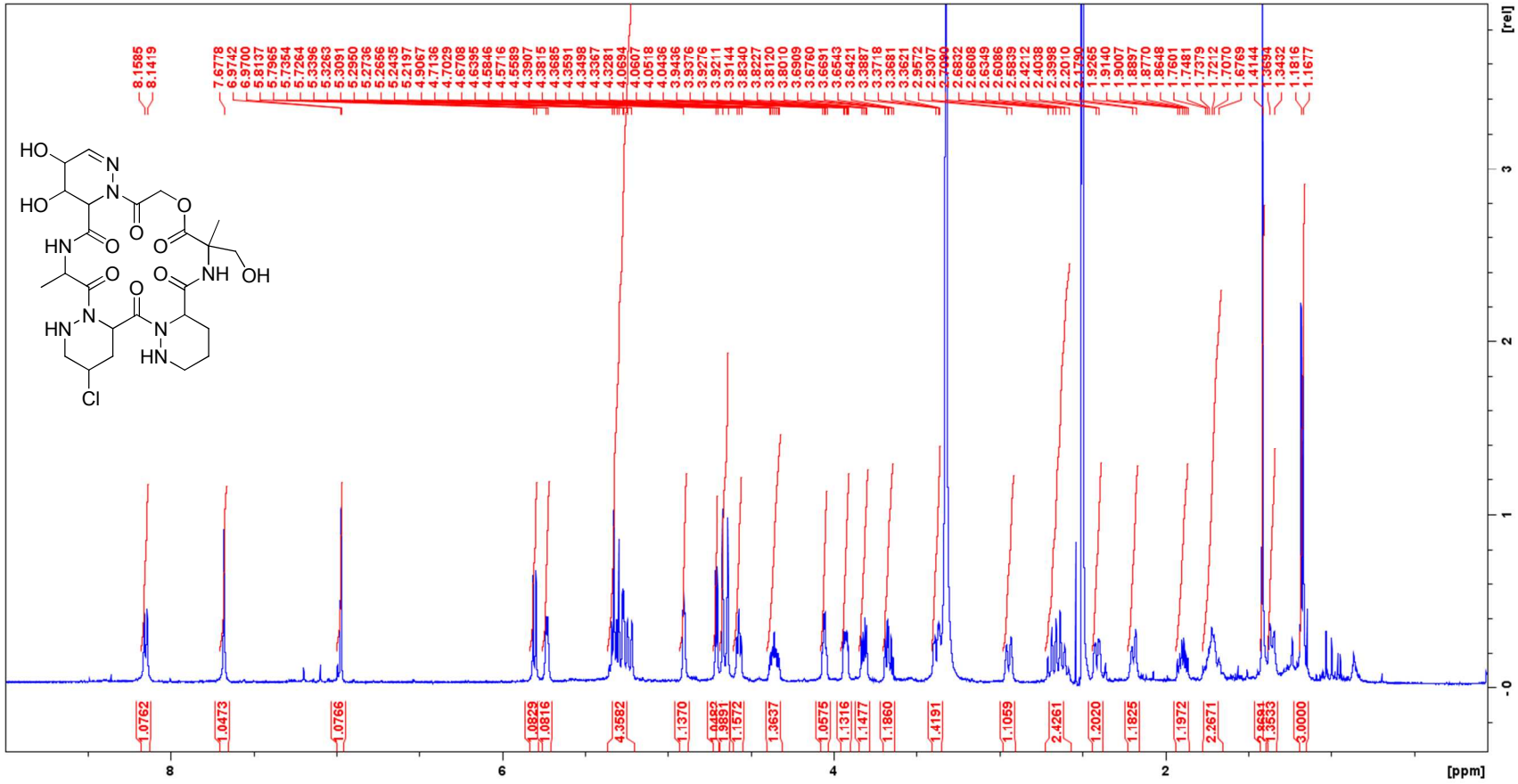



**Figure S4**. $^{1}$H NMR (500 MHz, DMSO-*d6*) spectrum of **1** (impurities are not peak picked)

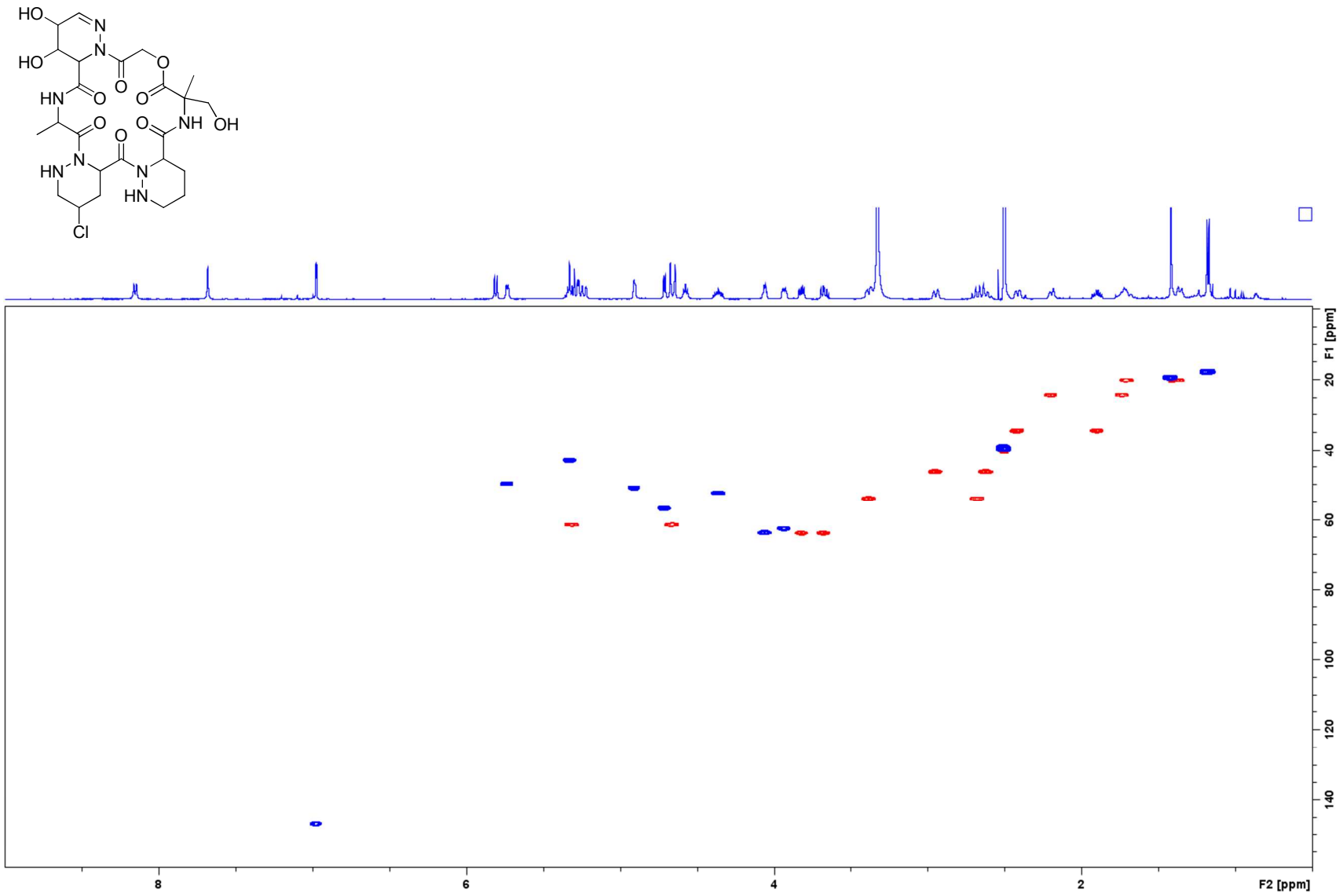



**Figure S5.** $^{1}H$, $^{13}C$ HSQC (500 MHz, DMSO-*d6*) spectrum of **1**

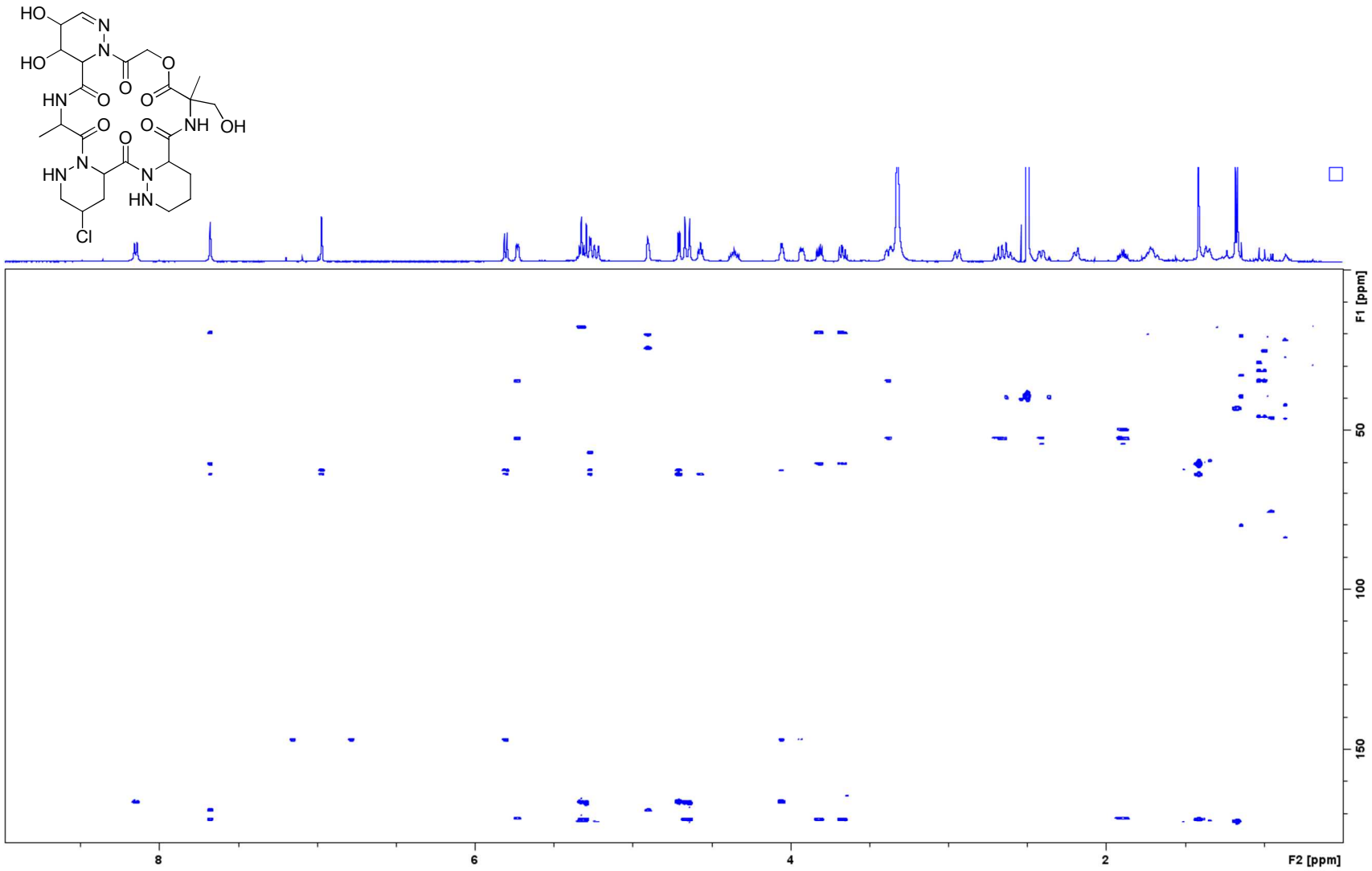



**Figure S6.** $^{1}$H, $^{13}$C HMBC (500 MHz, DMSO-*d6*) spectrum of **1**

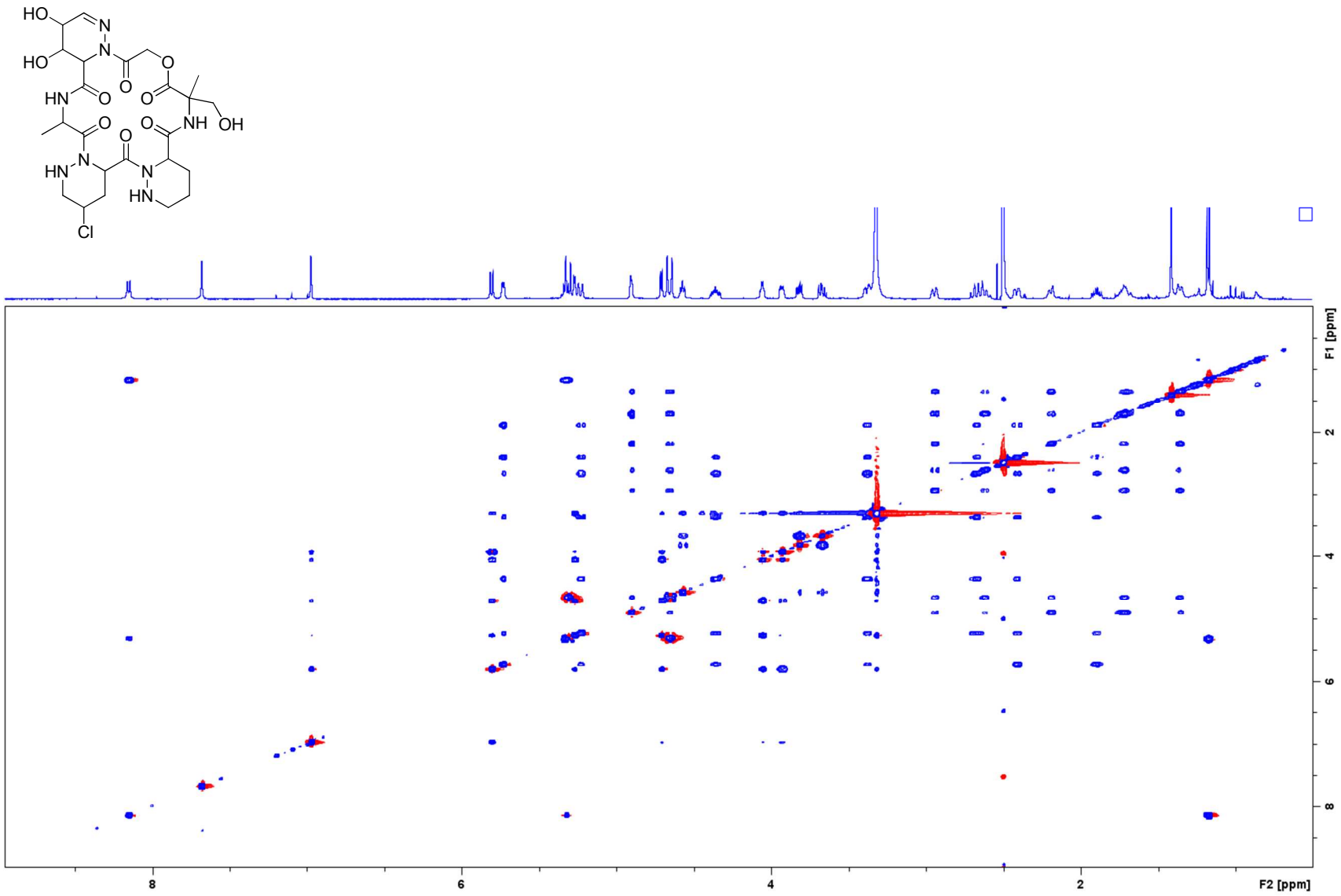



**Figure S7.** $^{1}$H, $^{1}$H TOCSY (500 MHz, DMSO-*d6*) spectrum of **1**

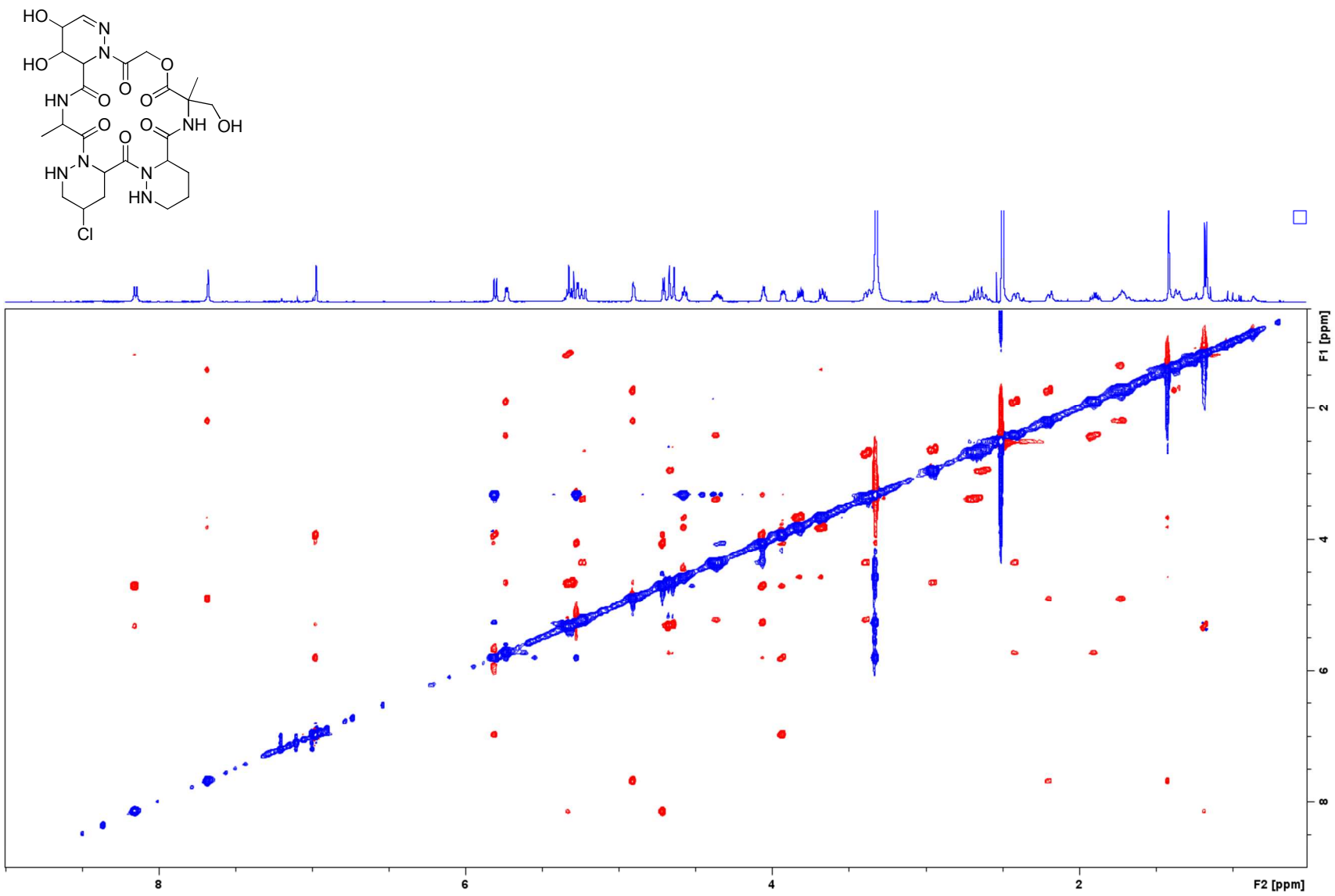



**Figure S 8.** $^{1}$H, $^{1}$H ROESY (500 MHz, DMSO-*d6*) spectrum of **1**

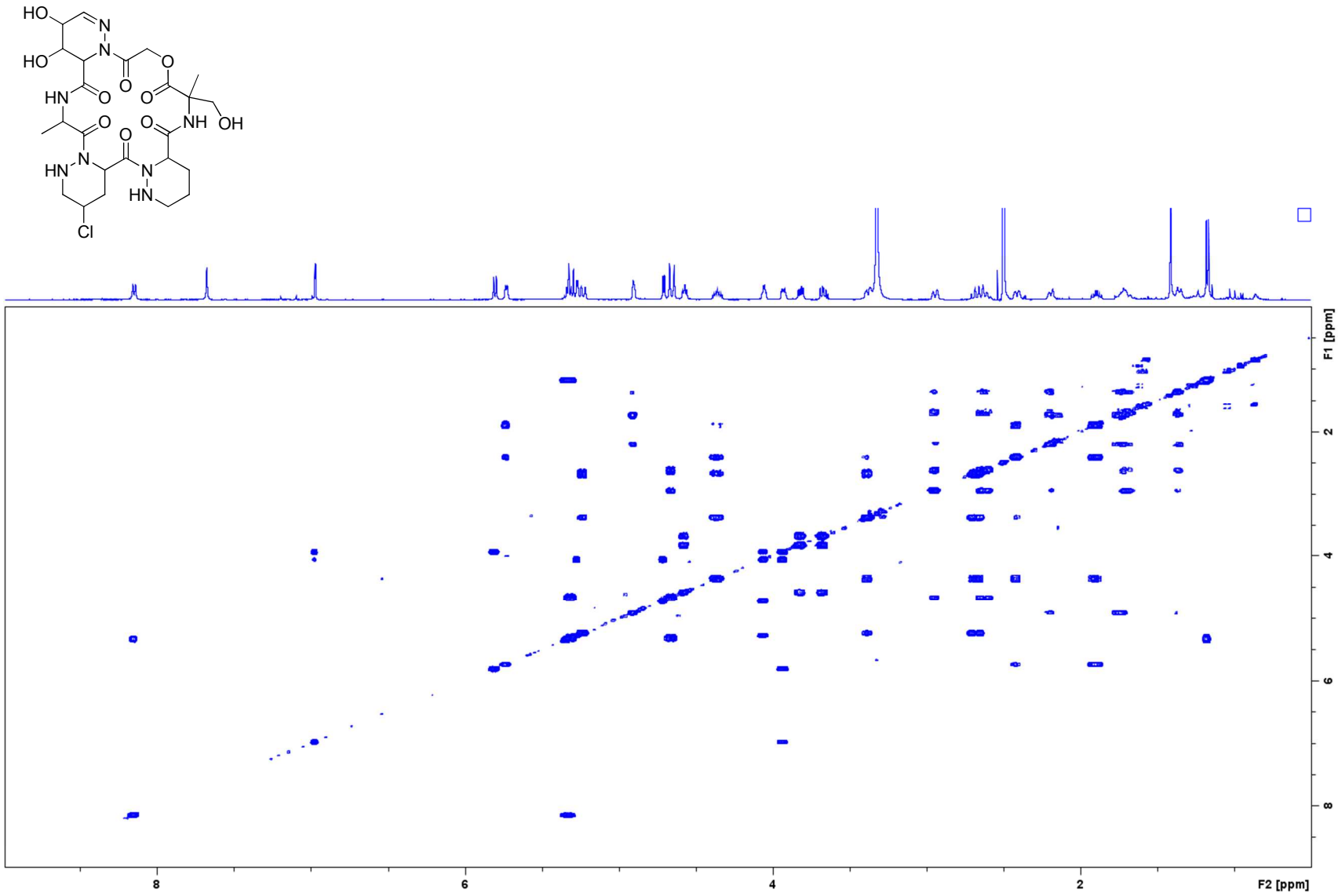



**Figure S 9.** $^{1}$H, $^{1}$H COSY (500 MHz, DMSO-*d6*) spectrum of **1**

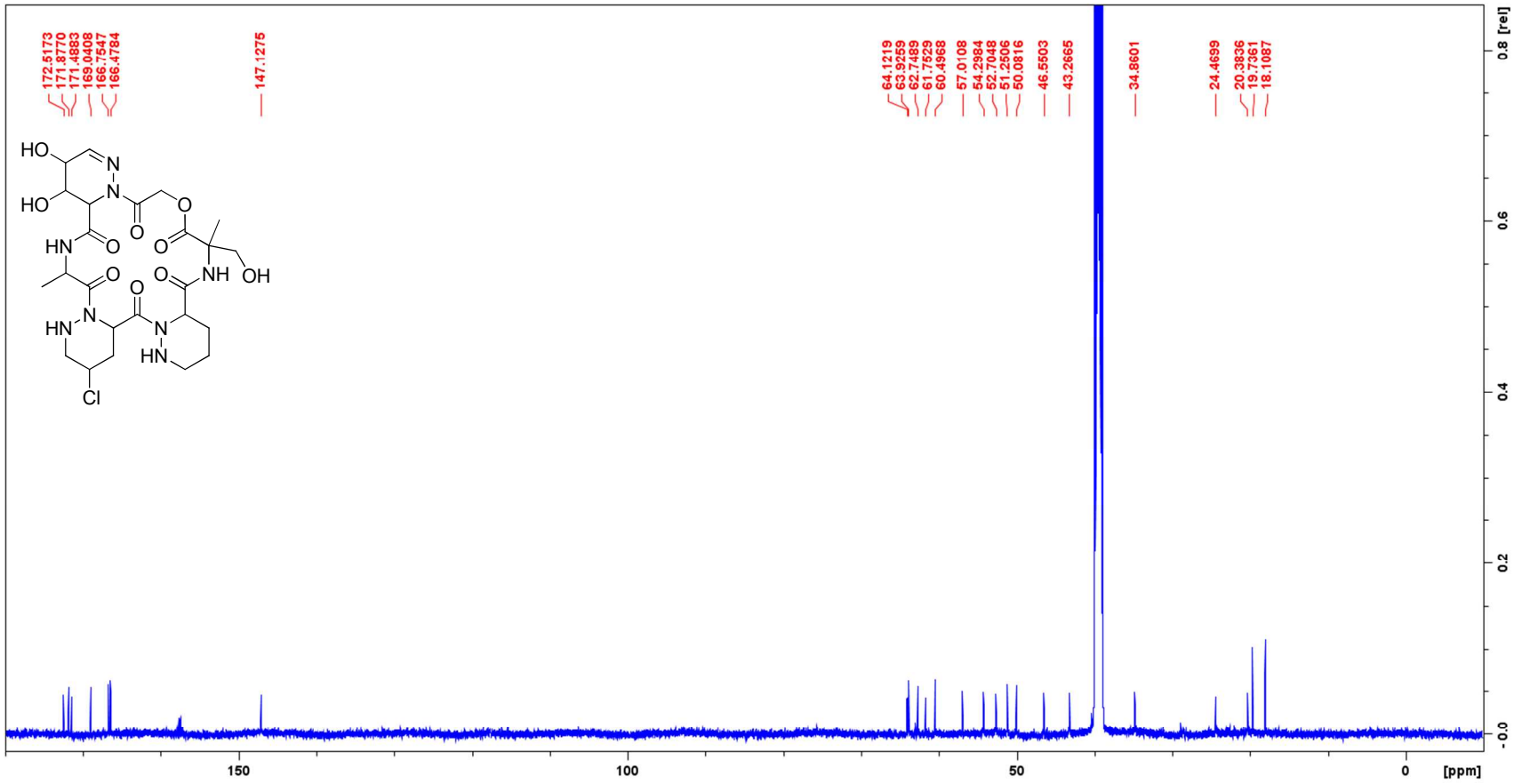



**Figure S 10.** $^{13}$C NMR (500 MHz, DMSO-*d6*) spectrum of **1**

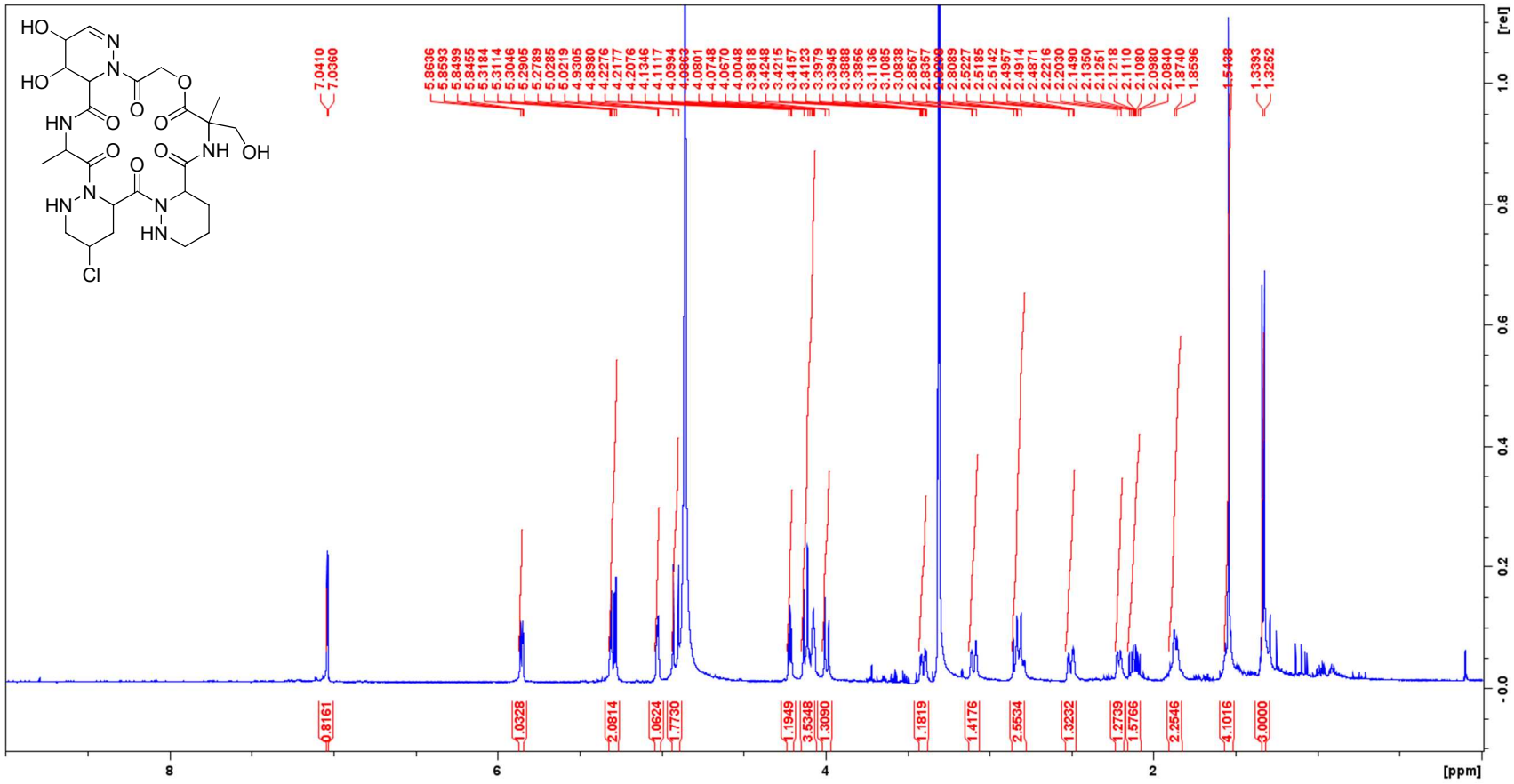



**Figure S 11.** $^{1}$H NMR (500 MHz, $CD_3OD$) spectrum of **1** (impurities are not peak picked)

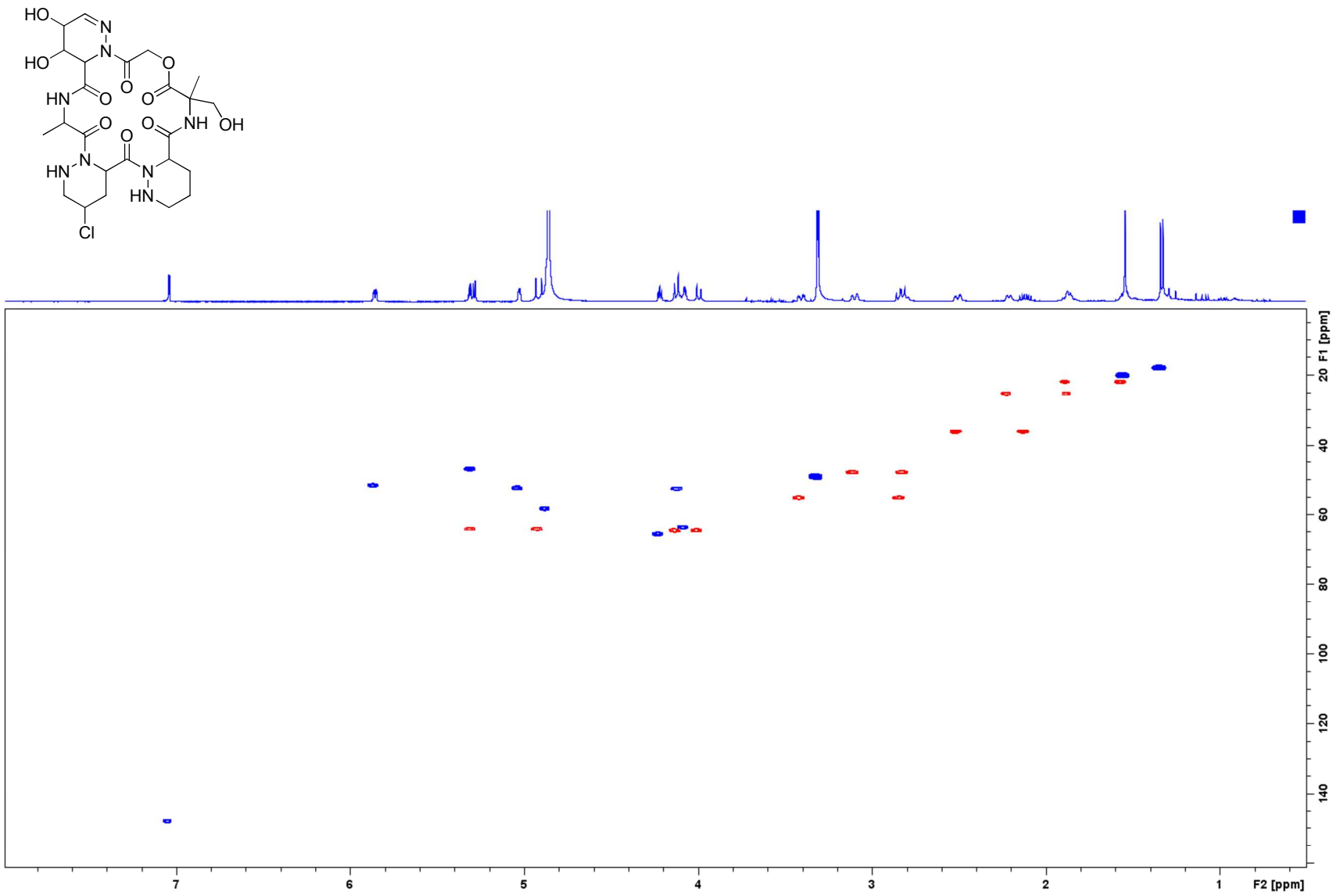



**Figure S 12.** $^{1}H$, $^{13}C$ HSQC (500 MHz, $CD_3OD$) spectrum of **1**

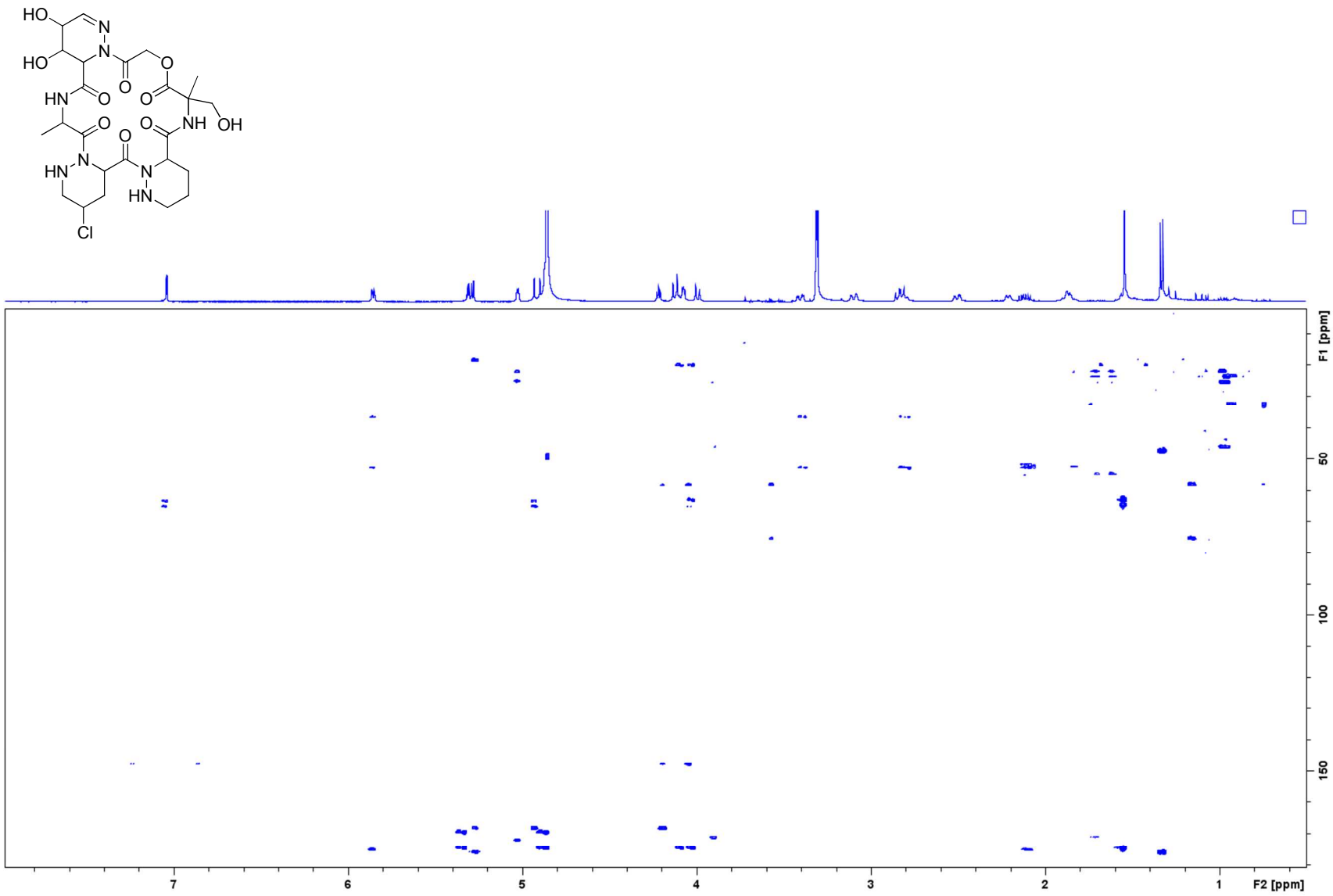



**Figure S 13.** $^{1}H$, $^{13}C$ HMBC (500 MHz, $CD_3OD$) spectrum of **1** (from another batch of **1**)

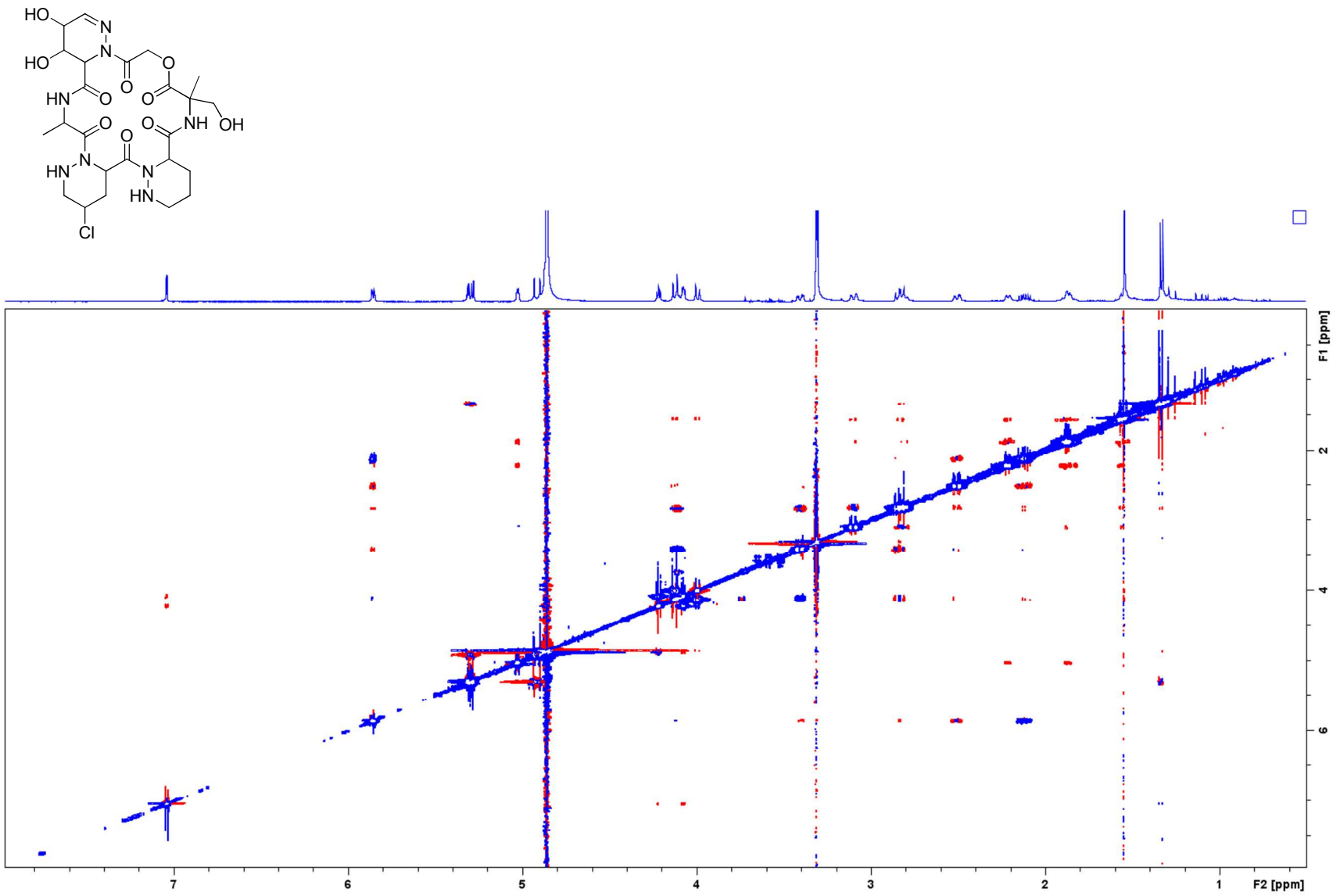



**Figure S 14.** $^{1}$H, $^{1}$H ROESY (500 MHz, $CD_3OD$) spectrum of **1**

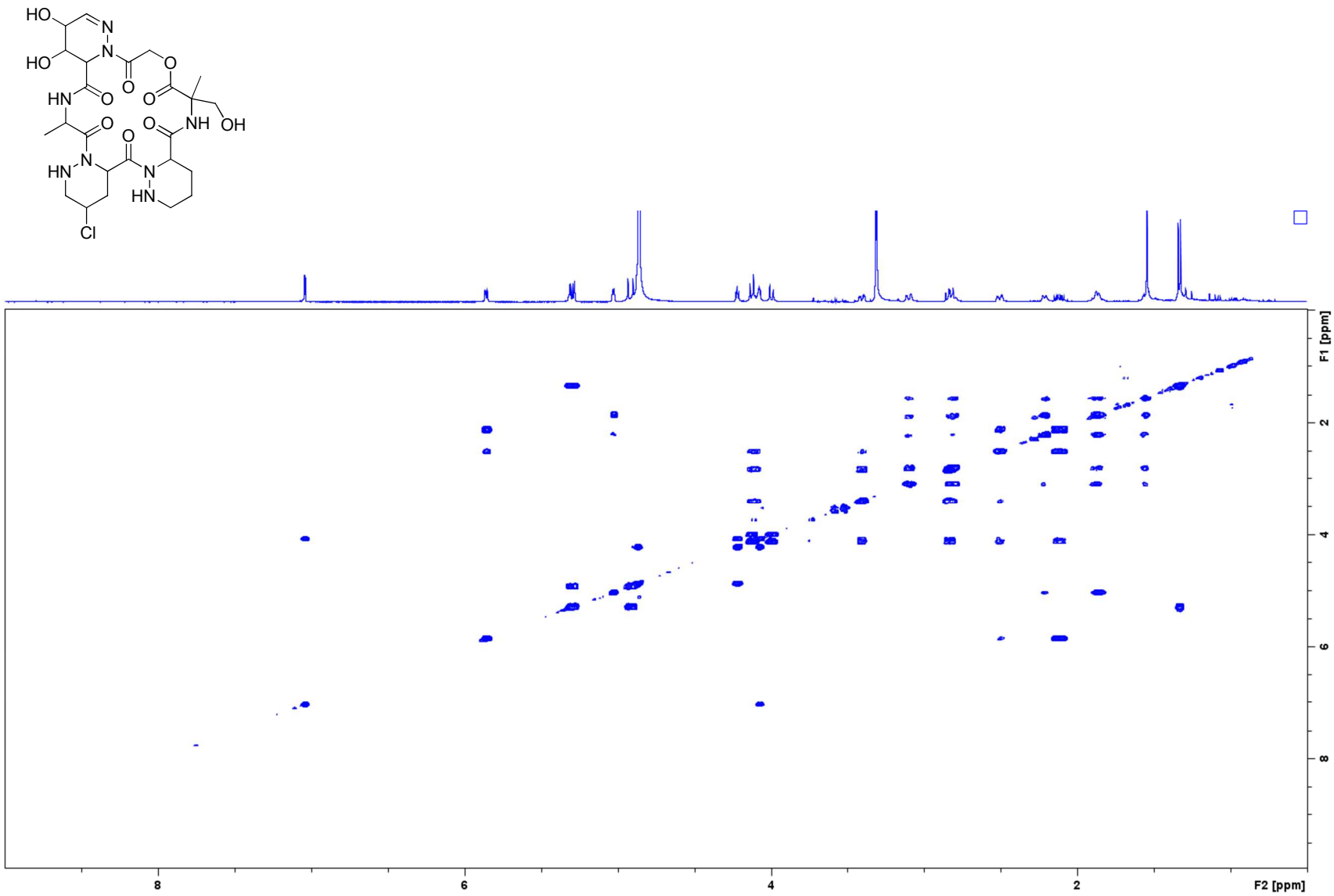



**Figure S 15.** $^{1}H$, $^{1}H$ COSY (500 MHz, $CD_3OD$) spectrum of **1**

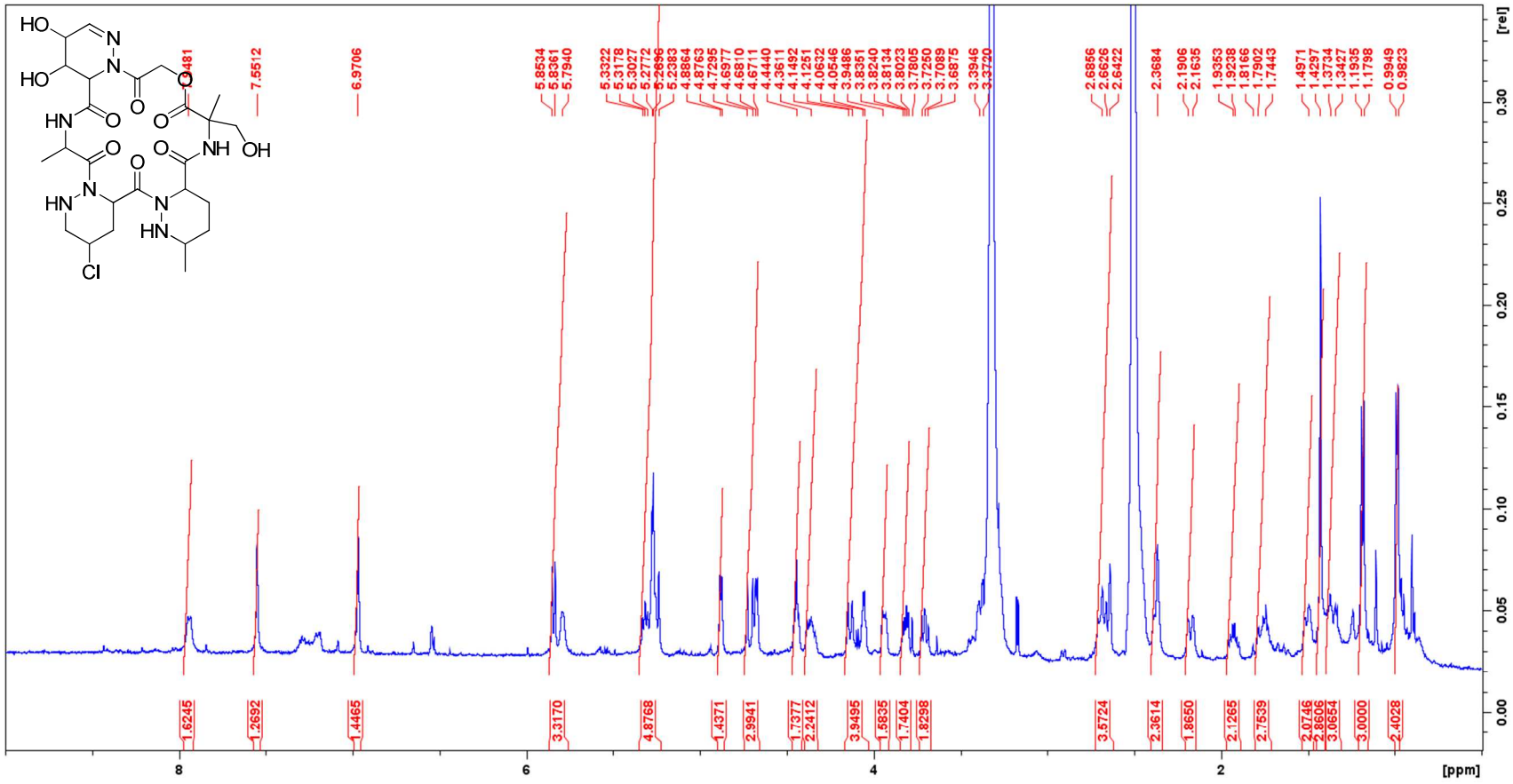



**Figure S 16.** $^{1}$H NMR (500 MHz, DMSO-*d6*) spectrum of **2** (impurities are not peak picked)

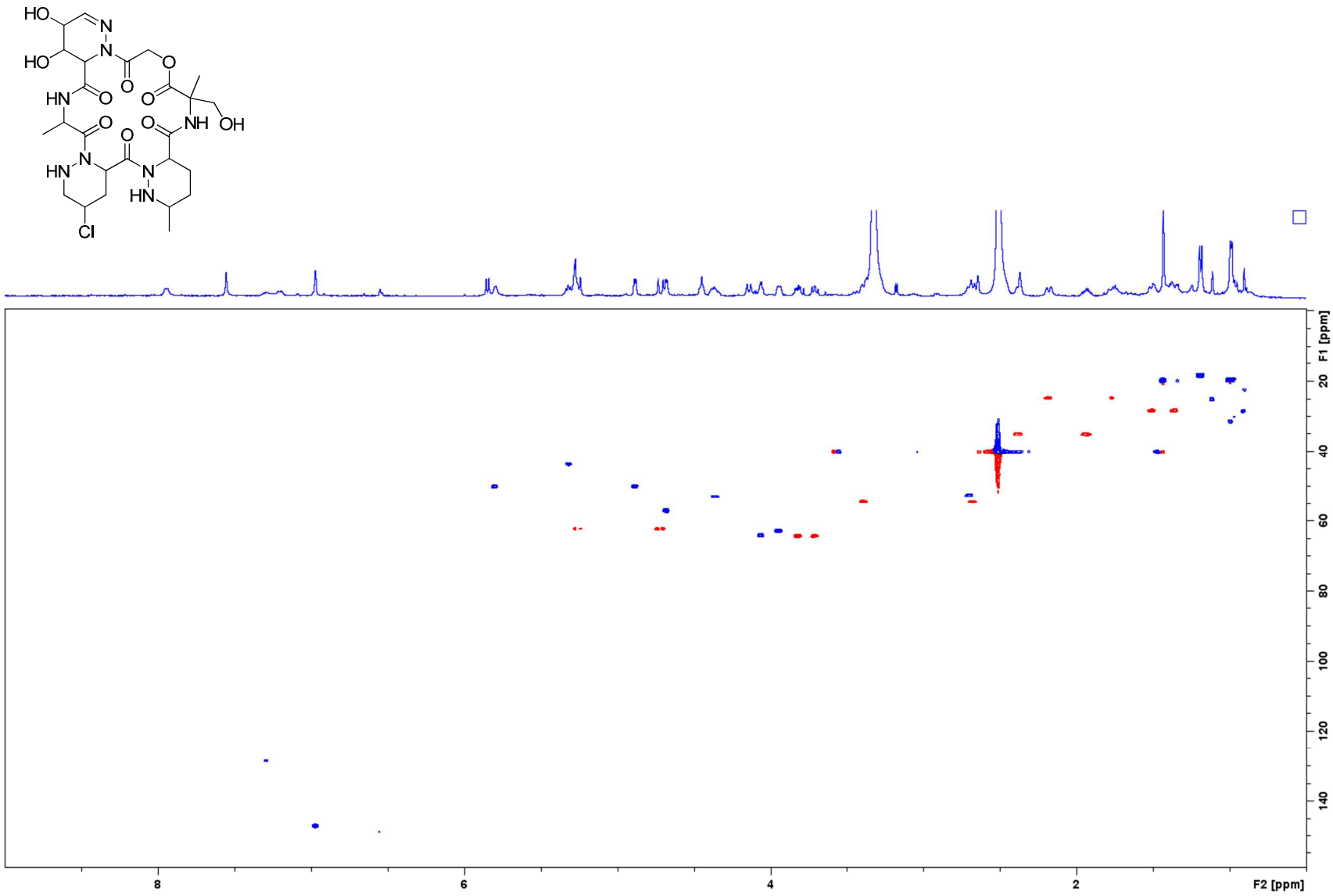



**Figure S 17.** $^{1}H$, $^{13}C$ HSQC (500 MHz, DMSO-*d6*) spectrum of **2**

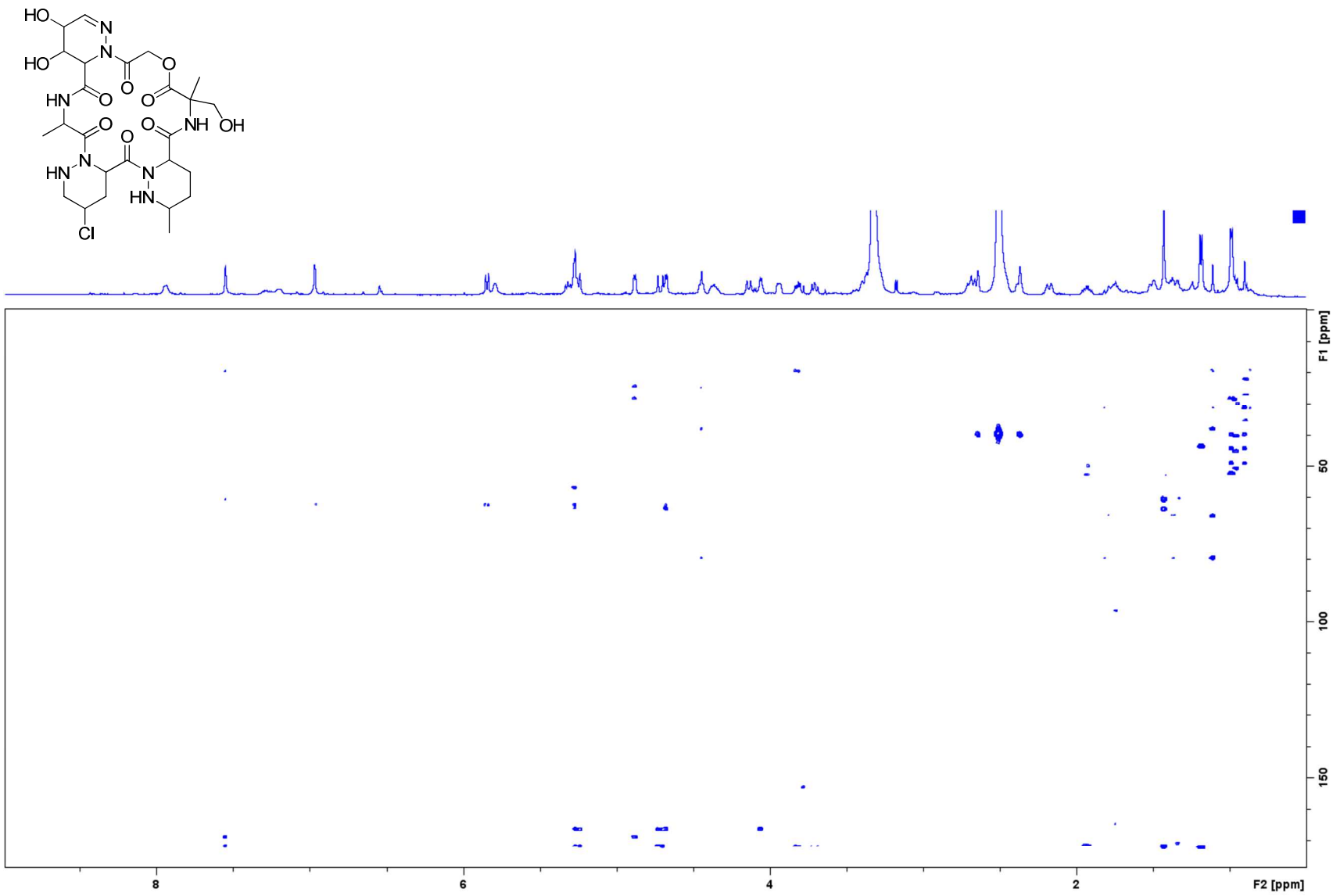



**Figure S 18.** $^{1}H$, $^{13}C$ HMBC (500 MHz, DMSO-*d6*) spectrum of **2**

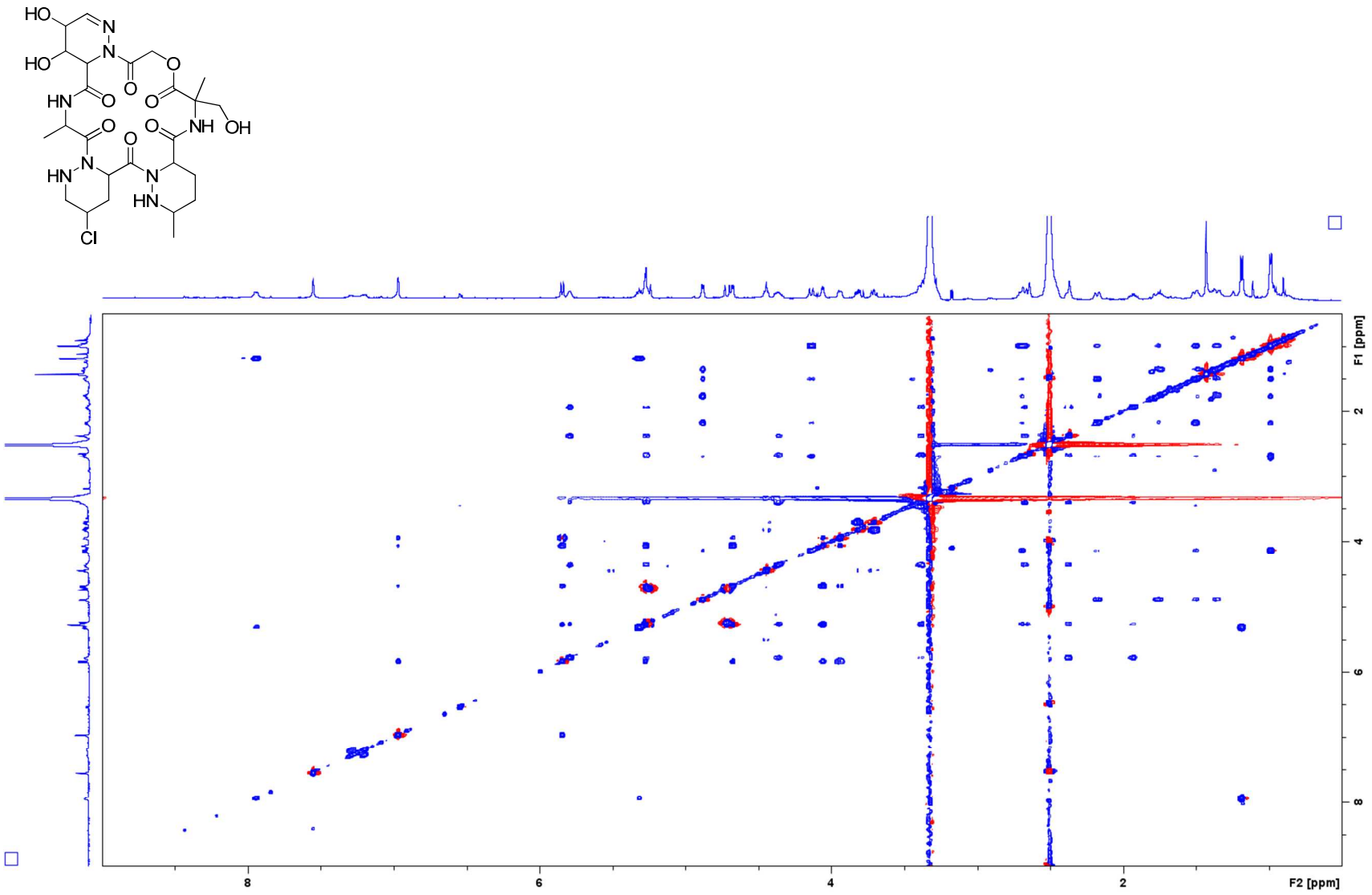



**Figure S 19.** $^{1}$H, $^{1}$H TOCSY (500 MHz, DMSO-*d6*) spectrum of **2**

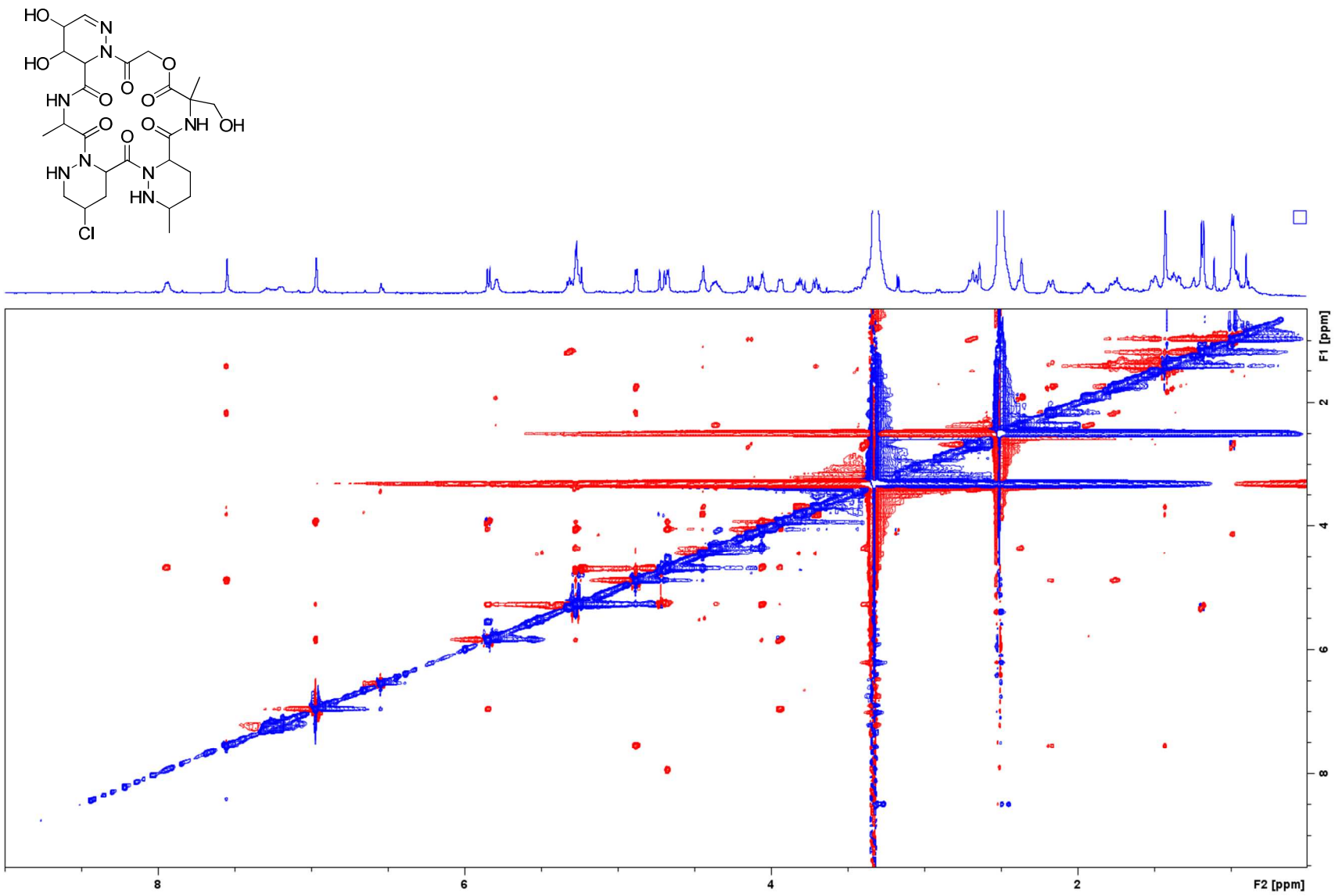



**Figure S 20.** $^{1}$H, $^{1}$H ROESY (500 MHz, DMSO-*d6*) spectrum of **2**

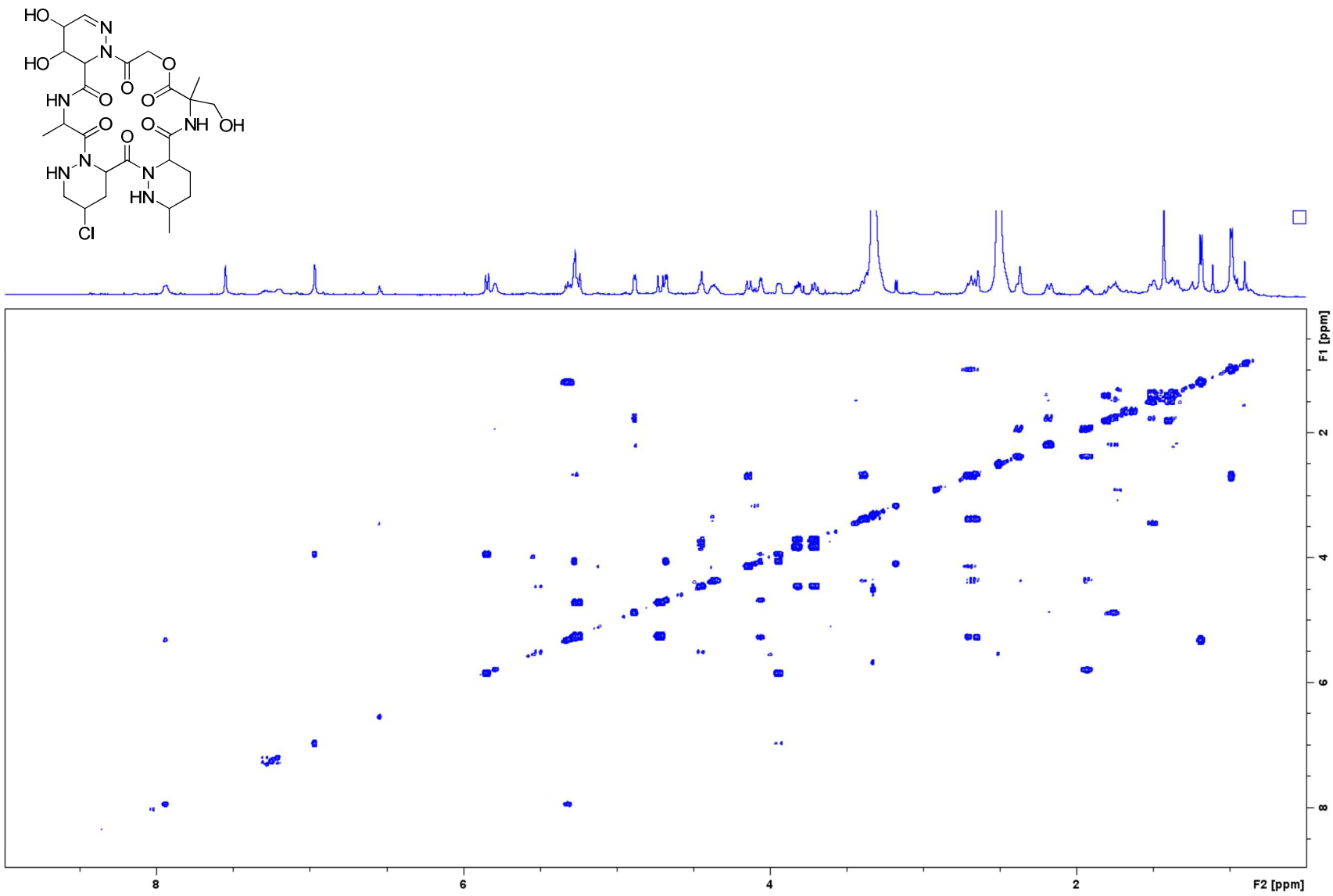



**Figure S 21.** $^{1}$H, $^{1}$H COSY (500 MHz, DMSO-*d6*) spectrum of **2**

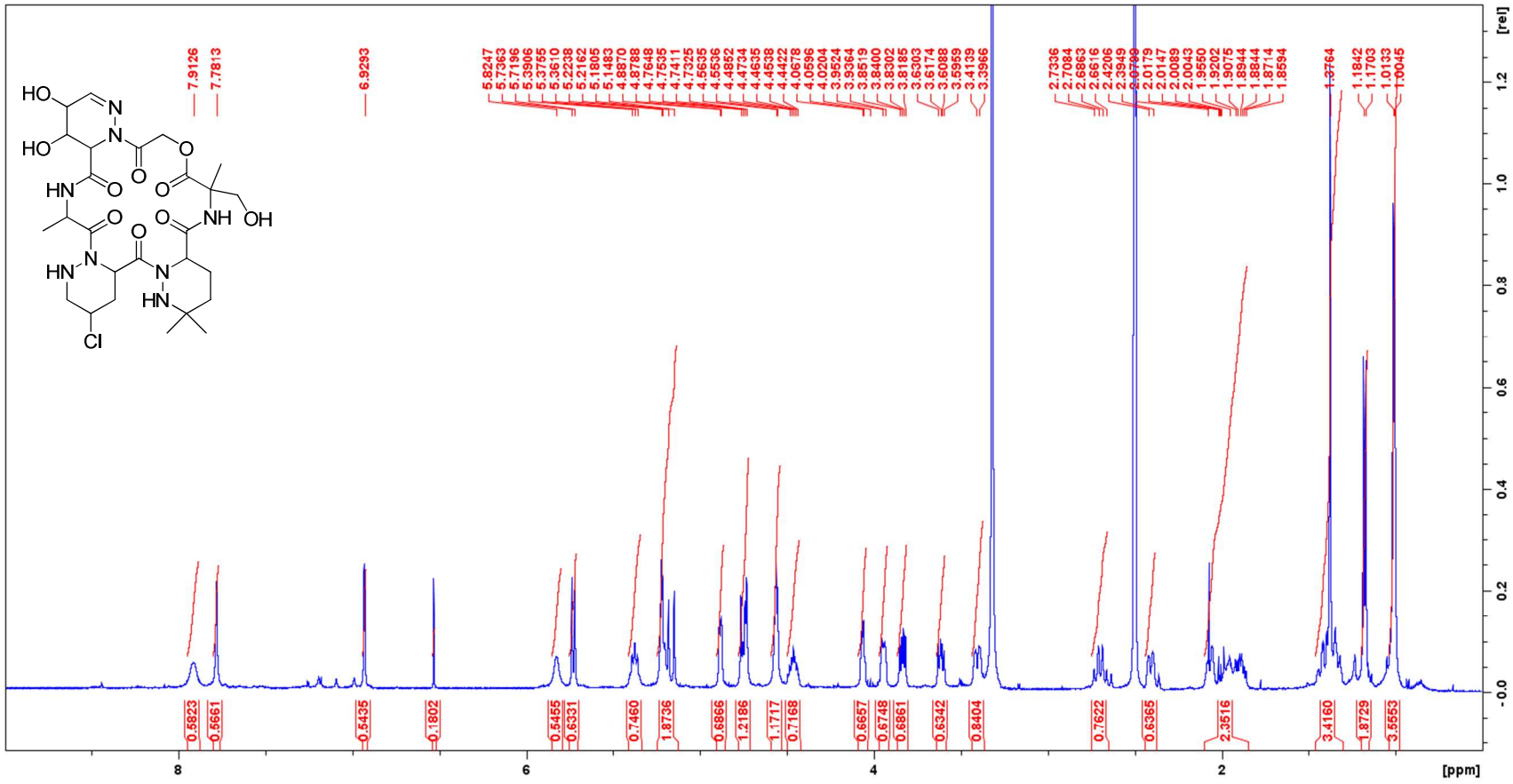



**Figure S 22.** $^{1}$H NMR (500 MHz, DMSO-*d6*) spectrum of **3** (impurities are not peak picked)

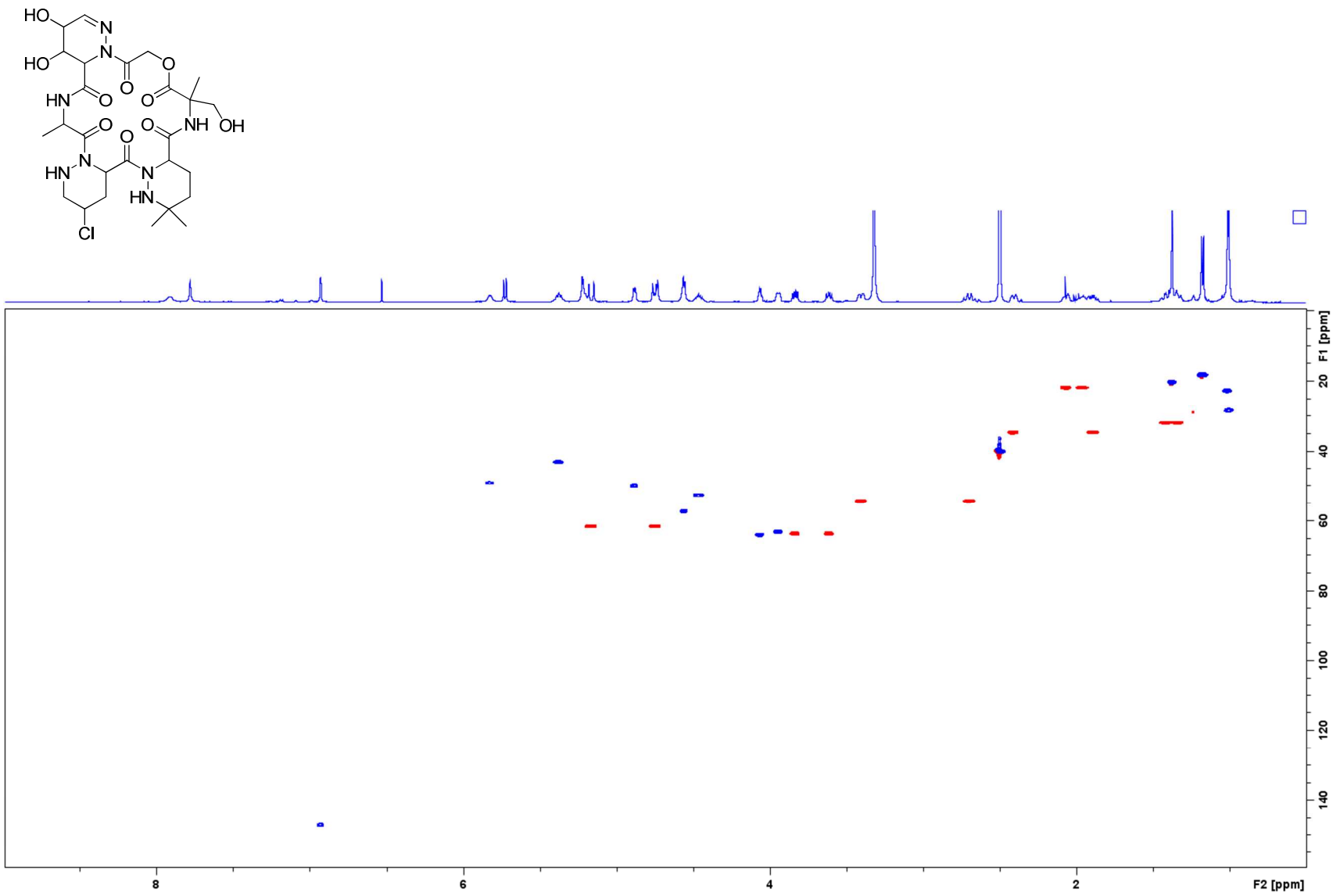



**Figure S 23.** $^{1}H$, $^{13}C$ HSQC (500 MHz, DMSO-*d6*) spectrum of **3**

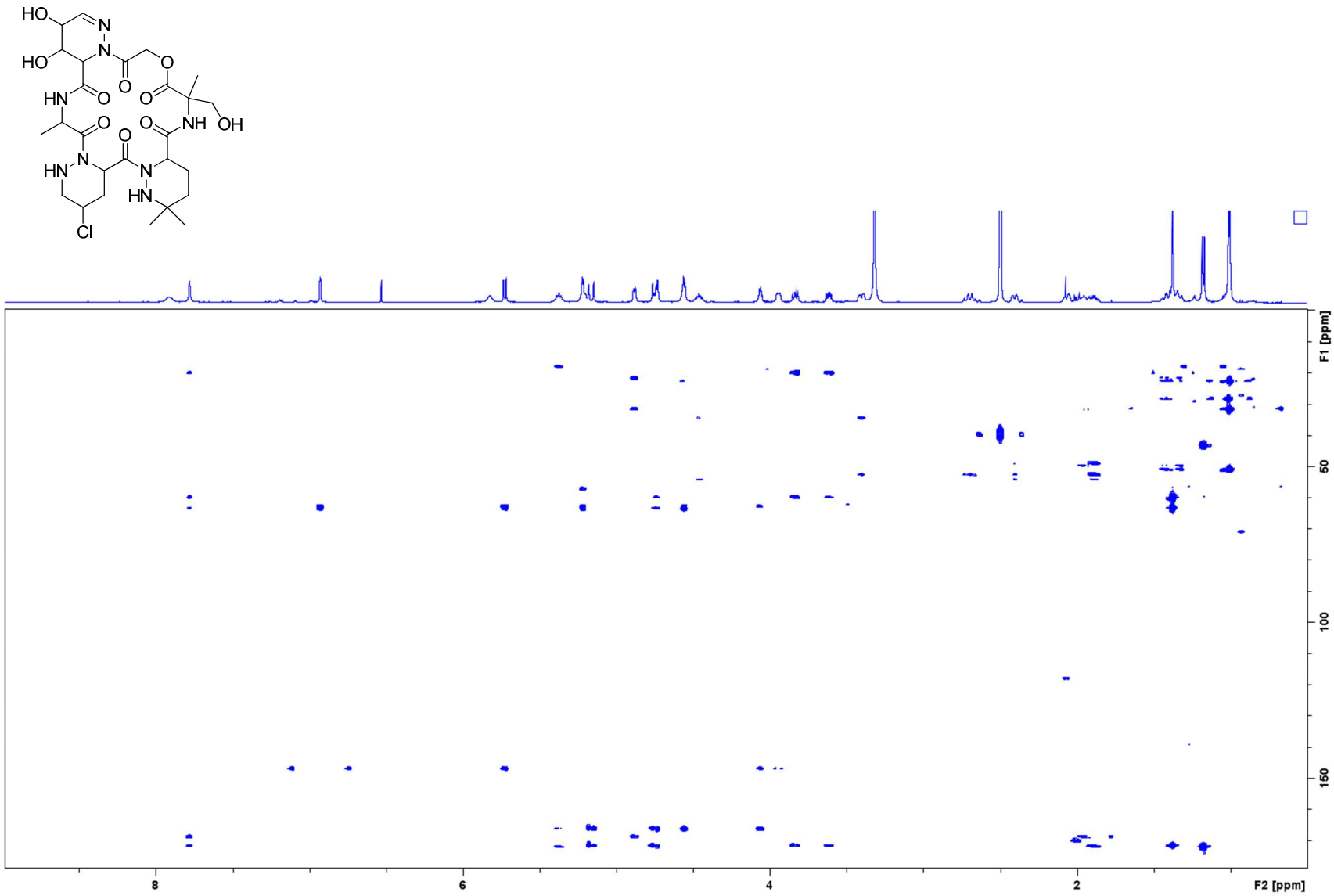



**Figure S 24.** $^{1}H$, $^{13}C$ HMBC (500 MHz, DMSO-*d6*) spectrum of **3**

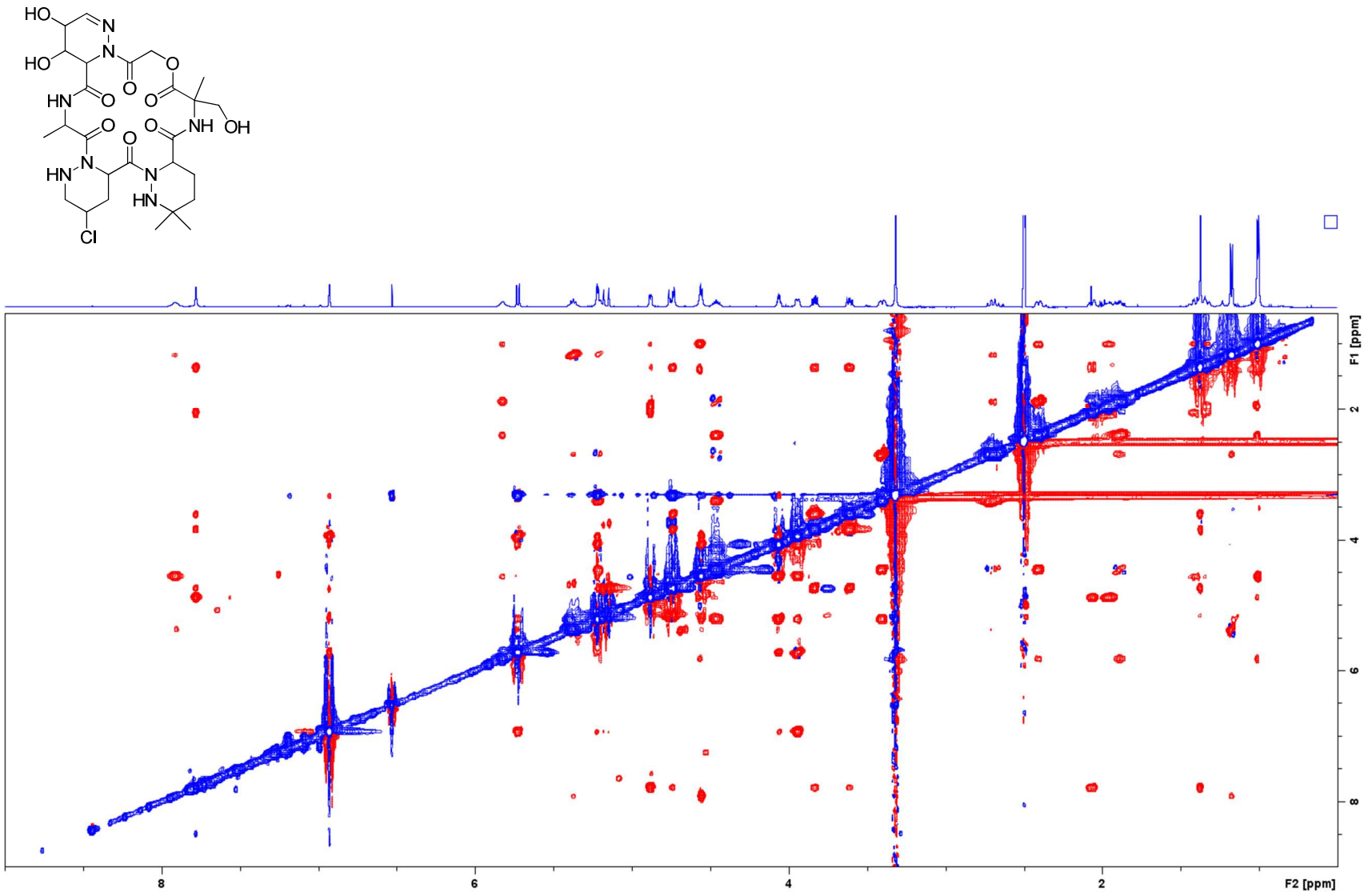



**Figure S 25.** $^{1}$H, $^{1}$H ROESY (500 MHz, DMSO-*d6*) spectrum of **3**

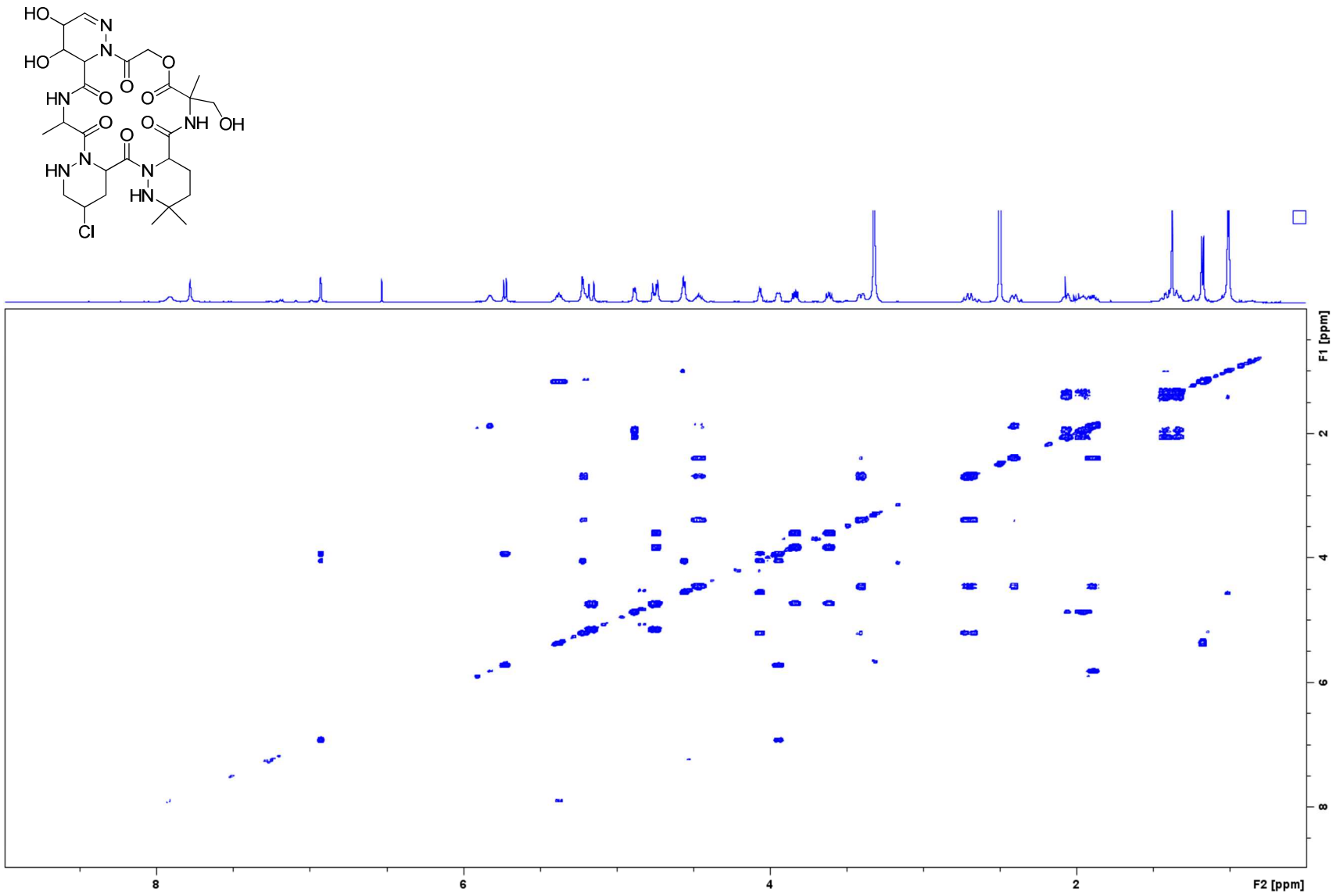



**Figure S 26.** $^{1}$H, $^{1}$H COSY (500 MHz, DMSO-*d6*) spectrum of **3**

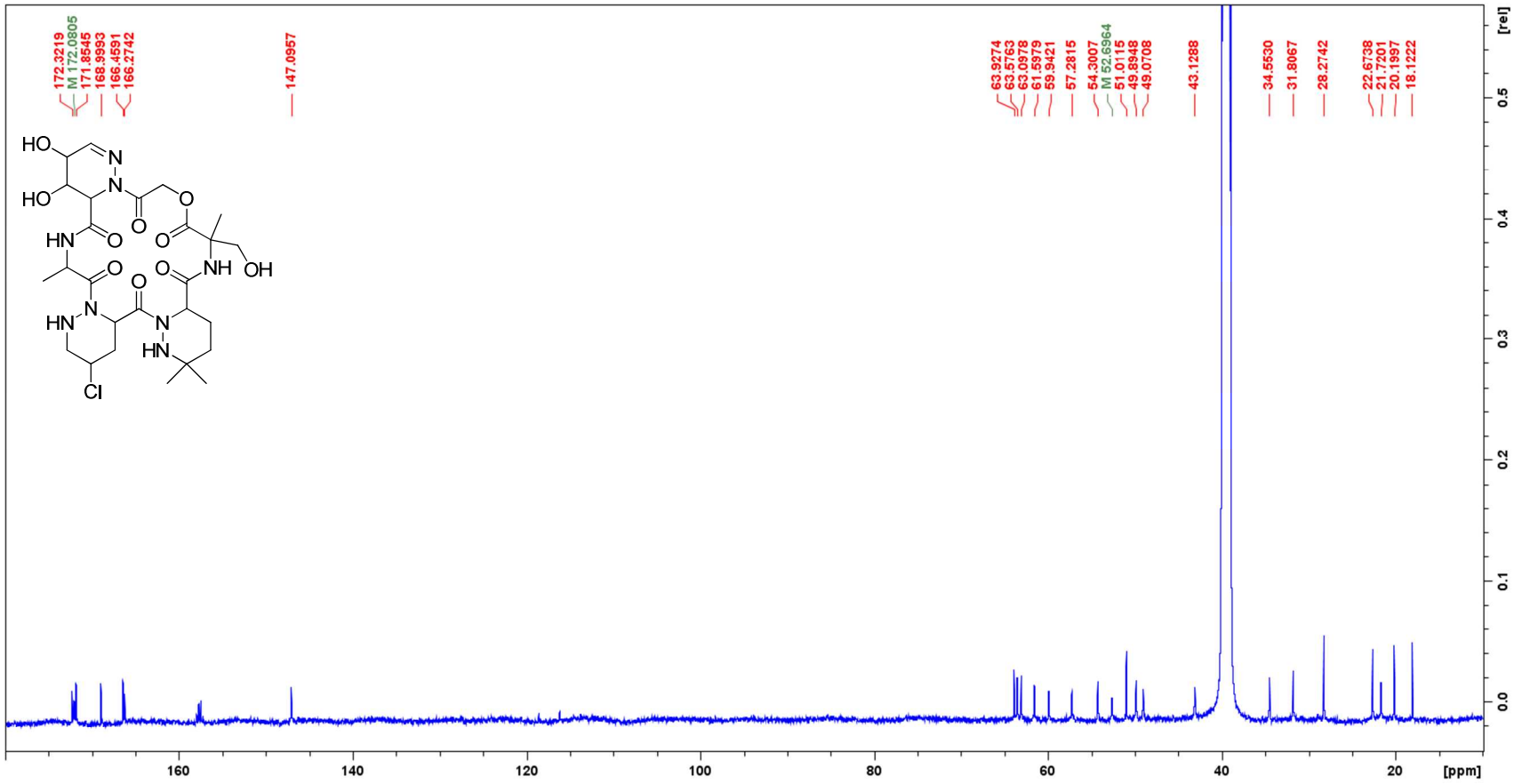



**Figure S 27.** $^{13}$C NMR (500 MHz, DMSO-*d6*) spectrum of **3**

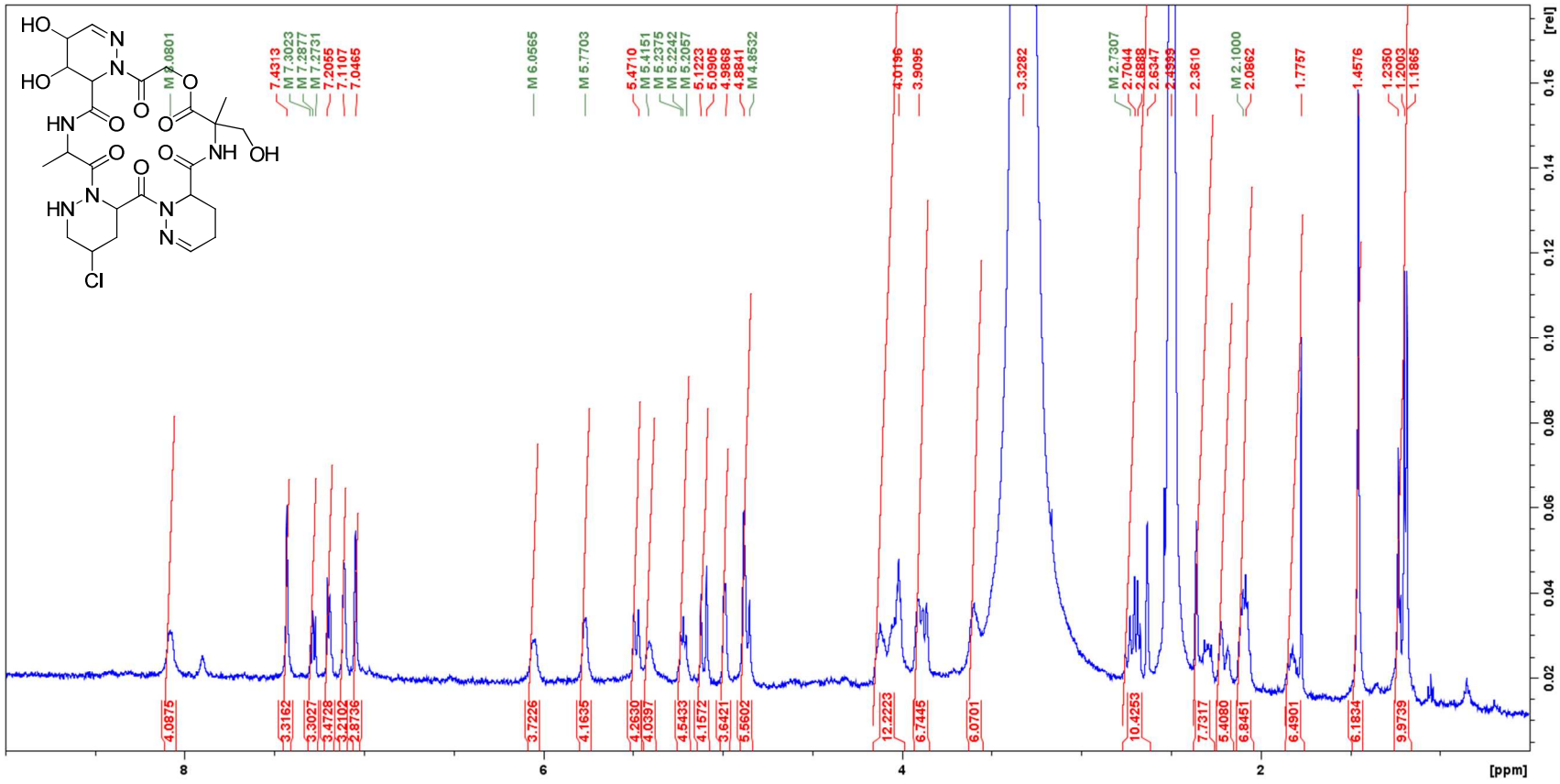



**Figure S 28.** $^{1}$H NMR (500 MHz, DMSO-*d6*) spectrum of **4**

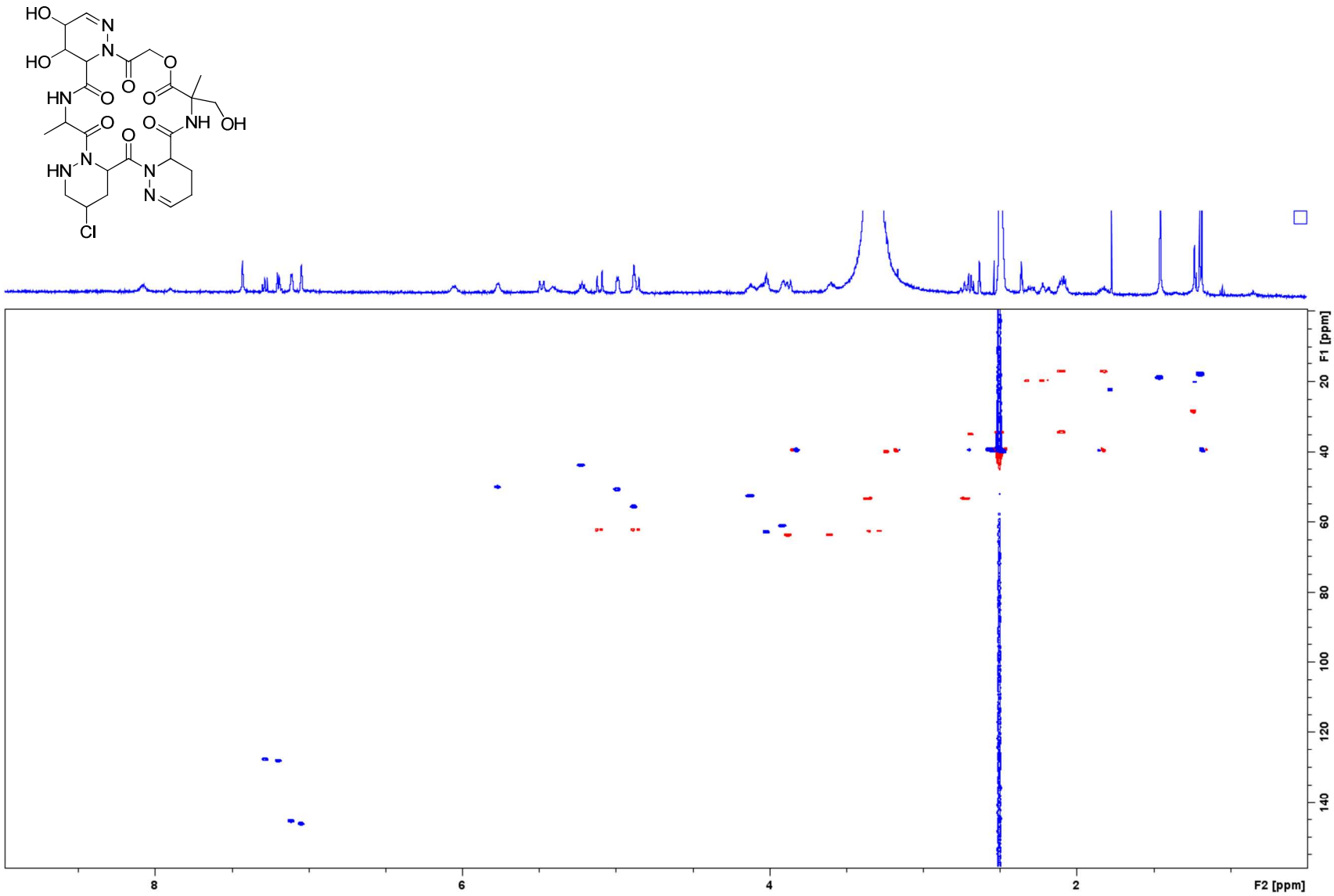



**Figure S 29.** $^{1}H$, $^{13}C$ HSQC (500 MHz, DMSO-*d6*) spectrum of **4**

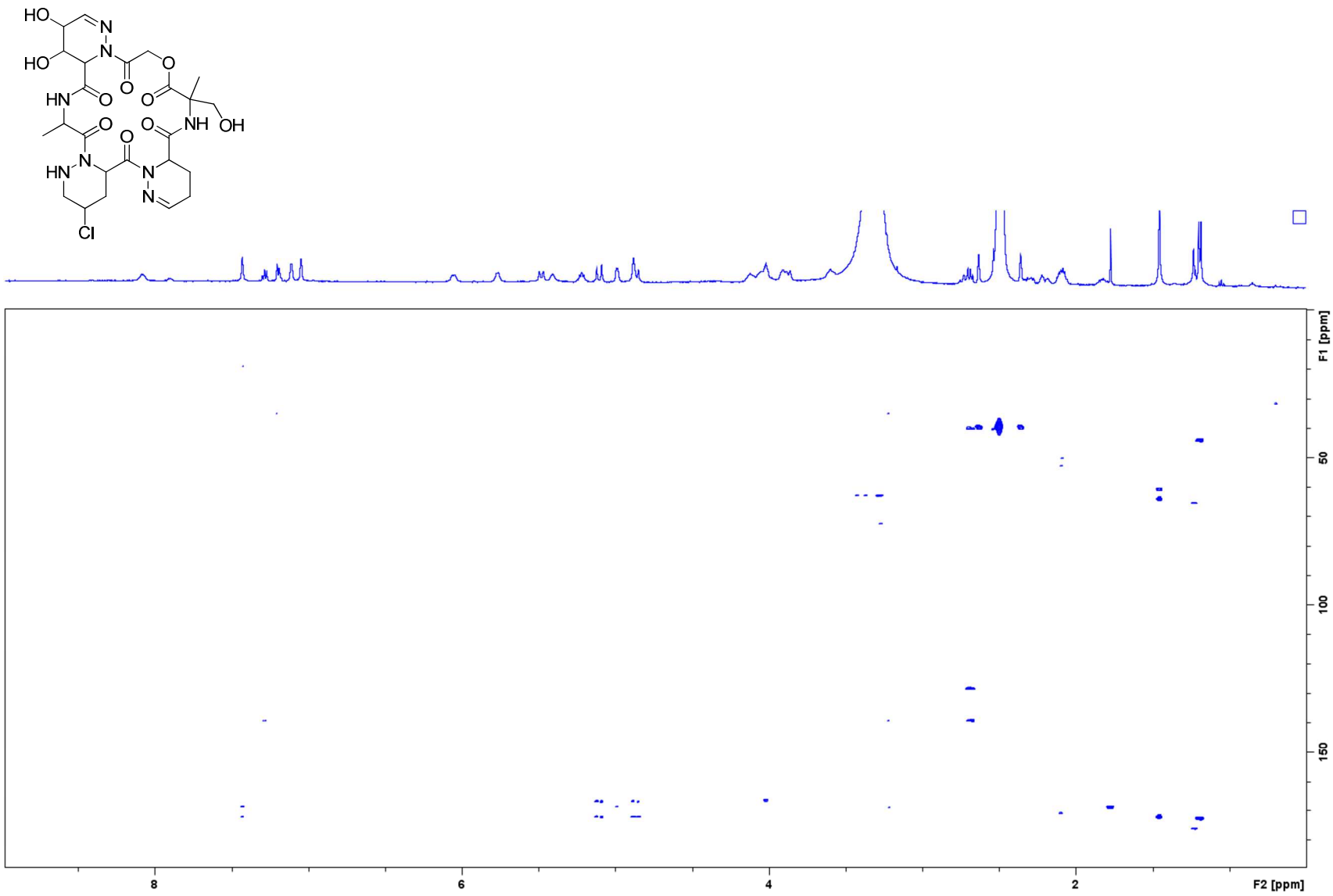



**Figure S 30.** $^{1}H$, $^{13}C$ HMBC (500 MHz, DMSO-*d6*) spectrum of **4**

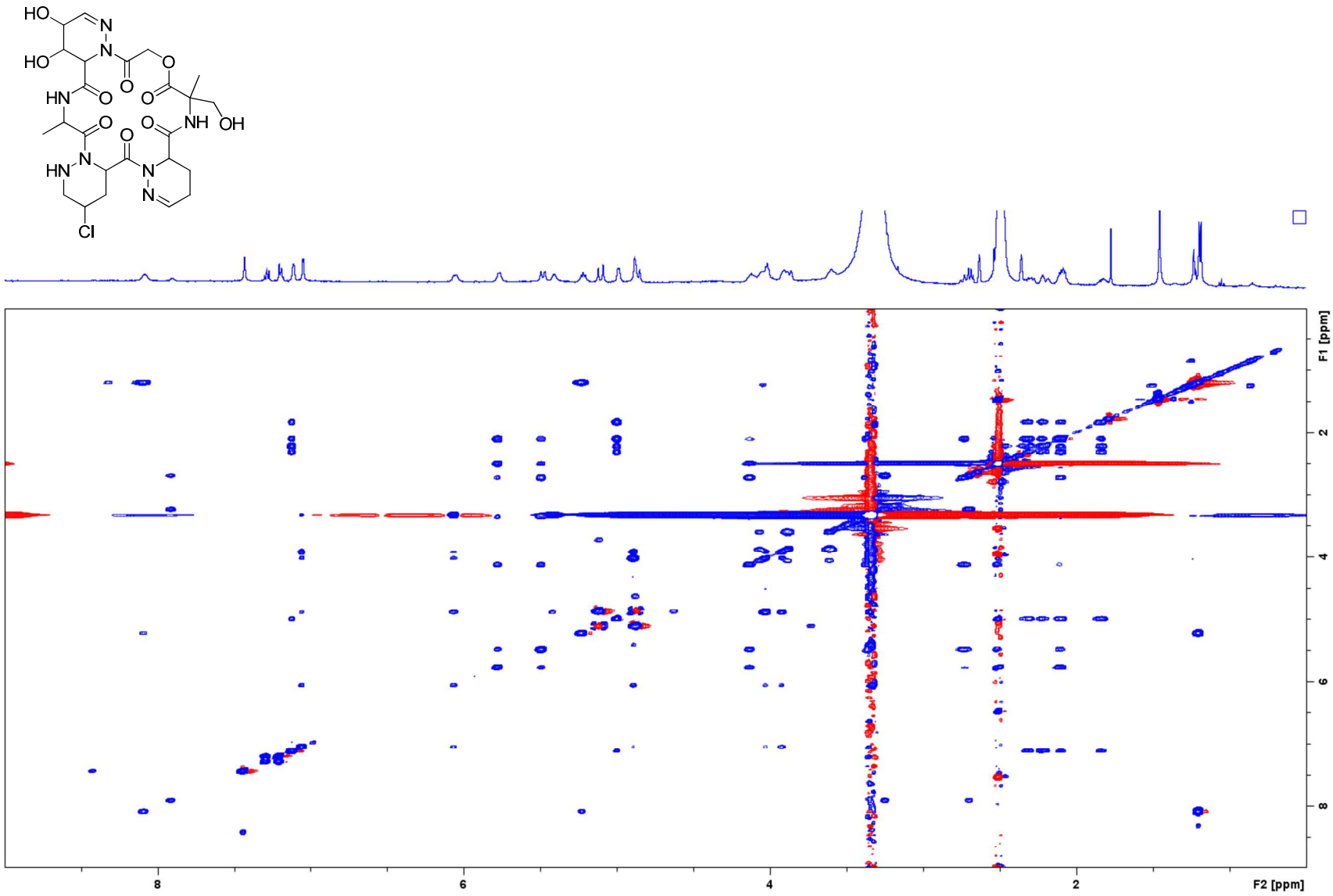



**Figure S 31.** $^{1}$H, $^{1}$H TOCSY (500 MHz, DMSO-*d6*) spectrum of **4**

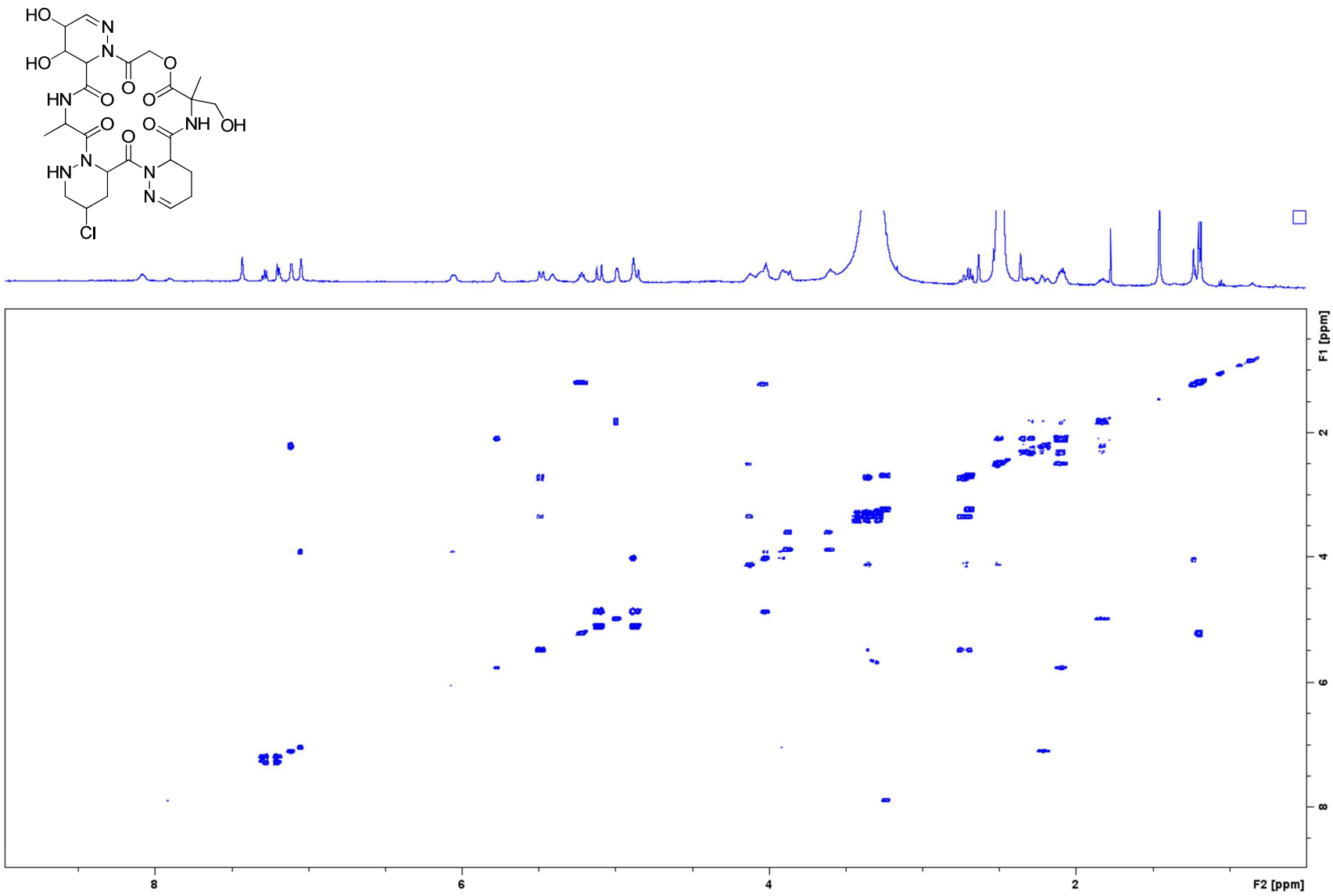



**Figure S 32.** $^{1}$H, $^{1}$H COSY (500 MHz, DMSO-*d6*) spectrum of **4**

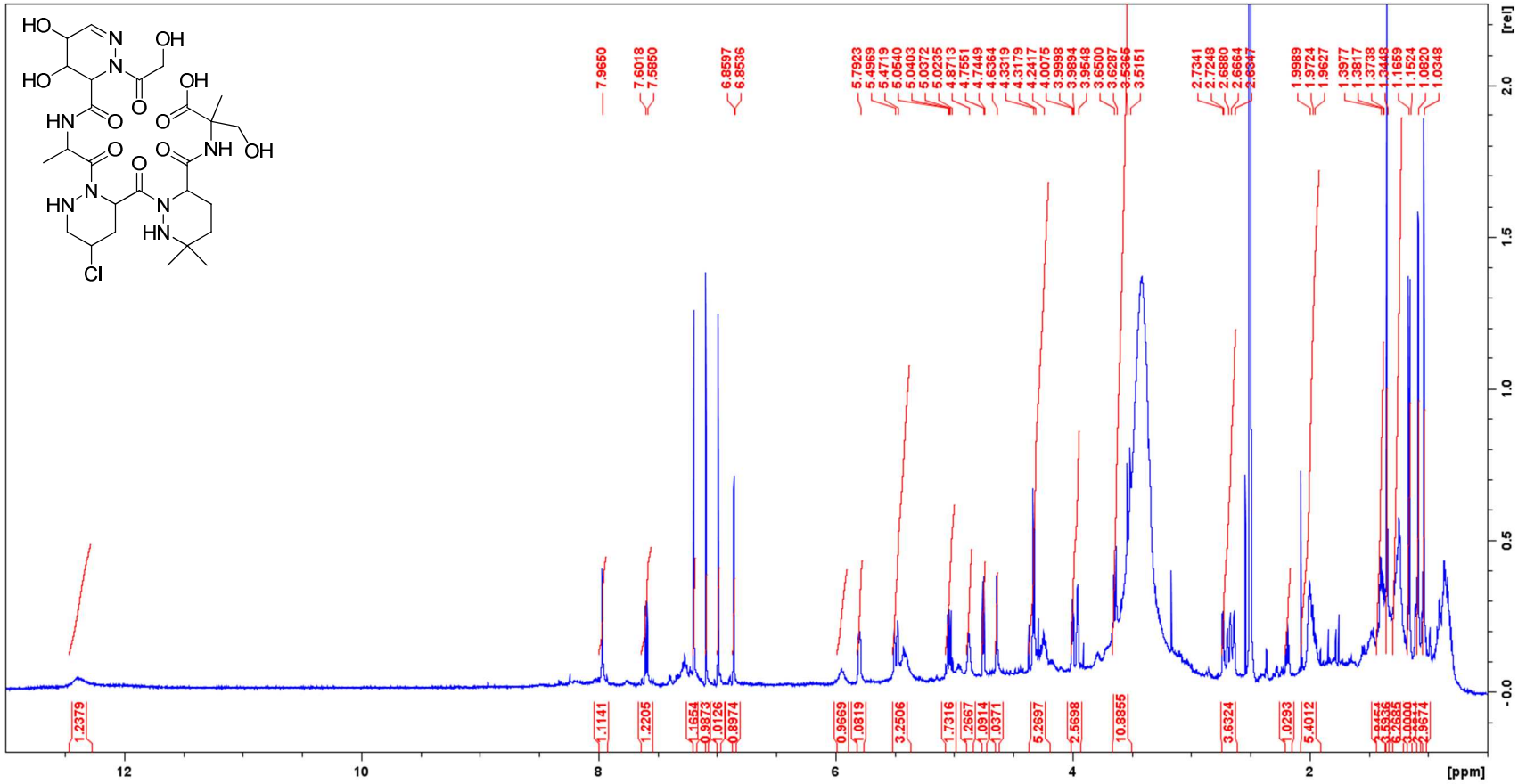



**Figure S 33.** $^{1}$H NMR (500 MHz, DMSO-*d6*) spectrum of **5** (impurities are not peak picked)

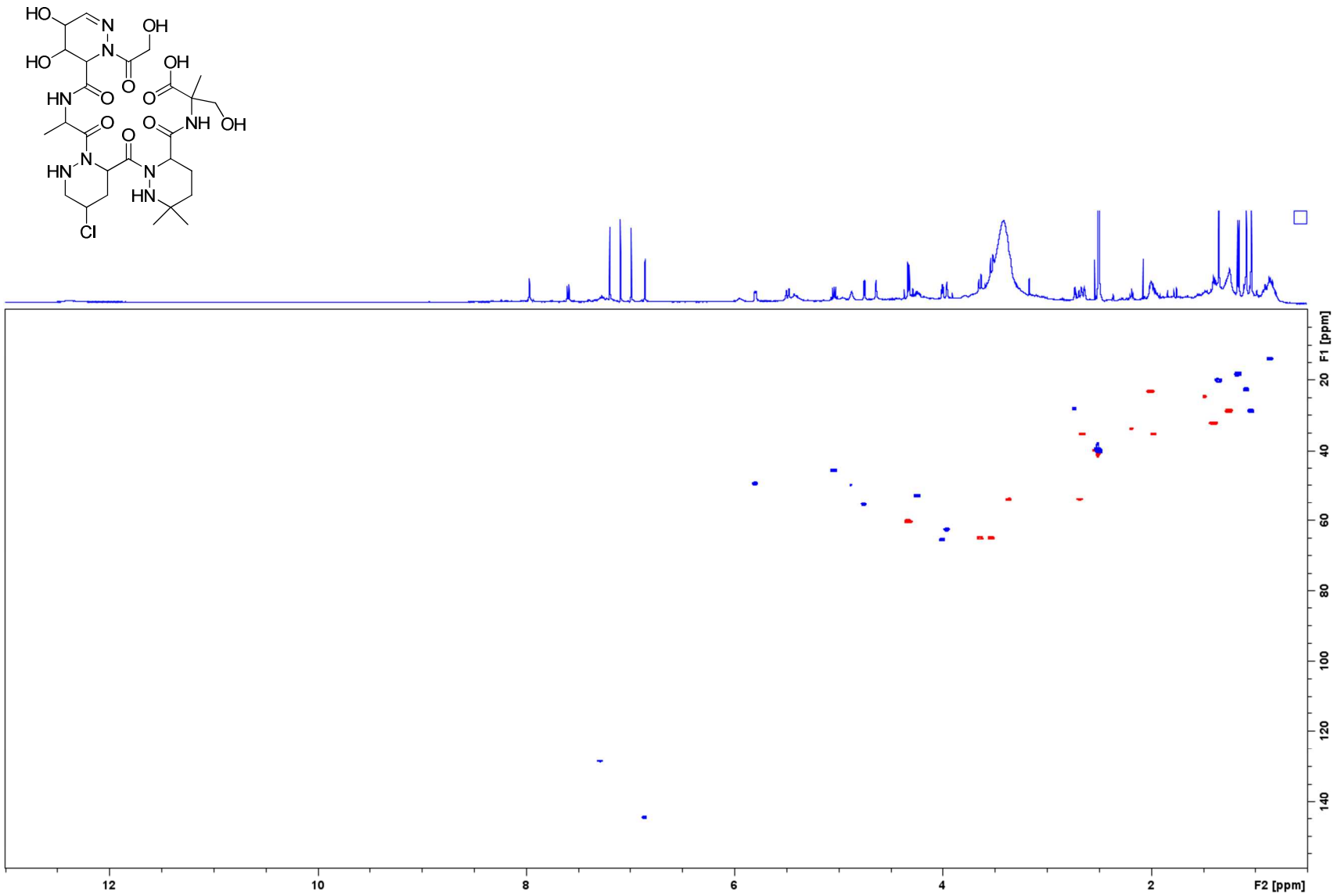



**Figure S 34.** $^{1}$H NMR (500 MHz, DMSO-*d6*) spectrum of **5**

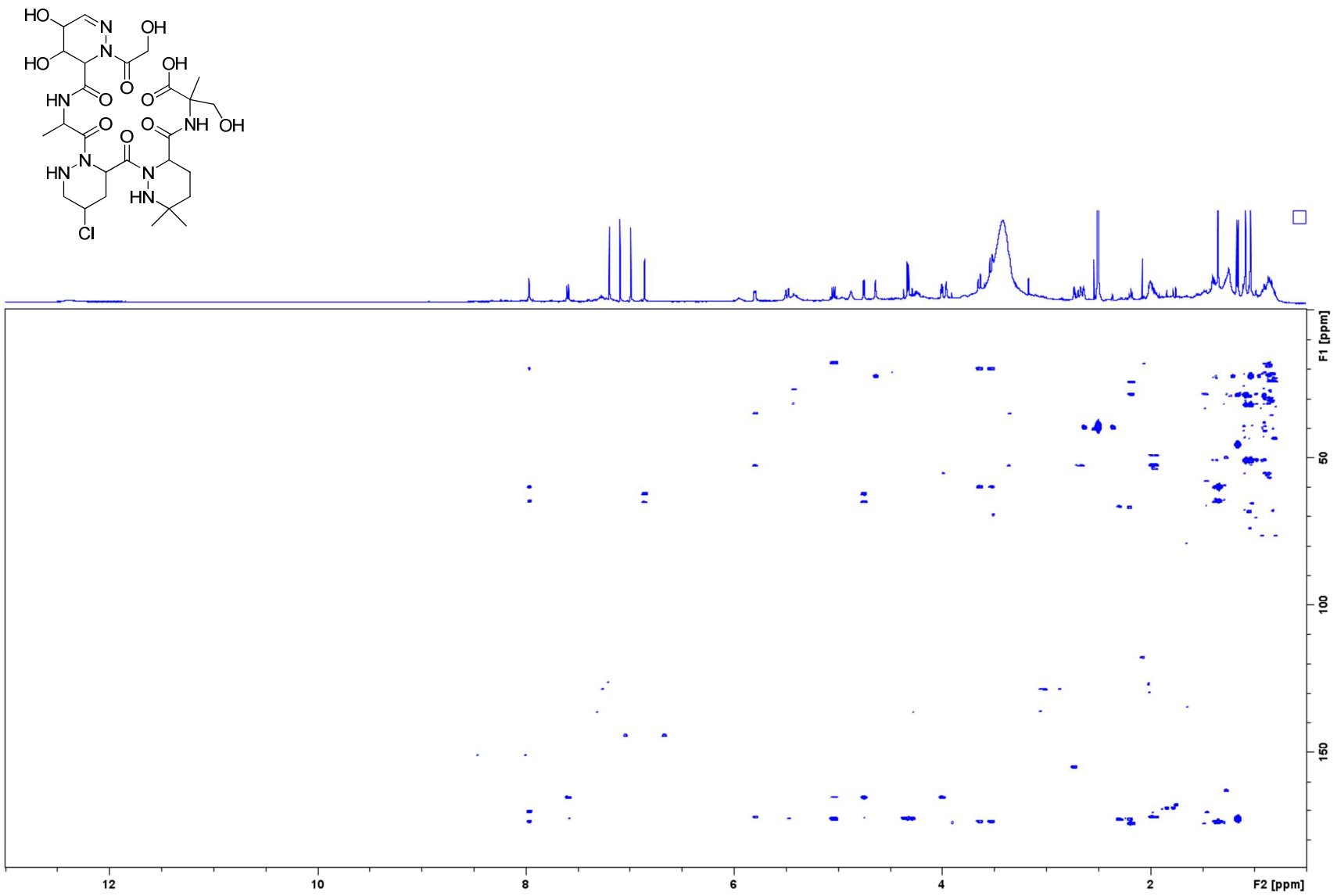



**Figure S 35.** $^{1}H$, $^{13}C$ HMBC (500 MHz, DMSO-*d6*) spectrum of **5**

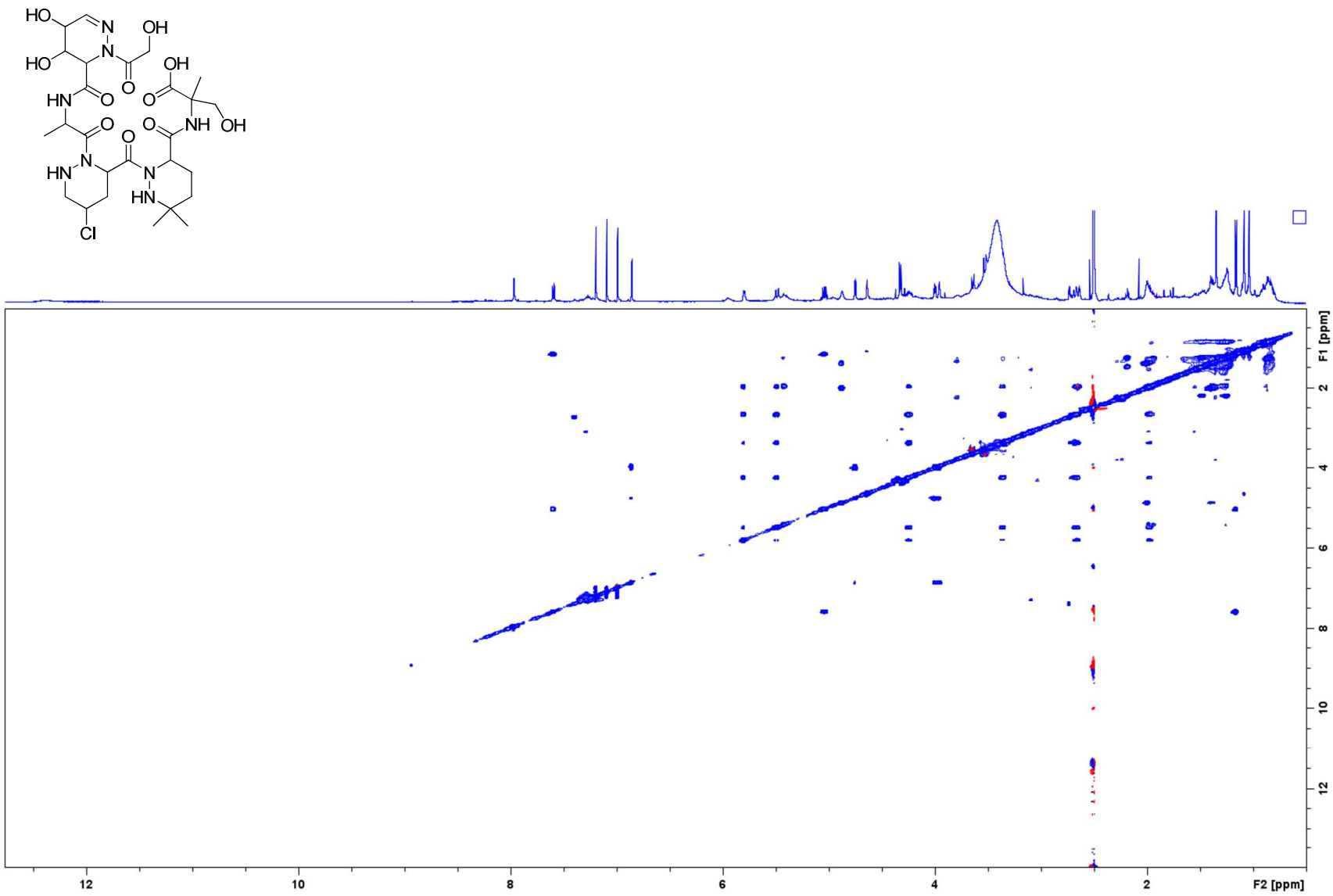



**Figure S 36.** $^{1}$H, $^{1}$H TOCSY (500 MHz, DMSO-*d6*) spectrum of **5**

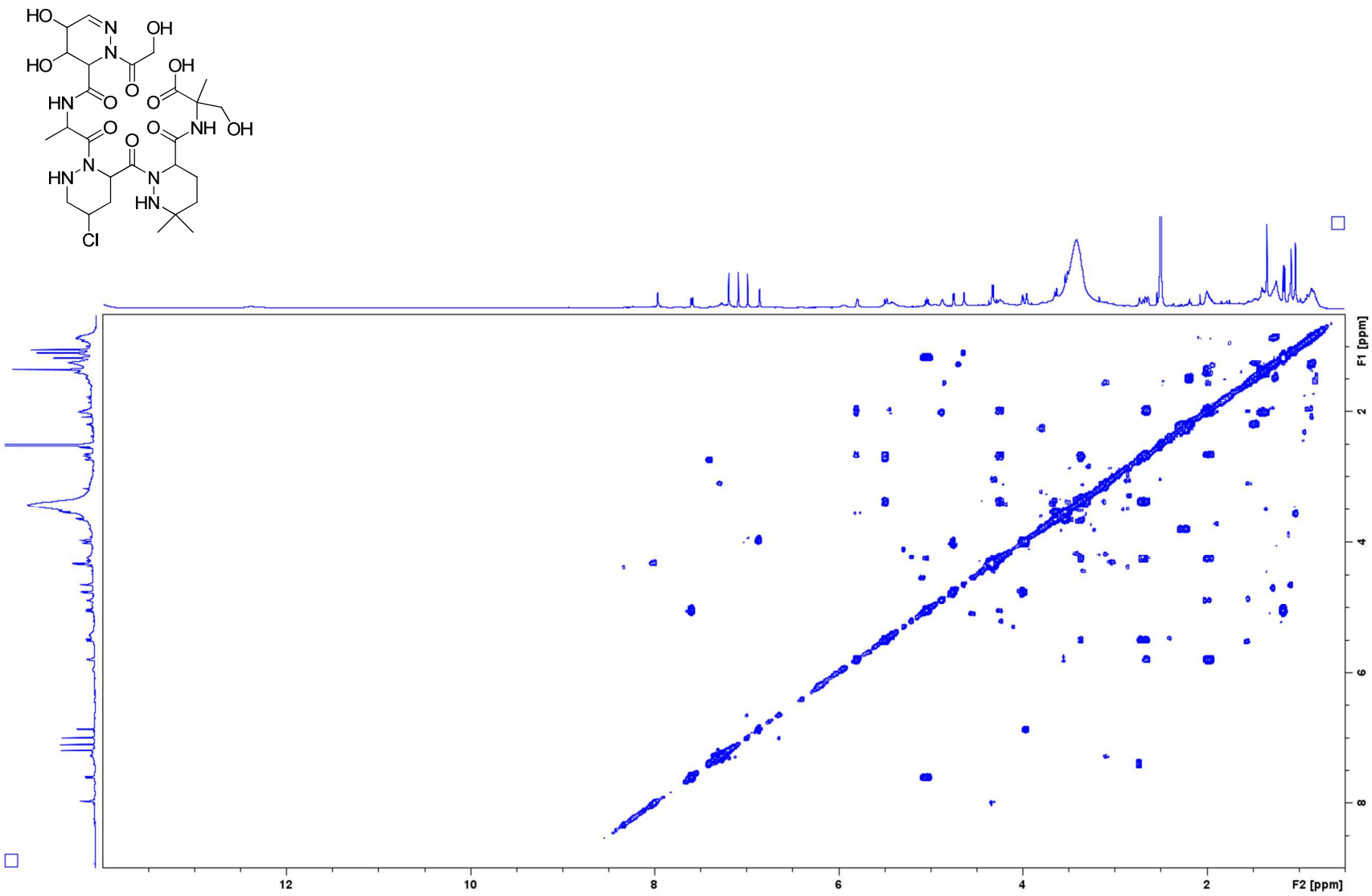



**Figure S 37.** $^{1}$H, $^{1}$H COSY (500 MHz, DMSO-*d6*) spectrum of **5**

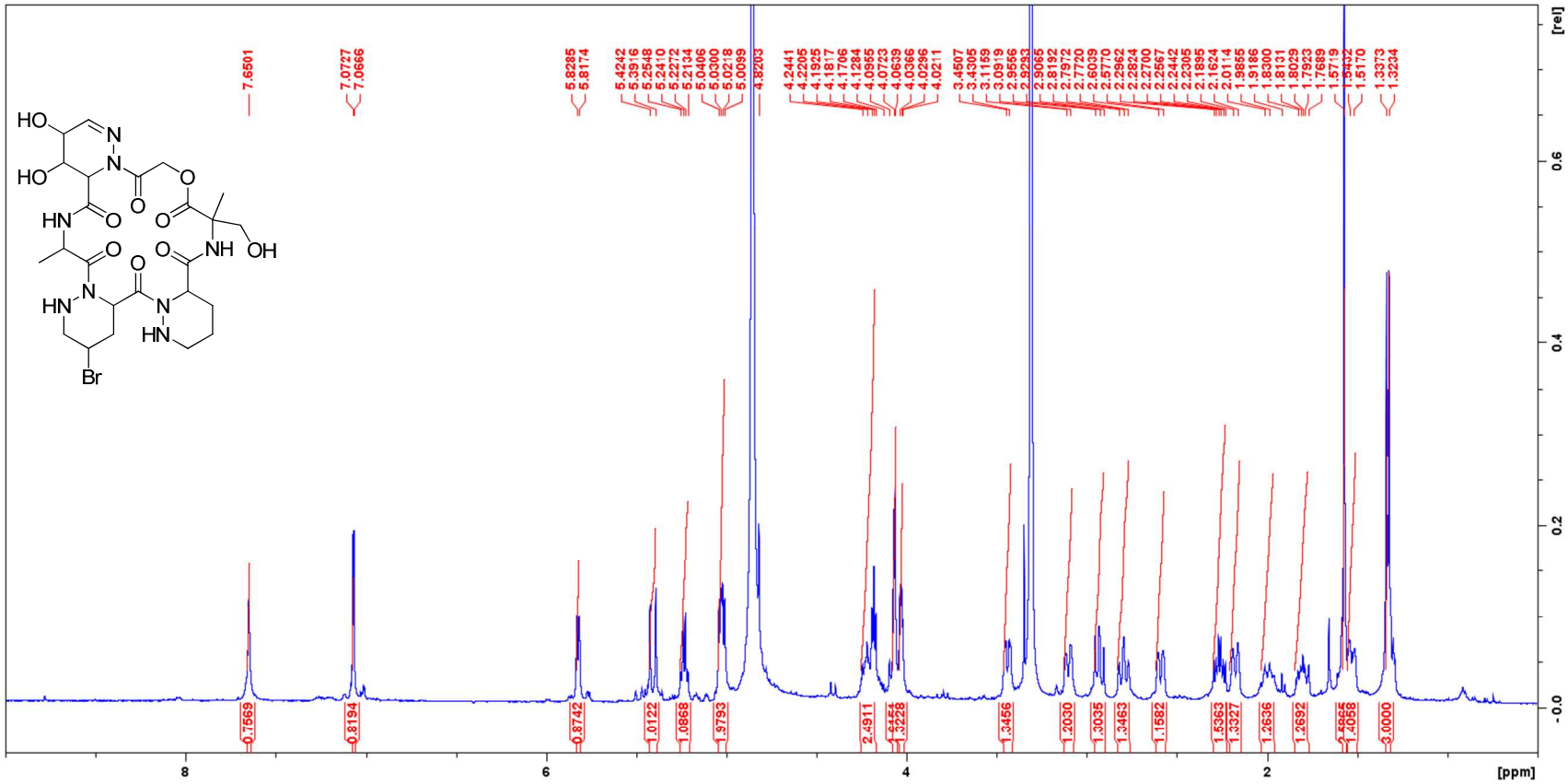



**Figure S 38.** $^{1}$H NMR (500 MHz, $CD_3OD$) spectrum of **6** (impurities are not peak picked)

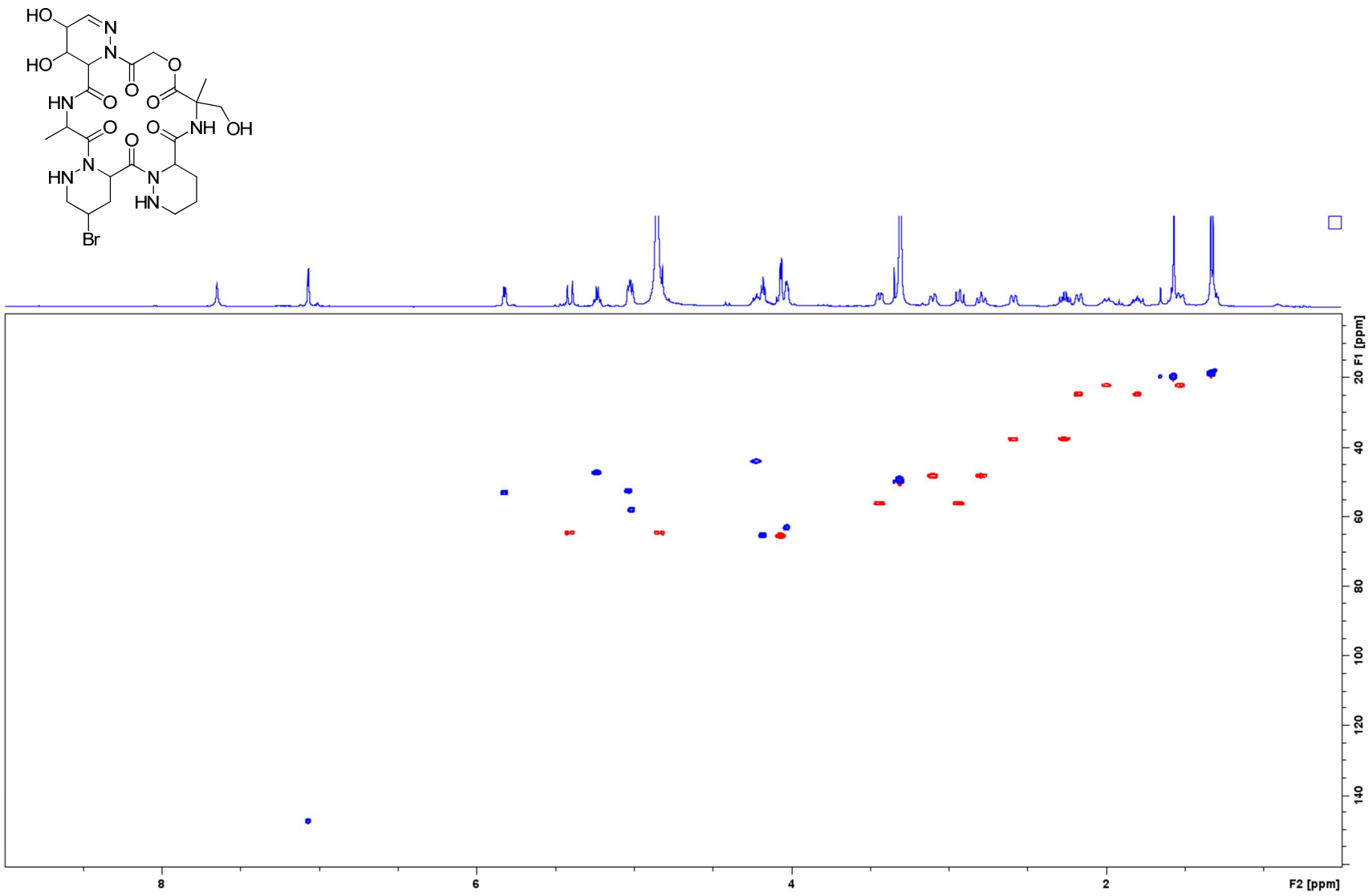



**Figure S 39.** $^{1}H$, $^{13}C$ HSQC (500 MHz, $CD_3OD$) spectrum of **6**

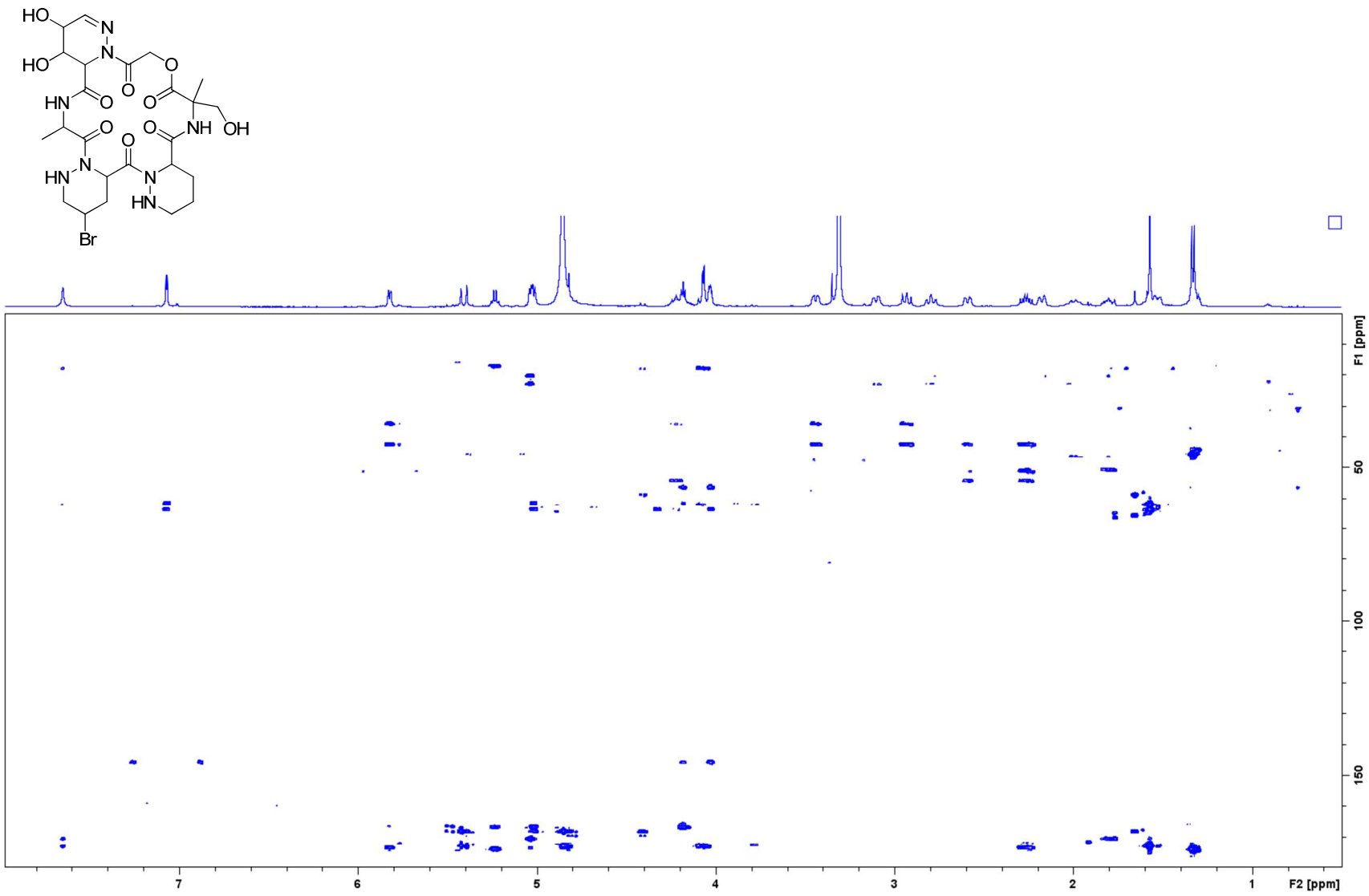



**Figure S 40.** $^{1}H$, $^{13}C$ HMBC (500 MHz, $CD_3OD$) spectrum of **6**

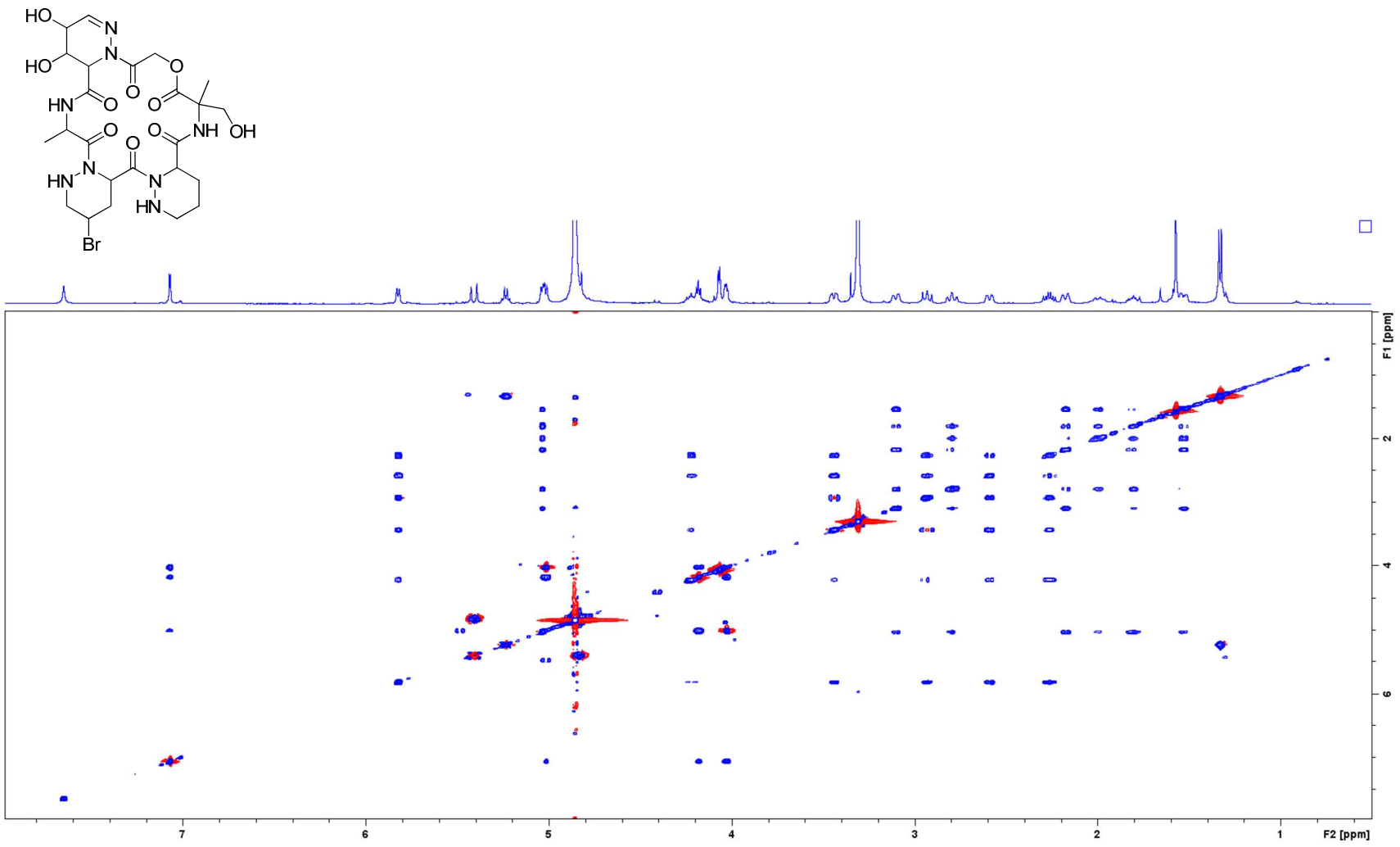



**Figure S 41.** $^{1}$H, $^{1}$H TOCSY (500 MHz, $CD_3OD$) spectrum of **6**

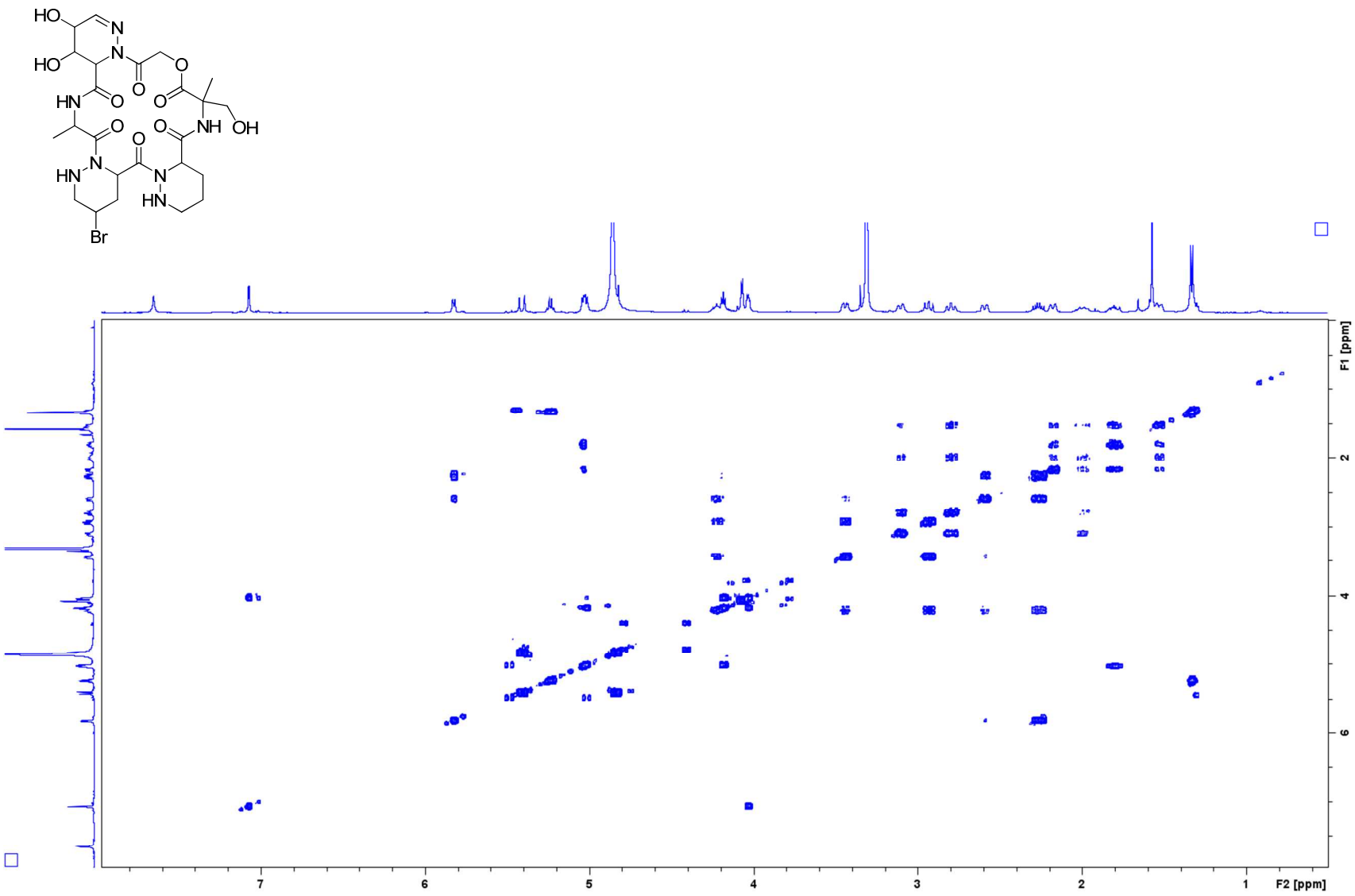



**Figure S 42.** $^{1}H$, $^{1}H$ COSY (500 MHz, $CD_3OD$) spectrum of **6**

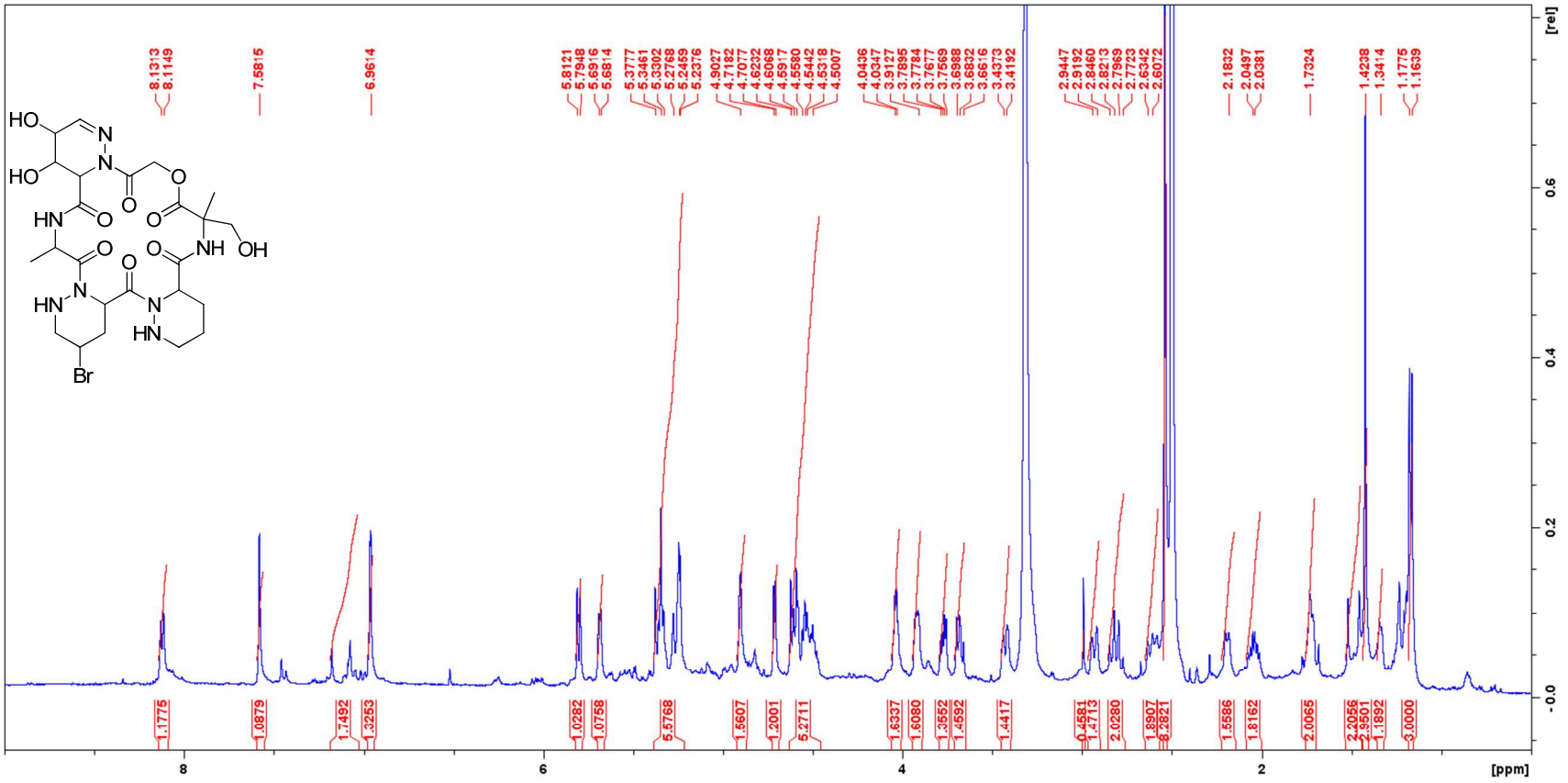



**Figure S 43.** $^{1}$H NMR (500 MHz, DMSO-*d6*) spectrum of **6** (impurities are not peak picked)

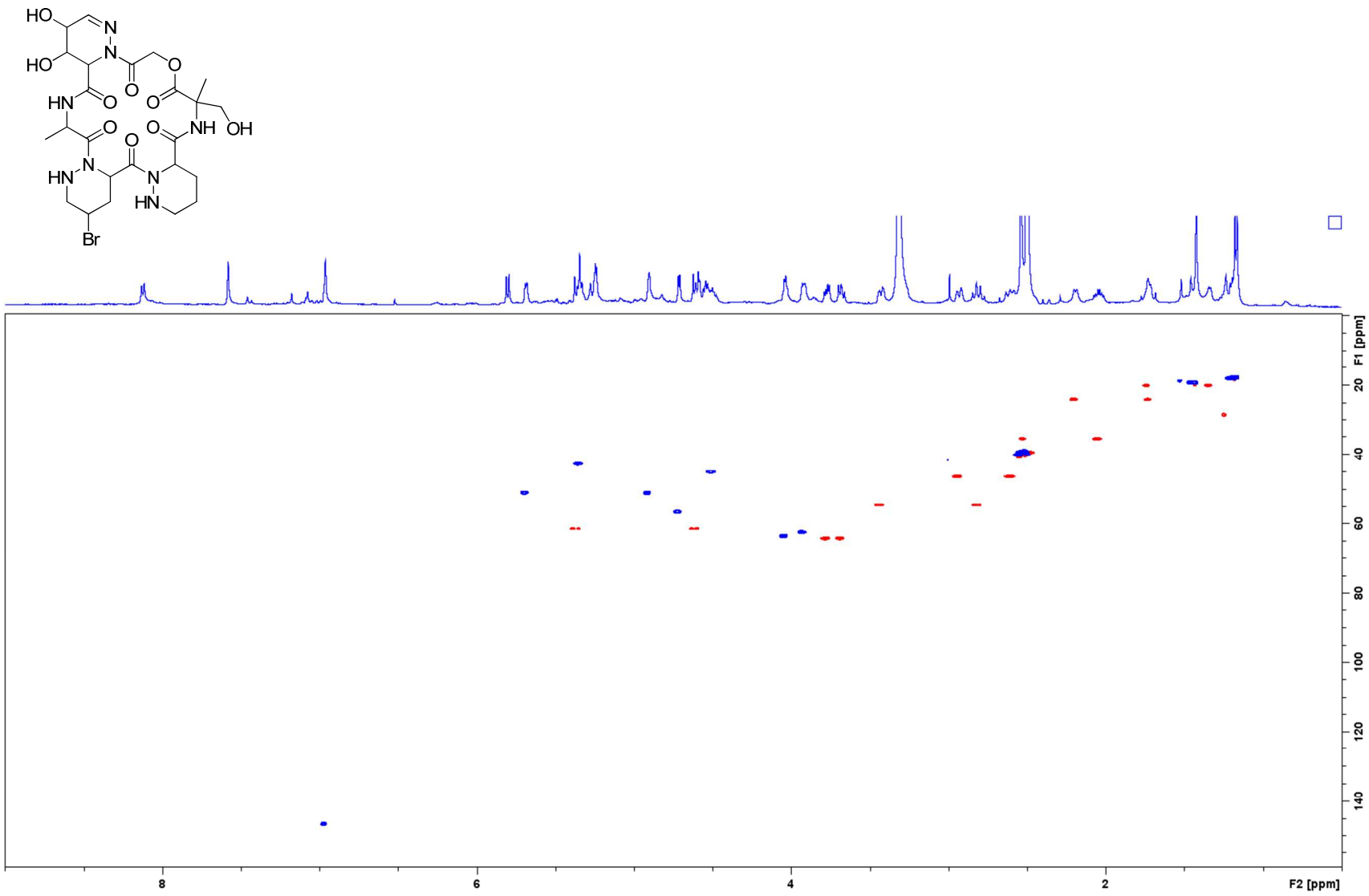



**Figure S 44.** $^{1}H$, $^{13}C$ HSQC (500 MHz, DMSO-*d6*) spectrum of **6**

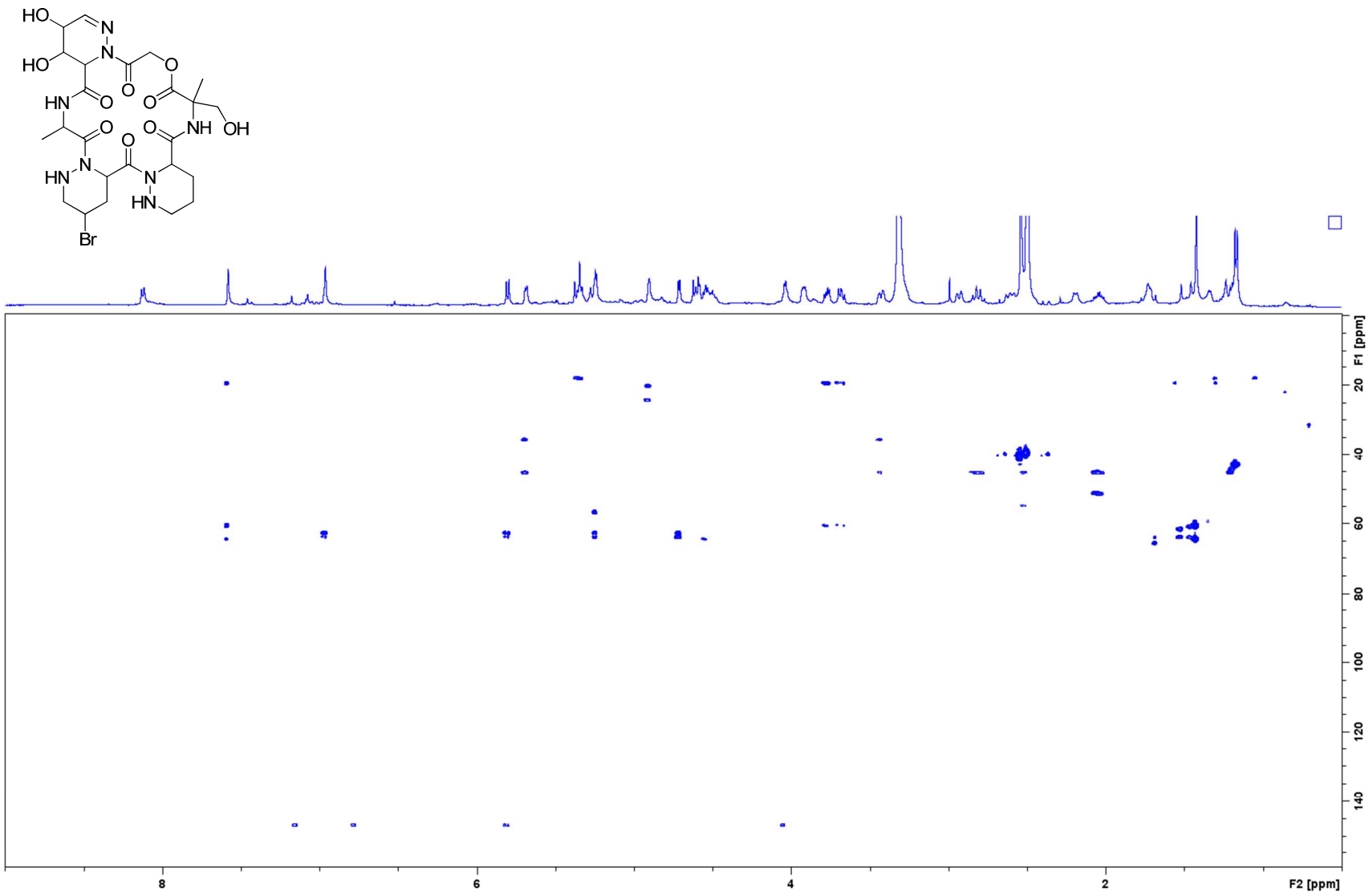



**Figure S 45.** $^{1}H$, $^{13}C$ HMBC (500 MHz, DMSO-*d6*) spectrum of **6**

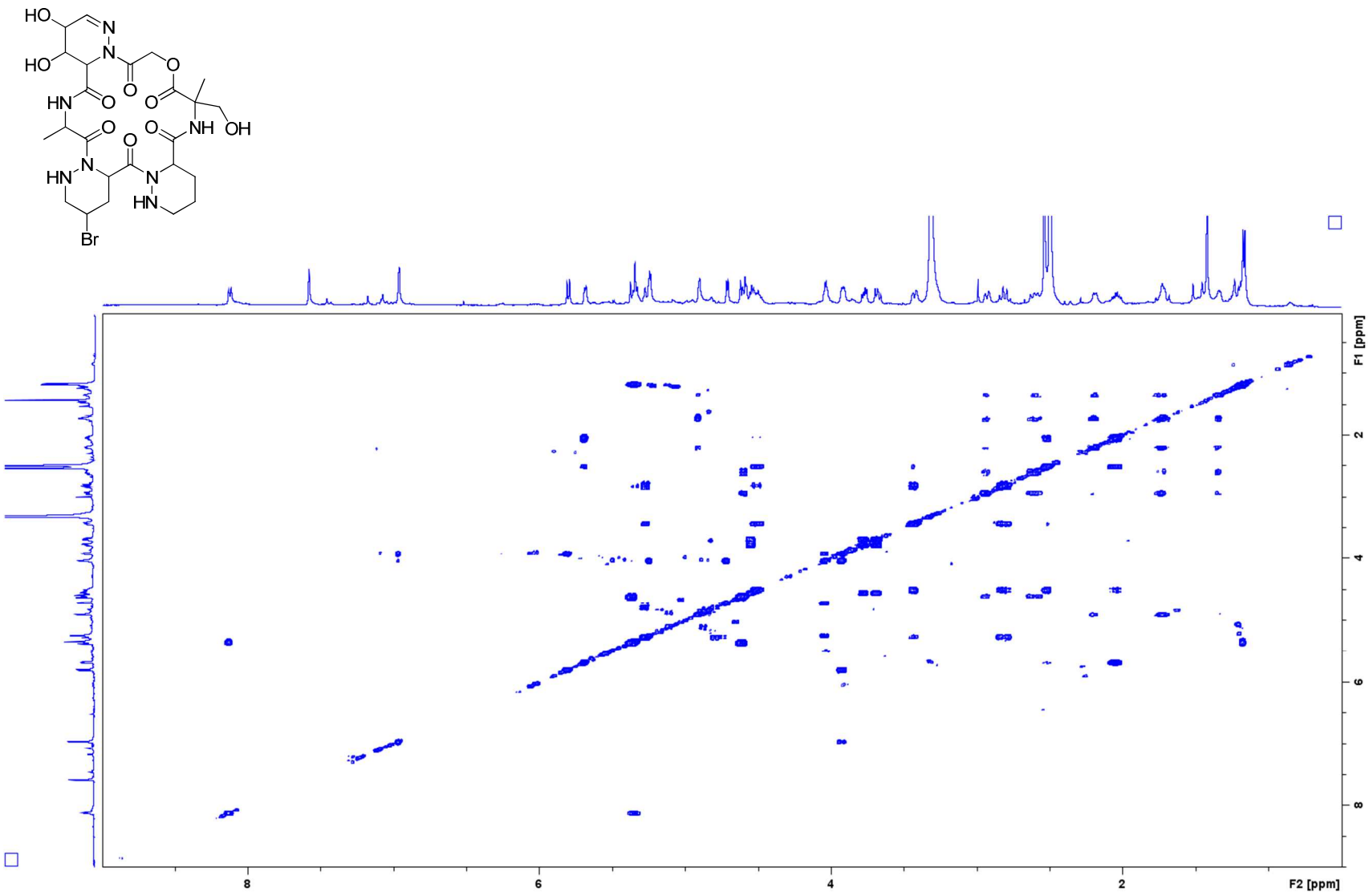



**Figure S 46.** $^{1}$H, $^{1}$H COSY (500 MHz, DMSO-*d6*) spectrum of **6**

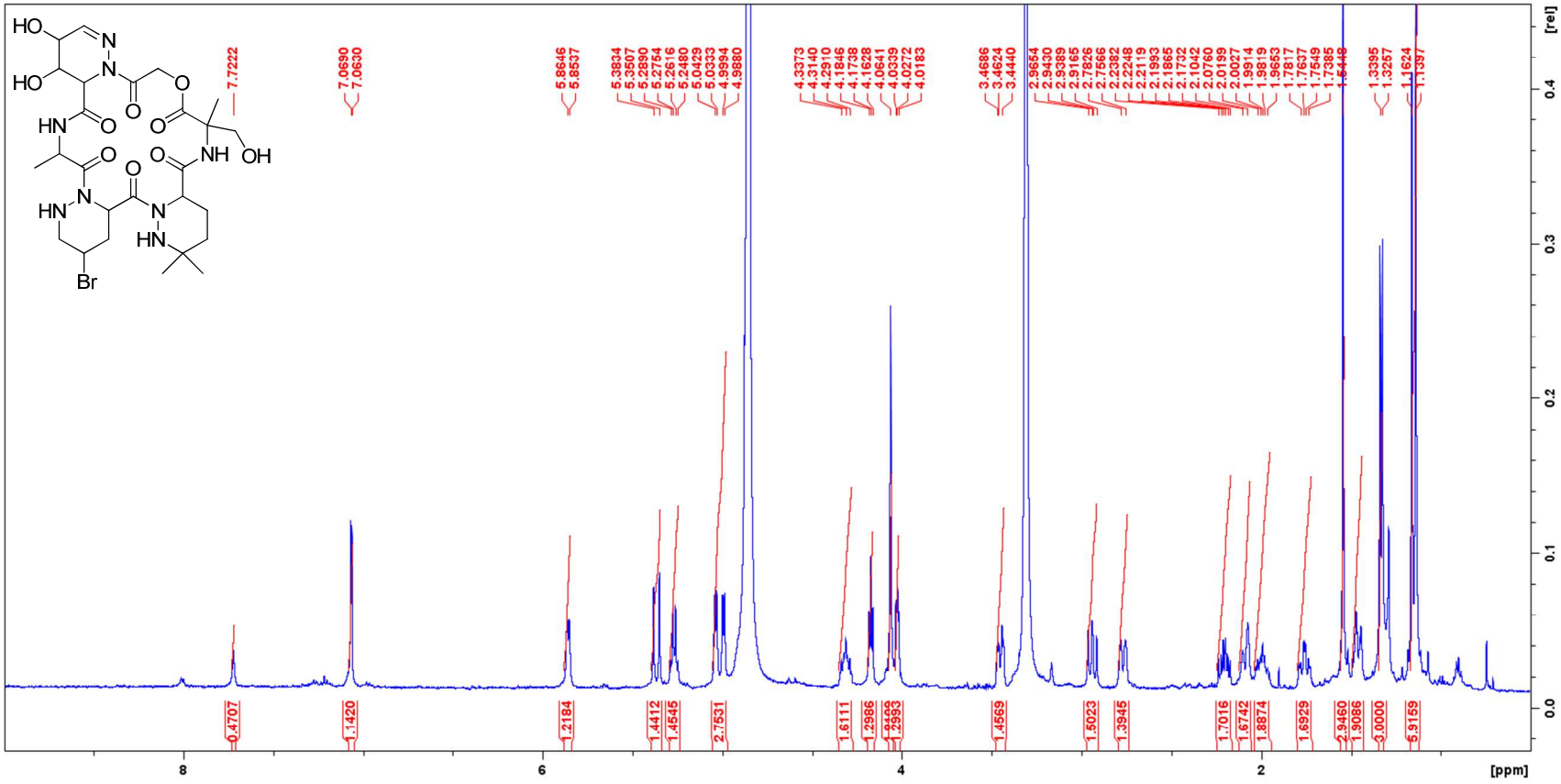



**Figure S 47.** $^{1}$H NMR (500 MHz, $CD_3OD$) spectrum of **7** (impurities are not peak picked)

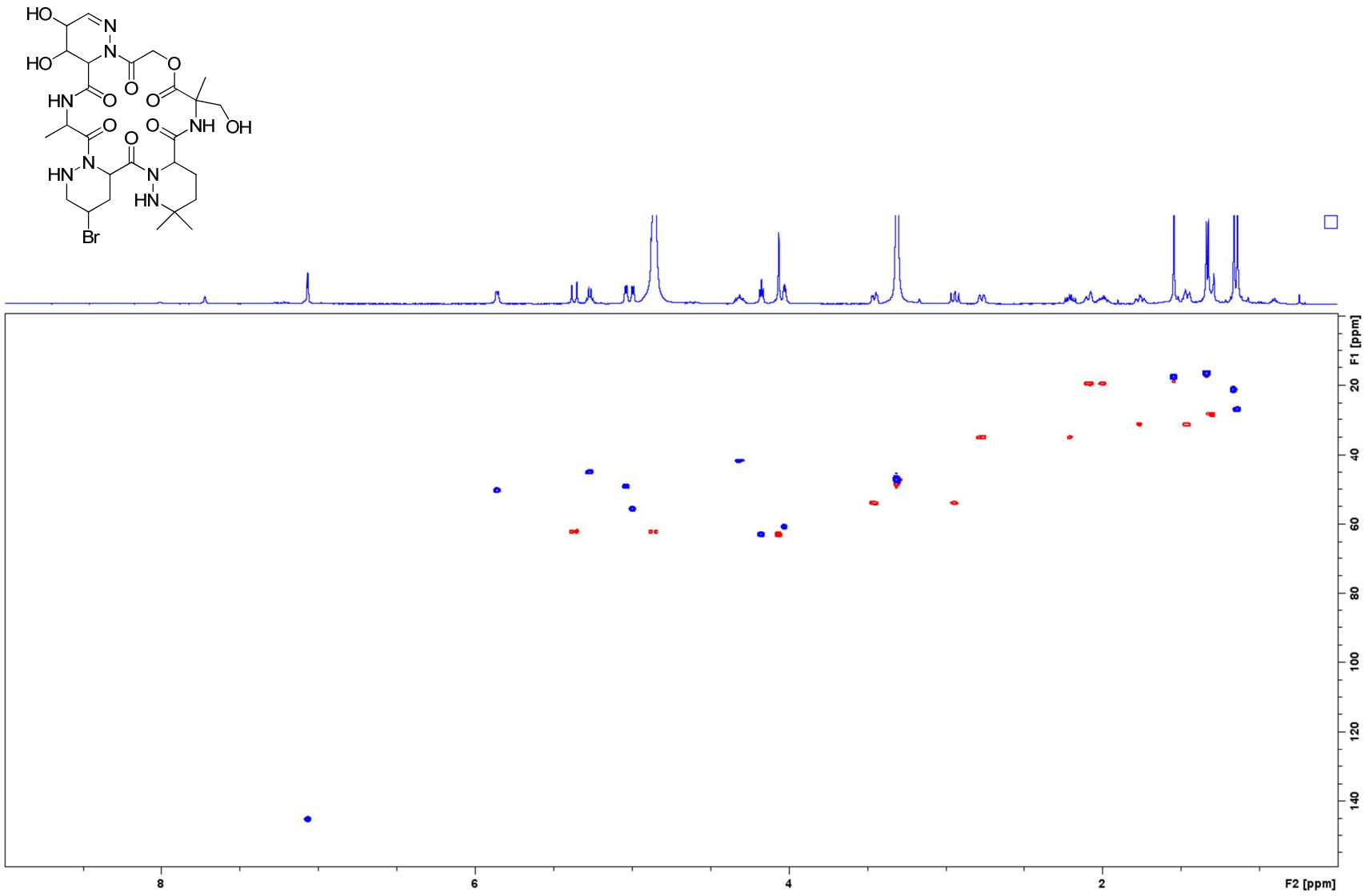



**Figure S 48.** $^{1}H$, $^{13}C$ HSQC (500 MHz, $CD_3OD$) spectrum of **7**

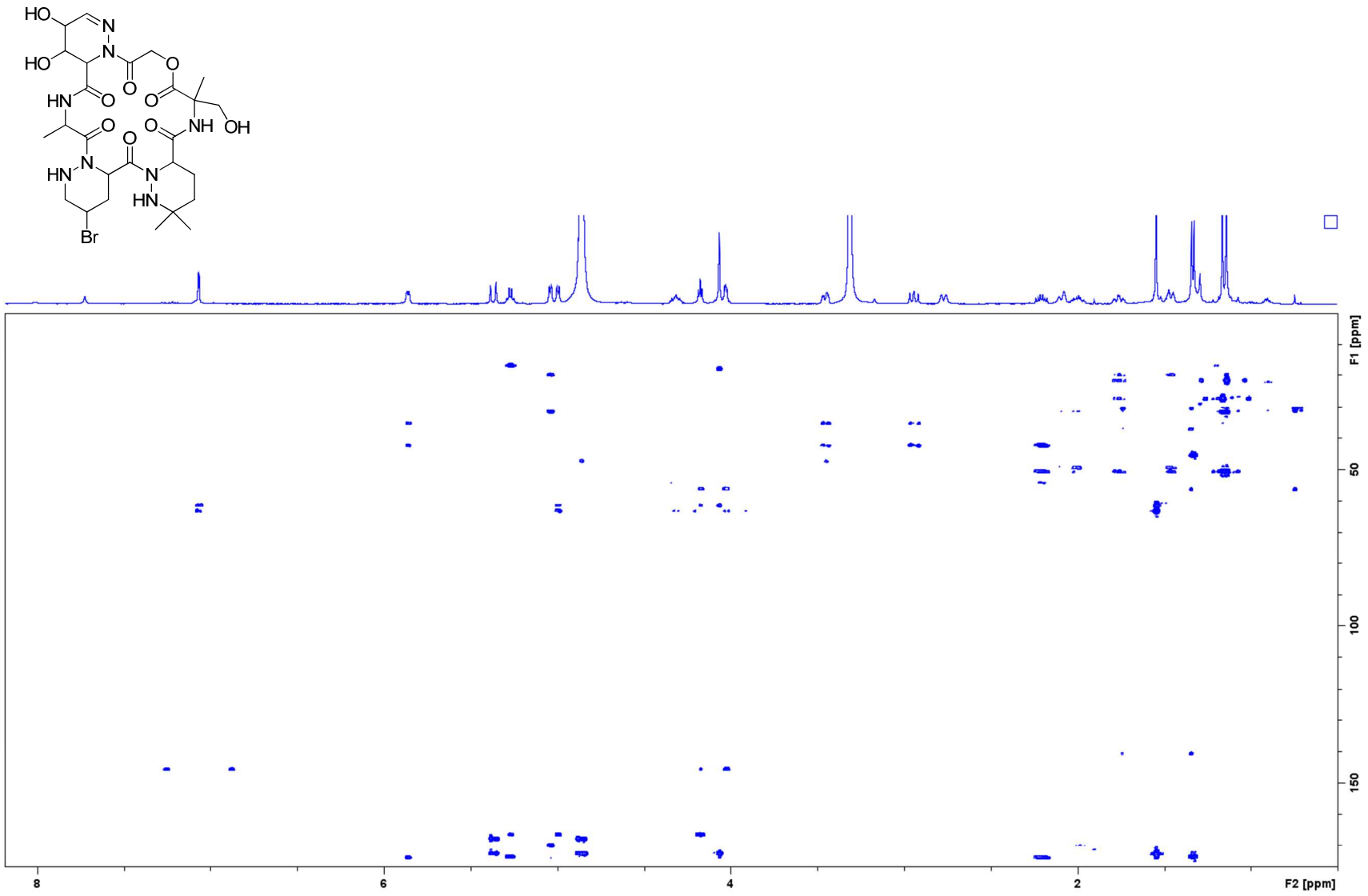



**Figure S 49.** $^{1}H$, $^{13}C$ HMBC (500 MHz, $CD_3OD$) spectrum of **7**

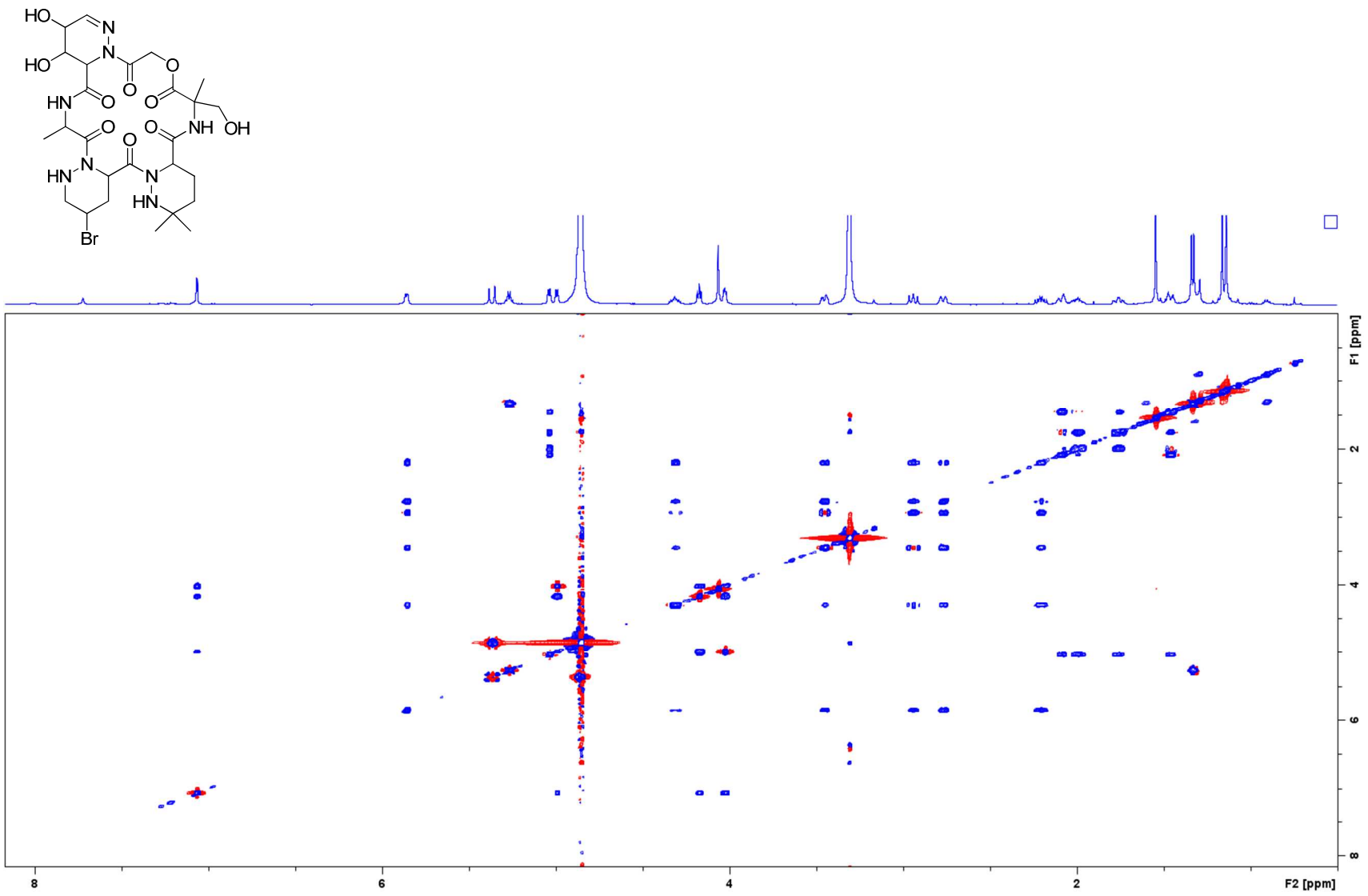



**Figure S 50.** $^{1}$H, $^{1}$H TOCSY (500 MHz, $CD_3OD$) spectrum of **7**

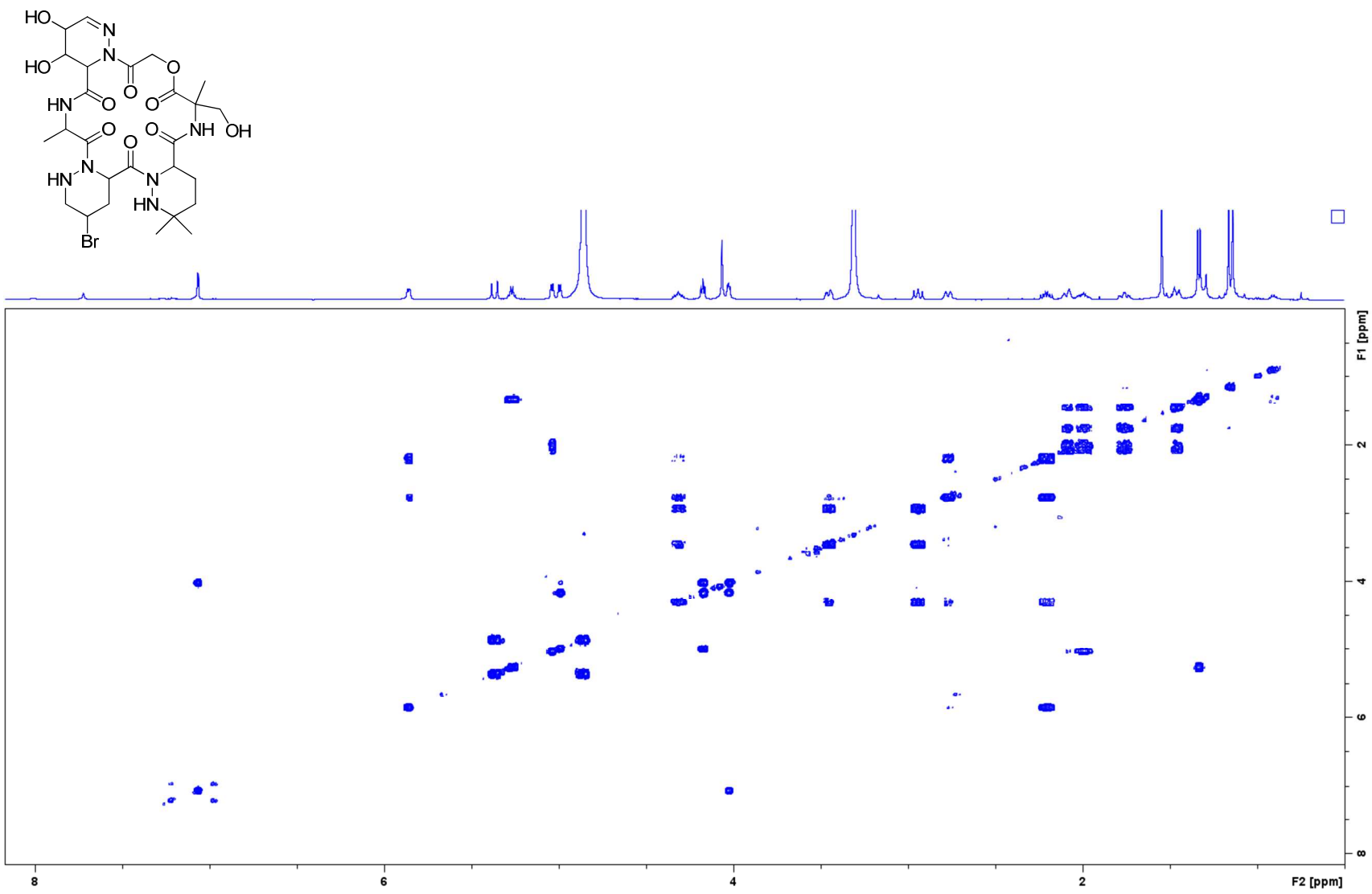



**Figure S 51.** $^{1}$H, $^{1}$H COSY (500 MHz, $CD_3OD$) spectrum of **7**

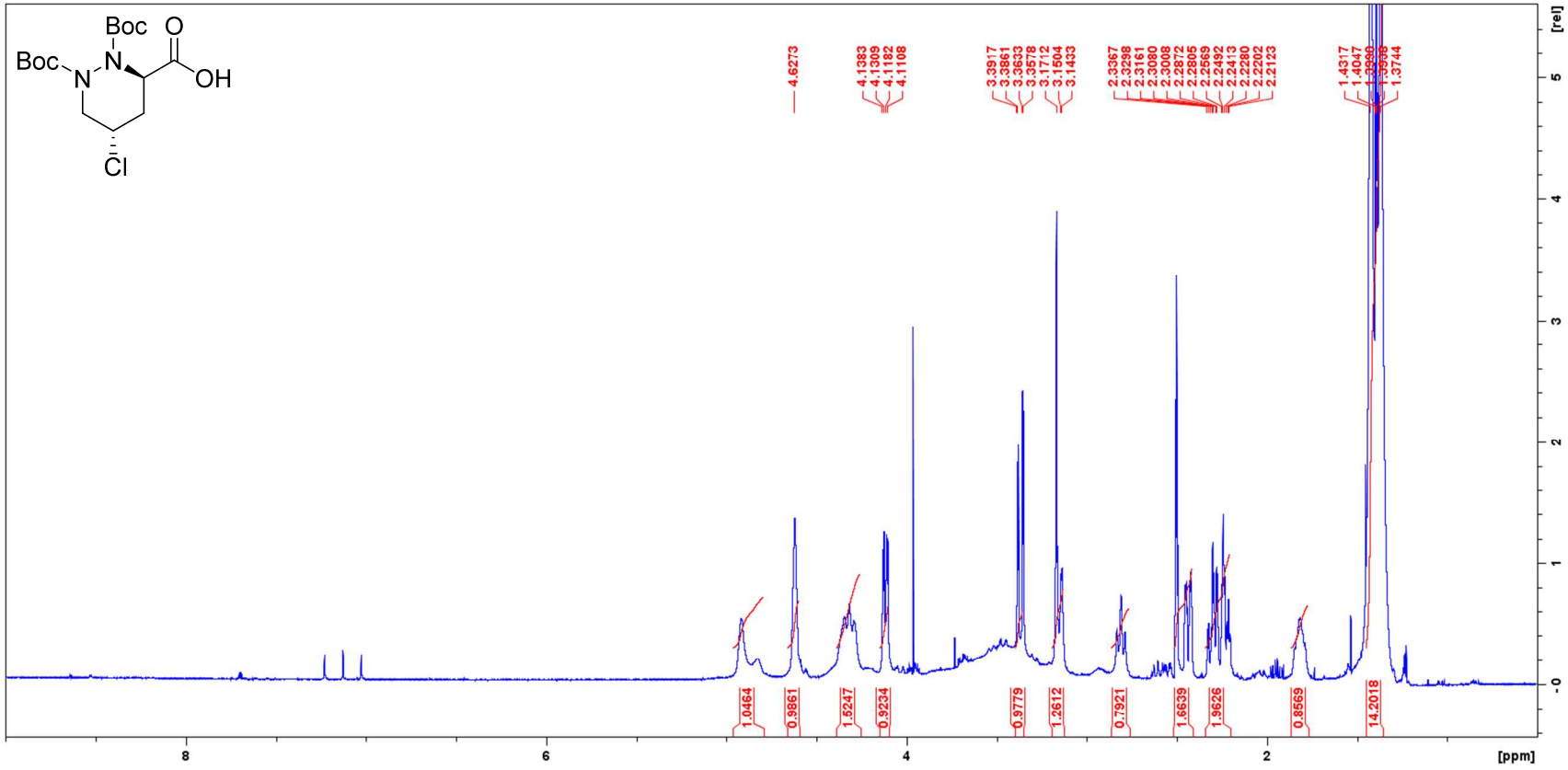



**Figure S52.** $^{1}$H NMR (500 MHz, DMSO-*d6*) spectrum of **20** (impurities are not peak picked)

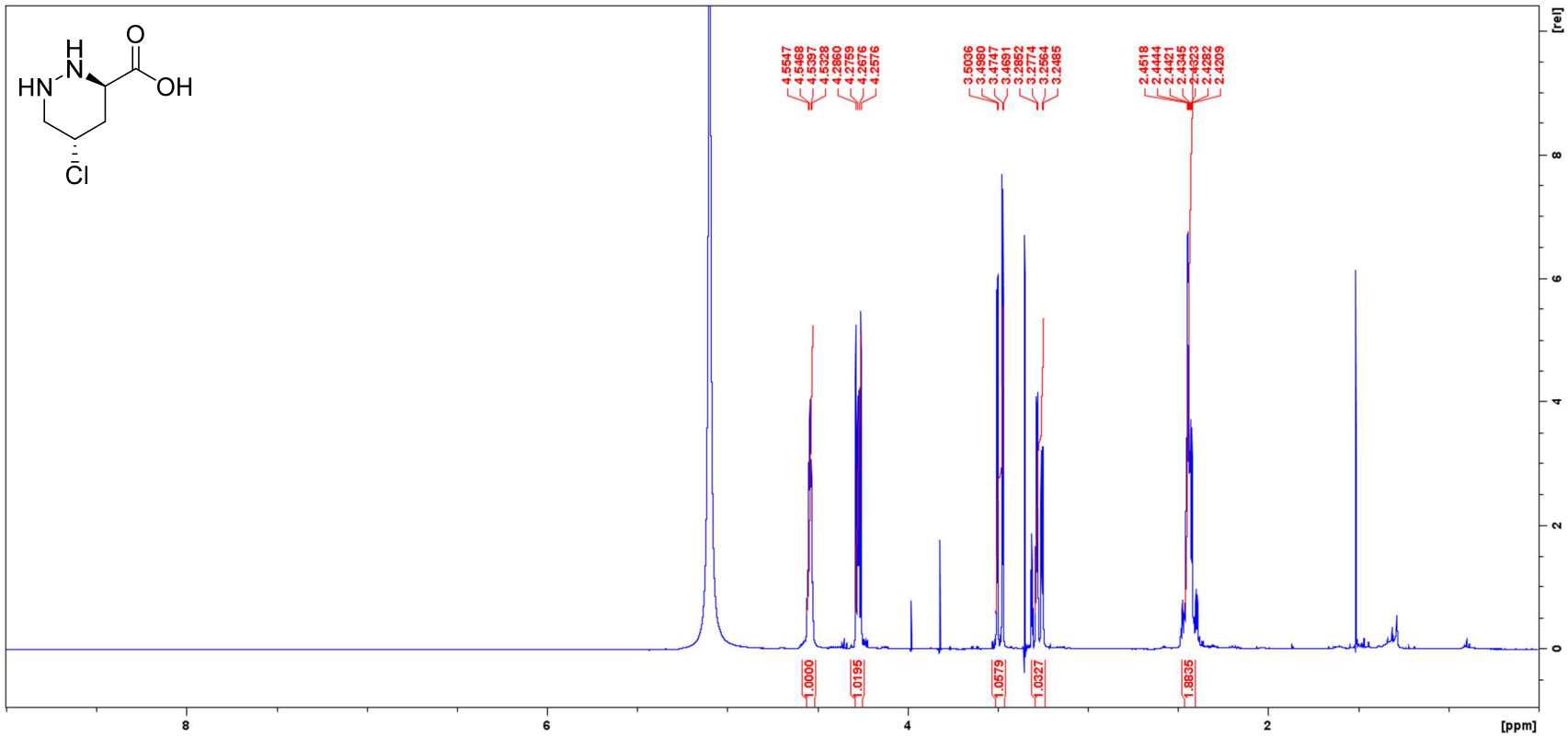



**Figure S53.** $^{1}$H NMR (500 MHz, $CD_3OD$) spectrum of **21** (impurities are not peak picked)

**Table S10.** Cartesian coordinates of the optimized geometries for the conformers of **1a-1h** and related energies computed at the M062X/6-31g(d,p) level. In details, for each compound, we have reported information about the conformers contributing at least the 99.9% to the final Boltzmann distribution.

Compound **1a**

**1a** conf_1

energy (M062X/6-31g(d,p)) = -2585.2965422 Hartree

| | | | |
|---|---|---|---|
| C | -0.9387344787 | -0.3530515476 | 0.8510068494 |
| O | -1.5844856823 | 0.1609631359 | 1.7376124188 |
| C | -0.5249453724 | 0.3452332103 | -0.4374219021 |
| N | -1.3109117819 | 1.5666129671 | -0.4932330774 |
| C | -1.0638460918 | 2.5532410205 | -1.3872057098 |
| O | -0.4357701066 | 2.3950012205 | -2.4291173048 |
| C | -1.6023051026 | 3.927312557 | -0.9532713559 |
| C | -1.6335791074 | 4.9575481365 | -2.0809736149 |
| C | -0.2433093756 | 5.4835934063 | -2.4385957701 |
| C | 0.500860289 | 5.9122875675 | -1.1790013718 |
| N | 0.5400864966 | 4.8644197589 | -0.1583674469 |
| N | -0.7530854844 | 4.4141465529 | 0.1426708239 |
| C | -1.0677736157 | 4.1495672645 | 1.4307775302 |
| O | -2.1132919947 | 3.5759189134 | 1.7462636446 |
| C | -0.0505870671 | 4.587505374 | 2.4898991141 |
| N | -0.3026344078 | 3.8645268415 | 3.7269133838 |
| N | -1.4102346652 | 4.2222532503 | 4.5104180006 |
| C | -1.3988381559 | 5.6451845702 | 4.8310380339 |
| C | -1.3039585844 | 6.485679023 | 3.562503567 |
| C | -0.0692737904 | 6.1007526443 | 2.7659678551 |
| C | 0.3379886735 | 2.7000586256 | 3.9757856985 |
| O | 1.1468076627 | 2.2158275156 | 3.1802315649 |
| C | 0.0989005228 | 2.0322404743 | 5.326630071 |
| C | 0.9037124929 | 2.7565644895 | 6.4115014341 |
| N | 0.511273024 | 0.6523841589 | 5.1668639503 |
| C | 0.2038825226 | -0.3128150554 | 6.0351827477 |
| O | -0.3792185038 | -0.117093961 | 7.1081736268 |
| C | 0.5680913925 | -2.7296485675 | 6.7586871048 |
| C | 0.644266527 | -1.7266959994 | 5.6012272545 |
| N | -0.1705537644 | -2.2027273264 | 4.4713942318 |
| N | -1.2279238385 | -3.0648735835 | 4.5917943 |
| C | -1.548185079 | -3.498579348 | 5.7476821278 |
| C | -0.8756561589 | -3.1372961983 | 7.031792995 |
| C | 0.1414793846 | -1.8097468725 | 3.2002310966 |
| O | 1.0939873968 | -1.078356995 | 2.9644659519 |
| C | -0.7737950615 | -2.3170486383 | 2.0952051583 |
| O | -0.4896159885 | -1.6124232063 | 0.8942187853 |
| O | -0.9449801575 | -4.2495265667 | 7.8956426705 |
| Cl | -1.2417382913 | 8.2414443792 | 3.993164981 |
| C | -0.7845238619 | -0.5689058671 | -1.639233537 |

```
C   1.0022837176   0.6819542517   -0.3551131384
O   1.2897188486   1.8595385714   0.3513941565
O   1.1865385187   -2.2343520987  7.9209390708
H   -2.3878661589  -4.1872894375  5.7805854482
H   -1.7502852778  1.8324501972   0.3844180816
H   -2.6001287974  3.7984982083   -0.5289224328
H   -2.2665373228  5.7885722289   -1.7503187044
H   -2.1149446394  4.5088211895   -2.9538113572
H   -0.3307100803  6.3312714479   -3.125879282
H   0.0224570589   6.7891673612   -0.7285916585
H   1.5386999716   6.1771402129   -1.3976907732
H   1.0767643747   4.0545568042   -0.4743431138
H   0.9446667335   4.3118780317   2.1480354443
H   -2.2333036641  3.9940848736   3.952078561
H   -0.5451602528  5.8547319616   5.4823526017
H   -2.3159289915  5.8641582473   5.3814932872
H   -2.2116420778  6.3684937587   2.9658241568
H   -0.0206312023  6.6423738783   1.8201083222
H   0.8240748975   6.3521672257   3.3460319694
H   -0.9606496687  2.0665792902   5.5839123875
H   0.7826934842   2.2286531364   7.358714356
H   1.9648858624   2.7792094536   6.1502793694
H   0.5446698058   3.7804678333   6.5329181235
H   0.9951220546   0.4144446724   4.3029362349
H   1.1175779688   -3.6309381032  6.472395892
H   1.674509879    -1.6727643843  5.2417576452
H   -1.4000982112  -2.2706580434  7.4634417041
H   -1.8202399694  -2.200167507   2.3720548961
H   -0.5765286126  -3.3680882508  1.8834903645
H   -0.4553022717  -3.9973857064  8.6923490771
H   -1.825035501   -0.902306956   -1.6544655755
H   -0.5777265551  -0.0122309427  -2.5529846998
H   -0.1380553783  -1.4477026203  -1.5976207928
H   1.3509392658   0.8469627224   -1.375292094
H   1.5287021366   -0.1871933603  0.0552552436
H   1.1772266891   1.7390232946   1.3114658083
H   0.7058153579   -1.4115232116  8.1298791837
H   0.3238471933   4.6999244441   -2.9476036449
```

**1a** conf_2

energy (M062X/6-31g(d,p)) = -2585.2786983 Hartree

```
C   -0.5968929173  -0.4429669881  0.8479593594
O   -1.3692762462  -0.0204160589  1.6789161299
C   -0.1068483986  0.3658808675   -0.3549862561
N   -0.9470652014  1.5531305545   -0.3838474466
C   -1.0892565769  2.4480491963   -1.3932450542
O   -0.8613598834  2.2372108731   -2.5757216962
C   -1.593239994   3.8233178252   -0.8973935201
C   -1.6427912707  4.8648052266   -2.0135378288
C   -0.2453971458  5.3376644719   -2.4125857965
C   0.5491038758   5.7494024477   -1.1775543877
N   0.5789147886   4.7070659856   -0.1477367034
```

| | | | |
|---|---|---|---|
| N | -0.7235921435 | 4.3001419633 | 0.1813885503 |
| C | -1.0722462641 | 4.154936128 | 1.4801551496 |
| O | -2.1387687605 | 3.6266218356 | 1.8083031923 |
| C | -0.0773692678 | 4.6545799625 | 2.5330453934 |
| N | -0.331830901 | 3.9701580718 | 3.7915209482 |
| N | -1.4736801509 | 4.314152868 | 4.5306815149 |
| C | -1.5031550689 | 5.7458508486 | 4.8092020163 |
| C | -1.4041393635 | 6.550267505 | 3.5168806223 |
| C | -0.1456427871 | 6.175586397 | 2.7522617247 |
| C | 0.3401531144 | 2.82752335 | 4.0833050914 |
| O | 1.2206633802 | 2.3887927584 | 3.3471772234 |
| C | 0.0128361436 | 2.1305587607 | 5.4015589508 |
| C | 0.7229760471 | 2.8434302286 | 6.5571848751 |
| N | 0.4588275606 | 0.758283216 | 5.2479278943 |
| C | 0.1013283247 | -0.2217705536 | 6.0794547087 |
| O | -0.5856848277 | -0.0458829044 | 7.0936317834 |
| C | 0.4981539092 | -2.6115961528 | 6.8688331969 |
| C | 0.6345906677 | -1.6214682403 | 5.7046574084 |
| N | -0.0459787323 | -2.1575609324 | 4.5139064652 |
| N | -1.0601749812 | -3.0771877491 | 4.5523523282 |
| C | -1.4695980226 | -3.5051007521 | 5.6819206406 |
| C | -0.9440618521 | -3.0839964117 | 7.0151227601 |
| C | 0.3856933845 | -1.7849434554 | 3.2714951661 |
| O | 1.3119005479 | -1.0000320869 | 3.1212522666 |
| C | -0.3481287519 | -2.3944616641 | 2.0836002517 |
| O | -0.03062263 | -1.6513279306 | 0.9106639054 |
| O | -1.0418359532 | -4.1804539343 | 7.8963201599 |
| Cl | -1.3954026776 | 8.3201695827 | 3.8945993013 |
| C | -0.1697829034 | -0.4571756748 | -1.641709586 |
| C | 1.3451260126 | 0.7760817111 | -0.0074903924 |
| O | 1.7708252511 | 1.7454307136 | -0.9462275351 |
| O | 0.9832600695 | -2.0744448236 | 8.0748738029 |
| H | -2.2705013989 | -4.2386055976 | 5.6498637707 |
| H | -1.2900406109 | 1.8318602846 | 0.5290174951 |
| H | -2.5829013192 | 3.6874842641 | -0.4538260865 |
| H | -2.2341122557 | 5.7137614065 | -1.6534703118 |
| H | -2.1660316112 | 4.4353725279 | -2.8705432088 |
| H | -0.3169417525 | 6.180163855 | -3.1079140998 |
| H | 0.1158113383 | 6.6472509958 | -0.7232964416 |
| H | 1.589509481 | 5.9740696806 | -1.4270866771 |
| H | 1.0740660033 | 3.8790648091 | -0.4919076618 |
| H | 0.9286190805 | 4.3922338284 | 2.2138591914 |
| H | -2.2729548396 | 4.054793598 | 3.9513948637 |
| H | -0.6668144853 | 5.9945819816 | 5.469307948 |
| H | -2.4356156219 | 5.9613484973 | 5.3348810548 |
| H | -2.2971850971 | 6.391478722 | 2.9080931389 |
| H | -0.0998769258 | 6.6885110646 | 1.7897217451 |
| H | 0.7307623317 | 6.4739960426 | 3.3358756167 |
| H | -1.0630137023 | 2.1414454558 | 5.5811341031 |
| H | 0.3403596995 | 3.8601305238 | 6.6685284216 |
| H | 0.5403575145 | 2.2971778899 | 7.4839946064 |
| H | 1.8001517296 | 2.8858041698 | 6.3758151714 |
| H | 1.0227140126 | 0.5453238224 | 4.4271648309 |
| H | 1.1125779611 | -3.4893076568 | 6.6487570696 |

| | | | |
|---|---|---|---|
| H | 1.6901924672 | -1.5251078433 | 5.4403795685 |
| H | -1.5477240227 | -2.235963705 | 7.3739328389 |
| H | -1.4231908151 | -2.412385806 | 2.2485345401 |
| H | 0.0037498287 | -3.4099856623 | 1.9000758693 |
| H | -0.6353958376 | -3.8893755715 | 8.7259691946 |
| H | 0.3895515369 | -1.3843111671 | -1.5073288595 |
| H | -1.2045371374 | -0.7016173736 | -1.8923696927 |
| H | 0.2599233935 | 0.1124804327 | -2.4622671734 |
| H | 1.9788598166 | -0.1172113906 | -0.0396528864 |
| H | 1.3691944154 | 1.1831011331 | 1.0108281373 |
| H | 2.712191403 | 1.9009216014 | -0.792550422 |
| H | 0.4489263619 | -1.2714672158 | 8.2231920886 |
| H | 0.2787896543 | 4.5286753664 | -2.9312243218 |

**1a** conf_3

energy (M062X/6-31g(d,p)) = -2585.2756221 Hartree

| | | | |
|---|---|---|---|
| C | -0.9553449973 | -0.4801368237 | 0.8647379361 |
| O | -1.5832853057 | 0.0925956725 | 1.7271234178 |
| C | -0.5271168375 | 0.1556438896 | -0.4547997936 |
| N | -0.982272583 | 1.5411098078 | -0.3544665422 |
| C | -0.6922825959 | 2.5422412749 | -1.1984542862 |
| O | 0.0223463569 | 2.4361974447 | -2.2026604671 |
| C | -1.3078262447 | 3.8874457599 | -0.7899021516 |
| C | -1.3987230961 | 4.897602891 | -1.9354204597 |
| C | -0.0722174282 | 5.5921919173 | -2.233925117 |
| C | 0.5323339286 | 6.1304400444 | -0.943830652 |
| N | 0.6811033413 | 5.0891415279 | 0.0758523572 |
| N | -0.5380107974 | 4.4458424297 | 0.3290322484 |
| C | -0.931736806 | 4.211029284 | 1.6088247945 |
| O | -1.9169740209 | 3.5206283447 | 1.8613547351 |
| C | -0.1330944149 | 4.9140107792 | 2.7137208374 |
| N | -0.2047405278 | 4.1586931061 | 3.9615834842 |
| N | -0.9204032858 | 4.6679968173 | 5.05176734 |
| C | -2.2180118415 | 5.164312095 | 4.6167720733 |
| C | -2.1096945712 | 6.2552295783 | 3.530716958 |
| C | -0.6928552444 | 6.3188934271 | 2.9659348901 |
| C | 0.3690510748 | 2.9340669744 | 4.0240265279 |
| O | 0.942402616 | 2.4531307295 | 3.0485346791 |
| C | 0.3538082116 | 2.2229157158 | 5.3717959938 |
| C | 1.4467880344 | 2.8004907473 | 6.2799724372 |
| N | 0.5741256955 | 0.8126033926 | 5.1092256078 |
| C | 0.3662677595 | -0.1232734838 | 6.0383065298 |
| O | -0.0334259953 | 0.132187962 | 7.1819819979 |
| C | 0.6581619706 | -2.5393182175 | 6.805129638 |
| C | 0.6990770755 | -1.5704365721 | 5.6155928679 |
| N | -0.1972934659 | -2.0624286938 | 4.5575584383 |
| N | -1.2745536961 | -2.8804058315 | 4.7753368693 |
| C | -1.5478031254 | -3.2422203221 | 5.9677138734 |
| C | -0.7839504343 | -2.8499556347 | 7.1903810836 |
| C | 0.0834721557 | -1.7713602978 | 3.2536815281 |
| O | 1.0335180044 | -1.0652757475 | 2.9432755513 |
| C | -0.8520269576 | -2.3672778752 | 2.2086420214 |

| | | | |
|---|---|---|---|
| O | -0.5790907737 | -1.7587531635 | 0.9524931618 |
| O | -0.8538919861 | -3.910308754 | 8.1165239657 |
| Cl | -2.5471329177 | 7.8943549825 | 4.1835188648 |
| C | -1.230183303 | -0.5713535938 | -1.6097366788 |
| C | 1.019640949 | 0.044293275 | -0.5886778748 |
| O | 1.4813330359 | 0.1904809854 | -1.9024995709 |
| O | 1.3908417285 | -2.0643129453 | 7.906237457 |
| H | -2.4095225573 | -3.8942301995 | 6.0807391821 |
| H | -1.5281277269 | 1.7616221843 | 0.476512643 |
| H | -2.305839847 | 3.6960241178 | -0.3921471301 |
| H | -2.1422557837 | 5.6486204417 | -1.6462884374 |
| H | -1.7821012745 | 4.3876448138 | -2.822854936 |
| H | -0.2321502427 | 6.4099068025 | -2.9437674085 |
| H | -0.0983102005 | 6.9188805992 | -0.5192732048 |
| H | 1.5271740793 | 6.5520994898 | -1.1087486855 |
| H | 1.3444722376 | 4.3868797259 | -0.2508756408 |
| H | 0.9061102555 | 4.997833799 | 2.3979838043 |
| H | -0.3786258251 | 5.4161059 | 5.4793648553 |
| H | -2.7512525908 | 5.5282589178 | 5.4961481484 |
| H | -2.7662412754 | 4.3156853088 | 4.2045495464 |
| H | -2.8389486833 | 6.0749996762 | 2.7419050391 |
| H | -0.6679114553 | 6.8960658548 | 2.0405246496 |
| H | -0.0355031717 | 6.8261249899 | 3.678062944 |
| H | -0.617933791 | 2.3536538213 | 5.8505775556 |
| H | 1.2485537707 | 3.8495528084 | 6.5086959076 |
| H | 1.4682812342 | 2.2416474212 | 7.2169832524 |
| H | 2.4239715623 | 2.7218578252 | 5.7962546038 |
| H | 0.9282353841 | 0.5523395847 | 4.1908392774 |
| H | 1.1280512418 | -3.478217378 | 6.4979061996 |
| H | 1.7054756417 | -1.570207797 | 5.1896990738 |
| H | -1.2333224166 | -1.9343214159 | 7.6053104746 |
| H | -1.8942809539 | -2.2281580567 | 2.4896442773 |
| H | -0.6549654161 | -3.4315120992 | 2.0785852283 |
| H | -0.2766357367 | -3.6553829977 | 8.8516742114 |
| H | -0.900914379 | -1.6106745005 | -1.6619859155 |
| H | -2.3139395438 | -0.5444722503 | -1.4736909072 |
| H | -0.9791961008 | -0.0806351395 | -2.5500197585 |
| H | 1.3190906516 | -0.9503584063 | -0.2556532164 |
| H | 1.4660626641 | 0.7791316585 | 0.0969927866 |
| H | 1.1134502381 | 1.043051536 | -2.2157755716 |
| H | 0.9911596747 | -1.1972853681 | 8.1120552354 |
| H | 0.6235616513 | 4.8855154322 | -2.695904656 |

**1a** conf_4

energy (M062X/6-31g(d,p)) = -2585.274681 Hartree

| | | | |
|---|---|---|---|
| C | 0.1172960095 | -2.5608495341 | -1.5917812232 |
| O | 0.3970051988 | -1.8114949508 | -2.4978757302 |
| C | 1.1216915705 | -3.2411780141 | -0.6672221719 |
| N | 2.4116881431 | -2.6433372932 | -0.9806608056 |
| C | 3.5341153948 | -2.8645249797 | -0.2617391672 |
| O | 3.6762460418 | -3.7860507987 | 0.5388428233 |
| C | 4.620307717 | -1.8029275348 | -0.4898107029 |

| | | | |
|---|---|---|---|
| C | 6.027488184 | -2.2601577916 | -0.1041682303 |
| C | 6.2611535485 | -2.2716142604 | 1.4056977591 |
| C | 5.8195857045 | -0.9464106677 | 2.0136382589 |
| N | 4.4367518218 | -0.6041142768 | 1.6703293339 |
| N | 4.2490694682 | -0.6067082488 | 0.2811309169 |
| C | 3.5073177345 | 0.3754876521 | -0.286104178 |
| O | 3.1394185263 | 0.3082419074 | -1.4611081321 |
| C | 3.1850929868 | 1.5933258547 | 0.5895287029 |
| N | 2.1512630725 | 2.3916213717 | -0.0466255112 |
| N | 2.4790536598 | 3.0891598543 | -1.2167772811 |
| C | 3.6241149547 | 3.9701423715 | -1.0054567406 |
| C | 4.812730186 | 3.2016990868 | -0.4366230281 |
| C | 4.4212915009 | 2.4770893468 | 0.8407285727 |
| C | 0.9015045042 | 2.4759176077 | 0.4859498954 |
| O | 0.5825860545 | 1.8799614547 | 1.5096952936 |
| C | -0.106034918 | 3.3828929634 | -0.223963172 |
| C | -0.207057618 | 4.7161331693 | 0.5133238047 |
| N | -1.3903796893 | 2.7080547026 | -0.2469544698 |
| C | -1.8537651436 | 2.1158641267 | -1.3573317165 |
| O | -1.2942519485 | 2.1871329741 | -2.4568095559 |
| C | -4.2051118282 | 2.263835725 | -2.143182217 |
| C | -3.2323778703 | 1.4591588588 | -1.2573178695 |
| N | -3.1755491782 | 0.0786698924 | -1.7438860935 |
| N | -4.1744194946 | -0.5240081467 | -2.4592576198 |
| C | -5.2515282896 | 0.1231640814 | -2.6837202758 |
| C | -5.5309807475 | 1.5235999938 | -2.2023675393 |
| C | -2.1945142341 | -0.7528048188 | -1.2920141232 |
| O | -1.3708082217 | -0.3681318157 | -0.4721423683 |
| C | -2.1750644094 | -2.1597354214 | -1.8775714896 |
| O | -1.1360006388 | -2.8981869573 | -1.2566204485 |
| O | -6.0865908425 | 1.5288694561 | -0.9000456077 |
| Cl | 6.1787865031 | 4.344693236 | -0.1107398888 |
| C | 1.1058275684 | -4.7529130333 | -0.9265830406 |
| C | 0.7289153516 | -2.9328998049 | 0.7975321977 |
| O | 0.7747529137 | -1.5588766838 | 1.0895773465 |
| O | -3.7631643559 | 2.3834183989 | -3.468665417 |
| H | -6.00442968 | -0.4187103198 | -3.2493602503 |
| H | 2.3759309103 | -1.7914761904 | -1.5330729524 |
| H | 4.6023381025 | -1.4995325707 | -1.5381717817 |
| H | 6.7367129846 | -1.5712194815 | -0.5764420956 |
| H | 6.2034951775 | -3.2503467272 | -0.5329604244 |
| H | 7.3212089737 | -2.4443889396 | 1.6172878198 |
| H | 6.4571918637 | -0.1285432088 | 1.6604495299 |
| H | 5.8766417513 | -0.96460131 | 3.1050393057 |
| H | 3.8024996418 | -1.296609934 | 2.0692400837 |
| H | 2.7886027689 | 1.2518740636 | 1.5439963779 |
| H | 2.6940238693 | 2.3803505317 | -1.9169018383 |
| H | 3.3325770372 | 4.7650453652 | -0.3124406611 |
| H | 3.8740884707 | 4.4245483742 | -1.9664625597 |
| H | 5.1992347637 | 2.5019441054 | -1.1814545184 |
| H | 5.2444684715 | 1.8695110612 | 1.2183716162 |
| H | 4.1630464087 | 3.2125725676 | 1.6091736495 |
| H | 0.1909133327 | 3.5411645877 | -1.2571284294 |
| H | -0.9537237727 | 5.3523263004 | 0.0326363952 |

| | | | |
|---|---|---|---|
| H | -0.494523476 | 4.5609369455 | 1.5571923306 |
| H | 0.7544765019 | 5.2354937945 | 0.4963658109 |
| H | -1.7724504631 | 2.4261031606 | 0.6453763907 |
| H | -4.3501484877 | 3.2414985848 | -1.6642475475 |
| H | -3.6130640071 | 1.4706568733 | -0.2316432492 |
| H | -6.1829574686 | 2.0340781388 | -2.9200030095 |
| H | -2.0386786933 | -2.1141009394 | -2.9595174481 |
| H | -3.0983284847 | -2.6920273521 | -1.6586225796 |
| H | -6.9608268417 | 1.117237609 | -0.9394837284 |
| H | 1.3640724844 | -4.964193374 | -1.9671676516 |
| H | 1.8402607172 | -5.2332359656 | -0.2794108438 |
| H | 0.1165527359 | -5.1656993195 | -0.7180291806 |
| H | 1.4576303485 | -3.4233233317 | 1.4440629914 |
| H | -0.2574727129 | -3.3673983751 | 0.994727872 |
| H | 0.0311183865 | -1.1238677303 | 0.6345266028 |
| H | -2.7836733132 | 2.3872604045 | -3.442061682 |
| H | 5.6940368072 | -3.0883364519 | 1.8603865654 |

**1a** conf_5

energy (M062X/6-31g(d,p)) = -2585.2740974 Hartree

| | | | |
|---|---|---|---|
| C | -1.0414456081 | -0.4401468464 | 0.8800133755 |
| O | -1.649821675 | 0.1434804347 | 1.7488301997 |
| C | -0.655684115 | 0.1754164533 | -0.4640572679 |
| N | -1.0975718289 | 1.5664192658 | -0.369732756 |
| C | -0.8220534039 | 2.554308477 | -1.2347131704 |
| O | -0.1428431219 | 2.4269617554 | -2.2602090021 |
| C | -1.3970722799 | 3.9177890719 | -0.8199201823 |
| C | -1.4684350591 | 4.9328760959 | -1.9614142515 |
| C | -0.1216648077 | 5.5809009613 | -2.2756829475 |
| C | 0.5237779712 | 6.0916105054 | -0.993746807 |
| N | 0.6508957318 | 5.0406919381 | 0.0201870081 |
| N | -0.5914423772 | 4.4490066131 | 0.2877288466 |
| C | -0.9473687827 | 4.1976383577 | 1.5706989008 |
| O | -1.9594526923 | 3.5482712619 | 1.8430628217 |
| C | -0.0306407077 | 4.7443609201 | 2.6709746265 |
| N | -0.2935552674 | 4.0293721677 | 3.9089474631 |
| N | -1.4865229522 | 4.294136804 | 4.5982944168 |
| C | -1.6146804484 | 5.7160942889 | 4.8946461546 |
| C | -1.5051303022 | 6.5467313753 | 3.6200478657 |
| C | -0.1957962885 | 6.2555305558 | 2.9053963832 |
| C | 0.4270715898 | 2.9180317748 | 4.2146713245 |
| O | 1.3590175026 | 2.5385276823 | 3.5103066283 |
| C | 0.0653526249 | 2.1816639105 | 5.5019610467 |
| C | 0.5890232198 | 2.9366350326 | 6.7271587567 |
| N | 0.6474702207 | 0.8589253481 | 5.3943686345 |
| C | 0.107094555 | -0.2048576477 | 6.0131977901 |
| O | -0.8320899401 | -0.1264251019 | 6.8016581791 |
| C | 0.8572403856 | -2.550859185 | 6.7551705446 |
| C | 0.727457022 | -1.5517085275 | 5.6031363428 |
| N | -0.1066089231 | -2.1399426825 | 4.5487086528 |
| N | -1.1178242599 | -3.0281722798 | 4.7881545684 |
| C | -1.299596825 | -3.4468934388 | 5.9807100345 |

| | | | |
|---|---|---|---|
| C | -0.5083302484 | -3.0540214857 | 7.1885267378 |
| C | 0.0833373181 | -1.749891058 | 3.2513099006 |
| O | 0.9743245423 | -0.9776091538 | 2.9351052392 |
| C | -0.8911188953 | -2.3298525824 | 2.2317443129 |
| O | -0.6575405121 | -1.71596174 | 0.9703774317 |
| O | -0.4078114733 | -4.1847830428 | 8.0283206749 |
| Cl | -1.6129563811 | 8.3076504901 | 4.0225171916 |
| C | -1.4061784302 | -0.5641153356 | -1.5806516009 |
| C | 0.8839268001 | 0.0508516008 | -0.6532610847 |
| O | 1.2986630657 | 0.1656802228 | -1.9857893138 |
| O | 1.4803696112 | -1.9782915989 | 7.8818363253 |
| H | -2.1075054594 | -4.161074429 | 6.1134298163 |
| H | -1.6274561352 | 1.7981504962 | 0.468383021 |
| H | -2.3948751553 | 3.7563167877 | -0.4083831873 |
| H | -2.1814338665 | 5.7084222568 | -1.6608566591 |
| H | -1.8801849942 | 4.4389134183 | -2.8450308066 |
| H | -0.2627595299 | 6.407511073 | -2.9790665936 |
| H | -0.0702229888 | 6.9005146717 | -0.5550450965 |
| H | 1.5305763762 | 6.4767251662 | -1.1738052252 |
| H | 1.2773501498 | 4.3134682012 | -0.3252924377 |
| H | 1.002044896 | 4.5445478703 | 2.3921760573 |
| H | -2.2440353153 | 3.9924967921 | 3.9848342453 |
| H | -0.8255091654 | 6.0026958152 | 5.5961871778 |
| H | -2.5814144339 | 5.8671361691 | 5.379364472 |
| H | -2.3613055221 | 6.3489631928 | 2.970770347 |
| H | -0.1380432705 | 6.7847040375 | 1.9528325758 |
| H | 0.6362546027 | 6.594082824 | 3.5304628118 |
| H | -1.0180333091 | 2.081270279 | 5.5852406455 |
| H | 0.1027048943 | 3.9100755544 | 6.8164313847 |
| H | 0.3706880219 | 2.3539625583 | 7.6246188374 |
| H | 1.6702576731 | 3.0822644909 | 6.6569932775 |
| H | 1.3087171266 | 0.7281330984 | 4.6362780694 |
| H | 1.4247547395 | -3.4162917193 | 6.3899200175 |
| H | 1.7117649065 | -1.3855140398 | 5.161134742 |
| H | -1.0272983607 | -2.2261588978 | 7.69145383 |
| H | -1.9215986133 | -2.1791296494 | 2.5518572923 |
| H | -0.7160783318 | -3.3952177961 | 2.0849942446 |
| H | 0.086863741 | -3.8943778682 | 8.8078956316 |
| H | -2.4839275638 | -0.5261876409 | -1.4051474154 |
| H | -1.1867201218 | -0.0912281579 | -2.5379065944 |
| H | -1.0869552023 | -1.6068220592 | -1.6274495327 |
| H | 1.1888355225 | -0.93880066 | -0.3107432493 |
| H | 1.3612843325 | 0.7958773177 | 0.0001088833 |
| H | 0.9302087136 | 1.0166333412 | -2.3016311725 |
| H | 2.436379594 | -1.9833242565 | 7.7395337722 |
| H | 0.5408874954 | 4.8522301035 | -2.7521331775 |

Compound **1b**

**1b** conf_1

energy (M062X/6-31g(d,p)) = -2585.3002203 Hartree

| | | | |
|---|---|---|---|
| C | 0.2110346258 | -0.3641122351 | 1.4280147969 |
| O | -0.4121259153 | 0.0371648846 | 2.386035508 |
| C | 0.3772155275 | 0.3988514103 | 0.1212425443 |
| N | -0.6225205949 | 1.4534303298 | 0.1504223872 |
| C | -0.6324053003 | 2.4756438757 | -0.7374017625 |
| O | -0.0657020188 | 2.4480012086 | -1.8252651824 |
| C | -1.3846683788 | 3.719060609 | -0.2343254325 |
| C | -1.6999158456 | 4.7336300466 | -1.3318354906 |
| C | -0.4684431342 | 5.521181077 | -1.780104308 |
| C | 0.2752318827 | 6.0747197406 | -0.5697481655 |
| N | 0.5953978684 | 5.0449124295 | 0.4194569459 |
| N | -0.5589349751 | 4.3491502491 | 0.8054433961 |
| C | -0.7116346406 | 4.0085353566 | 2.104803151 |
| O | -1.5974543969 | 3.2350450144 | 2.4783349943 |
| C | 0.2752536891 | 4.6277548486 | 3.0999869695 |
| N | 0.2692015946 | 3.8504858133 | 4.3295834961 |
| N | -0.836245463 | 3.9489441974 | 5.1879790159 |
| C | -1.1052834236 | 5.3366996462 | 5.5494521838 |
| C | -1.2689792933 | 6.2023048566 | 4.3047492811 |
| C | -0.036351202 | 6.099222719 | 3.4227891695 |
| C | 1.1722769931 | 2.8625839207 | 4.5203724833 |
| O | 2.0319827092 | 2.5898247034 | 3.6787861791 |
| C | 1.1402797115 | 2.1278257142 | 5.8587589061 |
| C | 1.6856187479 | 3.012867149 | 6.9837487418 |
| N | 1.9441830166 | 0.9349709059 | 5.6820315379 |
| C | 1.7652768943 | -0.1730052898 | 6.405543355 |
| O | 0.9659122959 | -0.2335331677 | 7.3498403028 |
| C | 2.9915778953 | -2.3872960163 | 6.9910072725 |
| C | 2.5837925717 | -1.3744492825 | 5.9122097697 |
| N | 1.7972696539 | -2.0600146584 | 4.8820093691 |
| N | 0.869251637 | -3.0179038468 | 5.1823073096 |
| C | 0.8552199218 | -3.520617318 | 6.357117175 |
| C | 1.7991163263 | -3.2114733742 | 7.4896444123 |
| C | 1.8146506843 | -1.5861450401 | 3.59743978 |
| O | 2.5575747203 | -0.6768586571 | 3.2595877678 |
| C | 0.8588746255 | -2.2574506064 | 2.622580029 |
| O | 0.8609237961 | -1.5332666467 | 1.4010024405 |
| O | 1.1435882723 | -2.5805149707 | 8.5714371095 |
| Cl | -1.5438641849 | 7.9235497874 | 4.788402412 |
| C | 0.1965033897 | -0.5402872519 | -1.0749300818 |
| C | 1.8173471192 | 1.0130667752 | 0.0949691819 |
| O | 1.9398156321 | 2.2074826547 | 0.8218364394 |
| O | 3.6421345059 | -1.7504710431 | 8.0567584875 |
| H | 0.0750209796 | -4.2556337737 | 6.5337530267 |
| H | -1.0333786667 | 1.6277087747 | 1.0643520884 |
| H | -2.3035593471 | 3.3996246217 | 0.2614657712 |

| | | | |
|---|---|---|---|
| H | -2.4525559575 | 5.4242515798 | -0.9354378536 |
| H | -2.1531168361 | 4.2081585523 | -2.1764635767 |
| H | -0.7699712885 | 6.3419867066 | -2.4388117968 |
| H | -0.3263304439 | 6.8379615302 | -0.0635873589 |
| H | 1.222388146 | 6.5376707743 | -0.8589718624 |
| H | 1.2516258132 | 4.3586902146 | 0.0427677179 |
| H | 1.2770685351 | 4.5683196132 | 2.6804240369 |
| H | -1.6257528938 | 3.5602000309 | 4.6714827928 |
| H | -0.2760050143 | 5.7117218837 | 6.1566935497 |
| H | -2.0116737133 | 5.3466764591 | 6.1580277514 |
| H | -2.169860123 | 5.91016996 | 3.7601112517 |
| H | -0.1643639607 | 6.6558933963 | 2.4931304392 |
| H | 0.8222602907 | 6.5208784157 | 3.9545219148 |
| H | 0.1172994876 | 1.8335945998 | 6.0990782475 |
| H | 1.0420795067 | 3.880710391 | 7.1364183999 |
| H | 1.7145673844 | 2.4343144728 | 7.9092704723 |
| H | 2.6975765137 | 3.3533394053 | 6.749789956 |
| H | 2.5117858572 | 0.9021304645 | 4.8392867324 |
| H | 3.6995910839 | -3.0720604496 | 6.5121100728 |
| H | 3.4859297901 | -1.0055181188 | 5.4227691162 |
| H | 2.1717365629 | -4.161780686 | 7.883862175 |
| H | -0.1451412079 | -2.311609776 | 3.0415964826 |
| H | 1.1971694563 | -3.2647329716 | 2.3788797962 |
| H | 0.8439294739 | -1.7063113013 | 8.2231077704 |
| H | 0.2243740463 | 0.0499947802 | -1.9906401713 |
| H | 0.9943913217 | -1.284924225 | -1.1015128484 |
| H | -0.7629826546 | -1.059889416 | -1.0170692921 |
| H | 2.0408153683 | 1.2640473221 | -0.9426024337 |
| H | 2.5274470877 | 0.2489652059 | 0.4298004991 |
| H | 1.9526110265 | 2.0434704067 | 1.7811870805 |
| H | 2.9639230465 | -1.6667412904 | 8.750603098 |
| H | 0.1971237887 | 4.8662119287 | -2.3484669238 |

**1b** conf_2

energy (M062X/6-31g(d,p)) = -2585.2908899 Hartree

| | | | |
|---|---|---|---|
| C | -0.7031463083 | -1.1889772407 | -1.0217277772 |
| O | -0.429254126 | -0.1877366689 | -1.6402803626 |
| C | 0.307195505 | -2.1855719448 | -0.4728147385 |
| N | 1.5845599821 | -1.8237432664 | -1.0638893314 |
| C | 2.7486537817 | -2.3646237316 | -0.6301259827 |
| O | 2.8271468011 | -3.4119589704 | 0.0000193239 |
| C | 3.9891088599 | -1.5090414168 | -0.9360610538 |
| C | 5.3037369805 | -2.2734027653 | -0.7826001146 |
| C | 5.6599751179 | -2.5403752165 | 0.6807635594 |
| C | 5.5389585082 | -1.2592823644 | 1.4998752885 |
| N | 4.2480423362 | -0.5934434232 | 1.3405102435 |
| N | 3.9748914874 | -0.3647519673 | -0.0145197745 |
| C | 3.3718211704 | 0.7942246664 | -0.3694230495 |
| O | 2.933868576 | 0.9813115045 | -1.5054168807 |
| C | 3.2687449445 | 1.873987637 | 0.7137763807 |
| N | 2.2560641004 | 2.8444344251 | 0.330643532 |
| N | 2.5296952997 | 3.7146800584 | -0.735455547 |

| | | | |
|---|---|---|---|
| C | 3.7658022112 | 4.4512938513 | -0.5045131817 |
| C | 4.9313441061 | 3.5072332277 | -0.2211989026 |
| C | 4.6010754472 | 2.6021378174 | 0.9543662562 |
| C | 0.9788662811 | 2.7087433828 | 0.7671577963 |
| O | 0.6425845641 | 1.8035283738 | 1.5286031624 |
| C | -0.0225724888 | 3.776118143 | 0.3395477788 |
| C | 0.2093952465 | 5.078147966 | 1.1118527192 |
| N | -1.3395142785 | 3.2261788188 | 0.5951473279 |
| C | -2.4067948794 | 3.645640659 | -0.0864129897 |
| O | -2.3615396776 | 4.6166734542 | -0.8507006844 |
| C | -4.9389441238 | 3.7553006544 | -0.1653286471 |
| C | -3.7267294844 | 2.8702054528 | 0.1766012332 |
| N | -3.7578910202 | 1.5996379465 | -0.5700057636 |
| N | -4.7633511121 | 1.2416086344 | -1.4492879356 |
| C | -5.8819859954 | 1.8389829539 | -1.3266015571 |
| C | -6.1954211791 | 2.9027984975 | -0.3062396646 |
| C | -2.9301055477 | 0.5710995542 | -0.212897344 |
| O | -2.2011837597 | 0.6220417857 | 0.7658488707 |
| C | -2.9766750875 | -0.6572684103 | -1.1135543274 |
| O | -1.9586475737 | -1.5642674847 | -0.7276479309 |
| O | -7.2885462266 | 3.686192736 | -0.6969672294 |
| Cl | 6.4235434022 | 4.4583624127 | 0.1193524009 |
| C | -0.1126653879 | -3.6132334852 | -0.8405220975 |
| C | 0.3689853454 | -2.0421874219 | 1.0862450842 |
| O | 1.1987876622 | -1.0006432679 | 1.5236983052 |
| O | -4.8540725905 | 4.4058065445 | -1.4056587421 |
| H | -6.6624403288 | 1.5475553316 | -2.0249351815 |
| H | 1.616686931 | -0.8963142797 | -1.4794676376 |
| H | 3.9008596461 | -1.0877149158 | -1.9397747696 |
| H | 6.0927728292 | -1.6740311191 | -1.2522483782 |
| H | 5.2319239431 | -3.2135670972 | -1.3358141169 |
| H | 6.680715225 | -2.9316294458 | 0.7512843288 |
| H | 6.3135673365 | -0.5406568147 | 1.2055358082 |
| H | 5.6634394192 | -1.4544809491 | 2.5688703481 |
| H | 3.4785120385 | -1.1505197581 | 1.7177592607 |
| H | 2.9446714801 | 1.4094030574 | 1.6427338467 |
| H | 2.6174237767 | 3.11948585 | -1.5605604325 |
| H | 3.622914484 | 5.123870683 | 0.3472409273 |
| H | 3.9606013227 | 5.0607393254 | -1.3900393668 |
| H | 5.1559342518 | 2.9174334555 | -1.1139875408 |
| H | 5.3916635908 | 1.8702875234 | 1.129323423 |
| H | 4.5039080539 | 3.2125997289 | 1.8580989644 |
| H | 0.0752259735 | 3.9808973027 | -0.7278860806 |
| H | 1.1875873157 | 5.4969186054 | 0.8675648807 |
| H | -0.5577066972 | 5.8008240903 | 0.8271843345 |
| H | 0.1518908581 | 4.9027864951 | 2.1895472583 |
| H | -1.3827415635 | 2.342743863 | 1.101200107 |
| H | -5.0592433915 | 4.4778596501 | 0.6549686181 |
| H | -3.7689140267 | 2.6251739334 | 1.2443895851 |
| H | -6.4573009991 | 2.4262097758 | 0.6468052043 |
| H | -2.8670808708 | -0.3594254288 | -2.1574810746 |
| H | -3.9159221126 | -1.1968362386 | -0.9973833313 |
| H | -6.9294851247 | 4.2984389448 | -1.360840044 |
| H | 0.674215971 | -4.2993867281 | -0.5274438981 |

```
H   -1.047948176   -3.8763841832  -0.3421988
H   -0.2551694872  -3.7076703607  -1.9200915924
H   0.8038622335   -2.9644267704  1.4740814156
H   -0.6527426288  -1.9461973689  1.4695167998
H   0.75164694     -0.1375673856  1.4699938824
H   -3.9415846616  4.7714286568   -1.4541414772
H   4.982949578    -3.2990095402  1.0804370762
```

**1b** conf_3

energy (M062X/6-31g(d,p)) = -2585.2878379 Hartree

```
C   0.3946904267   -0.4342684097  1.3539958399
O   -0.2993416154  -0.0789474513  2.2798094511
C   0.5949671348   0.3634224016   0.0698878488
N   -0.2927745964  1.5098881218   0.1861010126
C   -0.4901802141  2.4471011575   -0.7612602941
O   -0.1033723882  2.3587506778   -1.9279193256
C   -1.2132009032  3.7001739018   -0.23674266
C   -1.5078776733  4.7272684404   -1.3279909249
C   -0.25598434    5.4852303824   -1.7696189969
C   0.4944786839   6.0232115381   -0.5564285443
N   0.7889550386   4.9831723369   0.4327600567
N   -0.3823591263  4.3094995308   0.8095481552
C   -0.6003699728  4.0293066035   2.1153919882
O   -1.5045743163  3.2665000302   2.4677392405
C   0.3274405561   4.6913065718   3.1397259103
N   0.2852100943   3.9346490841   4.3805325445
N   -0.8698434964  4.0030022705   5.1732688437
C   -1.1900949674  5.3867060229   5.5079906869
C   -1.3157470224  6.2364433805   4.2471442816
C   -0.0423248826  6.157974825    3.4211125832
C   1.2205559126   2.9835679089   4.6300962773
O   2.1642410899   2.7851591851   3.8689016803
C   1.0827320283   2.1873355952   5.9270492649
C   1.5309234543   3.0181732568   7.132512045
N   1.906118565    1.0053083356   5.7554766929
C   1.6856523605   -0.1339454207  6.4149771242
O   0.8121196843   -0.2423739599  7.2872708961
C   2.9529956766   -2.3030261733  7.0579749167
C   2.5633255796   -1.3070950119  5.9556960101
N   1.8553046917   -2.022664198   4.8894809367
N   0.9615732804   -3.0257948646  5.139498105
C   0.9072085205   -3.5307912668  6.3120896465
C   1.7711986841   -3.1766353859  7.4936542438
C   1.9362321609   -1.5594151908  3.6032488027
O   2.6559117444   -0.6186010426  3.3070877522
C   1.0893996755   -2.2916723016  2.5705927282
O   1.1130063578   -1.5606534409  1.3496619608
O   1.0291553069   -2.5706921156  8.5332067731
Cl  -1.6566766612  7.9553937958   4.6984011053
C   0.2656434155   -0.5127686637  -1.1455590446
C   2.0873335633   0.8314261736   0.0791672899
O   2.3188037077   2.0044775861   -0.66255718
```

| | | | |
|---|---|---|---|
| O | 3.5151904402 | -1.6383749183 | 8.1567363505 |
| H | 0.1555798825 | -4.3035945742 | 6.44604665 |
| H | -0.6816961566 | 1.6684528657 | 1.1123009341 |
| H | -2.1378051096 | 3.3882988421 | 0.2539344825 |
| H | -2.2433637679 | 5.4327466056 | -0.9264003821 |
| H | -1.9714692133 | 4.2162193304 | -2.1751285684 |
| H | -0.5335848429 | 6.3111570266 | -2.4321527972 |
| H | -0.0923890082 | 6.7979759741 | -0.0511882867 |
| H | 1.452582443 | 6.4656311742 | -0.8412280484 |
| H | 1.4284685167 | 4.2889417843 | 0.039216016 |
| H | 1.3480401272 | 4.6512941185 | 2.7654627547 |
| H | -1.6201275604 | 3.5942729977 | 4.6154519232 |
| H | -0.3991162823 | 5.7864116459 | 6.1496260846 |
| H | -2.1249958127 | 5.3821222275 | 6.0721109409 |
| H | -2.1831471851 | 5.9163149592 | 3.6652570101 |
| H | -0.1476089307 | 6.6994409263 | 2.4792119034 |
| H | 0.779320848 | 6.6129286997 | 3.9828081698 |
| H | 0.0463073404 | 1.8781239377 | 6.070385355 |
| H | 0.8719676533 | 3.8772523986 | 7.270606 |
| H | 1.488613023 | 2.3989199021 | 8.0309299586 |
| H | 2.5563599249 | 3.3714305735 | 6.9963723933 |
| H | 2.540149414 | 1.0211303418 | 4.9615660064 |
| H | 3.7148994289 | -2.9575282165 | 6.6213965427 |
| H | 3.4753308828 | -0.9082144337 | 5.5102518018 |
| H | 2.1625468255 | -4.1079684241 | 7.9140866333 |
| H | 0.0680945402 | -2.421888165 | 2.9249218586 |
| H | 1.5162888157 | -3.2689205164 | 2.3445857229 |
| H | 0.7087175815 | -1.7137523068 | 8.1606324179 |
| H | 0.8925446407 | -1.4055463924 | -1.1393272825 |
| H | -0.7835630408 | -0.8177515943 | -1.1174752346 |
| H | 0.4346303841 | 0.0394465887 | -2.0690823849 |
| H | 2.7010406571 | -0.0052365326 | -0.2781064742 |
| H | 2.3935676859 | 1.0564956088 | 1.1039144015 |
| H | 1.8033279071 | 1.9604036146 | -1.4851376377 |
| H | 2.7959969051 | -1.5850606797 | 8.8113965635 |
| H | 0.3978458244 | 4.8153203929 | -2.335957503 |

**1b** conf_4

energy (M062X/6-31g(d,p)) = -2585.2865694 Hartree

| | | | |
|---|---|---|---|
| C | 0.2302918614 | -0.4571161173 | 1.4541475459 |
| O | -0.3797836472 | -0.0076614618 | 2.3982524785 |
| C | 0.3253058314 | 0.2189410545 | 0.0875418074 |
| N | -0.3838669684 | 1.4868189406 | 0.2559454291 |
| C | -0.4221116638 | 2.5047027086 | -0.6175423911 |
| O | 0.1497799069 | 2.5168653069 | -1.7136895202 |
| C | -1.2248413396 | 3.7173076588 | -0.1194054693 |
| C | -1.6064776091 | 4.702462411 | -1.2245398921 |
| C | -0.4548264448 | 5.6161206363 | -1.638595911 |
| C | 0.1848331097 | 6.2419849178 | -0.4056293336 |
| N | 0.6150313667 | 5.2347726203 | 0.568579059 |
| N | -0.4503139291 | 4.3972707925 | 0.927401503 |
| C | -0.6315826178 | 4.0700613348 | 2.2293454792 |

| | | | |
|---|---|---|---|
| O | -1.4620588124 | 3.2254962681 | 2.5718265199 |
| C | 0.2537472877 | 4.7798133628 | 3.2596670729 |
| N | 0.254151697 | 4.0113347651 | 4.4938521982 |
| N | -0.8968289061 | 4.023341447 | 5.2960106444 |
| C | -1.2754518257 | 5.387451306 | 5.6459308308 |
| C | -1.4531334691 | 6.2387091706 | 4.3926962995 |
| C | -0.1855354518 | 6.2239528452 | 3.55426729 |
| C | 1.2030144104 | 3.0614493563 | 4.6969683352 |
| O | 2.1187435112 | 2.8786893627 | 3.8991152641 |
| C | 1.1215341693 | 2.2549795941 | 5.9917502582 |
| C | 1.597999193 | 3.0892834685 | 7.1840575507 |
| N | 1.9556364711 | 1.0863933116 | 5.7843498114 |
| C | 1.7908130906 | -0.0501347597 | 6.4643427778 |
| O | 0.9700259089 | -0.1622103238 | 7.3860478144 |
| C | 3.135740064 | -2.1883141285 | 7.0474544999 |
| C | 2.6494950369 | -1.2184883503 | 5.9607890038 |
| N | 1.8668729903 | -1.961692945 | 4.9689286031 |
| N | 0.9979889727 | -2.9588358196 | 5.3119978691 |
| C | 1.0423460142 | -3.4408511136 | 6.4947343017 |
| C | 2.000503382 | -3.0625624694 | 7.5932742239 |
| C | 1.8423824431 | -1.5307460739 | 3.668650685 |
| O | 2.5391660567 | -0.6046955062 | 3.2862876233 |
| C | 0.8981236406 | -2.2811958223 | 2.7370770338 |
| O | 0.8746249605 | -1.6268730284 | 1.4751013501 |
| O | 1.3440045369 | -2.4433534999 | 8.6817088489 |
| Cl | -1.8678834902 | 7.9373260374 | 4.8577616929 |
| C | -0.3747674383 | -0.6669633531 | -0.9526704496 |
| C | 1.8259394154 | 0.418569161 | -0.2733869959 |
| O | 2.0550606567 | 0.6119976298 | -1.6410628129 |
| O | 3.7747036657 | -1.4955838109 | 8.0853419411 |
| H | 0.3066250628 | -4.21166665 | 6.7061630199 |
| H | -0.8612338549 | 1.6027037455 | 1.1479506278 |
| H | -2.1265707723 | 3.3487473673 | 0.3728354371 |
| H | -2.433317656 | 5.3120965454 | -0.8439719348 |
| H | -1.9857591176 | 4.1393334148 | -2.0807996316 |
| H | -0.8245923857 | 6.3998694312 | -2.3071207284 |
| H | -0.520498429 | 6.9086278733 | 0.1019681457 |
| H | 1.0710722351 | 6.8273424229 | -0.6630903082 |
| H | 1.3455869441 | 4.6553025629 | 0.1547761488 |
| H | 1.2753418365 | 4.795283163 | 2.8850876711 |
| H | -1.6339747984 | 3.583441731 | 4.7443455396 |
| H | -0.4960656163 | 5.8172826072 | 6.2821276717 |
| H | -2.2028329682 | 5.3360295858 | 6.2200057034 |
| H | -2.3109236899 | 5.8825840179 | 3.817269437 |
| H | -0.3239247826 | 6.7649595443 | 2.6168341738 |
| H | 0.6181827979 | 6.7146315759 | 4.1117399232 |
| H | 0.0953219778 | 1.929947268 | 6.1695908162 |
| H | 1.5952053312 | 2.4677180648 | 8.0817178838 |
| H | 2.6126433502 | 3.4586015002 | 7.0140104571 |
| H | 0.9311941099 | 3.9381757535 | 7.3460156248 |
| H | 2.5480677929 | 1.1098565085 | 4.9595898327 |
| H | 3.8676331873 | -2.844735065 | 6.564795388 |
| H | 3.5180471244 | -0.8184460252 | 5.4366998509 |
| H | 2.4322150021 | -3.9845600805 | 7.9943444572 |

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H   -0.1022547798  -2.3371981209  3.1648322089
H   1.2604022898   -3.2911450896  2.5458521574
H   0.9758557774   -1.6020488883  8.3180883316
H   -0.3706993372  -0.1612928437  -1.9182896549
H   0.1494089081   -1.6185948661  -1.0569694
H   -1.4091754875  -0.8573495419  -0.6566978329
H   2.3668870955   -0.4841137586  0.0136907144
H   2.2079638317   1.249822277    0.3373269551
H   1.4834355951   1.3649983842   -1.8978378322
H   3.1111355334   -1.4443003512  8.7967968899
H   0.297201855    5.0422790519   -2.1883586145
```

**1b** conf_5

energy (M062X/6-31g(d,p)) = -2585.2836836 Hartree

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C   0.5685636654   -0.3561485099  1.0086519086
O   -0.290949994   0.0156970037   1.7703654684
C   1.0900845443   0.4446417079   -0.1927492663
N   0.4746443301   1.7576525191   -0.1357191939
C   -0.7608778318  2.1087512565   -0.5630754037
O   -1.4543102002  1.4611292187   -1.3369288679
C   -1.3138983572  3.4360304814   -0.0126085216
C   -1.7693265251  4.3831789792   -1.1288771079
C   -0.6073068004  5.1894241726   -1.7004187004
C   0.1430000828   5.8796270224   -0.5671483421
N   0.6197520463   4.9324465783   0.4464374213
N   -0.4233796748  4.1192117051   0.9223203113
C   -0.6758690171  4.0653908146   2.2606398375
O   -1.6289825708  3.4317797892   2.7094624754
C   0.303586473    4.786581563    3.1945078012
N   0.3147149579   4.0890555042   4.4747001224
N   -0.8016992096  4.2059201716   5.3172501268
C   -1.0835449174  5.6080675145   5.6056679688
C   -1.2746516234  6.3967264741   4.3134863302
C   -0.0514477534  6.2657423258   3.4203654127
C   1.2266221303   3.1104488332   4.7040179125
O   2.144236758    2.8807484894   3.9203041254
C   1.0898739294   2.3067330552   5.9974910823
C   1.6068456707   3.0960227433   7.202709141
N   1.8539998594   1.0917278923   5.7841696892
C   1.5389752413   -0.078574775   6.3423112555
O   0.6165461591   -0.2055223091  7.1594127067
C   2.7273850962   -2.3002972301  6.9300829811
C   2.3869062078   -1.260523162   5.8503714763
N   1.6853148828   -1.9245170303  4.7458573064
N   0.7799750799   -2.9333458472  4.9350064609
C   0.689343091    -3.4765394506  6.0875123485
C   1.5195317837   -3.1664417275  7.3048068078
C   1.8137853229   -1.443490961   3.4763988496
O   2.5395047265   -0.4848434914  3.2353945359
C   1.0297612388   -2.1751171414  2.3930564315
O   1.2379801737   -1.513795003   1.154825631
O   0.752623767    -2.5765001495  8.3348393646
```

| | | | |
|---|---|---|---|
| Cl | -1.57400632 | 8.1400016623 | 4.6974366226 |
| C | 0.8809155896 | -0.305074294 | -1.5067999827 |
| C | 2.603682592 | 0.6854199172 | 0.0214190495 |
| O | 2.8518834675 | 1.4688814617 | 1.1616116529 |
| O | 3.2661077227 | -1.6786227358 | 8.0648108646 |
| H | -0.0702315618 | -4.2483834846 | 6.1729830233 |
| H | 0.8534066848 | 2.2969781365 | 0.6343457098 |
| H | -2.1821475938 | 3.1351102622 | 0.5778365865 |
| H | -2.5146236403 | 5.0681683063 | -0.7104610278 |
| H | -2.2649675671 | 3.7866628334 | -1.8977388739 |
| H | -0.9783978631 | 5.9322169175 | -2.4132464458 |
| H | -0.505653304 | 6.6061126124 | -0.0659507808 |
| H | 1.0243900135 | 6.4144385282 | -0.9297272853 |
| H | 1.3240716171 | 4.328840238 | 0.0243903997 |
| H | 1.3063785332 | 4.7247332874 | 2.7785303859 |
| H | -1.583619701 | 3.7925888242 | 4.8078773778 |
| H | -0.2502904503 | 6.0244053056 | 6.179593295 |
| H | -1.9832536113 | 5.6452018835 | 6.2233279649 |
| H | -2.1764872851 | 6.0576515424 | 3.7993159211 |
| H | -0.2090004362 | 6.7592670496 | 2.4592555875 |
| H | 0.8017387706 | 6.7462307311 | 3.9093076945 |
| H | 0.0463085798 | 2.0371465802 | 6.1640080823 |
| H | 0.996366929 | 3.9862106878 | 7.3650765744 |
| H | 1.553125185 | 2.4682270161 | 8.0948833786 |
| H | 2.6460076922 | 3.397956742 | 7.0482285354 |
| H | 2.5203533503 | 1.1267947351 | 5.0188901423 |
| H | 3.4913862872 | -2.9535743716 | 6.4958819723 |
| H | 3.3201983824 | -0.8751623903 | 5.4383824052 |
| H | 1.8838194579 | -4.1143861709 | 7.7118906834 |
| H | -0.0289873608 | -2.2154577486 | 2.6471703034 |
| H | 1.4048222615 | -3.1907170759 | 2.2683157936 |
| H | 0.4567901381 | -1.7049896485 | 7.9761065099 |
| H | 1.472082672 | -1.2235414005 | -1.4938996276 |
| H | -0.1666295721 | -0.5498446711 | -1.6693703472 |
| H | 1.2214590826 | 0.3180540545 | -2.3373588338 |
| H | 2.9729186093 | 1.2435511302 | -0.8430581746 |
| H | 3.118883703 | -0.2792769904 | 0.0623051854 |
| H | 2.7711042635 | 0.892914102 | 1.9440969386 |
| H | 2.527752915 | -1.6307056004 | 8.6984671718 |
| H | 0.082029024 | 4.5348930079 | -2.2490323199 |

**1b** conf_6

energy (M062X/6-31g(d,p)) = -2585.2783681 Hartree

| | | | |
|---|---|---|---|
| C | -0.8243726895 | -1.3599227158 | -1.1041289812 |
| O | -0.4947636933 | -0.4549797883 | -1.8348777707 |
| C | 0.1471039554 | -2.3066770609 | -0.4054763183 |
| N | 1.470184738 | -1.8242979473 | -0.809188894 |
| C | 2.6408023085 | -2.1787905797 | -0.2603710685 |
| O | 2.7785708232 | -3.0116710372 | 0.6437646698 |
| C | 3.8487901953 | -1.3880660782 | -0.7714955107 |
| C | 5.1606945774 | -2.1768051266 | -0.7826332853 |
| C | 5.7748294711 | -2.3543010507 | 0.6074569397 |

| | | | |
|---|---|---|---|
| C | 5.788160677 | -1.0255418895 | 1.3568200876 |
| N | 4.4654048252 | -0.3955728303 | 1.4034990127 |
| N | 3.9755616543 | -0.2153502322 | 0.1029170967 |
| C | 3.3560272094 | 0.9474030931 | -0.2365910758 |
| O | 2.8085710724 | 1.0825241812 | -1.3283378372 |
| C | 3.3674460003 | 2.0786891743 | 0.7986974104 |
| N | 2.3446739321 | 3.0490147731 | 0.445667406 |
| N | 2.5637883612 | 3.8610707368 | -0.6786908768 |
| C | 3.8117426914 | 4.5983209652 | -0.5518146794 |
| C | 4.9851098504 | 3.6516433146 | -0.3134172706 |
| C | 4.7251268589 | 2.7899599992 | 0.9118168443 |
| C | 1.0595453218 | 2.8406887689 | 0.8668185318 |
| O | 0.7766363558 | 1.9419889406 | 1.6461330204 |
| C | 0.0096215458 | 3.8282344368 | 0.3698356653 |
| C | 0.138406313 | 5.166868419 | 1.1021793845 |
| N | -1.2875671119 | 3.2165326749 | 0.5933929346 |
| C | -2.3366866869 | 3.5656806839 | -0.1556650509 |
| O | -2.2760581961 | 4.4873766755 | -0.9786675097 |
| C | -4.858130343 | 3.739610745 | -0.1811077772 |
| C | -3.6664340806 | 2.8103146722 | 0.1134545247 |
| N | -3.7562355673 | 1.565862762 | -0.6697839723 |
| N | -4.8255328777 | 1.2289146667 | -1.4771755721 |
| C | -5.9203772147 | 1.85395817 | -1.2933762965 |
| C | -6.1506591359 | 2.9350739008 | -0.26940566 |
| C | -2.9263410055 | 0.5220616855 | -0.3669696799 |
| O | -2.1285124133 | 0.5701014921 | 0.5541990789 |
| C | -3.061063837 | -0.7190114281 | -1.2468176005 |
| O | -2.0977166967 | -1.6733844308 | -0.8321575548 |
| O | -7.2265325064 | 3.7586801949 | -0.6253238459 |
| Cl | 6.509079645 | 4.5904735011 | -0.1048359585 |
| C | -0.0884410197 | -3.7367517415 | -0.9056166159 |
| C | -0.082012525 | -2.2172782055 | 1.1367058213 |
| O | 0.3620762244 | -3.3414055565 | 1.8347807073 |
| O | -4.7964291371 | 4.3857232162 | -1.4246242524 |
| H | -6.747634586 | 1.5743248652 | -1.9409002245 |
| H | 1.4516265711 | -1.0320570704 | -1.4472506366 |
| H | 3.6393849203 | -0.9977376241 | -1.7680304839 |
| H | 5.8613761085 | -1.6256505144 | -1.4209052651 |
| H | 4.9898321902 | -3.1479480401 | -1.2558529764 |
| H | 6.7950865823 | -2.7414980195 | 0.5148331824 |
| H | 6.4696145292 | -0.3126662951 | 0.8788611794 |
| H | 6.1162890796 | -1.1526491705 | 2.3923666496 |
| H | 3.821981138 | -1.0206890537 | 1.8917971201 |
| H | 3.1029208016 | 1.6608036558 | 1.7689738007 |
| H | 2.5986685977 | 3.2329471996 | -1.4829885555 |
| H | 3.7254940153 | 5.2982681024 | 0.2852162449 |
| H | 3.9550641593 | 5.1768909424 | -1.4674961994 |
| H | 5.1425222307 | 3.030219654 | -1.1995722028 |
| H | 5.5174812698 | 2.0535745007 | 1.0566201704 |
| H | 4.701803661 | 3.4327710386 | 1.7977094769 |
| H | 0.1325002691 | 4.005245135 | -0.699687225 |
| H | -0.6505055079 | 5.839479894 | 0.759857768 |
| H | 0.0441168241 | 5.0256975259 | 2.1822869615 |
| H | 1.1047106697 | 5.6259688652 | 0.8835108089 |

| | | | |
|---|---|---|---|
| H | -1.3066612113 | 2.3417986122 | 1.1132284665 |
| H | -4.9180840852 | 4.4658094228 | 0.6429825373 |
| H | -3.6950176166 | 2.5380361153 | 1.1751310069 |
| H | -6.3960677118 | 2.475821784 | 0.6962916366 |
| H | -2.9341161463 | -0.4511003893 | -2.297114773 |
| H | -4.0307739089 | -1.1963651377 | -1.1166040391 |
| H | -6.8689877469 | 4.3500543423 | -1.3085983823 |
| H | -1.0879672349 | -4.0729779305 | -0.625729186 |
| H | 0.0194564381 | -3.78591631 | -1.9924291358 |
| H | 0.6375956191 | -4.4043392253 | -0.442048214 |
| H | -1.1549739193 | -2.1399353688 | 1.3129126098 |
| H | 0.3774240266 | -1.2817841077 | 1.4884183655 |
| H | 1.3145628406 | -3.4169684964 | 1.6379292729 |
| H | -3.8666474274 | 4.6952127074 | -1.5209122984 |
| H | 5.1927366905 | -3.0855057541 | 1.1741043183 |

**1b** conf_7

energy (M062X/6-31g(d,p)) = -2585.2775984 Hartree

| | | | |
|---|---|---|---|
| C | -0.6766592929 | -1.520224002 | -0.7618422783 |
| O | -0.3031807734 | -0.6642671434 | -1.5211062991 |
| C | 0.2308614239 | -2.416632111 | 0.0900475917 |
| N | 1.590807184 | -1.9430981708 | -0.070456205 |
| C | 2.4428372701 | -2.2182034998 | -1.0919515715 |
| O | 2.3403777589 | -3.1469675931 | -1.8749905455 |
| C | 3.6480475968 | -1.2636842386 | -1.2182373305 |
| C | 4.9648755245 | -2.0382405327 | -1.3089212836 |
| C | 5.4277006428 | -2.4998327898 | 0.0710622724 |
| C | 5.4546012678 | -1.317284822 | 1.0353784821 |
| N | 4.1694709594 | -0.6169818983 | 1.1158620283 |
| N | 3.7130444988 | -0.2572170158 | -0.1626815477 |
| C | 3.4476408037 | 1.0531780216 | -0.4366082639 |
| O | 3.2098756502 | 1.4376627868 | -1.5770376103 |
| C | 3.3984420183 | 2.020131178 | 0.7528188263 |
| N | 2.4083043946 | 3.0520450208 | 0.4623633374 |
| N | 2.7072736676 | 4.0139468397 | -0.5168688998 |
| C | 3.9513047836 | 4.700387986 | -0.1946673409 |
| C | 5.0984879362 | 3.7085431483 | -0.0186304274 |
| C | 4.7502502721 | 2.6851424618 | 1.0510039148 |
| C | 1.1082521153 | 2.8394347243 | 0.808972576 |
| O | 0.775042923 | 1.878298469 | 1.4917038808 |
| C | 0.0795156157 | 3.8690460393 | 0.3497893455 |
| C | 0.1919010125 | 5.1674336962 | 1.1525167876 |
| N | -1.2173103312 | 3.2407864869 | 0.5237688411 |
| C | -2.2661279618 | 3.5864810926 | -0.2235731027 |
| O | -2.225453171 | 4.5300759591 | -1.0215163139 |
| C | -4.7935262713 | 3.6444986119 | -0.3549577054 |
| C | -3.5742926694 | 2.7849276137 | 0.0290545323 |
| N | -3.5870026225 | 1.4857848098 | -0.670288746 |
| N | -4.5698030475 | 1.1013300954 | -1.5691200717 |
| C | -5.6944811636 | 1.6929566477 | -1.482345595 |
| C | -6.0372211621 | 2.7731637148 | -0.4897249213 |
| C | -2.7851238766 | 0.4666285751 | -0.2478702897 |

| | | | |
|---|---|---|---|
| O | -2.0461661491 | 0.5787057436 | 0.723494668 |
| C | -2.8885847504 | -0.8336333656 | -1.043185286 |
| O | -1.9791032995 | -1.7786199492 | -0.5129334134 |
| O | -7.1360136994 | 3.5318194107 | -0.9103395753 |
| Cl | 6.6090042209 | 4.5861255789 | 0.4261017716 |
| C | 0.0271156293 | -3.892183773 | -0.2484051562 |
| C | -0.1143799223 | -2.1809433155 | 1.5826876199 |
| O | 0.2948073962 | -0.9177788751 | 2.0301646115 |
| O | -4.7006348533 | 4.2619481018 | -1.6110237778 |
| H | -6.4563922442 | 1.3834544006 | -2.1933885897 |
| H | 1.7031405291 | -1.0400739587 | 0.3770660995 |
| H | 3.4750744756 | -0.7101686154 | -2.1441959096 |
| H | 5.7233478186 | -1.3819938152 | -1.7508830271 |
| H | 4.8150410328 | -2.8820978272 | -1.9855467011 |
| H | 6.4210548615 | -2.9564051162 | 0.0083378414 |
| H | 6.2083085653 | -0.5869487107 | 0.7189967137 |
| H | 5.7057958125 | -1.6279096455 | 2.0537400699 |
| H | 3.4738024686 | -1.2335124488 | 1.534629268 |
| H | 3.0599388343 | 1.484053988 | 1.6369155648 |
| H | 2.8128693751 | 3.4968676256 | -1.3915986152 |
| H | 3.8112374224 | 5.2720777372 | 0.7282427685 |
| H | 4.1641988472 | 5.4036649942 | -1.0032357679 |
| H | 5.311306713 | 3.2173843895 | -0.9712171495 |
| H | 5.5277737127 | 1.9229654372 | 1.1386201829 |
| H | 4.6749291083 | 3.194239326 | 2.0174791088 |
| H | 0.2204118322 | 4.0978078941 | -0.7082331033 |
| H | 1.1604834608 | 5.6381224891 | 0.9743857784 |
| H | -0.5932570331 | 5.8553105626 | 0.8318347908 |
| H | 0.0774522823 | 4.9707386163 | 2.2219935518 |
| H | -1.2380358162 | 2.3689603631 | 1.0487539952 |
| H | -4.9333856242 | 4.3871164038 | 0.4441430748 |
| H | -3.6314067823 | 2.5723710254 | 1.1029337854 |
| H | -6.3029034436 | 2.3128971792 | 0.4702992173 |
| H | -2.6955803654 | -0.6375593013 | -2.0992448615 |
| H | -3.8786976056 | -1.2760959456 | -0.9422167535 |
| H | -6.7776884503 | 4.135265457 | -1.5826160951 |
| H | -0.9917114859 | -4.1847874354 | 0.0176958849 |
| H | 0.2022772761 | -4.0915750967 | -1.3038422581 |
| H | 0.7305917383 | -4.4970442734 | 0.3292772413 |
| H | 0.4464380052 | -2.9166430141 | 2.1668150927 |
| H | -1.1842553608 | -2.355742583 | 1.7361626901 |
| H | -0.3245434472 | -0.2420744296 | 1.7078932984 |
| H | -3.7917838881 | 4.6378246647 | -1.6575119967 |
| H | 4.7478898258 | -3.2708800547 | 0.4566072799 |

**1b** conf_8

energy (M062X/6-31g(d,p)) = -2585.2769394 Hartree

| | | | |
|---|---|---|---|
| C | 0.3142584814 | -0.3970684448 | 0.9934452863 |
| O | -0.3911672715 | 0.0802804305 | 1.8473821261 |
| C | 0.6445380889 | 0.2437095719 | -0.3623663769 |
| N | 0.2476784846 | 1.6359905033 | -0.3161013574 |
| C | -1.0117595957 | 2.1229811753 | -0.3742539906 |

| | | | |
|---|---|---|---|
| O | -2.0043884465 | 1.4996728114 | -0.7378456584 |
| C | -1.1641761091 | 3.6106811167 | -0.011025445 |
| C | -0.7916570685 | 4.581329993 | -1.1514811321 |
| C | 0.7156691896 | 4.817930336 | -1.2844237649 |
| C | 1.3487752133 | 5.116064272 | 0.0740021694 |
| N | 0.9678822057 | 4.0308913611 | 0.972572049 |
| N | -0.4189561149 | 4.007615958 | 1.181795123 |
| C | -1.0590906387 | 4.5193486922 | 2.2649213977 |
| O | -2.2799037679 | 4.4225323715 | 2.4122937151 |
| C | -0.2122895734 | 5.1599007412 | 3.3662328326 |
| N | -0.1468237321 | 4.2355002602 | 4.5005657725 |
| N | -1.2788924546 | 4.0827794582 | 5.3110313934 |
| C | -1.7199873975 | 5.3678406865 | 5.8476205538 |
| C | -2.0043694913 | 6.3529353366 | 4.7213454665 |
| C | -0.7829999637 | 6.5109967454 | 3.8303137354 |
| C | 0.8852869159 | 3.3638035786 | 4.6125636583 |
| O | 1.798705163 | 3.3288196976 | 3.7859234514 |
| C | 0.9067483837 | 2.462122188 | 5.8403583668 |
| C | 1.3775861442 | 3.2451291629 | 7.070603537 |
| N | 1.7952018674 | 1.3566118954 | 5.5358886505 |
| C | 1.7067511259 | 0.1839679381 | 6.169587409 |
| O | 0.8966200189 | -0.0116670898 | 7.0856358394 |
| C | 3.2081607541 | -1.8530334408 | 6.70388261 |
| C | 2.6324682926 | -0.9148887611 | 5.6321435627 |
| N | 1.8775108796 | -1.7092008657 | 4.6583735512 |
| N | 1.0677382556 | -2.7514524738 | 5.0229222114 |
| C | 1.175389683 | -3.229980986 | 6.2022763795 |
| C | 2.1459519564 | -2.8047021946 | 7.2717051112 |
| C | 1.8291403233 | -1.317569234 | 3.3540605631 |
| O | 2.4903815688 | -0.363595556 | 2.9575229855 |
| C | 0.9190835924 | -2.1298372812 | 2.4414100162 |
| O | 0.9587875222 | -1.5727954901 | 1.1389543002 |
| O | 1.4855883171 | -2.2418655756 | 8.3874437496 |
| Cl | -2.4598717881 | 7.9599534075 | 5.4225479825 |
| C | 0.0084928721 | -0.5503619735 | -1.5058061958 |
| C | 2.1793317772 | 0.2392170143 | -0.5393896338 |
| O | 2.839876485 | 0.9653962899 | 0.4666692254 |
| O | 3.8188989523 | -1.1206978461 | 7.7305582713 |
| H | 0.486554994 | -4.0367443985 | 6.436303517 |
| H | 0.9242507651 | 2.257599753 | 0.1373932831 |
| H | -2.2176752756 | 3.7274809702 | 0.2345865964 |
| H | -1.2868563317 | 5.5338396731 | -0.9300509152 |
| H | -1.2127543649 | 4.2122623279 | -2.0914369719 |
| H | 0.8961375185 | 5.648508383 | -1.9730799838 |
| H | 1.0196028024 | 6.0953953277 | 0.4544514895 |
| H | 2.4390895155 | 5.1214387425 | 0.0056295894 |
| H | 1.46450072 | 3.9528176476 | 1.8573738493 |
| H | 0.8111409104 | 5.3320927151 | 3.0422699162 |
| H | -2.0175746204 | 3.6875235609 | 4.7287257941 |
| H | -0.9369529164 | 5.7575697872 | 6.5044909736 |
| H | -2.6143930058 | 5.1840380246 | 6.4461985042 |
| H | -2.8672892629 | 6.0290719044 | 4.1419887645 |
| H | -1.0144805322 | 7.1266463274 | 2.9578708346 |
| H | 0.0033589194 | 7.0197021604 | 4.39683867 |

| | | | |
|---|---|---|---|
| H | -0.0912845453 | 2.0659300323 | 6.029931204 |
| H | 0.669940753 | 4.0403279418 | 7.31226255 |
| H | 1.4411726133 | 2.5664255984 | 7.9231727408 |
| H | 2.3623223593 | 3.6849695734 | 6.8934900597 |
| H | 2.4043589691 | 1.471104523 | 4.733638807 |
| H | 3.9716643394 | -2.4564164707 | 6.2016157377 |
| H | 3.458200413 | -0.4558186144 | 5.0882904403 |
| H | 2.646700383 | -3.7028316811 | 7.6453965978 |
| H | -0.0964902584 | -2.1413190415 | 2.837900404 |
| H | 1.2751244219 | -3.1554693642 | 2.3495511719 |
| H | 1.039194037 | -1.4333031265 | 8.0395468054 |
| H | -1.0741793176 | -0.5895787981 | -1.4037219938 |
| H | 0.248480472 | -0.065081456 | -2.4556900633 |
| H | 0.4128719604 | -1.565155558 | -1.5196584799 |
| H | 2.4025250527 | 0.7311420571 | -1.4900124574 |
| H | 2.5284050198 | -0.7970724234 | -0.5964483538 |
| H | 2.779958689 | 0.4543165907 | 1.2966483427 |
| H | 3.1740858072 | -1.129924342 | 8.4611080207 |
| H | 1.2001198952 | 3.9322258728 | -1.7084349427 |

Compound **1c**

**1c** conf_1

energy (M062X/6-31g(d,p)) = -2585.2800955 Hartree

| | | | |
|---|---|---|---|
| C | -0.9736551714 | -0.1871825248 | 0.8582411779 |
| O | -1.617317559 | 0.3636110383 | 1.7227210065 |
| C | -0.4671113015 | 0.4946295001 | -0.4083816394 |
| N | -1.0090526851 | 1.8438883812 | -0.3640771993 |
| C | -0.8720457025 | 2.7747192628 | -1.3290085183 |
| O | -0.4569180313 | 2.5500642469 | -2.466960697 |
| C | -1.2328129061 | 4.1955061689 | -0.8600066504 |
| C | -1.1507524392 | 5.2369565246 | -1.9744024549 |
| C | 0.2913978174 | 5.5842350069 | -2.3436945459 |
| C | 1.0991128361 | 5.9035811451 | -1.0905721289 |
| N | 1.0151468495 | 4.8482443947 | -0.0775595379 |
| N | -0.3228654137 | 4.5629192755 | 0.2316676932 |
| C | -0.6894163458 | 4.4015381369 | 1.5245258256 |
| O | -1.7997749036 | 3.956804067 | 1.8287879378 |
| C | 0.3376128539 | 4.7825405632 | 2.5959831579 |
| N | 0.0002127737 | 4.1130560389 | 3.8414011838 |
| N | -1.1158295224 | 4.5569794848 | 4.5653404327 |
| C | -1.0102608049 | 5.9809718924 | 4.8642912816 |
| C | -0.8053008525 | 6.7902117885 | 3.5871448013 |
| C | 0.4209788013 | 6.3000505897 | 2.8348652557 |
| C | 0.5725591413 | 2.9190918494 | 4.1447090188 |
| O | 1.4330238586 | 2.4145125268 | 3.427738356 |
| C | 0.1446678203 | 2.2444351085 | 5.4460628153 |
| C | 0.8195360261 | 2.9156912787 | 6.6464044982 |
| N | 0.5259466666 | 0.8517453597 | 5.3200951514 |
| C | -0.0417691914 | -0.1199705139 | 6.0490185454 |
| O | -0.8499987015 | 0.0803623003 | 6.9535987968 |
| C | 0.3072773218 | -2.5346044555 | 6.8001249851 |
| C | 0.4080591558 | -1.5390329465 | 5.6510547371 |
| N | -0.3835747467 | -2.0230187227 | 4.5103124651 |
| N | -1.5034623575 | -2.8033336361 | 4.6329592369 |
| C | -1.8540534757 | -3.1930245857 | 5.7987903718 |
| C | -1.1512391586 | -2.8873016653 | 7.0938072895 |
| C | -0.02642253 | -1.6532487314 | 3.2418742707 |
| O | 0.961969072 | -0.9683364193 | 3.0279152227 |
| C | -0.9320360977 | -2.1427706851 | 2.1189071517 |
| O | -0.5893745139 | -1.4653246786 | 0.9146467981 |
| O | -1.235569012 | -3.9761360967 | 7.9814908357 |
| Cl | -0.62087898 | 8.5437545195 | 3.9953207973 |
| C | -0.9380095745 | -0.2882197743 | -1.6412127023 |
| C | 1.0911715903 | 0.5361592727 | -0.2901472825 |
| O | 1.6873726225 | 1.5759518682 | -1.0279016397 |
| O | 1.0325795954 | -3.7224093909 | 6.523133272 |
| H | -2.7400493453 | -3.8213739625 | 5.8360082671 |
| H | -1.392323943 | 2.13034472 | 0.5329761904 |
| H | -2.2350287519 | 4.1761951139 | -0.426279363 |
| H | -1.6683416777 | 6.1362081895 | -1.6231236193 |
| H | -1.695389635 | 4.8637035714 | -2.844888231 |

| | | | |
|---|---|---|---|
| H | 0.3063063529 | 6.4414978817 | -3.0242179223 |
| H | 0.7419987801 | 6.8296901022 | -0.6270552676 |
| H | 2.1596727429 | 6.035268451 | -1.320098154 |
| H | 1.4403253957 | 3.9846580399 | -0.4236353596 |
| H | 1.3155183762 | 4.4220574384 | 2.2846464212 |
| H | -1.9273017992 | 4.3817704841 | 3.9719993666 |
| H | -0.1671900043 | 6.1371577452 | 5.5439677024 |
| H | -1.927439 | 6.2811272539 | 5.3751935763 |
| H | -1.6995203075 | 6.7350471411 | 2.962113978 |
| H | 0.5330921892 | 6.8183964842 | 1.8806882362 |
| H | 1.3139426838 | 6.5001191721 | 3.4350462795 |
| H | -0.9381414786 | 2.3085471168 | 5.5657029949 |
| H | 1.9067615535 | 2.9000434629 | 6.533316487 |
| H | 0.4858127726 | 3.9506044708 | 6.7448932673 |
| H | 0.5514476188 | 2.3746681044 | 7.5559714464 |
| H | 1.1176102735 | 0.6155511819 | 4.5283751025 |
| H | 0.7691546235 | -2.1049824775 | 7.6899515397 |
| H | 1.4462543831 | -1.5066582584 | 5.3137265558 |
| H | -1.6326626827 | -2.0258595168 | 7.5652349813 |
| H | -1.9808169821 | -1.9854119201 | 2.3643691908 |
| H | -0.7659652454 | -3.2025385896 | 1.9252511091 |
| H | -0.5260247894 | -4.581328575 | 7.7070127486 |
| H | -2.0298328324 | -0.2908686364 | -1.6916116992 |
| H | -0.5567788567 | 0.1706606621 | -2.5523965645 |
| H | -0.5851402895 | -1.3187705685 | -1.5816173644 |
| H | 1.4757087749 | -0.4473905064 | -0.5881158143 |
| H | 1.3739928848 | 0.7056008692 | 0.7518136125 |
| H | 1.2409050339 | 1.6443021623 | -1.8881838095 |
| H | 0.8109922745 | -4.0250035692 | 5.6296802507 |
| H | 0.749328083 | 4.7406699979 | -2.868725509 |

**1c** conf_2

energy (M062X/6-31g(d,p)) = -2585.2792363 Hartree

| | | | |
|---|---|---|---|
| C | -1.2800504997 | -0.0757870507 | 0.922703766 |
| O | -1.9178372922 | 0.5007533771 | 1.7753316588 |
| C | -0.7267640527 | 0.5720275337 | -0.3397604405 |
| N | -1.3315431562 | 1.891964536 | -0.4066511599 |
| C | -0.9229997948 | 2.8401179488 | -1.2824002075 |
| O | -0.2817115639 | 2.6057208422 | -2.3021743558 |
| C | -1.2846330717 | 4.2714648811 | -0.8527341862 |
| C | -1.1891039912 | 5.2988064411 | -1.9796175448 |
| C | 0.2541954555 | 5.6531859909 | -2.3393694672 |
| C | 1.0486752881 | 5.9800546039 | -1.0800214089 |
| N | 0.9625939948 | 4.9279852162 | -0.0662003395 |
| N | -0.3753878253 | 4.6442989744 | 0.2403283267 |
| C | -0.7135538077 | 4.4079149441 | 1.5279635899 |
| O | -1.8241412556 | 3.9726137065 | 1.8422881369 |
| C | 0.3568902336 | 4.6979376391 | 2.5861101621 |
| N | -0.0059887403 | 4.0328079978 | 3.8272268392 |
| N | -1.0691253885 | 4.5493117245 | 4.5824664852 |
| C | -0.8588342858 | 5.9583071134 | 4.8959060396 |
| C | -0.6108180694 | 6.7693056233 | 3.6279232433 |

| | | | |
|---|---|---|---|
| C | 0.5644248039 | 6.1982072403 | 2.852773886 |
| C | 0.4879683341 | 2.8065577689 | 4.1189893583 |
| O | 1.2745379827 | 2.2260011706 | 3.3672061968 |
| C | 0.0858050554 | 2.1854132478 | 5.452358833 |
| C | 0.8229640756 | 2.8609865348 | 6.6131756748 |
| N | 0.4009840139 | 0.7743229974 | 5.3691665035 |
| C | -0.3190478699 | -0.1451002655 | 6.0292039626 |
| O | -1.2013601206 | 0.1326961192 | 6.8373972554 |
| C | -0.2408917418 | -2.4636210115 | 6.9673668535 |
| C | 0.0422214222 | -1.6185775156 | 5.7138147995 |
| N | -0.7413476805 | -2.0654833315 | 4.5475336683 |
| N | -1.7197809688 | -3.0270715814 | 4.5914818565 |
| C | -1.6857887737 | -3.8621433709 | 5.5576098294 |
| C | -0.5956640173 | -3.8880597998 | 6.5932116323 |
| C | -0.4184812793 | -1.6090825602 | 3.3012297322 |
| O | 0.5540408413 | -0.8958885963 | 3.1003356018 |
| C | -1.336671223 | -2.0520519667 | 2.1696956542 |
| O | -0.965032937 | -1.3745222291 | 0.9780428505 |
| O | 0.5997492305 | -4.4521935297 | 6.0615666308 |
| Cl | -0.2877823076 | 8.4966006217 | 4.0598091131 |
| C | -1.0739797244 | -0.2869505228 | -1.5607892453 |
| C | 0.8277167422 | 0.6897511976 | -0.2069091953 |
| O | 1.2524266644 | 1.7973756971 | 0.5422918905 |
| O | 0.8609925779 | -2.4217405514 | 7.8378865146 |
| H | -2.4800279757 | -4.6024283054 | 5.5673842402 |
| H | -1.7560806809 | 2.2115129166 | 0.4603251705 |
| H | -2.2888859427 | 4.2712138522 | -0.4247057585 |
| H | -1.7148672312 | 6.2006373846 | -1.6465007944 |
| H | -1.7241210926 | 4.9151449991 | -2.8524164758 |
| H | 0.2685708042 | 6.5098435768 | -3.0209480055 |
| H | 0.6815002906 | 6.9050063569 | -0.6213561305 |
| H | 2.110337847 | 6.1184020542 | -1.3009231991 |
| H | 1.3897048775 | 4.0614234825 | -0.3969275528 |
| H | 1.2987427946 | 4.2696161303 | 2.2495509735 |
| H | -1.9044953322 | 4.4336079134 | 4.0080980977 |
| H | 0.0011914414 | 6.0454810843 | 5.5666155889 |
| H | -1.7461729137 | 6.3144497001 | 5.4230801185 |
| H | -1.5143702824 | 6.7928595631 | 3.014181227 |
| H | 0.7084063741 | 6.7205778875 | 1.9058872973 |
| H | 1.4767665906 | 6.3151451139 | 3.4459207242 |
| H | -0.9888382709 | 2.2969160036 | 5.6046703656 |
| H | 1.9051584519 | 2.7942872346 | 6.473442792 |
| H | 0.5373066976 | 3.9112954821 | 6.6950897639 |
| H | 0.5581786862 | 2.3551270563 | 7.5441786023 |
| H | 0.976714153 | 0.4805820486 | 4.5854611085 |
| H | -1.0852115656 | -2.0104815305 | 7.4901803208 |
| H | 1.0999698289 | -1.7038796567 | 5.4524697545 |
| H | -0.918930621 | -4.4325793369 | 7.4849502629 |
| H | -2.3794098566 | -1.8576656504 | 2.4218155252 |
| H | -1.2146886256 | -3.1137192772 | 1.9579717595 |
| H | 0.5181638382 | -5.4152898913 | 6.0681814815 |
| H | -0.5584460621 | -1.2479518907 | -1.5106809833 |
| H | -2.150029895 | -0.470662672 | -1.6112810323 |
| H | -0.7629602013 | 0.2424622892 | -2.4611088152 |

| | | | |
|---|---|---|---|
| H | 1.2253445119 | 0.8315221612 | -1.2126427891 |
| H | 1.2151380381 | -0.2545960174 | 0.1905567128 |
| H | 1.1368320324 | 1.6509702821 | 1.4979120483 |
| H | 1.4934904925 | -3.0681872818 | 7.4831320111 |
| H | 0.7211535216 | 4.8101391305 | -2.8553334045 |

**1c** conf_3

energy (M062X/6-31g(d,p)) = -2585.2783766 Hartree

| | | | |
|---|---|---|---|
| C | -1.2163971877 | -0.1777365887 | 0.8721320905 |
| O | -1.7001027713 | 0.471409155 | 1.7721590468 |
| C | -0.8554342362 | 0.3876210962 | -0.5007094876 |
| N | -1.0888813294 | 1.8259178181 | -0.3766848148 |
| C | -0.7613330498 | 2.770367494 | -1.2717367032 |
| O | -0.1929512518 | 2.556467307 | -2.3483158458 |
| C | -1.1287594757 | 4.1964270887 | -0.8277205388 |
| C | -1.0682556592 | 5.2263952328 | -1.9561597022 |
| C | 0.3552810951 | 5.673565165 | -2.2819684459 |
| C | 1.0803223922 | 6.0749404275 | -1.0039215411 |
| N | 1.0638146581 | 5.0091792851 | 0.0020369329 |
| N | -0.2470445603 | 4.5959574467 | 0.2766961302 |
| C | -0.6257848427 | 4.395973781 | 1.5619832644 |
| O | -1.7174188098 | 3.8953465255 | 1.8420837895 |
| C | 0.3687495016 | 4.8014597746 | 2.6550197254 |
| N | 0.0334681424 | 4.1077921289 | 3.8878187578 |
| N | -1.0961746917 | 4.5209642071 | 4.6097865484 |
| C | -1.0256024311 | 5.9421542213 | 4.9272291808 |
| C | -0.8357258064 | 6.7692731931 | 3.6599376456 |
| C | 0.4076227716 | 6.3177686341 | 2.9118458459 |
| C | 0.5862793218 | 2.8929573766 | 4.1464629512 |
| O | 1.4167027412 | 2.3889553927 | 3.395363359 |
| C | 0.1842945535 | 2.2025080421 | 5.4470231874 |
| C | 0.9008023254 | 2.8519874256 | 6.6353499876 |
| N | 0.5428192286 | 0.8065643634 | 5.2925405728 |
| C | -0.0059641722 | -0.1608516099 | 6.0421186294 |
| O | -0.7620791192 | 0.0498527978 | 6.9883798442 |
| C | 0.3369641223 | -2.5961655596 | 6.7418531746 |
| C | 0.378447435 | -1.5853667306 | 5.6018553561 |
| N | -0.5185268999 | -2.0290451581 | 4.525694174 |
| N | -1.6673717814 | -2.7448577622 | 4.7391297026 |
| C | -1.9348688594 | -3.1346960495 | 5.9267489779 |
| C | -1.1037805755 | -2.8953929497 | 7.1582454875 |
| C | -0.2516512768 | -1.6666821375 | 3.2321628287 |
| O | 0.751782723 | -1.0390663256 | 2.9333928791 |
| C | -1.2894984105 | -2.089408446 | 2.1993259949 |
| O | -0.9805506553 | -1.4899979424 | 0.9473142734 |
| O | -1.1558059723 | -4.0049348694 | 8.0229112444 |
| Cl | -0.6998160503 | 8.5229754794 | 4.0844914772 |
| C | -1.798282083 | -0.2328854934 | -1.5423349547 |
| C | 0.6275625357 | 0.0483625914 | -0.8245223239 |
| O | 0.9363102634 | 0.1153306203 | -2.1888392989 |
| O | 0.9836579297 | -3.8066288752 | 6.380317663 |
| H | -2.8489796869 | -3.7126329173 | 6.0347873915 |

| | | | |
|---|---|---|---|
| H | -1.5419071199 | 2.1200807226 | 0.4866432599 |
| H | -2.1353752617 | 4.1688724309 | -0.4061017571 |
| H | -1.6561796558 | 6.0936495426 | -1.6362586917 |
| H | -1.5587825588 | 4.8086337018 | -2.8386335133 |
| H | 0.3298083292 | 6.516868793 | -2.9791579787 |
| H | 0.6138307559 | 6.9579378022 | -0.5541579413 |
| H | 2.1305385844 | 6.311675079 | -1.1920306549 |
| H | 1.581331174 | 4.2035617323 | -0.3497676565 |
| H | 1.3622038634 | 4.4736526077 | 2.3562494793 |
| H | -1.9016029588 | 4.3339224645 | 4.011818633 |
| H | -0.1889592544 | 6.1100424881 | 5.6119968811 |
| H | -1.9518878618 | 6.2133521581 | 5.4378584191 |
| H | -1.7247534016 | 6.6955151541 | 3.0292761368 |
| H | 0.514715017 | 6.8488470954 | 1.9644588569 |
| H | 1.2900973811 | 6.5350098103 | 3.5215713469 |
| H | -0.8937422041 | 2.2790492461 | 5.5982428702 |
| H | 0.5810756437 | 3.8892740839 | 6.7541184407 |
| H | 0.6528914631 | 2.303499882 | 7.5459640192 |
| H | 1.9840849146 | 2.8266447473 | 6.4905851184 |
| H | 1.0911007264 | 0.5698073952 | 4.4709621435 |
| H | 0.894233082 | -2.204154429 | 7.5937355375 |
| H | 1.3860235609 | -1.5788190976 | 5.181092668 |
| H | -1.5031699964 | -2.0290928101 | 7.6926600037 |
| H | -2.2914715566 | -1.8106785165 | 2.523289369 |
| H | -1.2563435508 | -3.1659033073 | 2.033125378 |
| H | -0.4995775917 | -4.6300279523 | 7.6711879579 |
| H | -1.6335093696 | -1.3096841936 | -1.6103821051 |
| H | -2.8402966373 | -0.0454222952 | -1.272274284 |
| H | -1.5997428627 | 0.2112540651 | -2.5176864034 |
| H | 0.8168496825 | -0.97838765 | -0.5083403965 |
| H | 1.2624442332 | 0.7113859305 | -0.2184511125 |
| H | 0.6654224689 | 1.0125917513 | -2.4742803684 |
| H | 0.6725752601 | -4.0793451076 | 5.503787476 |
| H | 0.8992356069 | 4.8592620192 | -2.7703855892 |

**1c** conf_4

energy (M062X/6-31g(d,p)) = -2585.2750679 Hartree

| | | | |
|---|---|---|---|
| C | -0.4508198595 | -0.8942982083 | -0.0577437632 |
| O | -0.5233797395 | -2.0781044084 | -0.2864278003 |
| C | 0.3106578625 | 0.1101088236 | -0.9249011157 |
| N | -0.1518557995 | 1.4680584992 | -0.706803089 |
| C | -1.386565836 | 1.9105278044 | -1.0390424058 |
| O | -2.1723356343 | 1.2901012637 | -1.7461150163 |
| C | -1.8076704805 | 3.2740978592 | -0.4702652385 |
| C | -2.307562038 | 4.2171211774 | -1.5710664307 |
| C | -1.1478973688 | 4.885506878 | -2.304130049 |
| C | -0.2139050906 | 5.5457122183 | -1.2965698975 |
| N | 0.2759823226 | 4.6075241943 | -0.2799048828 |
| N | -0.7829408961 | 3.9254021636 | 0.3423739664 |
| C | -0.940868764 | 4.0214147029 | 1.6931268663 |
| O | -1.9070954546 | 3.5226978685 | 2.2655552979 |
| C | 0.1680945606 | 4.7288029732 | 2.4863521706 |

| | | | |
|---|---|---|---|
| N | 0.1340633281 | 4.2346573134 | 3.8582359918 |
| N | -0.9039078926 | 4.6638137605 | 4.7012769411 |
| C | -0.9405559249 | 6.118375592 | 4.7809116513 |
| C | -1.0767601067 | 6.726329531 | 3.388904673 |
| C | 0.0597823184 | 6.2624416426 | 2.493395273 |
| C | 0.8199591094 | 3.1017948446 | 4.1668938214 |
| O | 1.5927413984 | 2.5804633944 | 3.367994801 |
| C | 0.6328984367 | 2.4975006541 | 5.5571263606 |
| C | 1.6394088615 | 3.1033063672 | 6.5376285114 |
| N | 0.8116418961 | 1.0668158685 | 5.3876146598 |
| C | 0.1403039619 | 0.1656116091 | 6.1233029209 |
| O | -0.519977835 | 0.4489018621 | 7.1199116393 |
| C | -0.0585440806 | -2.3359546798 | 6.6397684209 |
| C | 0.23446571 | -1.2747178916 | 5.5821833524 |
| N | -0.6990462403 | -1.4262512376 | 4.4571522845 |
| N | -1.9789304145 | -1.8966298325 | 4.5911983259 |
| C | -2.3580147323 | -2.3086605709 | 5.738584059 |
| C | -1.5407569731 | -2.3466320613 | 7.0013474937 |
| C | -0.3143978543 | -1.0624208224 | 3.2050878795 |
| O | 0.8305970075 | -0.6746037335 | 2.9778802561 |
| C | -1.3719592652 | -1.1365032468 | 2.1134675005 |
| O | -0.9274273663 | -0.3059102349 | 1.0525363027 |
| O | -1.8660171479 | -3.4759385112 | 7.7746602381 |
| Cl | -1.074486395 | 8.5328098695 | 3.5015145177 |
| C | 0.2953391684 | -0.3183876406 | -2.3870771399 |
| C | 1.7791886985 | 0.0858596153 | -0.4056453166 |
| O | 1.9412768021 | 0.7753767791 | 0.802461912 |
| O | 0.2064555172 | -3.6294502598 | 6.1244024053 |
| H | -3.3776241538 | -2.6820287246 | 5.7878732156 |
| H | 0.3153507723 | 1.9121677186 | 0.077710215 |
| H | -2.6278196407 | 3.0483127604 | 0.2151112233 |
| H | -2.9354797179 | 4.9832423015 | -1.1034904169 |
| H | -2.9386523717 | 3.6427786313 | -2.2524323208 |
| H | -1.5262546546 | 5.6318059622 | -3.0094442147 |
| H | 0.6704587167 | 5.9683374559 | -1.7800449152 |
| H | -0.7310994408 | 6.3600335193 | -0.7775595887 |
| H | 0.8711298398 | 3.9146324764 | -0.7311434879 |
| H | 1.1302790398 | 4.4509807146 | 2.0610256077 |
| H | -1.7694719084 | 4.3139583972 | 4.2888270248 |
| H | -0.0194121332 | 6.4685862437 | 5.2557773416 |
| H | -1.7857971293 | 6.3950600525 | 5.4145094043 |
| H | -2.0481782118 | 6.4674584329 | 2.9611845464 |
| H | -0.064838773 | 6.629356259 | 1.4737862346 |
| H | 1.0024361523 | 6.6625671078 | 2.8799032426 |
| H | -0.3771234477 | 2.6781240851 | 5.9230343517 |
| H | 1.4592024267 | 4.1746972356 | 6.6576213754 |
| H | 1.5322298272 | 2.6208860338 | 7.5116116539 |
| H | 2.6615264909 | 2.954164922 | 6.1797827567 |
| H | 1.2853453055 | 0.7719675947 | 4.5389093163 |
| H | 0.5386440878 | -2.1316319588 | 7.5327949847 |
| H | 1.2339360086 | -1.445909893 | 5.17660842 |
| H | -1.7608127067 | -1.4549011725 | 7.5939226115 |
| H | -2.3262011949 | -0.7487934746 | 2.4638519977 |
| H | -1.506715208 | -2.1650277035 | 1.7713251492 |

H  -1.3754448376  -4.2079254487  7.364306925
H  0.7853170629  -1.2887019394  -2.4920256818
H  -0.7236428026  -0.3926569211  -2.7630215107
H  0.8390895413  0.4179747275  -2.9834858101
H  2.3948347037  0.6007492514  -1.1482583978
H  2.1125270725  -0.9575744449  -0.3470400198
H  1.5282190197  0.2688019194  1.5303834764
H  1.1426347662  -3.8322884061  6.2495958939
H  -0.5887702711  4.1451244944  -2.890668953

**1c** conf_5

energy (M062X/6-31g(d,p)) = -2585.2723471 Hartree

C  -0.4064621258  0.1714548173  0.8225671657
O  0.5826150094  0.8646746569  0.8042526927
C  -1.8022618435  0.5997147851  0.3430145999
N  -1.7670057839  2.0167821134  0.0089516848
C  -1.0880517685  2.5994927728  -1.000254578
O  -0.6385234118  2.0171527029  -1.9882280352
C  -0.9233554257  4.1159670109  -0.815510912
C  -0.3672532581  4.827905074  -2.0479995876
C  1.1397264689  4.6414843307  -2.2101290225
C  1.8482602005  4.9752097266  -0.9032130091
N  1.3200621775  4.2137470991  0.2292294551
N  -0.0668849757  4.3747556574  0.3518543777
C  -0.6201876521  4.5534475737  1.5739064717
O  -1.841467496  4.4312012411  1.7443164505
C  0.3002043843  4.9283238484  2.7329428952
N  -0.1120594075  4.198375902  3.9240240687
N  -1.3030934907  4.5628392237  4.5676731596
C  -1.2855377167  5.9807493949  4.9203995373
C  -1.0276532356  6.8459688167  3.6904715414
C  0.2729735859  6.4420257339  3.0147114652
C  0.5848287102  3.1050766163  4.332178888
O  1.6116779307  2.7413519243  3.7665380972
C  0.0542843047  2.3426429997  5.5431304415
C  0.5466522476  2.9811686711  6.8447570113
N  0.5250435147  0.9792799796  5.3948084929
C  -0.137896096  -0.066773052  5.9098819645
O  -1.1341995209  0.0359957815  6.6222739223
C  -0.0690196115  -2.5581629152  6.4218785475
C  0.4639605377  -1.4367659356  5.5385222051
N  0.2184988537  -1.7606096131  4.1236417322
N  -0.8280830741  -2.5351156347  3.69581599
C  -1.6182058033  -3.0354024186  4.5672460472
C  -1.516482606  -2.8904316122  6.0613199983
C  1.0969468753  -1.3088791938  3.1713495725
O  2.0876947704  -0.6616178393  3.4820529547
C  0.7963950688  -1.656291539  1.7173092876
O  -0.4372215627  -1.0904377277  1.2691097509
O  -1.938508307  -4.06805993  6.7066664744
Cl  -0.9536440891  8.5886387116  4.1773008042
C  -2.8315879188  0.429858501  1.4653914128

| | | | |
|---|---|---|---|
| C | -2.1987328193 | -0.3064163416 | -0.8488185998 |
| O | -1.147763777 | -0.5902376551 | -1.7305057844 |
| O | 0.7245011633 | -3.72961208 | 6.3158858434 |
| H | -2.4182753059 | -3.6550253635 | 4.1704168682 |
| H | -2.0548779038 | 2.6522904594 | 0.7499033005 |
| H | -1.9039187882 | 4.5258827302 | -0.5622018245 |
| H | -0.5941338897 | 5.8941880001 | -1.9414844534 |
| H | -0.9031245079 | 4.4661916338 | -2.9286864504 |
| H | 1.5107423167 | 5.2853513143 | -3.0136627104 |
| H | 1.7387172436 | 6.037715488 | -0.6610880108 |
| H | 2.9173266425 | 4.7544314937 | -0.956311053 |
| H | 1.5001098195 | 3.2167528454 | 0.1082238988 |
| H | 1.3159938329 | 4.6227899735 | 2.496903604 |
| H | -2.0537970594 | 4.3910698596 | 3.8988458028 |
| H | -0.5019592988 | 6.1473822175 | 5.6656098728 |
| H | -2.250270324 | 6.2209645305 | 5.3720651377 |
| H | -1.8682379747 | 6.7749499765 | 2.9985670472 |
| H | 0.422529848 | 6.9968846398 | 2.0850779872 |
| H | 1.1101270715 | 6.671726437 | 3.6814654162 |
| H | -1.0357736998 | 2.3361269358 | 5.5391759663 |
| H | 0.1463022915 | 3.9915259493 | 6.9540548168 |
| H | 0.2074172288 | 2.3797191114 | 7.6908701442 |
| H | 1.6387748544 | 3.0276463544 | 6.8600720966 |
| H | 1.3318430267 | 0.8302855625 | 4.7944410708 |
| H | -0.0100723032 | -2.2497311246 | 7.4658066935 |
| H | 1.5491125642 | -1.3866937409 | 5.6548714105 |
| H | -2.1604482748 | -2.0725924603 | 6.3963578912 |
| H | 0.6894944584 | -2.731581687 | 1.587635287 |
| H | 1.6237816939 | -1.2730972363 | 1.1226099537 |
| H | -1.1698926178 | -4.6624585705 | 6.6744849906 |
| H | -2.8321620294 | -0.5967310323 | 1.8307952816 |
| H | -2.6104147728 | 1.0936500887 | 2.3061256383 |
| H | -3.8275800215 | 0.6734536864 | 1.0859239276 |
| H | -3.0557641753 | 0.1677379559 | -1.3484545978 |
| H | -2.5336528582 | -1.2612480282 | -0.4387109744 |
| H | -0.8437452065 | 0.2846139081 | -2.0542801238 |
| H | 0.8631030116 | -3.9311778285 | 5.3781131081 |
| H | 1.3585420814 | 3.6065337419 | -2.4912524894 |

**1c** conf_6

energy (M062X/6-31g(d,p)) = -2585.2718609 Hartree

| | | | |
|---|---|---|---|
| C | -1.2477344743 | -0.1779012142 | 0.8586550574 |
| O | -1.8744023581 | 0.4137017825 | 1.7090740134 |
| C | -0.7690176526 | 0.4451555422 | -0.4518054871 |
| N | -1.1340583642 | 1.8573368025 | -0.3418525628 |
| C | -0.7696086226 | 2.8415566491 | -1.1779453834 |
| O | -0.077644759 | 2.6853323299 | -2.1914188886 |
| C | -1.2287735484 | 4.2373073413 | -0.7346035603 |
| C | -1.2845451573 | 5.2671955714 | -1.8646586848 |
| C | 0.0881895 | 5.8144623661 | -2.2551219444 |
| C | 0.8595273151 | 6.2378707915 | -1.0115045977 |
| N | 0.9588964915 | 5.1575535161 | -0.0254208129 |

| | | | |
|---|---|---|---|
| N | -0.3144580092 | 4.6882671017 | 0.3229804655 |
| C | -0.6036928312 | 4.4457986364 | 1.6251167253 |
| O | -1.6601147818 | 3.9097063292 | 1.9634158707 |
| C | 0.4564833596 | 4.8402381618 | 2.660659265 |
| N | 0.1716909179 | 4.1575613318 | 3.9122032158 |
| N | -0.8990952853 | 4.6147225523 | 4.6960722309 |
| C | -0.7571409794 | 6.0298019918 | 5.0113808265 |
| C | -0.6175648797 | 6.850947228 | 3.7343233705 |
| C | 0.5589508989 | 6.3543844104 | 2.9114000861 |
| C | 0.6440781016 | 2.8938792456 | 4.1023897167 |
| O | 1.3621789483 | 2.343086262 | 3.273679322 |
| C | 0.3233505944 | 2.2218463547 | 5.4319429601 |
| C | 1.3362046702 | 2.6872944748 | 6.4846062158 |
| N | 0.381179669 | 0.7898801189 | 5.2086887821 |
| C | -0.1623019569 | -0.0697976386 | 6.0713804803 |
| O | -0.6718877226 | 0.2894925345 | 7.138937092 |
| C | -0.6310470286 | -2.3155267709 | 6.9813041914 |
| C | -0.075437951 | -1.5890353634 | 5.7485262305 |
| N | -0.8242882359 | -2.0048735564 | 4.5437182237 |
| N | -1.7036036494 | -3.063046291 | 4.5275966891 |
| C | -1.7110628009 | -3.8897415787 | 5.4985825755 |
| C | -0.816811364 | -3.7879543723 | 6.7002611804 |
| C | -0.4333749448 | -1.6222727037 | 3.2883635626 |
| O | 0.5520803533 | -0.9297017152 | 3.0850754758 |
| C | -1.3040364754 | -2.126822834 | 2.1413428335 |
| O | -0.9245637674 | -1.4701638875 | 0.93761732 |
| O | 0.4135443985 | -4.4242621981 | 6.3992517912 |
| Cl | -0.3903468959 | 8.5986874923 | 4.1452163568 |
| C | -1.5167024995 | -0.225836882 | -1.613127008 |
| C | 0.7674111521 | 0.2354696517 | -0.5848695167 |
| O | 1.2401129958 | 0.3509388707 | -1.8980625425 |
| O | 0.2605937231 | -2.1712303272 | 8.0582219458 |
| H | -2.4217630666 | -4.7052704962 | 5.4089007008 |
| H | -1.6463414136 | 2.1077513135 | 0.5008137337 |
| H | -2.2096443825 | 4.1508947594 | -0.2651015531 |
| H | -1.9163549057 | 6.091766433 | -1.516687835 |
| H | -1.7855371216 | 4.8181132437 | -2.7262140054 |
| H | -0.0321960252 | 6.6682238479 | -2.929402684 |
| H | 0.3712949056 | 7.0858117005 | -0.5192035613 |
| H | 1.8821605126 | 6.5370315954 | -1.2549630723 |
| H | 1.4824237547 | 4.3806503339 | -0.4298606524 |
| H | 1.4224184824 | 4.4837623834 | 2.3069029413 |
| H | -1.7457548424 | 4.4570119377 | 4.1485337876 |
| H | 0.1265666468 | 6.1638982022 | 5.6421943629 |
| H | -1.6388519793 | 6.3330573999 | 5.5797361037 |
| H | -1.5468916955 | 6.8109493168 | 3.1610292491 |
| H | 0.6267100108 | 6.8793332132 | 1.9576593871 |
| H | 1.4841971228 | 6.5421061616 | 3.465027595 |
| H | -0.6798828033 | 2.4883202503 | 5.7635320327 |
| H | 1.2404671117 | 3.7621478404 | 6.6563372094 |
| H | 1.1462425808 | 2.1652650078 | 7.4238983464 |
| H | 2.3559135394 | 2.470548113 | 6.155380607 |
| H | 0.7799070627 | 0.448723637 | 4.3368538528 |
| H | -1.6088960746 | -1.8868731467 | 7.2259154808 |

| | | | |
|---|---|---|---|
| H | 0.9756804765 | -1.8681332564 | 5.6198890532 |
| H | -1.3001266681 | -4.2613252328 | 7.5638075007 |
| H | -2.3598959995 | -1.9644119291 | 2.3560794294 |
| H | -1.136093721 | -3.1877036617 | 1.9616836582 |
| H | 1.002465027 | -4.2195723228 | 7.1420763566 |
| H | -1.2549987402 | -1.2837643815 | -1.6723775732 |
| H | -2.59653329 | -0.13024735 | -1.4765728788 |
| H | -1.2344194149 | 0.2541611418 | -2.5500145952 |
| H | 1.0024108159 | -0.7767247222 | -0.2532170467 |
| H | 1.2603622103 | 0.9392751452 | 0.1019146233 |
| H | 0.928207186 | 1.2242297052 | -2.2130382984 |
| H | 0.1835280239 | -1.2389888163 | 8.3209646721 |
| H | 0.6560705803 | 5.0486745248 | -2.7910700112 |

**1c** conf_7

energy (M062X/6-31g(d,p)) = -2585.2711356 Hartree

| | | | |
|---|---|---|---|
| C | 0.0342491989 | -0.8170505014 | 0.0048185042 |
| O | 0.3083705877 | -1.940598694 | -0.344550249 |
| C | 0.714792726 | 0.4416449763 | -0.5351631956 |
| N | -0.0786925996 | 1.6268382799 | -0.2887058637 |
| C | -1.2867293128 | 1.8903976802 | -0.8254272724 |
| O | -1.861114572 | 1.1607108145 | -1.6263514427 |
| C | -1.9465297495 | 3.1977255125 | -0.3470803818 |
| C | -2.5557826172 | 3.9898414719 | -1.5062296913 |
| C | -1.4854150995 | 4.7462809925 | -2.2892227795 |
| C | -0.6230828212 | 5.5699722582 | -1.337619293 |
| N | -0.0276922574 | 4.7549941445 | -0.2717205188 |
| N | -1.0189656912 | 4.0299549642 | 0.4118284069 |
| C | -1.1002792106 | 4.1131819564 | 1.7672785542 |
| O | -2.0124373919 | 3.5852278304 | 2.3989954423 |
| C | 0.0612198227 | 4.8098587643 | 2.485487648 |
| N | 0.2377097955 | 4.1548916995 | 3.7792706958 |
| N | -0.6694360736 | 4.4542520782 | 4.8110804783 |
| C | -0.7442408162 | 5.8889110647 | 5.0524913663 |
| C | -1.1267069361 | 6.6259477541 | 3.7738256424 |
| C | -0.1210580401 | 6.3231777918 | 2.6768907784 |
| C | 0.9482027681 | 3.0006577601 | 3.8370475992 |
| O | 1.5022378624 | 2.5331056429 | 2.8373074174 |
| C | 1.1075611257 | 2.3121106814 | 5.1875224061 |
| C | 2.5185951335 | 2.5780844556 | 5.7189293841 |
| N | 0.8545859552 | 0.8954539813 | 5.0053252499 |
| C | 0.1619511443 | 0.1684769118 | 5.9029206733 |
| O | -0.2929220526 | 0.6221795484 | 6.9492279747 |
| C | -0.5422786744 | -2.1517796738 | 6.6871119741 |
| C | -0.0045164855 | -1.3194872995 | 5.5257626174 |
| N | -0.8703072954 | -1.4873973232 | 4.3506033232 |
| N | -2.2143166635 | -1.7386199565 | 4.4343125058 |
| C | -2.7341866608 | -1.89465615 | 5.5897731428 |
| C | -2.0211037703 | -1.8592407047 | 6.9145625303 |
| C | -0.3126052375 | -1.4048951419 | 3.1094069437 |
| O | 0.8881765609 | -1.1844226628 | 2.9713086692 |
| C | -1.2122556365 | -1.5472053587 | 1.8902666871 |

| | | | |
|---|---|---|---|
| O | -0.8202711297 | -0.5138705804 | 0.994667965 |
| O | -2.5899486301 | -2.7809147134 | 7.8125651072 |
| Cl | -1.1875896435 | 8.4069764547 | 4.0816231971 |
| C | 1.0862381594 | 0.2985477974 | -2.0071029163 |
| C | 2.0016670893 | 0.5756886949 | 0.3443719046 |
| O | 2.5339911051 | 1.8773815393 | 0.2899299463 |
| O | -0.4787383545 | -3.5336994459 | 6.377152102 |
| H | -3.802299421 | -2.0960993691 | 5.5986779282 |
| H | 0.2507572179 | 2.2288874007 | 0.4508692301 |
| H | -2.7312785079 | 2.9003253465 | 0.3526714892 |
| H | -3.2784362611 | 4.6994236553 | -1.0897157862 |
| H | -3.1023200883 | 3.294524271 | -2.1466043583 |
| H | -1.9526092808 | 5.3999909911 | -3.0321223927 |
| H | -1.2197380189 | 6.3536614691 | -0.8590642385 |
| H | 0.2064374146 | 6.0532269664 | -1.8598681303 |
| H | 0.6204497392 | 4.0847195692 | -0.6869298676 |
| H | 0.9717582414 | 4.6543184632 | 1.9116832701 |
| H | -1.5755001808 | 4.1057852087 | 4.4956648871 |
| H | 0.227361431 | 6.2380435603 | 5.4138876089 |
| H | -1.4857855551 | 6.050880418 | 5.8372605625 |
| H | -2.139470455 | 6.350643558 | 3.471603115 |
| H | -0.4179822256 | 6.7729626718 | 1.7275102915 |
| H | 0.8482833014 | 6.7458284735 | 2.9588972406 |
| H | 0.3689426956 | 2.6876870848 | 5.8912305822 |
| H | 2.6794921271 | 3.6499078076 | 5.8646605125 |
| H | 2.6452910995 | 2.0745571754 | 6.6799619734 |
| H | 3.2702187614 | 2.2027396245 | 5.019820008 |
| H | 1.2247730976 | 0.4325289732 | 4.1807489306 |
| H | 0.0243564504 | -1.9175292319 | 7.5915363212 |
| H | 0.9741648907 | -1.7092339937 | 5.2348521011 |
| H | -2.1166729896 | -0.8618206023 | 7.3523269501 |
| H | -2.2612615451 | -1.3986814061 | 2.1261606607 |
| H | -1.0629417563 | -2.5297853826 | 1.4358623414 |
| H | -2.2134415065 | -3.6399377786 | 7.5571343854 |
| H | 1.7227758001 | 1.1382449414 | -2.2967338142 |
| H | 1.6344245429 | -0.6325515698 | -2.1614364505 |
| H | 0.1943168867 | 0.2937981411 | -2.6339451475 |
| H | 2.7342814632 | -0.1386477652 | -0.0434115514 |
| H | 1.7640500513 | 0.2994791472 | 1.3746335485 |
| H | 2.3789207414 | 2.2781577122 | 1.1614498276 |
| H | 0.3914792335 | -3.870913962 | 6.6267231501 |
| H | -0.8491430066 | 4.0412431348 | -2.8394884119 |

**1c** conf_8

energy (M062X/6-31g(d,p)) = -2585.2702046 Hartree

| | | | |
|---|---|---|---|
| C | -0.8715227112 | -0.8926144843 | 0.2374793646 |
| O | -0.543240127 | -2.0542984469 | 0.2152872208 |
| C | -0.5164290262 | 0.0912869527 | -0.8790452197 |
| N | -0.986632156 | 1.4301743769 | -0.5073242329 |
| C | -0.6826536619 | 2.5822026694 | -1.1251607062 |
| O | 0.109480835 | 2.687393054 | -2.07062409 |
| C | -1.3568963824 | 3.8235973072 | -0.5331739523 |

| | | | |
|---|---|---|---|
| C | -1.7355908514 | 4.8760334958 | -1.5809039125 |
| C | -0.5460920542 | 5.7000364015 | -2.0730997379 |
| C | 0.2740906249 | 6.2016967895 | -0.8903138176 |
| N | 0.6760867835 | 5.1195551193 | 0.0155387503 |
| N | -0.4454070524 | 4.4057497335 | 0.4574809306 |
| C | -0.5970732592 | 4.1255035193 | 1.7764768198 |
| O | -1.506158104 | 3.4024652988 | 2.1831417606 |
| C | 0.4265773087 | 4.7390321329 | 2.7440371756 |
| N | 0.29117419 | 4.0915398962 | 4.0401587031 |
| N | -0.8252074919 | 4.4111243152 | 4.8282206376 |
| C | -0.9019236646 | 5.8446661541 | 5.0752947891 |
| C | -0.9134320558 | 6.6158383382 | 3.7601589406 |
| C | 0.3057730187 | 6.2615257315 | 2.9253428794 |
| C | 0.9894616386 | 2.9523012205 | 4.2925080718 |
| O | 1.8051088385 | 2.504913252 | 3.4911002939 |
| C | 0.7752218942 | 2.2622345156 | 5.6367700865 |
| C | 1.8133702505 | 2.7610676522 | 6.645023286 |
| N | 0.8941909518 | 0.8389169353 | 5.378533855 |
| C | 0.2446432343 | -0.0787767248 | 6.1125562164 |
| O | -0.3491517703 | 0.1722825688 | 7.1585674393 |
| C | 0.1409440429 | -2.6069020835 | 6.526154469 |
| C | 0.2671485099 | -1.4898024975 | 5.4976654494 |
| N | -0.8259540064 | -1.6008779233 | 4.5199552084 |
| N | -2.0703162519 | -2.0898838277 | 4.8210951661 |
| C | -2.2736540487 | -2.5695398138 | 5.9882562191 |
| C | -1.2722679542 | -2.6624524817 | 7.1080840927 |
| C | -0.651480948 | -1.1089966589 | 3.2545603849 |
| O | 0.4162514856 | -0.6492657763 | 2.8816187531 |
| C | -1.8749424662 | -1.1541383769 | 2.3473746183 |
| O | -1.6135366107 | -0.3450394565 | 1.2090199773 |
| O | -1.4613527458 | -3.839713782 | 7.8556074407 |
| Cl | -0.9416326471 | 8.3954968736 | 4.088667925 |
| C | -1.223602903 | -0.3882125763 | -2.1540083638 |
| C | 1.0305677529 | 0.0193941547 | -1.0515453159 |
| O | 1.4860009242 | 0.4076010806 | -2.315480087 |
| O | 0.4665829203 | -3.8661562825 | 5.9586344508 |
| H | -3.2721264073 | -2.9602481245 | 6.166060478 |
| H | -1.5933211367 | 1.4832331261 | 0.3005809314 |
| H | -2.2473185711 | 3.5233200236 | 0.0194896047 |
| H | -2.4666999853 | 5.5428764956 | -1.1104292926 |
| H | -2.2423411698 | 4.3824378091 | -2.4148743289 |
| H | -0.9058291459 | 6.5497756603 | -2.6620339959 |
| H | -0.3004534985 | 6.9247644006 | -0.3010453749 |
| H | 1.1924597918 | 6.6948709405 | -1.2189250907 |
| H | 1.2761995787 | 4.4672885193 | -0.4894128488 |
| H | 1.4234083336 | 4.5133327409 | 2.367281298 |
| H | -1.6446297267 | 4.0922629199 | 4.3102976367 |
| H | -0.0394257725 | 6.1437971445 | 5.6779858514 |
| H | -1.8105762135 | 6.0341950077 | 5.650525087 |
| H | -1.8383582736 | 6.4128176639 | 3.2148013396 |
| H | 0.2737357104 | 6.748484827 | 1.950832696 |
| H | 1.2048017694 | 6.6082169683 | 3.4443540287 |
| H | -0.2241472159 | 2.4640010711 | 6.0197920144 |
| H | 1.6807322966 | 3.8294348225 | 6.8353055554 |

| | | | |
|---|---|---|---|
| H | 1.6904806104 | 2.2221624952 | 7.5868683639 |
| H | 2.8252735217 | 2.5918724806 | 6.2680622084 |
| H | 1.2984061278 | 0.5721364213 | 4.4868623474 |
| H | 0.8644779385 | -2.4454677075 | 7.3264237475 |
| H | 1.1960627756 | -1.6361850667 | 4.9425417432 |
| H | -1.4110799588 | -1.8090324899 | 7.777460127 |
| H | -2.7442944751 | -0.7212610835 | 2.8372163156 |
| H | -2.101512573 | -2.1793493161 | 2.0504261873 |
| H | -1.0009338222 | -4.534067725 | 7.3545882062 |
| H | -0.8970882994 | -1.3994307151 | -2.4035419543 |
| H | -2.3072166143 | -0.3847540311 | -2.0136067144 |
| H | -0.9693302835 | 0.274869047 | -2.9808890011 |
| H | 1.3192505252 | -1.0242733833 | -0.9176924029 |
| H | 1.4869404098 | 0.6075014346 | -0.2419298161 |
| H | 1.1532685478 | 1.3212067815 | -2.4365568148 |
| H | 0.0019605704 | -3.9595620202 | 5.1130834972 |
| H | 0.0877003814 | 5.0918145151 | -2.7235935698 |

Compound **1d**

**1d** conf_1

energy (M062X/6-31g(d,p)) = -2585.2797614 Hartree

| | | | |
|---|---|---|---|
| C | -1.1728740067 | -0.1756281548 | 0.8141900302 |
| O | -1.66559501 | 0.4542785025 | 1.7229064603 |
| C | -0.7892020246 | 0.419441184 | -0.5396396893 |
| N | -1.0464218452 | 1.8517701118 | -0.3962733106 |
| C | -0.7081952906 | 2.8169397806 | -1.2649365084 |
| O | -0.1096323422 | 2.6306397742 | -2.330250259 |
| C | -1.1054099016 | 4.2292964542 | -0.8033774035 |
| C | -1.035309475 | 5.2814698658 | -1.9104111119 |
| C | 0.3878499915 | 5.7572708632 | -2.1947276179 |
| C | 1.0773342156 | 6.1445236705 | -0.8928248833 |
| N | 1.0563532369 | 5.0581078883 | 0.0907376069 |
| N | -0.2535164337 | 4.6190637497 | 0.3278497213 |
| C | -0.6560808284 | 4.3833973812 | 1.5994798532 |
| O | -1.7460947142 | 3.8611037239 | 1.8445873552 |
| C | 0.3092282802 | 4.7762629188 | 2.7228467145 |
| N | -0.042527293 | 4.0467532364 | 3.9302518083 |
| N | -1.1957131825 | 4.4226439085 | 4.63530483 |
| C | -1.1564440848 | 5.8368012424 | 4.9889856221 |
| C | -0.9496976032 | 6.6984687349 | 3.7475784434 |
| C | 0.3183953124 | 6.2859235465 | 3.0185906462 |
| C | 0.5314839301 | 2.8413659343 | 4.1803140122 |
| O | 1.3968723341 | 2.3704532817 | 3.4471529429 |
| C | 0.1027472642 | 2.1128332933 | 5.4520550034 |
| C | 0.7555773461 | 2.7506113188 | 6.6820549324 |
| N | 0.5111634067 | 0.7316586996 | 5.2779293981 |
| C | -0.0366939526 | -0.2736505338 | 5.9645921496 |
| O | -0.8648867411 | -0.0956401697 | 6.8676215267 |
| C | 0.4355256549 | -2.7406847313 | 6.6065046427 |
| C | 0.4148055864 | -1.6673623826 | 5.5117281053 |
| N | -0.4631569269 | -2.1164981114 | 4.4257088049 |
| N | -1.6493094335 | -2.7650378472 | 4.6501832604 |
| C | -1.8838605739 | -3.2335463641 | 5.8167737568 |
| C | -0.9774539999 | -3.1776119849 | 7.020653578 |
| C | -0.2089453742 | -1.7124480063 | 3.1411993053 |
| O | 0.7919662686 | -1.0755322638 | 2.8545613083 |
| C | -1.2493135551 | -2.1129312267 | 2.1029297184 |
| O | -0.9395425238 | -1.4897884604 | 0.8631386145 |
| O | -1.5501151745 | -2.3987194031 | 8.0425281941 |
| Cl | -0.8528744244 | 8.4425189413 | 4.2192560351 |
| C | -1.6947811923 | -0.1947907872 | -1.6170271545 |
| C | 0.707180317 | 0.107352791 | -0.8294244647 |
| O | 1.0507071622 | 0.2023648771 | -2.1836375233 |
| O | 1.1972039837 | -3.8441012836 | 6.1593729903 |
| H | -2.8524377554 | -3.7128530707 | 5.9309388581 |
| H | -1.520609934 | 2.1249753234 | 0.4626140007 |
| H | -2.1204469734 | 4.1800527597 | -0.4046295094 |
| H | -1.6442802947 | 6.1331536182 | -1.5881022877 |
| H | -1.4987733252 | 4.8730562468 | -2.8117051642 |

| | | | |
|---|---|---|---|
| H | 0.3644563756 | 6.6137373227 | -2.8757372684 |
| H | 0.5860990139 | 7.0102959849 | -0.4360374221 |
| H | 2.1273565168 | 6.402171677 | -1.0522958754 |
| H | 1.5939762463 | 4.2680748891 | -0.2663306621 |
| H | 1.3138974958 | 4.4706906714 | 2.4382012142 |
| H | -1.9831748176 | 4.237896052 | 4.0131990799 |
| H | -0.3398302687 | 6.0010194085 | 5.698326863 |
| H | -2.0993865208 | 6.0799466606 | 5.4829488579 |
| H | -1.8220204811 | 6.6268151242 | 3.0937669367 |
| H | 0.4390560777 | 6.8423631565 | 2.0875523338 |
| H | 1.1827145143 | 6.5008658017 | 3.6545178357 |
| H | -0.981930625 | 2.150849425 | 5.5628165873 |
| H | 0.4005034113 | 3.7744999648 | 6.813592118 |
| H | 0.4909802679 | 2.1730787964 | 7.5697878823 |
| H | 1.8435990899 | 2.760461901 | 6.5774750415 |
| H | 1.1138541382 | 0.5421776341 | 4.4820140642 |
| H | 0.9500640809 | -2.3492876236 | 7.4862941992 |
| H | 1.4180754251 | -1.6010705766 | 5.0884831284 |
| H | -0.8831004247 | -4.193636617 | 7.4167173296 |
| H | -2.2496454207 | -1.8383129065 | 2.4356709391 |
| H | -1.219205557 | -3.1861945824 | 1.9157963578 |
| H | -1.4664861918 | -1.4684841494 | 7.7345547723 |
| H | -2.7462855639 | -0.0289124222 | -1.3706658345 |
| H | -1.478677317 | 0.2717279373 | -2.5781357814 |
| H | -1.5112968611 | -1.2673155969 | -1.7020787004 |
| H | 0.9035950701 | -0.9216463627 | -0.5250482706 |
| H | 1.3155039894 | 0.7694180032 | -0.1957087004 |
| H | 0.7748502412 | 1.1007348634 | -2.460650857 |
| H | 0.7933412143 | -4.1902521709 | 5.3501365705 |
| H | 0.9559187807 | 4.9615588936 | -2.6863160812 |

**1d** conf_2

energy (M062X/6-31g(d,p)) = -2585.2770746 Hartree

| | | | |
|---|---|---|---|
| C | -0.6857423486 | -0.2324654886 | 0.4853784885 |
| O | -1.4851021846 | 0.3756467139 | 1.1550920008 |
| C | 0.1537550152 | 0.3677037687 | -0.6511564715 |
| N | -0.0795896723 | 1.8002989017 | -0.6493341716 |
| C | -1.138964327 | 2.4577625943 | -1.1779216 |
| O | -1.9112437705 | 2.0019610879 | -2.011432449 |
| C | -1.3690393269 | 3.8922227727 | -0.668802262 |
| C | -1.471363403 | 4.9058447733 | -1.8134858222 |
| C | -0.0961053554 | 5.3652898953 | -2.287386433 |
| C | 0.7189963404 | 5.8542532053 | -1.0952048423 |
| N | 0.8470547939 | 4.8356953967 | -0.0471510025 |
| N | -0.4092057467 | 4.3358228105 | 0.3386468723 |
| C | -0.7780760146 | 4.3856012834 | 1.6498482795 |
| O | -1.9022712578 | 4.0478148388 | 2.0143244914 |
| C | 0.2821868929 | 4.8258056113 | 2.6669854104 |
| N | -0.0207543179 | 4.1903323405 | 3.9443129466 |
| N | -1.1225136019 | 4.6500753558 | 4.682850378 |
| C | -1.0067999589 | 6.0810071563 | 4.9406314867 |
| C | -0.8480575316 | 6.8552113241 | 3.6353851494 |

| | | | |
|---|---|---|---|
| C | 0.3557936267 | 6.3492881439 | 2.8570346562 |
| C | 0.5294716565 | 2.9864450438 | 4.2437799436 |
| O | 1.3986720124 | 2.4779342853 | 3.540433271 |
| C | 0.0466508953 | 2.2817886579 | 5.5117911703 |
| C | 0.6756403951 | 2.8981095783 | 6.7638268657 |
| N | 0.4241247212 | 0.8900312281 | 5.3479717356 |
| C | -0.2342775057 | -0.1209390439 | 5.9180243121 |
| O | -1.1718748743 | 0.0436969655 | 6.7091326977 |
| C | 0.1713919901 | -2.5881627597 | 6.5846564535 |
| C | 0.2654751364 | -1.5098422071 | 5.4972307516 |
| N | -0.4683234487 | -1.9645663131 | 4.3093177978 |
| N | -1.6365990193 | -2.6815739017 | 4.3736833583 |
| C | -2.0013225314 | -3.1653329257 | 5.499448096 |
| C | -1.2707240816 | -3.0622258948 | 6.814688779 |
| C | -0.0640653885 | -1.5673571579 | 3.0690257624 |
| O | 0.9233178611 | -0.8543657102 | 2.9237219181 |
| C | -0.8904855327 | -2.0787965479 | 1.8944422982 |
| O | -0.3734077027 | -1.5238271038 | 0.6954176719 |
| O | -2.0009092364 | -2.2853378145 | 7.7314411168 |
| Cl | -0.6573400075 | 8.6199025277 | 3.9886227702 |
| C | -0.1214275949 | -0.3235898724 | -1.9851561511 |
| C | 1.6453452662 | 0.1863298311 | -0.2827496012 |
| O | 1.9843635528 | 0.8888479861 | 0.8862679641 |
| O | 1.0132123549 | -3.6703983255 | 6.2438616184 |
| H | -2.9499936993 | -3.6948758909 | 5.4820555588 |
| H | 0.360455456 | 2.2336741583 | 0.1544935584 |
| H | -2.3298085059 | 3.8372127758 | -0.1521720946 |
| H | -2.0379032829 | 5.7706556376 | -1.4516929189 |
| H | -2.0465878602 | 4.4488764603 | -2.6215309216 |
| H | -0.1994767703 | 6.1666768873 | -3.0254172863 |
| H | 0.2479789112 | 6.7356198887 | -0.6468207155 |
| H | 1.7361327869 | 6.1304902024 | -1.3841150751 |
| H | 1.3971432757 | 4.0592177336 | -0.4115213336 |
| H | 1.2561583915 | 4.4649105929 | 2.3445773922 |
| H | -1.9455202626 | 4.4645884575 | 4.1082524984 |
| H | -0.1406130622 | 6.2533629418 | 5.5863763932 |
| H | -1.9057505089 | 6.3952063137 | 5.4749506424 |
| H | -1.7616767688 | 6.7789232383 | 3.0418432801 |
| H | 0.4336320072 | 6.8400066209 | 1.8850383467 |
| H | 1.2663687542 | 6.5746581 | 3.4209152309 |
| H | -1.0398447049 | 2.3448001519 | 5.5865372276 |
| H | 0.3531813829 | 3.9345474712 | 6.8797892233 |
| H | 0.3584459132 | 2.3330276126 | 7.6429057919 |
| H | 1.7664739829 | 2.8674670908 | 6.7006069482 |
| H | 1.1073998695 | 0.7051505859 | 4.619036209 |
| H | 0.5583675282 | -2.1838345893 | 7.5219618223 |
| H | 1.3125142073 | -1.4353642449 | 5.1998649445 |
| H | -1.2020436862 | -4.0685938273 | 7.2392173618 |
| H | -1.9420348883 | -1.8263943027 | 2.026149442 |
| H | -0.7933932721 | -3.1603287541 | 1.8015376968 |
| H | -1.8845161013 | -1.3537164827 | 7.4372383466 |
| H | -1.1738774715 | -0.272641545 | -2.2559878456 |
| H | 0.4601643794 | 0.164333786 | -2.7712355552 |
| H | 0.1883002066 | -1.3690331158 | -1.9190757005 |

```
H   2.2392346566   0.6076270084   -1.0981825622
H   1.8680278396   -0.8822181779  -0.2027463832
H   1.6642652989   0.3750242917   1.6502659934
H   0.7087487187   -4.0513443321  5.4074139091
H   0.4351805091   4.541344244    -2.7810251306
```

**1d** conf_3

energy (M062X/6-31g(d,p)) = -2585.2696298 Hartree

```
C   -1.4661767766  -0.229703851   0.5902570394
O   -2.2814309619  0.2604167626   1.336117477
C   -0.8299557801  0.4735225098   -0.6039426262
N   -1.3080383097  1.8471500115   -0.5491833592
C   -0.8445692261  2.8377522394   -1.3417943368
O   -0.1834712497  2.6604177872   -2.362476422
C   -1.1774362921  4.2417752062   -0.8134697996
C   -1.0967622218  5.338734521    -1.8746744812
C   0.3385727894   5.7380248492   -2.2136299104
C   1.1201084523   6.015418905    -0.9354685045
N   1.0671024697   4.896408343    0.0091450468
N   -0.2591641064  4.5427389936   0.2950433002
C   -0.6037681528  4.2463931517   1.5713227108
O   -1.6928780082  3.7348031212   1.8418845627
C   0.4069953537   4.6093584151   2.6668545872
N   0.0308442168   3.9537395744   3.9073132002
N   -1.1219260905  4.3959925387   4.5698670622
C   -1.0489876194  5.8263636963   4.8532969606
C   -0.7701929867  6.6247801243   3.5836406197
C   0.4959045744   6.1282036346   2.9047121803
C   0.7576604153   2.9176670067   4.4054897135
O   1.7750107908   2.5065340335   3.855542725
C   0.2750113539   2.2892702034   5.7137664656
C   0.9624889779   2.9593939038   6.9028651423
N   0.5741053037   0.8718641332   5.6601301979
C   -0.4063015831  -0.0477621398  5.5676248648
O   -1.6021466775  0.1951987939   5.671304065
C   -0.3066350442  -2.2387426239  6.7226099127
C   0.060941882    -1.5070862202  5.4247056806
N   -0.6297215664  -2.1201439862  4.2819232631
N   -1.3827018354  -3.2659343143  4.3330674457
C   -1.2629645556  -4.0187255345  5.3553930728
C   -0.3470458303  -3.7452290047  6.5055267766
C   -0.4993860966  -1.5374358787  3.0602478307
O   0.2343950746   -0.5684982069  2.905173326
C   -1.308252193   -2.1498079626  1.9234957087
O   -0.9850749546  -1.4741412302  0.7191951378
O   -0.8318571639  -4.4163971945  7.6410300656
Cl  -0.6106590604  8.3819144632   3.9899468971
C   -1.2462311885  -0.2337250152  -1.8995000623
C   0.7080825451   0.4316228247   -0.4292789651
O   1.1378918504   1.1065607026   0.7255003114
O   0.5391837096   -1.8750343193  7.7860631239
H   -1.8751861875  -4.9156398774  5.3715580606
```

| | | | |
|---|---|---|---|
| H | -1.7599768657 | 2.1183375013 | 0.3197275127 |
| H | -2.1768284787 | 4.2225282217 | -0.3748259018 |
| H | -1.634726684 | 6.2109752746 | -1.4868488194 |
| H | -1.6280869078 | 5.0010194769 | -2.7683877253 |
| H | 0.3376722237 | 6.6280381469 | -2.8509616238 |
| H | 0.7205738502 | 6.8970522138 | -0.4223498797 |
| H | 2.1772929204 | 6.2017055173 | -1.1415180217 |
| H | 1.5228640608 | 4.0802533886 | -0.399623621 |
| H | 1.3882932312 | 4.231644027 | 2.3852398408 |
| H | -1.9025207077 | 4.1934855721 | 3.946062566 |
| H | -0.2507907688 | 6.0003374679 | 5.5812579796 |
| H | -1.9982973596 | 6.1239665628 | 5.3035576116 |
| H | -1.6264326905 | 6.5657074201 | 2.9074986714 |
| H | 0.6664684552 | 6.6455364789 | 1.9597843856 |
| H | 1.3541814833 | 6.3204924554 | 3.5561269856 |
| H | -0.8043812154 | 2.3850546487 | 5.8033592906 |
| H | 0.6977993871 | 4.0185763076 | 6.9529377803 |
| H | 0.6467898801 | 2.4780357951 | 7.831338352 |
| H | 2.0499784544 | 2.8779197494 | 6.8183661055 |
| H | 1.4969106984 | 0.6286283618 | 5.3256059359 |
| H | -1.3095723703 | -1.9246484056 | 7.0233717226 |
| H | 1.1411450508 | -1.5688741529 | 5.2528473529 |
| H | 0.6635548074 | -4.1012723152 | 6.2380284588 |
| H | -2.3751350995 | -2.0824001 | 2.1433191314 |
| H | -1.0432948594 | -3.1936398847 | 1.7660538264 |
| H | -0.3090946865 | -4.0931842302 | 8.3901016011 |
| H | -0.9045939 | -1.2708181202 | -1.8952679979 |
| H | -2.3333447288 | -0.220830601 | -2.0097450232 |
| H | -0.802422288 | 0.2878747865 | -2.7480191541 |
| H | 1.1491587242 | 0.9427473416 | -1.2859465379 |
| H | 1.0328976975 | -0.6149307732 | -0.4443362996 |
| H | 0.8967690954 | 0.5661255452 | 1.4997266708 |
| H | 1.4528777957 | -2.0958801503 | 7.5503159709 |
| H | 0.8238937538 | 4.9314233819 | -2.7699932142 |

**1d** conf_4

energy (M062X/6-31g(d,p)) = -2585.2671877 Hartree

| | | | |
|---|---|---|---|
| C | -1.4608911785 | -0.0701101501 | 0.8560946018 |
| O | -1.8270026992 | 0.60243575 | 1.794494903 |
| C | -1.084976198 | 0.4867763407 | -0.5163711307 |
| N | -1.1646216595 | 1.9393213471 | -0.3660692074 |
| C | -0.7491053467 | 2.8555508571 | -1.2550125536 |
| O | -0.219318697 | 2.5960001068 | -2.3408742205 |
| C | -0.9706510236 | 4.3095160442 | -0.8016440516 |
| C | -0.7234883201 | 5.3370428369 | -1.9063798114 |
| C | 0.75961977 | 5.6196783907 | -2.1348259717 |
| C | 1.4387295389 | 5.9343018843 | -0.8079049061 |
| N | 1.2387018904 | 4.8735029444 | 0.1829522159 |
| N | -0.1236556982 | 4.5989662214 | 0.362684024 |
| C | -0.6069459537 | 4.4252109431 | 1.6153445223 |
| O | -1.7585829851 | 4.0240063581 | 1.8057579362 |
| C | 0.3363548117 | 4.7241814229 | 2.786339465 |

| | | | |
|---|---|---|---|
| N | -0.165978761 | 4.0574960029 | 3.9757945089 |
| N | -1.3238663893 | 4.5684079885 | 4.5834756461 |
| C | -1.1475795569 | 5.9725368102 | 4.9356302456 |
| C | -0.7572419585 | 6.7907783872 | 3.7085598397 |
| C | 0.5004180302 | 6.2270958721 | 3.0681136693 |
| C | 0.2547874352 | 2.7904309185 | 4.2679430246 |
| O | 1.1553519867 | 2.2543841694 | 3.638391088 |
| C | -0.454965122 | 2.094010312 | 5.4382924613 |
| C | 0.0719910998 | 2.5921586314 | 6.7833268117 |
| N | -0.3890407434 | 0.6530686061 | 5.2655784127 |
| C | 0.6095180076 | -0.1721231443 | 5.6046533042 |
| O | 1.6305843513 | 0.1371897319 | 6.2238084503 |
| C | 0.0925959311 | -2.2553574262 | 6.7624440199 |
| C | 0.3829793728 | -1.670539462 | 5.3661936984 |
| N | -0.6726509721 | -1.9975169411 | 4.41176232 |
| N | -1.7436656608 | -2.8236940771 | 4.6807180477 |
| C | -1.6695250896 | -3.5728859309 | 5.7105306287 |
| C | -0.4909457077 | -3.6495600545 | 6.6297624466 |
| C | -0.4828479735 | -1.6603532166 | 3.0942817106 |
| O | 0.5322947605 | -1.0990792242 | 2.7245390839 |
| C | -1.6253408897 | -2.0061492329 | 2.1468703717 |
| O | -1.3754479258 | -1.4023888432 | 0.8843440495 |
| O | -0.9192084707 | -4.166102087 | 7.8653196704 |
| Cl | -0.4913411028 | 8.5182378076 | 4.1800938016 |
| C | -2.1095932058 | -0.0144017393 | -1.5448487061 |
| C | 0.34907756 | 0.0034351068 | -0.8822715109 |
| O | 0.6256303341 | 0.0452271262 | -2.2540240238 |
| O | 1.2730260715 | -2.324505847 | 7.5156967979 |
| H | -2.5291786876 | -4.2059267622 | 5.9108911522 |
| H | -1.5919568955 | 2.2693181622 | 0.4975574715 |
| H | -1.9992882672 | 4.3911545168 | -0.4444391265 |
| H | -1.2278094895 | 6.2631763351 | -1.6097132884 |
| H | -1.2001896035 | 4.9852426023 | -2.8240807988 |
| H | 0.8768380278 | 6.4609382792 | -2.8250752468 |
| H | 1.0435234198 | 6.8622342865 | -0.3806134466 |
| H | 2.5187937542 | 6.0539286372 | -0.9241343392 |
| H | 1.6933063776 | 4.0191287708 | -0.1395209516 |
| H | 1.312863118 | 4.3004689396 | 2.5615318324 |
| H | -2.0752888 | 4.4700105806 | 3.8997721278 |
| H | -0.3678776308 | 6.0490643295 | 5.6993518107 |
| H | -2.0877224937 | 6.3298400591 | 5.3611461228 |
| H | -1.5854101787 | 6.8142697642 | 2.9962155807 |
| H | 0.7440433966 | 6.753583347 | 2.1436067881 |
| H | 1.3401037429 | 6.3506447059 | 3.7589047511 |
| H | -1.5144753245 | 2.3467235713 | 5.3867067891 |
| H | -0.1877115164 | 3.6470548862 | 6.8908248502 |
| H | -0.4019083413 | 2.0348302087 | 7.5950473749 |
| H | 1.151473924 | 2.4734871641 | 6.8626215468 |
| H | -1.1273631271 | 0.2531989485 | 4.7048996722 |
| H | -0.6616768858 | -1.6333082968 | 7.2672569058 |
| H | 1.3325882851 | -2.0798316979 | 5.0116170936 |
| H | 0.2714625277 | -4.3002135354 | 6.1698134246 |
| H | -2.582092367 | -1.6792528885 | 2.5544833347 |
| H | -1.6675640675 | -3.078761704 | 1.9601308241 |

H  -0.1448612914  -4.1713695614  8.4460594085
H  -2.0549195493  -1.100293677   -1.6407065672
H  -3.1212525473  0.2684575765   -1.2437802416
H  -1.8924424402  0.4304834007   -2.5160222123
H  0.4443692913   -1.0376201004  -0.5719183209
H  1.0621477303   0.5981592739   -0.2928736333
H  0.4499162542   0.9702467141   -2.5246420887
H  1.7042204772   -1.4534547783  7.4154940781
H  1.2391575154   4.7492063998   -2.5939783618

**1d** conf_5

energy (M062X/6-31g(d,p)) = -2585.2663732 Hartree

C  -1.2735629437  -0.1473702175  0.8545871712
O  -1.8759586621  0.4797178855   1.6963876408
C  -0.7728183859  0.4379494349   -0.4656174548
N  -1.0704532608  1.866860542    -0.3704680901
C  -0.6561419497  2.8270434157   -1.2112521581
O  0.0425237298   2.6353839346   -2.2135327448
C  -1.0829189382  4.2425917568   -0.7941325421
C  -1.0257958252  5.2694895412   -1.9261983952
C  0.3892538233   5.7621722804   -2.2233699175
C  1.0806669403   6.1775229731   -0.9309519301
N  1.0762694009   5.1058398946   0.0694601825
N  -0.2303033598  4.6670564246   0.3244381018
C  -0.6219226947  4.4442987732   1.6022115559
O  -1.7099474648  3.9256179492   1.8610988538
C  0.3524595329   4.8489817609   2.7147400202
N  -0.0129102588  4.1563713406   3.9394936816
N  -1.1647978173  4.5695355629   4.6256611812
C  -1.1020860857  5.9901420461   4.9469202864
C  -0.8724084983  6.8189765056   3.6872189784
C  0.3904091166   6.3646875795   2.9742511263
C  0.5327480589   2.9412717987   4.2170007675
O  1.4005057229   2.4451972551   3.5041379653
C  0.0608131107   2.2410014729   5.4873784077
C  0.701430309    2.8801130787   6.7234057362
N  0.4250503126   0.8439082787   5.3551480987
C  -0.2532471693  -0.1191285845  5.9961715373
O  -1.1495892241  0.1005605399   6.8066315641
C  -0.0101249988  -2.4491768672  6.8903301336
C  0.1723113882   -1.5676017837  5.6527993388
N  -0.6405267405  -2.0569708966  4.5224506389
N  -1.6866877489  -2.9509856842  4.6553362049
C  -1.5752465902  -3.7999347059  5.6022400541
C  -0.3830065089  -3.8739517177  6.4975691876
C  -0.3835789601  -1.5976390997  3.2651781111
O  0.5682284639   -0.8701089714  3.0209575395
C  -1.3490687073  -2.0660654234  2.1814641809
O  -1.0012880216  -1.450946182   0.9487059709
O  -0.6834309324  -4.6545242211  7.6248361867
Cl  -0.7433499088  8.5716863982   4.1187000736
C  -1.5568716232  -0.2098219214  -1.6160142298

| | | | |
|---|---|---|---|
| C | 0.7509353778 | 0.1539185909 | -0.6034407762 |
| O | 1.2225576561 | 0.2327957092 | -1.9196585761 |
| O | 1.1079126239 | -2.4153014667 | 7.7469403612 |
| H | -2.3939555936 | -4.5012376072 | 5.7344971743 |
| H | -1.5982006146 | 2.146726661 | 0.4539253037 |
| H | -2.096247924 | 4.1927137778 | -0.3924784885 |
| H | -1.6476566918 | 6.1188487258 | -1.6228198288 |
| H | -1.4843411773 | 4.8353313948 | -2.8182644265 |
| H | 0.3490684105 | 6.6091230133 | -2.9154927309 |
| H | 0.5825567365 | 7.0446371639 | -0.4841831658 |
| H | 2.1268681524 | 6.444197332 | -1.1005831493 |
| H | 1.6103192274 | 4.3126801811 | -0.2862403036 |
| H | 1.3508375941 | 4.5167316749 | 2.437076829 |
| H | -1.9514008063 | 4.3828806528 | 4.0029700313 |
| H | -0.2860816335 | 6.1560700549 | 5.6566703091 |
| H | -2.0428932325 | 6.2623182131 | 5.4297256964 |
| H | -1.7429010991 | 6.7496515695 | 3.0305930937 |
| H | 0.5264921284 | 6.8965183274 | 2.0312170436 |
| H | 1.2559376048 | 6.577315946 | 3.6093952387 |
| H | -1.0241300527 | 2.3145432678 | 5.575024389 |
| H | 0.3785446734 | 3.9176753661 | 6.8301237105 |
| H | 0.3939290073 | 2.3260926538 | 7.6127282453 |
| H | 1.7917987003 | 2.8512034306 | 6.6495693794 |
| H | 1.0320038129 | 0.6023559964 | 4.5780696304 |
| H | -0.8357392933 | -2.0415001619 | 7.4774706905 |
| H | 1.2157735752 | -1.5879223275 | 5.3256003675 |
| H | 0.4481156684 | -4.3151248274 | 5.9168374766 |
| H | -2.3771293097 | -1.8320179251 | 2.4603859522 |
| H | -1.2628757943 | -3.1385843741 | 2.0120905389 |
| H | 0.0295239677 | -4.4904243997 | 8.2607048249 |
| H | -1.3488782779 | -1.2803449495 | -1.6618244058 |
| H | -2.630091953 | -0.0584272664 | -1.4777793302 |
| H | -1.2541639096 | 0.2429722535 | -2.5601675426 |
| H | 0.938555643 | -0.8645211483 | -0.2615753739 |
| H | 1.2805078629 | 0.8402990192 | 0.0734906356 |
| H | 0.958372532 | 1.1205640777 | -2.2382511286 |
| H | 1.8807149144 | -2.743092544 | 7.2628061018 |
| H | 0.9667348631 | 4.9685817974 | -2.7065268117 |

Compound **1e**

**1e** conf_1

energy (M062X/6-31g(d,p)) = -2585.2738195 Hartree

| | | | |
|---|---|---|---|
| C | -0.6139132845 | -0.5812197005 | 0.871350576 |
| O | 0.2413052532 | -0.2045391454 | 1.643005393 |
| C | -1.0369506058 | 0.1582763969 | -0.3918019385 |
| N | -0.727204637 | 1.5767823836 | -0.1700663197 |
| C | -0.7462070064 | 2.5043508469 | -1.1417251929 |
| O | -0.8375563559 | 2.2491857798 | -2.3488607672 |
| C | -0.7115242426 | 3.9798174929 | -0.72538771 |
| C | 0.1072129035 | 4.8241653582 | -1.7078758401 |
| C | 1.6041129375 | 4.656221153 | -1.4630860951 |
| C | 1.9216477303 | 4.9312867566 | 0.0026250331 |
| N | 1.1153975236 | 4.1233077104 | 0.9223983026 |
| N | -0.2506940101 | 4.2141706713 | 0.6328227207 |
| C | -1.1165825915 | 4.6555725523 | 1.5932253322 |
| O | -2.3161729021 | 4.7655355535 | 1.3810502171 |
| C | -0.4884367215 | 5.1785897105 | 2.8913044227 |
| N | 0.079136848 | 4.1690454163 | 3.7864752104 |
| N | 0.7377434461 | 4.6635662194 | 4.9176669117 |
| C | -0.1653519115 | 5.4685748423 | 5.7331427261 |
| C | -0.882846163 | 6.5632364631 | 4.9521955645 |
| C | -1.4990590294 | 6.0180906111 | 3.6714085026 |
| C | -0.1219834122 | 2.8352034147 | 3.6649188549 |
| O | -0.8321017032 | 2.3643177176 | 2.7804039281 |
| C | 0.6377063903 | 1.9421576382 | 4.6515067106 |
| C | 2.117033553 | 1.864453498 | 4.2663232594 |
| N | 0.0634137171 | 0.6150142586 | 4.6686043698 |
| C | -0.6711436401 | 0.1682564102 | 5.6933347571 |
| O | -0.9650652058 | 0.8549193806 | 6.6799691872 |
| C | -0.341683734 | -1.8697588024 | 6.9926442863 |
| C | -1.0651757504 | -1.3118776025 | 5.7484273584 |
| N | -0.7488049466 | -2.0883332657 | 4.5530140244 |
| N | 0.0453499217 | -3.2132597283 | 4.5386617812 |
| C | 0.247842489 | -3.8099065293 | 5.6478262614 |
| C | -0.3379554586 | -3.3862038215 | 6.9567740994 |
| C | -1.3898340843 | -1.7780473412 | 3.3820683595 |
| O | -2.2628090511 | -0.9284535222 | 3.3452088349 |
| C | -0.9063910193 | -2.5126429381 | 2.1384717741 |
| O | -1.2575722793 | -1.7465094693 | 0.99184243 |
| O | 0.4323830365 | -3.9354431465 | 7.996502998 |
| Cl | 0.3064339622 | 7.8917375862 | 4.5518466006 |
| C | -2.5311441702 | -0.0204824044 | -0.6722096308 |
| C | -0.1760519419 | -0.4841853852 | -1.5325082959 |
| O | -0.7205790216 | -0.3510131298 | -2.8096648009 |
| O | -0.9810085032 | -1.4460378437 | 8.1646666104 |
| H | 0.8845592454 | -4.6893049486 | 5.6165653176 |
| H | -0.7279881108 | 1.8950611928 | 0.7994282869 |
| H | -1.7568812758 | 4.3024903948 | -0.744077793 |
| H | -0.1753169895 | 5.8725796826 | -1.5638292612 |
| H | -0.1654376739 | 4.5406619269 | -2.7254759436 |

| | | | |
|---|---|---|---|
| H | 2.1727941523 | 5.3368671235 | -2.1044456912 |
| H | 1.7317515101 | 5.9842989569 | 0.2387792112 |
| H | 2.9688488516 | 4.7225143895 | 0.236577763 |
| H | 1.3873741614 | 3.1439332307 | 0.8569381342 |
| H | 0.3544879752 | 5.8102488418 | 2.5883729609 |
| H | 1.5341692742 | 5.2184591278 | 4.6093838812 |
| H | 0.409709712 | 5.8849898033 | 6.5622025174 |
| H | -0.9252220604 | 4.7997168052 | 6.1514811891 |
| H | -1.6370006861 | 7.046001323 | 5.5739894285 |
| H | -2.3532166024 | 5.3893890335 | 3.943016644 |
| H | -1.8785958201 | 6.8309439738 | 3.0497700003 |
| H | 0.5394399647 | 2.347661849 | 5.6569649867 |
| H | 2.5709314166 | 2.8563970626 | 4.2833227891 |
| H | 2.6471542486 | 1.2259735844 | 4.9768571761 |
| H | 2.2350459403 | 1.442175631 | 3.2643615319 |
| H | 0.1689590197 | 0.0575824299 | 3.8296654057 |
| H | 0.7088528953 | -1.5431908269 | 6.97696027 |
| H | -2.1421675381 | -1.3524862598 | 5.9337358312 |
| H | -1.3824501319 | -3.7369957032 | 7.0080401627 |
| H | -1.4191168886 | -3.4679751347 | 2.0254119446 |
| H | 0.1682338046 | -2.6846533849 | 2.175723577 |
| H | 0.0672090047 | -3.5856885157 | 8.8221035856 |
| H | -2.7645725374 | -1.0647344361 | -0.8821301895 |
| H | -3.1210354826 | 0.3097199776 | 0.1859572546 |
| H | -2.8052741018 | 0.5752678268 | -1.5433791307 |
| H | -0.1114342869 | -1.5571306066 | -1.3335249679 |
| H | 0.8373741474 | -0.0647820646 | -1.4561325016 |
| H | -0.8122449921 | 0.6183688225 | -2.9299660629 |
| H | -1.0628224819 | -0.4755893959 | 8.0704588175 |
| H | 1.9159660078 | 3.6363062412 | -1.7226079327 |

**1e** conf_2

energy (M062X/6-31g(d,p)) = -2585.2737395 Hartree

| | | | |
|---|---|---|---|
| C | -0.9725468799 | 0.0995695968 | 0.7474666077 |
| O | -0.2316364822 | 0.7622627392 | 1.4335839605 |
| C | -2.0119706266 | 0.6704181004 | -0.2187236945 |
| N | -1.6641831959 | 2.0475529655 | -0.5373012977 |
| C | -0.4481351388 | 2.4060410433 | -1.032728649 |
| O | 0.3609365782 | 1.6119080483 | -1.4980537497 |
| C | -0.1627248036 | 3.904954505 | -0.9059364036 |
| C | 0.7319654035 | 4.47891808 | -2.0066370716 |
| C | 2.2108505296 | 4.14328543 | -1.8261912185 |
| C | 2.6415597647 | 4.4556582327 | -0.3982735941 |
| N | 1.7988413364 | 3.7867770126 | 0.5944383538 |
| N | 0.4480972263 | 4.1174132198 | 0.4152573744 |
| C | -0.3406468942 | 4.3576261048 | 1.4922262984 |
| O | -1.5716520268 | 4.4083501748 | 1.3898916595 |
| C | 0.3533528208 | 4.6146699313 | 2.8284803113 |
| N | -0.3753420932 | 3.942437697 | 3.8962181881 |
| N | -1.6169221173 | 4.4521045299 | 4.3015934241 |
| C | -1.5032257541 | 5.8595248685 | 4.6765749933 |
| C | -0.9026229714 | 6.6804100449 | 3.5398954506 |

| | | | |
|---|---|---|---|
| C | 0.4512963517 | 6.1205443095 | 3.1352555111 |
| C | 0.0868729461 | 2.7690009076 | 4.3990549731 |
| O | 1.1340603041 | 2.2599400259 | 4.0088912841 |
| C | -0.719416183 | 2.0962126944 | 5.5074246371 |
| C | -0.2387777134 | 2.5947483012 | 6.872791214 |
| N | -0.4985747863 | 0.6722977529 | 5.3275006946 |
| C | -1.256839555 | -0.2675766712 | 5.895758998 |
| O | -2.1326916648 | -0.0450485068 | 6.7378752843 |
| C | -0.0504734388 | -2.21887773 | 6.7541780796 |
| C | -0.9216305701 | -1.7261837251 | 5.5867601367 |
| N | -0.2678392783 | -1.9331249549 | 4.2980764452 |
| N | 0.8556577608 | -2.7037266493 | 4.110463167 |
| C | 1.251581426 | -3.4349864774 | 5.0781053746 |
| C | 0.5681854264 | -3.5597861192 | 6.4058190288 |
| C | -0.9548077569 | -1.5620989232 | 3.1681128243 |
| O | -2.0497274473 | -1.0334880067 | 3.2465866889 |
| C | -0.2702295557 | -1.8411100682 | 1.835875997 |
| O | -1.0304018614 | -1.2407122569 | 0.7954103963 |
| O | 1.5199387113 | -3.9731970323 | 7.3556784837 |
| Cl | -0.7272547466 | 8.4059047857 | 4.0616581543 |
| C | -3.3578291733 | 0.6845198838 | 0.5159851816 |
| C | -2.1310894051 | -0.1613187756 | -1.5139935329 |
| O | -3.0933207903 | 0.3875093256 | -2.3851330636 |
| O | -0.8325927504 | -2.3665645243 | 7.9108465939 |
| H | 2.1497011701 | -4.020479952 | 4.9035107611 |
| H | -2.1309420332 | 2.7656616844 | 0.007958055 |
| H | -1.1100531086 | 4.4457735515 | -0.8912451971 |
| H | 0.6046517551 | 5.5670995942 | -1.9910838614 |
| H | 0.3645214557 | 4.126693923 | -2.9745520892 |
| H | 2.8115756941 | 4.7212023899 | -2.5356326914 |
| H | 2.5886697791 | 5.5313415355 | -0.1993865815 |
| H | 3.66776496 | 4.1311479325 | -0.2074677397 |
| H | 1.8802367682 | 2.775231959 | 0.4891152563 |
| H | 1.3521462146 | 4.188215679 | 2.7983041753 |
| H | -2.2377710864 | 4.365623698 | 3.4969254022 |
| H | -0.8727558841 | 5.9357395526 | 5.5674418616 |
| H | -2.504247873 | 6.2149797793 | 4.929663966 |
| H | -1.5867981352 | 6.7027745912 | 2.6905584788 |
| H | 0.8539228201 | 6.6506670424 | 2.2684623483 |
| H | 1.1550987275 | 6.2479464857 | 3.9639033245 |
| H | -1.7826661664 | 2.3086818775 | 5.3957186316 |
| H | -0.4460797562 | 3.6618148598 | 6.9845105814 |
| H | -0.7644879628 | 2.0527608985 | 7.6606401651 |
| H | 0.8362519546 | 2.4292596875 | 6.9811053895 |
| H | 0.2387225676 | 0.4221052584 | 4.6791060846 |
| H | 0.7735883965 | -1.5095303737 | 6.9213202947 |
| H | -1.8701740751 | -2.270315062 | 5.6099012953 |
| H | -0.2448295958 | -4.2988915728 | 6.3138231484 |
| H | -0.260125192 | -2.9100181423 | 1.6234458366 |
| H | 0.7547715294 | -1.4700785491 | 1.839281861 |
| H | 1.0534399654 | -4.0558080135 | 8.1994967469 |
| H | -4.1269457994 | 1.0600895923 | -0.1616085269 |
| H | -3.6210386015 | -0.3252396217 | 0.832739853 |
| H | -3.3115814464 | 1.3206463011 | 1.4037525194 |

| | | | |
|---|---|---|---|
| H | -2.470491933 | -1.1664756745 | -1.2613576539 |
| H | -1.1494132883 | -0.231802848 | -1.9921754255 |
| H | -2.813169687 | 1.2947465871 | -2.5746490335 |
| H | -1.3933814128 | -1.5723816394 | 7.9789733071 |
| H | 2.3807983543 | 3.0830570977 | -2.0342640384 |

**1e** conf_3

energy (M062X/6-31g(d,p)) = -2585.2691808 Hartree

| | | | |
|---|---|---|---|
| C | -0.6398906181 | -0.3692345896 | 0.7376298383 |
| O | 0.1096663038 | 0.2139749883 | 1.4883802742 |
| C | -1.3151538085 | 0.2808141826 | -0.4679016023 |
| N | -0.9349496612 | 1.6862464072 | -0.3733933193 |
| C | -1.3257620045 | 2.6737731089 | -1.2057102102 |
| O | -1.9229826394 | 2.4955651536 | -2.2623377305 |
| C | -1.0178962137 | 4.1058969943 | -0.7294817646 |
| C | -0.5480766377 | 5.0020015729 | -1.8785795528 |
| C | 0.927837879 | 4.7795194309 | -2.1947764494 |
| C | 1.7524086385 | 4.9151364022 | -0.9201303081 |
| N | 1.2969359234 | 4.0139298801 | 0.1434930147 |
| N | -0.0784122897 | 4.158142199 | 0.3894618119 |
| C | -0.5089534914 | 4.509661221 | 1.6359122795 |
| O | -1.6951725629 | 4.7447058029 | 1.8621918836 |
| C | 0.5344843976 | 4.551572737 | 2.7562194964 |
| N | -0.0519634152 | 3.9628564306 | 3.9542808475 |
| N | -1.043142953 | 4.6742016108 | 4.6460484584 |
| C | -0.5551475068 | 6.0006455024 | 5.0177396279 |
| C | -0.0662109575 | 6.7663137719 | 3.7915744133 |
| C | 1.0125549642 | 5.9810217568 | 3.0624090554 |
| C | 0.2774918721 | 2.699931985 | 4.3303234384 |
| O | 1.1371416339 | 2.0479680153 | 3.7451256897 |
| C | -0.4537030124 | 2.104308641 | 5.5303325177 |
| C | 0.2542476426 | 2.4872044587 | 6.8323805196 |
| N | -0.4587470812 | 0.6670168914 | 5.3130837194 |
| C | -1.3108190622 | -0.1459859851 | 5.9381227478 |
| O | -2.1179331023 | 0.2305057446 | 6.7977366135 |
| C | -0.5109300175 | -2.2102149627 | 6.9604964279 |
| C | -1.205462915 | -1.6517252287 | 5.7026853732 |
| N | -0.519267576 | -2.0551127293 | 4.4779514724 |
| N | 0.4917601581 | -2.9895767596 | 4.4266372319 |
| C | 0.7037341666 | -3.7065829034 | 5.459744831 |
| C | -0.08966801 | -3.6487152569 | 6.7273303733 |
| C | -1.0972020836 | -1.7220276609 | 3.2764572836 |
| O | -2.0995681237 | -1.0315714496 | 3.2288363463 |
| C | -0.4171943354 | -2.2799870738 | 2.0312248371 |
| O | -0.9647765258 | -1.6554846816 | 0.8742707358 |
| O | 0.7064815811 | -4.1463932888 | 7.7747589726 |
| Cl | 0.5817608854 | 8.3793744901 | 4.2989350298 |
| C | -2.8342923725 | 0.0951248996 | -0.4006950353 |
| C | -0.7460839015 | -0.3614738283 | -1.7491594648 |
| O | 0.6606502008 | -0.3141965673 | -1.7958449261 |
| O | -1.3853374007 | -2.1675434186 | 8.0562624757 |
| H | 1.5179309961 | -4.4223476904 | 5.3904037937 |

| | | | |
|---|---|---|---|
| H | -0.4977919227 | 1.9396179728 | 0.50421988 |
| H | -1.9658990082 | 4.4822503342 | -0.3354957958 |
| H | -0.707889789 | 6.0448099804 | -1.5848155 |
| H | -1.1791988546 | 4.7998982042 | -2.7460578797 |
| H | 1.2682635009 | 5.5028283427 | -2.9420828897 |
| H | 1.6935116283 | 5.9383106052 | -0.5339998952 |
| H | 2.8067510146 | 4.6840366209 | -1.0914796177 |
| H | 1.465423358 | 3.0489946484 | -0.1355075149 |
| H | 1.3890917252 | 3.9403705165 | 2.4795881798 |
| H | -1.8255997246 | 4.7698717881 | 3.9984092151 |
| H | 0.2610286226 | 5.8850737616 | 5.7371743011 |
| H | -1.3758358188 | 6.5296675519 | 5.5067218805 |
| H | -0.9051099521 | 6.9880034344 | 3.1299989866 |
| H | 1.3070437986 | 6.4837069447 | 2.1378959718 |
| H | 1.8984161722 | 5.9091103303 | 3.7013268864 |
| H | -1.4842544827 | 2.457696466 | 5.5630082775 |
| H | 0.2081627189 | 3.5676011312 | 6.9868930838 |
| H | -0.2407899649 | 1.9944239435 | 7.6712242639 |
| H | 1.3019112971 | 2.1763201319 | 6.8044098937 |
| H | 0.1923947683 | 0.3195819084 | 4.6182973989 |
| H | 0.4023483036 | -1.629868579 | 7.1594511647 |
| H | -2.2318202164 | -2.0299737013 | 5.6835546222 |
| H | -1.0001634742 | -4.2573797245 | 6.5996887569 |
| H | -0.6322310208 | -3.3432251838 | 1.9239643839 |
| H | 0.6618439495 | -2.1383173992 | 2.0755979573 |
| H | 0.1723804083 | -4.0894500208 | 8.5798602909 |
| H | -3.0921287562 | -0.9637088625 | -0.4614448926 |
| H | -3.2270045214 | 0.4969616038 | 0.5360587529 |
| H | -3.2978581658 | 0.6244647252 | -1.2345326058 |
| H | -1.2054632428 | 0.1346204423 | -2.6099639086 |
| H | -1.025401018 | -1.4165913172 | -1.7624647569 |
| H | 0.9167440211 | 0.6140487696 | -1.8823151185 |
| H | -1.8069208238 | -1.286257861 | 8.0362408482 |
| H | 1.0796585057 | 3.7802622865 | -2.6238556888 |

**1e** conf_4

energy (M062X/6-31g(d,p)) = -2585.2672102 Hartree

| | | | |
|---|---|---|---|
| C | -1.2243006796 | 0.3665950561 | 0.6391807066 |
| O | -0.2564821801 | 0.8553180855 | 1.1754183458 |
| C | -2.1870943308 | 1.0924864237 | -0.3026299094 |
| N | -1.5948293652 | 2.3558336349 | -0.7084483406 |
| C | -0.3245253491 | 2.4455491347 | -1.1965348085 |
| O | 0.2721884334 | 1.5133607116 | -1.7172468636 |
| C | 0.2912804488 | 3.83528101 | -0.9942995212 |
| C | 1.5891432513 | 4.0521397908 | -1.7704956881 |
| C | 2.7895480214 | 3.3676802235 | -1.1197808303 |
| C | 2.8572845254 | 3.7386933409 | 0.3565192016 |
| N | 1.6139794237 | 3.4476608933 | 1.0665554149 |
| N | 0.5139039899 | 4.0441689191 | 0.4452225406 |
| C | -0.4459371733 | 4.6147759536 | 1.2130729647 |
| O | -1.5331183113 | 4.9470014984 | 0.7320262675 |
| C | -0.0933744931 | 4.8905761145 | 2.6761144803 |

| | | | |
|---|---|---|---|
| N | -0.1806327958 | 3.6961712398 | 3.5077319539 |
| N | -1.5007518355 | 3.2306405751 | 3.6150451793 |
| C | -2.322078616 | 4.1406144067 | 4.4041546076 |
| C | -2.3959819557 | 5.4337143571 | 3.6006511331 |
| C | -1.0076066475 | 5.9734309093 | 3.2799744157 |
| C | 0.7940483302 | 3.4759561252 | 4.4477211162 |
| O | 1.8655437967 | 4.0652891199 | 4.411489259 |
| C | 0.5053011057 | 2.4734290832 | 5.577021159 |
| C | 1.7064429686 | 2.3605778997 | 6.5073968997 |
| N | 0.08018408 | 1.1605465512 | 5.0996281497 |
| C | -0.6870732417 | 0.3861775569 | 5.8949392327 |
| O | -1.2191478848 | 0.8021667721 | 6.9259086097 |
| C | 0.0486270173 | -1.8060857992 | 6.6643227028 |
| C | -0.817741232 | -1.1034960947 | 5.5977421098 |
| N | -0.4448204924 | -1.5072178704 | 4.2460413397 |
| N | 0.4084556252 | -2.5485455228 | 3.9505147263 |
| C | 0.7361477526 | -3.3441092047 | 4.8913705557 |
| C | 0.2342774452 | -3.2674904461 | 6.2986306395 |
| C | -1.201542813 | -1.0311551975 | 3.205376098 |
| O | -2.0817218513 | -0.2079748825 | 3.393415565 |
| C | -0.8756350326 | -1.6008212638 | 1.8318822445 |
| O | -1.6163697062 | -0.8980143571 | 0.8455794797 |
| O | 1.1607459598 | -3.9097642353 | 7.1382516591 |
| Cl | -3.3333687646 | 6.6708228024 | 4.5381503298 |
| C | -3.4651916376 | 1.4028261692 | 0.485887227 |
| C | -2.5250465956 | 0.235356463 | -1.5433655716 |
| O | -3.3859811898 | 0.9301553662 | -2.4148293101 |
| O | -0.5696014913 | -1.7392688365 | 7.9200813134 |
| H | 1.4215366212 | -4.14471587 | 4.62837296 |
| H | -1.932559434 | 3.1885059738 | -0.2303163537 |
| H | -0.4502321753 | 4.5808591314 | -1.2909932963 |
| H | 1.769001079 | 5.1316438607 | -1.8211545465 |
| H | 1.4446407526 | 3.6974137909 | -2.7942105542 |
| H | 3.7116557864 | 3.6689207863 | -1.6271601418 |
| H | 3.0617095092 | 4.8085869456 | 0.4761605972 |
| H | 3.6493550876 | 3.1903236986 | 0.8732434411 |
| H | 1.4366165882 | 2.4444309406 | 1.1045747672 |
| H | 0.9448287627 | 5.2147550251 | 2.7283422553 |
| H | -1.510935258 | 2.2631486081 | 3.917543485 |
| H | -1.9129087031 | 4.3453518201 | 5.4052391896 |
| H | -3.3135503613 | 3.6972693953 | 4.5160830847 |
| H | -2.9576455799 | 5.2666564113 | 2.6841027929 |
| H | -1.0798055778 | 6.8267925252 | 2.6024694457 |
| H | -0.5345954465 | 6.3168343331 | 4.2060787767 |
| H | -0.3447585798 | 2.8598807067 | 6.1485667508 |
| H | 1.9690145214 | 3.338336085 | 6.9138992681 |
| H | 1.4575169706 | 1.6922406129 | 7.3344768642 |
| H | 2.5748664905 | 1.9662192729 | 5.9753724122 |
| H | 0.6062447759 | 0.7159098997 | 4.3583760301 |
| H | 1.0469489262 | -1.3445162816 | 6.6865614159 |
| H | -1.8637796269 | -1.3650736635 | 5.7820321176 |
| H | -0.7511933664 | -3.7597837099 | 6.346023739 |
| H | -1.1949884503 | -2.6407691232 | 1.7642297888 |
| H | 0.1944845016 | -1.5458721806 | 1.6326621182 |

H  0.8110314738  -3.8458369662  8.0385198596
H  -3.9083916456  0.4793214711  0.8603448649
H  -3.2478251699  2.0544432493  1.3363267706
H  -4.1787065738  1.8954550446  -0.1776904472
H  -3.0527200004  -0.6650973897  -1.2263761271
H  -1.5964887553  -0.056846507  -2.0438455187
H  -2.9345105149  1.7551336515  -2.6470752948
H  -0.8485396202  -0.8129674479  8.0463154061
H  2.6965364833  2.281993423  -1.2204827055

**1e** conf_5

energy (M062X/6-31g(d,p)) = -2585.2670317 Hartree

C  -0.6582606882  -0.4446697287  0.5967334703
O  0.2444416547  0.0214625634  1.2571666596
C  -1.4242537074  0.330553027  -0.4730407375
N  -0.84420707  1.6680852348  -0.4119544807
C  -1.1608601471  2.7295156775  -1.1569453533
O  -1.9105971882  2.7197982005  -2.1436438271
C  -0.5420330568  4.0685167971  -0.739388305
C  0.5223461698  4.557401345  -1.739925999
C  1.8577944353  3.8299187859  -1.5654509875
C  2.2905417893  3.8264138425  -0.1008741545
N  1.1913696066  3.2680181938  0.6806726217
N  0.0448500432  4.0750286061  0.5937047335
C  -0.426440526  4.8907999849  1.5700735172
O  -1.4970491016  5.4929605565  1.4591653479
C  0.3801028458  4.9956836134  2.8665422839
N  -0.2712574339  4.1885524455  3.9020981705
N  -1.4504902912  4.6673546403  4.4853362083
C  -1.2633498762  6.0015681692  5.0490209128
C  -0.76422395  6.9712895899  3.986322236
C  0.513506628  6.4507596032  3.348617733
C  0.1490445153  2.9226916194  4.1560393176
O  1.0662316786  2.4030767644  3.5183180601
C  -0.49749809  2.1901777421  5.3211848304
C  0.2150944976  2.5909962527  6.618679706
N  -0.3935647804  0.7635939674  5.0650686185
C  -1.1480320606  -0.1042153598  5.7461867809
O  -1.9346576339  0.239730921  6.6375966734
C  -0.098288558  -2.0551257635  6.7680983593
C  -0.9477816989  -1.6063477932  5.5623842303
N  -0.3553687508  -2.0314895369  4.2966646758
N  0.6566554352  -2.9583667077  4.188291245
C  0.9993797452  -3.6096765774  5.2294693129
C  0.3580338161  -3.4893177975  6.5760121212
C  -1.0484059292  -1.748189393  3.1457376432
O  -2.0441986135  -1.0459815989  3.1700965075
C  -0.5218739348  -2.3738723224  1.8594930376
O  -1.1035859712  -1.6932537676  0.7506982101
O  1.2915025574  -3.8851300261  7.5510847366
Cl  -0.4553670466  8.5892204338  4.74039987
C  -2.9114739073  0.3625006967  -0.0952263557

| | | | |
|---|---|---|---|
| C | -1.2217364326 | -0.3450763858 | -1.8550547858 |
| O | -2.130607788 | 0.1019721612 | -2.8221703547 |
| O | -0.8503754207 | -1.9830873833 | 7.9498929869 |
| H | 1.8131649126 | -4.3186677523 | 5.1063048377 |
| H | -0.0689118271 | 1.7914656103 | 0.2429617481 |
| H | -1.3737844082 | 4.7731129613 | -0.7152031789 |
| H | 0.6634167784 | 5.6295835221 | -1.5657370317 |
| H | 0.1362685074 | 4.4378866718 | -2.7555121177 |
| H | 2.6235341518 | 4.3091733106 | -2.1822146611 |
| H | 2.5514882081 | 4.8432429503 | 0.2306979781 |
| H | 3.1594119167 | 3.181549603 | 0.0499032974 |
| H | 1.388236586 | 3.0249375077 | 1.6502269987 |
| H | 1.3863449981 | 4.6001914224 | 2.7472364751 |
| H | -2.1621293071 | 4.7003368181 | 3.7557931964 |
| H | -0.5434302085 | 5.934646952 | 5.8698729686 |
| H | -2.2235309252 | 6.323086938 | 5.4573224741 |
| H | -1.5317381479 | 7.1385591488 | 3.2325300716 |
| H | 0.8163625251 | 7.0833808236 | 2.5109199031 |
| H | 1.315943578 | 6.4759927546 | 4.092541953 |
| H | -1.5516308917 | 2.4546777886 | 5.3952800125 |
| H | -0.2124342374 | 2.0288255698 | 7.4502766317 |
| H | 1.2840493586 | 2.3730938943 | 6.5505314478 |
| H | 0.0825280656 | 3.6571185744 | 6.8158109905 |
| H | 0.2504925785 | 0.4611522428 | 4.3447826013 |
| H | 0.8029532076 | -1.4269293182 | 6.8306477977 |
| H | -1.9424532279 | -2.051459758 | 5.6618733722 |
| H | -0.5339687853 | -4.1368187326 | 6.5981616753 |
| H | -0.8554354971 | -3.4092791315 | 1.7829222203 |
| H | 0.5646097433 | -2.3416068032 | 1.8120581796 |
| H | 0.8493234021 | -3.8007637545 | 8.4078748248 |
| H | -3.0386814592 | 0.7513415457 | 0.9170224375 |
| H | -3.4465752276 | 1.0031896069 | -0.7959003244 |
| H | -3.3358698429 | -0.6414551813 | -0.144971283 |
| H | -1.3782166002 | -1.420529555 | -1.74023224 |
| H | -0.1765301538 | -0.1844260431 | -2.1591485532 |
| H | -2.1112854605 | 1.0836720303 | -2.784544324 |
| H | -1.3487832182 | -1.1437504093 | 7.9151293068 |
| H | 1.7682051431 | 2.7916268982 | -1.9043951632 |

**1e** conf_6

energy (M062X/6-31g(d,p)) = -2585.2658839 Hartree

| | | | |
|---|---|---|---|
| C | -2.1108721854 | -0.0399055632 | 1.1434951027 |
| O | -2.7871709376 | 0.8628664605 | 1.5785347888 |
| C | -1.1003075234 | 0.1021730814 | 0.0041176701 |
| N | -0.9841629072 | 1.5440857471 | -0.2063820142 |
| C | -0.0430099278 | 2.1673765764 | -0.9267768551 |
| O | 0.8388301203 | 1.5988050452 | -1.5837171215 |
| C | -0.1346816695 | 3.7027695463 | -0.8845957807 |
| C | 0.7821624244 | 4.3842415161 | -1.9012371958 |
| C | 2.2430950343 | 4.4041380635 | -1.4542505643 |
| C | 2.3470538115 | 4.9564522305 | -0.0377567639 |
| N | 1.4843913293 | 4.2475344184 | 0.9068663484 |

| | | | |
|---|---|---|---|
| N | 0.1615029589 | 4.210196877 | 0.4592034623 |
| C | -0.8381003919 | 4.3654106027 | 1.3668654327 |
| O | -2.0019761857 | 4.0754249825 | 1.1003020486 |
| C | -0.4708082534 | 5.1099825275 | 2.6568377851 |
| N | -0.1593036863 | 4.2442873886 | 3.804370064 |
| N | 0.0964378527 | 4.8929839726 | 5.0184132237 |
| C | -1.021725772 | 5.731123073 | 5.4275159468 |
| C | -1.4433113131 | 6.7238378564 | 4.3545941682 |
| C | -1.64898028 | 6.0162961713 | 3.0274661416 |
| C | 0.0064974417 | 2.9018798531 | 3.7426981823 |
| O | -0.0939291209 | 2.2681179121 | 2.6940538968 |
| C | 0.3500054811 | 2.1804425573 | 5.0437752714 |
| C | 1.8632235054 | 2.1938901467 | 5.2808130032 |
| N | -0.1545320668 | 0.8262970634 | 4.904070214 |
| C | -0.4273682699 | 0.060178614 | 5.9615786822 |
| O | -0.2607427225 | 0.4232406343 | 7.1327954968 |
| C | 0.4321991411 | -2.2111742733 | 6.0957973277 |
| C | -0.8258343596 | -1.3960485963 | 5.7354279584 |
| N | -1.3191076155 | -1.7122438674 | 4.3961940963 |
| N | -0.879328083 | -2.7834597733 | 3.6474138898 |
| C | -0.1431089063 | -3.6570622813 | 4.2138820262 |
| C | 0.2623629391 | -3.6512688637 | 5.6539896655 |
| C | -2.5147021545 | -1.14159806 | 4.0136494763 |
| O | -3.094875283 | -0.361901471 | 4.7490315399 |
| C | -3.0862137716 | -1.5479129166 | 2.6590095724 |
| O | -2.179598726 | -1.3010457613 | 1.5825440104 |
| O | 1.4501915648 | -4.3932975508 | 5.7859571782 |
| Cl | -0.1633963098 | 8.0158179864 | 4.1912949693 |
| C | -1.6864730778 | -0.5856880629 | -1.23857994 |
| C | 0.2486477433 | -0.5576474934 | 0.4143182502 |
| O | 1.0632617482 | -0.9033716417 | -0.672092967 |
| O | 0.6457645216 | -2.1878231433 | 7.4815124317 |
| H | 0.1914431665 | -4.4795938331 | 3.5877680278 |
| H | -1.6222088176 | 2.1224185143 | 0.3401752345 |
| H | -1.1740089651 | 3.976449886 | -1.0797357116 |
| H | 0.425537213 | 5.4128102362 | -2.0251332123 |
| H | 0.675791407 | 3.8816887975 | -2.8653256717 |
| H | 2.8358531157 | 5.0180123067 | -2.1400218938 |
| H | 2.0565212705 | 6.0125991537 | -0.0134342431 |
| H | 3.3668474437 | 4.8833476789 | 0.3491701284 |
| H | 1.8013832584 | 3.2880116861 | 1.0407466916 |
| H | 0.4229109354 | 5.7064269304 | 2.4558737625 |
| H | 0.9369770018 | 5.4589453659 | 4.9088418825 |
| H | -0.7391643777 | 6.237463559 | 6.3521928236 |
| H | -1.8749971668 | 5.0795417985 | 5.6429477733 |
| H | -2.3440946546 | 7.2601407165 | 4.6531812479 |
| H | -2.5496070334 | 5.4001063678 | 3.1095689473 |
| H | -1.8197362028 | 6.7397190182 | 2.2269544011 |
| H | -0.1528520965 | 2.6510871449 | 5.8873672826 |
| H | 2.2218569219 | 3.2149750728 | 5.4262023906 |
| H | 2.0911775675 | 1.6151026452 | 6.1782792523 |
| H | 2.3875213163 | 1.7499811927 | 4.4303779504 |
| H | -0.2781768804 | 0.4855096071 | 3.9590775117 |
| H | 1.2979082573 | -1.8017034468 | 5.5535575246 |

| | | | |
|---|---|---|---|
| H | -1.6030102478 | -1.6210083593 | 6.4718064713 |
| H | -0.550916111 | -4.0992166763 | 6.2486230867 |
| H | -4.0046463244 | -0.9802455887 | 2.5193929615 |
| H | -3.2869114507 | -2.6175949979 | 2.630468392 |
| H | 1.6883850722 | -4.3708673888 | 6.7237127865 |
| H | -1.8000713733 | -1.6575533793 | -1.0641685876 |
| H | -2.6601559382 | -0.1567383426 | -1.4874062471 |
| H | -1.0097689123 | -0.4418444819 | -2.0810220406 |
| H | 0.0266482611 | -1.483140662 | 0.946659767 |
| H | 0.7506110824 | 0.1263958474 | 1.1130931343 |
| H | 1.1903772687 | -0.0672056977 | -1.1676055853 |
| H | 0.52213754 | -1.259750796 | 7.7620707482 |
| H | 2.6514323357 | 3.3893285399 | -1.4832571067 |

**1e** conf_7

energy (M062X/6-31g(d,p)) = -2585.2657816 Hartree

| | | | |
|---|---|---|---|
| C | -1.017972925 | 0.1520803563 | 0.726323218 |
| O | -0.2123522748 | 0.7840705962 | 1.3679882771 |
| C | -2.072141604 | 0.7658643883 | -0.1969914951 |
| N | -1.6701386496 | 2.1224225644 | -0.5398567821 |
| C | -0.4498362914 | 2.4141826198 | -1.0696887499 |
| O | 0.2884139865 | 1.5825418879 | -1.5830132898 |
| C | -0.0654387486 | 3.8895321423 | -0.9139545258 |
| C | 0.9113135262 | 4.4054355293 | -1.9715445004 |
| C | 2.3537393415 | 3.9646668526 | -1.7328534377 |
| C | 2.7464825022 | 4.2451557525 | -0.2880822078 |
| N | 1.8204084779 | 3.6344511033 | 0.6668414147 |
| N | 0.5030487784 | 4.053599983 | 0.4345320611 |
| C | -0.3102749191 | 4.3383638377 | 1.4809590519 |
| O | -1.5333315463 | 4.4538644353 | 1.3308646427 |
| C | 0.3401374426 | 4.5639712265 | 2.8444389177 |
| N | -0.4298802148 | 3.8777717312 | 3.8736148078 |
| N | -1.687573428 | 4.3820259727 | 4.2315667385 |
| C | -1.5895851544 | 5.7836669704 | 4.6334429339 |
| C | -0.9353107123 | 6.6242132723 | 3.541559361 |
| C | 0.4313699695 | 6.0644545765 | 3.180832451 |
| C | 0.0315687 | 2.7257688432 | 4.4270569787 |
| O | 1.1150517981 | 2.2399892239 | 4.1132475141 |
| C | -0.8382844698 | 2.0519604141 | 5.4858595708 |
| C | -0.5907254241 | 2.6724530951 | 6.8632888447 |
| N | -0.4851166682 | 0.6466177273 | 5.4507625075 |
| C | -1.346664453 | -0.3167671299 | 5.8205827087 |
| O | -2.4149767418 | -0.1058069359 | 6.3816375736 |
| C | 0.1555243355 | -2.1442352023 | 6.6616780522 |
| C | -0.8690211977 | -1.7579616192 | 5.5849689812 |
| N | -0.2785317948 | -1.9533360021 | 4.253695296 |
| N | 0.8092489115 | -2.7491594776 | 3.9946415637 |
| C | 1.2951540131 | -3.4545590477 | 4.9391727625 |
| C | 0.7636111389 | -3.5015671427 | 6.338686127 |
| C | -0.9849945665 | -1.529869552 | 3.1553920582 |
| O | -2.0544175654 | -0.9587899443 | 3.2732905846 |
| C | -0.3543456574 | -1.8126262102 | 1.7965997715 |

| | | | |
|---|---|---|---|
| O | -1.1366997152 | -1.1825369177 | 0.790304737 |
| O | 1.8214533276 | -3.8169962273 | 7.2097453596 |
| Cl | -0.7706743199 | 8.3362497203 | 4.1113283079 |
| C | -3.3822069216 | 0.8527276308 | 0.5950986657 |
| C | -2.2876626787 | -0.0681144414 | -1.4783356254 |
| O | -3.2503417189 | 0.5285316673 | -2.3168454923 |
| O | -0.3934157808 | -2.105548317 | 7.9552343321 |
| H | 2.1623479769 | -4.0599529973 | 4.6913802443 |
| H | -2.0729761562 | 2.8640383278 | 0.0267028594 |
| H | -0.9748261276 | 4.4924782455 | -0.932669255 |
| H | 0.8608974751 | 5.4997965409 | -1.9535789124 |
| H | 0.5602629928 | 4.0835477764 | -2.9558096107 |
| H | 3.0229648316 | 4.497526434 | -2.4156511047 |
| H | 2.7586617228 | 5.3218014015 | -0.0877715625 |
| H | 3.739522941 | 3.8514136494 | -0.0566348749 |
| H | 1.8368475091 | 2.6193369094 | 0.5665835862 |
| H | 1.3368117404 | 4.1313077641 | 2.8417192715 |
| H | -2.2737507709 | 4.309554598 | 3.4004112013 |
| H | -1.001259518 | 5.8440279277 | 5.5540377035 |
| H | -2.6006801549 | 6.1372149371 | 4.8460946596 |
| H | -1.5821592537 | 6.6723813803 | 2.664854244 |
| H | 0.8702264185 | 6.6089697936 | 2.3409028086 |
| H | 1.1023929082 | 6.1730595314 | 4.038891264 |
| H | -1.8937866712 | 2.1540098505 | 5.2312063453 |
| H | 0.4694063615 | 2.6154625569 | 7.1243525079 |
| H | -0.9055329469 | 3.7182518152 | 6.8799424702 |
| H | -1.1675147904 | 2.1232624028 | 7.610332448 |
| H | 0.3663975176 | 0.4271025202 | 4.9476251527 |
| H | 0.9705752977 | -1.4143914291 | 6.6713665332 |
| H | -1.763190536 | -2.3836091536 | 5.6789459056 |
| H | -0.0283451969 | -4.2692644949 | 6.3886251137 |
| H | -0.3786211814 | -2.8792992803 | 1.5748868012 |
| H | 0.6783167603 | -1.4660058985 | 1.7646010239 |
| H | 1.4707289732 | -3.714615023 | 8.1071999807 |
| H | -4.1614761258 | 1.2556381955 | -0.054686847 |
| H | -3.6796088683 | -0.1383701715 | 0.9396787687 |
| H | -3.2673383135 | 1.4992174005 | 1.4691495563 |
| H | -2.6732458885 | -1.0505636588 | -1.2034632192 |
| H | -1.3309336465 | -0.1976138061 | -1.9933010335 |
| H | -2.9296715656 | 1.4198976705 | -2.5178348109 |
| H | -1.1840188973 | -2.6651740005 | 7.9760289795 |
| H | 2.4549650753 | 2.8948023314 | -1.9361882648 |

**1e** conf_8

energy (M062X/6-31g(d,p)) = -2585.2646488 Hartree

| | | | |
|---|---|---|---|
| C | -0.9316394445 | -0.8691157857 | 0.1109336068 |
| O | -1.3121416408 | -2.0154873867 | 0.1222971868 |
| C | -1.5659866083 | 0.2008080671 | -0.7776241716 |
| N | -0.9342496236 | 1.494582602 | -0.5090978198 |
| C | -1.203769216 | 2.6389377476 | -1.1466398833 |
| O | -1.9275634682 | 2.7488157157 | -2.1467069976 |
| C | -0.5497980513 | 3.9193366118 | -0.6241877423 |

| | | | |
|---|---|---|---|
| C | 0.6168843151 | 4.3648087645 | -1.5294872089 |
| C | 1.8855455625 | 3.5496129105 | -1.2741366616 |
| C | 2.2069826174 | 3.4993361151 | 0.2166767696 |
| N | 1.0224578072 | 3.0008638013 | 0.9159829848 |
| N | -0.0692477021 | 3.8729222483 | 0.749633678 |
| C | -0.4990080409 | 4.7870729071 | 1.6613451431 |
| O | -1.5167776859 | 5.4572303242 | 1.4808592508 |
| C | 0.2968771191 | 4.936125985 | 2.9620847079 |
| N | -0.3753309421 | 4.2111140578 | 4.0430637743 |
| N | -1.5421285219 | 4.7458410923 | 4.5997727059 |
| C | -1.3254168042 | 6.1097474931 | 5.0783346485 |
| C | -0.7984071995 | 7.0008849005 | 3.9611535788 |
| C | 0.467341747 | 6.4121892785 | 3.3589700137 |
| C | 0.0409382928 | 2.9746702516 | 4.3968137372 |
| O | 0.9777473088 | 2.4191337111 | 3.8146639813 |
| C | -0.6530109786 | 2.2830485973 | 5.5671893972 |
| C | -0.1396687684 | 2.8211598577 | 6.9053187088 |
| N | -0.3718950209 | 0.8725930509 | 5.3994980137 |
| C | -1.1943469014 | -0.0972386474 | 5.8073388675 |
| O | -2.1671422842 | 0.0768994543 | 6.5468093106 |
| C | -0.1870089029 | -2.149312164 | 6.6900915294 |
| C | -0.8261830676 | -1.5323069411 | 5.4339665185 |
| N | 0.0495694218 | -1.6433350244 | 4.2706677474 |
| N | 1.1917839915 | -2.4082656408 | 4.2256841164 |
| C | 1.4004112568 | -3.2315920091 | 5.1775094671 |
| C | 0.4806262565 | -3.4653987364 | 6.3367876769 |
| C | -0.3969636759 | -1.1398999582 | 3.0745167873 |
| O | -1.4818684686 | -0.5923045367 | 2.9850691318 |
| C | 0.5476714222 | -1.2780843653 | 1.8870608531 |
| O | 0.0801900909 | -0.4118868452 | 0.8622806398 |
| O | 1.2367430105 | -3.9834234136 | 7.4036173549 |
| Cl | -0.4486797806 | 8.6512172568 | 4.6206526822 |
| C | -3.0562328007 | 0.2464650942 | -0.4095458115 |
| C | -1.3798064757 | -0.2656691716 | -2.2505565402 |
| O | -2.3019189494 | 0.2907753388 | -3.1433149199 |
| O | -1.1691891645 | -2.3846768852 | 7.6642515679 |
| H | 2.3168177839 | -3.81183606 | 5.1201939137 |
| H | -0.2197541965 | 1.549335526 | 0.2173966482 |
| H | -1.3382406712 | 4.6708656148 | -0.649360359 |
| H | 0.808549093 | 5.4220611482 | -1.3151585525 |
| H | 0.30403291 | 4.2940041437 | -2.5743796573 |
| H | 2.7247140614 | 3.9870160725 | -1.8225765544 |
| H | 2.5043343158 | 4.4950118317 | 0.5811607468 |
| H | 3.0225482597 | 2.8014389342 | 0.4203118071 |
| H | 1.1558441387 | 2.7912214818 | 1.9056416125 |
| H | 1.2907993132 | 4.5031912407 | 2.8693406245 |
| H | -2.2596842535 | 4.7438860299 | 3.875731136 |
| H | -0.6103078046 | 6.0769591123 | 5.9054943995 |
| H | -2.2791444521 | 6.478359177 | 5.4607993274 |
| H | -1.5593336873 | 7.144052146 | 3.1960001499 |
| H | 0.7873269659 | 6.9878375062 | 2.4874780079 |
| H | 1.2686165294 | 6.4595005511 | 4.1030560773 |
| H | -1.7312048169 | 2.4373733084 | 5.5066874006 |
| H | -0.6058620687 | 2.2565299403 | 7.715272543 |

| | | | |
|---|---|---|---|
| H | 0.9452209156 | 2.7089173714 | 6.9764580713 |
| H | -0.3976528641 | 3.8754751415 | 7.0227900282 |
| H | 0.4073878345 | 0.6611938555 | 4.7878704047 |
| H | 0.595444244 | -1.4761306008 | 7.0705841078 |
| H | -1.7684430272 | -2.0514107554 | 5.235933374 |
| H | -0.3026791856 | -4.1761750176 | 6.0257331516 |
| H | 0.5826322482 | -2.3104507063 | 1.5358093196 |
| H | 1.5539080623 | -0.9489003479 | 2.1388387737 |
| H | 0.6208696604 | -4.1303371548 | 8.1355383162 |
| H | -3.5587419527 | 1.0017792752 | -1.0129303254 |
| H | -3.5164405547 | -0.7235429665 | -0.6039028801 |
| H | -3.1734144552 | 0.4921305478 | 0.6482197081 |
| H | -1.5265064752 | -1.3477278219 | -2.2727756116 |
| H | -0.3390594347 | -0.055529686 | -2.5400601675 |
| H | -2.2541043669 | 1.2606206606 | -2.9963811225 |
| H | -1.7159981316 | -1.5788245333 | 7.7136564802 |
| H | 1.7561360311 | 2.5249093104 | -1.640069281 |

**1e** conf_9

energy (M062X/6-31g(d,p)) = -2585.2642137 Hartree

| | | | |
|---|---|---|---|
| C | -1.1973246536 | -0.9388626819 | 0.1219368267 |
| O | -1.5908244908 | -2.0806309202 | 0.1023835312 |
| C | -1.5285137022 | 0.0847450308 | -0.9605965662 |
| N | -1.5074268113 | 1.4307073755 | -0.3862185901 |
| C | -1.5939538324 | 2.5535764962 | -1.1361363077 |
| O | -1.9414830107 | 2.5685447297 | -2.3129110709 |
| C | -1.2434071854 | 3.8725307005 | -0.4440741541 |
| C | -0.5258317522 | 4.8317403083 | -1.4078985372 |
| C | 0.9138192701 | 4.3870560985 | -1.6803754211 |
| C | 1.6609716352 | 4.086476361 | -0.3836581052 |
| N | 0.8522972278 | 3.133977933 | 0.3799386603 |
| N | -0.395287223 | 3.6931525222 | 0.7309904065 |
| C | -0.6092734117 | 4.5086149177 | 1.8137373196 |
| O | -1.6969862655 | 5.0530130356 | 1.9961241672 |
| C | 0.4968226834 | 4.6779221155 | 2.8540494585 |
| N | 0.0324283663 | 4.1032405649 | 4.1152450188 |
| N | -0.9272583546 | 4.7920836987 | 4.8676681145 |
| C | -0.4797289486 | 6.1489207777 | 5.1674357097 |
| C | -0.1620447268 | 6.9064359637 | 3.8837662523 |
| C | 0.8765098524 | 6.1551039007 | 3.0655326511 |
| C | 0.3010540753 | 2.8030915654 | 4.3912209615 |
| O | 0.9698961388 | 2.1084707073 | 3.625662202 |
| C | -0.2208868242 | 2.2423810666 | 5.7137538496 |
| C | 0.6413133541 | 2.7120668175 | 6.8879226848 |
| N | -0.2039835493 | 0.8049246402 | 5.5601822498 |
| C | -1.1389050135 | -0.0049024029 | 6.0667208451 |
| O | -1.9805628664 | 0.3330683142 | 6.9033627625 |
| C | -0.4428173404 | -2.2086044257 | 6.8725506316 |
| C | -1.0679010702 | -1.478097919 | 5.6708409793 |
| N | -0.323544877 | -1.7197875427 | 4.4400415126 |
| N | 0.6990198348 | -2.6310645963 | 4.3146918408 |
| C | 0.850637136 | -3.4894045228 | 5.246486307 |

| | | | |
|---|---|---|---|
| C | -0.0180126634 | -3.6062285161 | 6.4616213211 |
| C | -0.7803180838 | -1.1434294917 | 3.2787701474 |
| O | -1.7984239093 | -0.4751229411 | 3.2605728972 |
| C | 0.0869629062 | -1.354312594 | 2.0495166925 |
| O | -0.347352412 | -0.4547478244 | 1.0382907592 |
| O | 0.7142226988 | -4.2601735524 | 7.4684866712 |
| Cl | 0.4619487439 | 8.5563522061 | 4.2891237387 |
| C | -2.8796532331 | -0.2582781295 | -1.5811662286 |
| C | -0.3934472501 | -0.018874924 | -2.0172325892 |
| O | 0.8604761438 | 0.3583461383 | -1.5047168519 |
| O | -1.3741754214 | -2.3001314755 | 7.9178120018 |
| H | 1.671963008 | -4.1901789037 | 5.1280447425 |
| H | -1.1503750665 | 1.5261608055 | 0.554709102 |
| H | -2.1748847973 | 4.3222596306 | -0.0942007348 |
| H | -0.5299616509 | 5.8248339784 | -0.9454503528 |
| H | -1.0945049875 | 4.8940501075 | -2.3370237411 |
| H | 1.4437240902 | 5.1607189454 | -2.2432842169 |
| H | 1.8485505022 | 5.0129376427 | 0.1808052366 |
| H | 2.6239604067 | 3.6112985294 | -0.5851741268 |
| H | 1.2936160256 | 2.7520130145 | 1.2105511216 |
| H | 1.3991973776 | 4.1366364158 | 2.5840255563 |
| H | -1.7762320854 | 4.8335176061 | 4.3027081728 |
| H | 0.4083136875 | 6.0907525869 | 5.8036112273 |
| H | -1.2763863612 | 6.6420587307 | 5.7279055972 |
| H | -1.0712471747 | 7.0703881864 | 3.3061631552 |
| H | 1.0336799926 | 6.639817235 | 2.0987484823 |
| H | 1.8294809658 | 6.1714097985 | 3.6033289606 |
| H | -1.2512434925 | 2.5614470549 | 5.8741541222 |
| H | 0.5815263634 | 3.7964174936 | 7.0002709918 |
| H | 0.2773754371 | 2.2460942996 | 7.8061683663 |
| H | 1.6859055677 | 2.4260371332 | 6.7397452588 |
| H | 0.4365164543 | 0.4607745571 | 4.8554492365 |
| H | 0.4621426161 | -1.6728142665 | 7.195252058 |
| H | -2.0992801376 | -1.8227283852 | 5.5548804876 |
| H | -0.9226902075 | -4.1773146878 | 6.1948701624 |
| H | 0.0235774894 | -2.3839387334 | 1.6958560296 |
| H | 1.1274806514 | -1.1118119917 | 2.2618914069 |
| H | 0.1343698874 | -4.3177899829 | 8.2411290692 |
| H | -3.1084547713 | 0.4569652719 | -2.370284522 |
| H | -2.855036983 | -1.2668346608 | -1.9969755592 |
| H | -3.6658727663 | -0.2158140048 | -0.823869268 |
| H | -0.6884503828 | 0.596208972 | -2.8742173102 |
| H | -0.3106553425 | -1.0569943495 | -2.3488905639 |
| H | 0.7537823142 | 1.2006319854 | -1.0264984736 |
| H | -1.7612640485 | -1.4115461197 | 8.0246837265 |
| H | 0.9093262343 | 3.4814465794 | -2.297538151 |

**1e** conf_10

energy (M062X/6-31g(d,p)) = -2585.2635966 Hartree

| | | | |
|---|---|---|---|
| C | -0.9544635489 | -0.8516191894 | 0.3038449903 |
| O | -1.2883822962 | -2.0064602838 | 0.4224173052 |
| C | -1.5317678202 | 0.0653379264 | -0.773645657 |

| | | | |
|---|---|---|---|
| N | -1.1405734658 | 1.448431738 | -0.4830193482 |
| C | -1.3276425109 | 2.5065524061 | -1.2886489919 |
| O | -1.7044945313 | 2.4394611274 | -2.4622928212 |
| C | -1.0919303102 | 3.8867141466 | -0.6589395407 |
| C | -0.5846120344 | 4.9010571951 | -1.686250078 |
| C | 0.890347569 | 4.6714221396 | -2.0027881103 |
| C | 1.697782874 | 4.642162678 | -0.7101281893 |
| N | 1.1828810929 | 3.6753520816 | 0.2666595218 |
| N | -0.1934983158 | 3.8375179086 | 0.4920102161 |
| C | -0.6414217232 | 4.1974366489 | 1.7311639567 |
| O | -1.8313781088 | 4.4245280275 | 1.9411767878 |
| C | 0.3973921548 | 4.2938074811 | 2.8490570648 |
| N | -0.1869673188 | 3.8044662233 | 4.0900055029 |
| N | -1.1719519318 | 4.5705197687 | 4.7298382674 |
| C | -0.6871376649 | 5.9251190466 | 4.9877164821 |
| C | -0.1896004103 | 6.5852070575 | 3.7054457475 |
| C | 0.8900402196 | 5.7381931461 | 3.0510797627 |
| C | 0.167315786 | 2.5926953147 | 4.5845322374 |
| O | 1.0075379204 | 1.8865217597 | 4.0286489338 |
| C | -0.5040893664 | 2.1253946335 | 5.8809752709 |
| C | 0.1312383399 | 2.783681425 | 7.1063609902 |
| N | -0.3494114307 | 0.6854924772 | 5.9045001207 |
| C | -1.4036849949 | -0.1583288556 | 5.9554098362 |
| O | -2.5266275113 | 0.1475664307 | 6.3284476707 |
| C | -0.4039399257 | -2.3044660184 | 6.7953103019 |
| C | -1.0633411891 | -1.6130384571 | 5.5924553998 |
| N | -0.1724442462 | -1.6841351197 | 4.4258152036 |
| N | 0.9363230884 | -2.4888634487 | 4.3282276596 |
| C | 1.1162541864 | -3.3854462792 | 5.2171326816 |
| C | 0.1959722997 | -3.638425225 | 6.3702296915 |
| C | -0.527241137 | -1.0036976518 | 3.2880481218 |
| O | -1.5714277027 | -0.3797108004 | 3.2206794531 |
| C | 0.474983937 | -1.0500431824 | 2.1425906199 |
| O | -0.0253341145 | -0.2620126364 | 1.0687467799 |
| O | 0.9300105582 | -4.2299771082 | 7.4125413088 |
| Cl | 0.4621442042 | 8.2318418742 | 4.0823678827 |
| C | -3.0568333547 | -0.0789078217 | -0.7473410305 |
| C | -0.9545964347 | -0.4496462192 | -2.1283729678 |
| O | -1.7255863524 | -0.1157879703 | -3.2446174671 |
| O | -1.2905520087 | -2.4434278633 | 7.8769673016 |
| H | 2.0072211765 | -3.9978965502 | 5.1131255486 |
| H | -0.8825699893 | 1.644105103 | 0.4750645999 |
| H | -2.0623960644 | 4.2051497809 | -0.2666542643 |
| H | -0.7243527155 | 5.903034443 | -1.2667123774 |
| H | -1.2008106763 | 4.8251308017 | -2.5834306548 |
| H | 1.2657631267 | 5.4623314611 | -2.659239648 |
| H | 1.6873999052 | 5.6293215013 | -0.2359689446 |
| H | 2.7417393363 | 4.3731916933 | -0.8892737932 |
| H | 1.32893099 | 2.7268655269 | -0.0741628336 |
| H | 1.2444877434 | 3.6550199259 | 2.6141472049 |
| H | -1.9620615116 | 4.6080572316 | 4.0861591056 |
| H | 0.125479708 | 5.8741808506 | 5.7187121666 |
| H | -1.5111888132 | 6.492473827 | 5.4252352353 |
| H | -1.0234197209 | 6.7548124045 | 3.0222981366 |

| | | | |
|---|---|---|---|
| H | 1.1996832959 | 6.1682993958 | 2.0958563084 |
| H | 1.7678824856 | 5.7050640115 | 3.7038438746 |
| H | -1.5706363233 | 2.3497708767 | 5.855229222 |
| H | -0.0234321645 | 3.8641179963 | 7.0907808241 |
| H | -0.3272008177 | 2.3794557406 | 8.0118616689 |
| H | 1.2052200312 | 2.5804141031 | 7.1418263952 |
| H | 0.4875572953 | 0.368142766 | 5.4278753215 |
| H | 0.4149843359 | -1.6844013945 | 7.1713022756 |
| H | -2.0142783313 | -2.1008615676 | 5.3554272758 |
| H | -0.6164626313 | -4.3051599606 | 6.0314620505 |
| H | 0.6612032334 | -2.0712619534 | 1.8136097678 |
| H | 1.4132082399 | -0.5877795812 | 2.446884777 |
| H | 0.3406114481 | -4.2455877025 | 8.1815091427 |
| H | -3.4949944029 | 0.5539228425 | -1.5190662627 |
| H | -3.3376434084 | -1.1149752109 | -0.9413823018 |
| H | -3.4498420268 | 0.2197980388 | 0.2274277904 |
| H | -0.9341653965 | -1.5403248512 | -2.0752917378 |
| H | 0.0816989104 | -0.0906734621 | -2.21034727 |
| H | -1.7916093245 | 0.8620528655 | -3.2245344926 |
| H | -2.0849840374 | -2.907066357 | 7.5726603481 |
| H | 1.0156846241 | 3.7227888719 | -2.5395933281 |

Compound **1f**

**1f** conf_1

energy (M062X/6-31g(d,p)) = -2585.2740608 Hartree

| | | | |
|---|---|---|---|
| C | -0.8171053702 | -0.58963739 | 0.8747542763 |
| O | -0.0035782054 | -0.1664790114 | 1.6675453894 |
| C | -1.2688757267 | 0.1412757903 | -0.3820186498 |
| N | -0.9454283522 | 1.5581609015 | -0.1707586496 |
| C | -0.9985875918 | 2.4887111109 | -1.1380015061 |
| O | -1.1573960815 | 2.2366768018 | -2.3386834002 |
| C | -0.9133175059 | 3.9613704536 | -0.7195336766 |
| C | -0.1534740052 | 4.7969381482 | -1.7555272635 |
| C | 1.3535703467 | 4.594969175 | -1.6241885648 |
| C | 1.7864243792 | 4.8530078927 | -0.185022904 |
| N | 1.0315956798 | 4.0613645208 | 0.79082557 |
| N | -0.349978939 | 4.1803714652 | 0.6028631855 |
| C | -1.1272128285 | 4.6753820373 | 1.6123639967 |
| O | -2.3334285975 | 4.8312078023 | 1.482328863 |
| C | -0.3890064356 | 5.1963594453 | 2.852657055 |
| N | 0.2055648334 | 4.1822966523 | 3.7251682884 |
| N | 0.9596325026 | 4.6695183707 | 4.7981881997 |
| C | 0.1489846629 | 5.5257800988 | 5.6573400557 |
| C | -0.5821162615 | 6.6321982496 | 4.9061857153 |
| C | -1.3100055565 | 6.0867796463 | 3.6854903835 |
| C | -0.0743024593 | 2.8593823782 | 3.659923595 |
| O | -0.8698354107 | 2.4034766808 | 2.8414030576 |
| C | 0.6996475891 | 1.9468135555 | 4.6155676355 |
| C | 2.1471756879 | 1.7816803417 | 4.1424473859 |
| N | 0.0290549297 | 0.6676332816 | 4.6746709781 |
| C | -0.4219984933 | 0.1439253956 | 5.8260181793 |
| O | -0.29490113 | 0.6737105962 | 6.9268727548 |
| C | -0.9586918072 | -2.045482535 | 6.9687604931 |
| C | -1.1792776503 | -1.1954913819 | 5.7234193307 |
| N | -0.8306806981 | -1.9794853332 | 4.5435083326 |
| N | 0.2326492716 | -2.8468625375 | 4.5237569933 |
| C | 0.8396492443 | -3.0860146107 | 5.6232651071 |
| C | 0.4853897308 | -2.5501832816 | 6.9895131736 |
| C | -1.5314095264 | -1.8002154658 | 3.3752134843 |
| O | -2.5022423403 | -1.0648985092 | 3.324959782 |
| C | -1.0046881917 | -2.5253605377 | 2.142930924 |
| O | -1.3925539134 | -1.7902804151 | 0.9853322022 |
| O | 0.6590142409 | -3.5441889414 | 7.9693560619 |
| Cl | 0.6225935464 | 7.9062845636 | 4.3917616683 |
| C | -2.7733680595 | -0.0368200029 | -0.6070284031 |
| C | -0.4509725492 | -0.5028389927 | -1.5518340652 |
| O | -1.0406873771 | -0.3650267259 | -2.8087243418 |
| O | -1.8484556804 | -3.1456639123 | 7.0242477197 |
| H | 1.6675281697 | -3.7870146444 | 5.5566297572 |
| H | -0.8781210812 | 1.871589351 | 0.7973443485 |
| H | -1.9514495903 | 4.3018381664 | -0.6594547122 |
| H | -0.5066480568 | 4.5277712063 | -2.7520278325 |
| H | -0.4025643045 | 5.8496155094 | -1.5835110377 |

H 1.8878769495 5.2677496761 -2.3023898715
H 1.6424418429 5.9094973243 0.0679249237
H 2.8425488844 4.6168446832 -0.0311527126
H 1.2783530104 3.0767038671 0.7108467048
H 0.4516217289 5.7911633397 2.4780846538
H 1.7559761739 5.1831848359 4.4254535349
H 0.7977223221 5.9353467136 6.4337232601
H -0.6037879088 4.8961368647 6.1438473914
H -1.2706136572 7.1551704787 5.5702008485
H -2.1641273992 5.4956670132 4.0315066427
H -1.704452227 6.901574319 3.0757816312
H 0.6872960428 2.3644009868 5.6211001494
H 2.1768542187 1.3416281188 3.141887162
H 2.6595978037 2.7449357528 4.1188697218
H 2.680307459 1.1192511922 4.8284886425
H -0.1548115311 0.2182781653 3.7858011
H -1.156891728 -1.4420984423 7.8525937523
H -2.2419447067 -0.9545219125 5.6352574042
H 1.1577473509 -1.7232225962 7.2424090413
H -1.4772511498 -3.5030856695 2.0454110235
H 0.0755225958 -2.646933979 2.1787735915
H -0.1624730125 -4.0644374597 7.9459015314
H -3.0788563134 0.5527645985 -1.471743834
H -3.0134054857 -1.0828808123 -0.8003999253
H -3.3316915022 0.2996871608 0.2697492086
H -0.3823313104 -1.5758974659 -1.3567489572
H 0.5654709813 -0.0855624291 -1.5118225029
H -1.1387965978 0.604353656 -2.9232138387
H -1.8816897358 -3.5692394236 6.1530505831
H 1.6216718634 3.5703960831 -1.9124897959

**1f** conf_2

energy (M062X/6-31g(d,p)) = -2585.2723297 Hartree

C -1.1175475234 -0.2549225854 0.8801015401
O -0.6514725351 0.3886497536 1.7941810866
C -1.6392806029 0.3688167784 -0.4152915627
N -1.5939295663 1.7993410527 -0.1629704975
C -1.7240761097 2.7679805021 -1.0901951004
O -2.1622339939 2.593494511 -2.2229644263
C -1.2934010818 4.1679698044 -0.6078922024
C -0.8033307021 5.0325198772 -1.7706161445
C 0.5691129076 4.5698885058 -2.255233505
C 1.538027836 4.4676512263 -1.0812902937
N 1.0231591473 3.6344220132 0.012344873
N -0.2513664644 4.0685385583 0.4143523238
C -0.461737057 4.5280952745 1.6783213062
O -1.551685635 4.9907914328 2.0193969949
C 0.6944303502 4.4111270784 2.6756733419
N 0.1666519096 3.8909116068 3.9323562481
N -0.6526365097 4.7175203114 4.7147586418
C 0.037255885 5.9677985181 5.0304055748
C 0.5009229044 6.6750507703 3.7602883069

| | | | |
|---|---|---|---|
| C | 1.3861895903 | 5.7624983924 | 2.9262523467 |
| C | 0.4424731547 | 2.6206011716 | 4.3289421588 |
| O | 1.2081390368 | 1.8918247194 | 3.7055187936 |
| C | -0.2415281766 | 2.1109167379 | 5.5958705515 |
| C | 0.6185967948 | 2.4031834575 | 6.827402399 |
| N | -0.4334121473 | 0.6851967692 | 5.3902241307 |
| C | -1.3504657705 | -0.0189454087 | 6.0696322138 |
| O | -2.0462696448 | 0.4416734135 | 6.9714070067 |
| C | -1.0762187957 | -2.3847527856 | 6.882159794 |
| C | -1.5092493299 | -1.5038785391 | 5.7071626468 |
| N | -0.8144713453 | -1.9100012283 | 4.4932125158 |
| N | 0.4347410159 | -2.4717023371 | 4.4886985764 |
| C | 1.0130072594 | -2.6784035527 | 5.6084494329 |
| C | 0.4465012967 | -2.3993992136 | 6.9783795942 |
| C | -1.4596500798 | -1.797161131 | 3.2843229637 |
| O | -2.6065287989 | -1.3940307259 | 3.2079203817 |
| C | -0.6516783941 | -2.1954399742 | 2.0542521363 |
| O | -1.2068882585 | -1.5841468607 | 0.8894349157 |
| O | 0.8889329851 | -3.3553581193 | 7.9087527518 |
| Cl | 1.408667052 | 8.1802501084 | 4.2008646827 |
| C | -3.0528587773 | -0.1211305087 | -0.7357258991 |
| C | -0.6648189718 | -0.0060248875 | -1.5432125366 |
| O | 0.6102456232 | 0.5016029707 | -1.1948398079 |
| O | -1.447262102 | -3.7341284898 | 6.677943278 |
| H | 2.0009821228 | -3.1278055541 | 5.5542479738 |
| H | -1.1697281819 | 2.0427672174 | 0.7237429626 |
| H | -2.1560171964 | 4.6326199975 | -0.1234991434 |
| H | -0.749201547 | 6.0696886361 | -1.4227322258 |
| H | -1.5404951208 | 4.9860384243 | -2.5743429825 |
| H | 0.9616981149 | 5.2636187167 | -3.0053060013 |
| H | 1.7464316266 | 5.4607342718 | -0.669077896 |
| H | 2.492094498 | 4.0286903175 | -1.3848135558 |
| H | 0.9322287125 | 2.6659474664 | -0.303875601 |
| H | 1.4227662468 | 3.6939301126 | 2.3066807437 |
| H | -1.4740444186 | 4.9205765355 | 4.1450993006 |
| H | 0.8973275673 | 5.7414332538 | 5.6677348506 |
| H | -0.6562165024 | 6.5946618022 | 5.5949997602 |
| H | -0.3608432888 | 7.0164578923 | 3.1855084145 |
| H | 1.6478299932 | 6.2336146534 | 1.9753140979 |
| H | 2.315740846 | 5.56705381 | 3.4703190839 |
| H | -1.2172248875 | 2.5810706398 | 5.7187413131 |
| H | 0.7136940003 | 3.4807068175 | 6.981283019 |
| H | 0.1451739559 | 1.9667068777 | 7.7090399133 |
| H | 1.6161516069 | 1.9720964459 | 6.708352072 |
| H | 0.0934528938 | 0.2739746519 | 4.6290735736 |
| H | -1.5122223643 | -1.9819471239 | 7.7997404375 |
| H | -2.5762879396 | -1.650570329 | 5.5293407483 |
| H | 0.8036668701 | -1.4231343712 | 7.3248018563 |
| H | -0.7238198999 | -3.2700494137 | 1.884465929 |
| H | 0.3955565315 | -1.9199595822 | 2.1600707349 |
| H | 0.3208659008 | -4.129715951 | 7.7580204008 |
| H | -3.416728134 | 0.4008163884 | -1.6218182476 |
| H | -3.055498412 | -1.1963491995 | -0.9239406429 |
| H | -3.7254239156 | 0.0908363375 | 0.0983945652 |

| | | | |
|---|---|---|---|
| H | -1.0326715916 | 0.4321998647 | -2.4756270929 |
| H | -0.64871067 | -1.0971630199 | -1.6441439505 |
| H | 1.216238688 | 0.3134200927 | -1.9231539715 |
| H | -2.3579168687 | -3.8556700571 | 6.9772509732 |
| H | 0.4780943884 | 3.5898144092 | -2.7386429453 |

**1f** conf_3

energy (M062X/6-31g(d,p)) = -2585.2709199 Hartree

| | | | |
|---|---|---|---|
| C | -1.0699215124 | -0.8302985254 | 0.4559695715 |
| O | -1.4967587929 | -1.9483811598 | 0.6189754319 |
| C | -1.6426956612 | 0.122477401 | -0.5914966704 |
| N | -1.1743306845 | 1.486498442 | -0.3165218986 |
| C | -1.370876213 | 2.5474527373 | -1.1180352921 |
| O | -1.8064044007 | 2.4808764333 | -2.2712386657 |
| C | -1.077864193 | 3.929404671 | -0.5200388993 |
| C | -0.6059741864 | 4.9200580208 | -1.5872173109 |
| C | 0.8440891325 | 4.6522537512 | -1.9788543426 |
| C | 1.7198511585 | 4.6244881603 | -0.7319119667 |
| N | 1.2355482538 | 3.6884212659 | 0.2897630518 |
| N | -0.1230846103 | 3.8868679774 | 0.5850387157 |
| C | -0.4906877721 | 4.3386358265 | 1.8211798394 |
| O | -1.6598879342 | 4.6170504866 | 2.0810095309 |
| C | 0.6059531623 | 4.4685894079 | 2.8780174192 |
| N | 0.0957457574 | 3.9788500032 | 4.1524635584 |
| N | -0.8584122638 | 4.7356860908 | 4.8467777547 |
| C | -0.3709714713 | 6.0935143158 | 5.0769906306 |
| C | 0.0371193655 | 6.7588999608 | 3.7660219494 |
| C | 1.0819299778 | 5.9232405555 | 3.0429852999 |
| C | 0.4326319504 | 2.7418530876 | 4.5871490292 |
| O | 1.2083139065 | 2.0226280226 | 3.9584229033 |
| C | -0.1703602289 | 2.2559402873 | 5.9102365806 |
| C | 0.5799520775 | 2.836238877 | 7.1097091827 |
| N | -0.06920026 | 0.8126152765 | 5.8449228612 |
| C | -1.0581822271 | -0.0282339866 | 6.1688578298 |
| O | -2.0246294205 | 0.2534228303 | 6.8811170676 |
| C | -0.2698670368 | -2.2218843891 | 6.9359774329 |
| C | -0.8758360927 | -1.4795994319 | 5.7337510918 |
| N | -0.0469087203 | -1.6312773766 | 4.5424543587 |
| N | 0.9201360644 | -2.5892124226 | 4.3948194862 |
| C | 1.0364195005 | -3.4918936825 | 5.2904205385 |
| C | 0.1645332863 | -3.6143549424 | 6.5112778699 |
| C | -0.4378822225 | -0.9810107503 | 3.392811867 |
| O | -1.436905954 | -0.2860500013 | 3.3703743463 |
| C | 0.4695333304 | -1.1479829248 | 2.1818236218 |
| O | -0.0277263565 | -0.3256557303 | 1.1322266789 |
| O | -0.966702419 | -4.3942153949 | 6.1735954476 |
| Cl | 0.6956961277 | 8.4111030178 | 4.1030599859 |
| C | -3.1705222009 | 0.0537603909 | -0.5055271038 |
| C | -1.1433734311 | -0.4176648878 | -1.9698071865 |
| O | -1.9504383304 | -0.0633107027 | -3.0529785993 |
| O | -1.2461423997 | -2.357976906 | 7.9401393835 |
| H | 1.8199303785 | -4.2217168225 | 5.113680843 |

H -0.8669422987 1.6737582809 0.629151101
H -2.0220917991 4.270691138 -0.0852865915
H -0.700309775 5.9293872598 -1.1724826491
H -1.271282179 4.8488317719 -2.4488555191
H 1.2008273982 5.4239780996 -2.6678254281
H 1.7594065003 5.6191613741 -0.2753758318
H 2.7457440648 4.3265811663 -0.9622087318
H 1.3413576309 2.7301956862 -0.0376374842
H 1.4504614669 3.8429913363 2.60277912
H -1.6842093433 4.7681631836 4.2486069002
H 0.4858244378 6.0486154629 5.7559456901
H -1.1712368206 6.6523595875 5.5664559363
H -0.8400391775 6.9200632666 3.1374008773
H 1.3199433393 6.3548718135 2.0679105674
H 2.0027430351 5.9081914152 3.634612146
H -1.2239021563 2.5307095782 5.9705230238
H 0.470877949 3.922083203 7.1435794807
H 0.1687860326 2.4158577481 8.0303246586
H 1.6432358155 2.5872338352 7.0572827649
H 0.6516270417 0.4926641184 5.2069545225
H 0.6075737012 -1.6726240046 7.3035136554
H -1.8725795461 -1.8878946711 5.5462225001
H 0.7349097484 -4.0809948053 7.3246368244
H 0.5201829336 -2.1887429242 1.8642219533
H 1.4734270939 -0.7878478713 2.4040890184
H -1.6046597681 -4.2248570609 6.8874044803
H -3.6082324126 0.7120448178 -1.2557428307
H -3.5107753189 -0.9656437304 -0.6915544285
H -3.5082869057 0.3656409958 0.4857384018
H -1.1570496426 -1.508492063 -1.9131516684
H -0.100125944 -0.0944864809 -2.0980164588
H -1.983375151 0.9160353228 -3.0317865444
H -1.7670668153 -1.5333553359 7.9536767493
H 0.919400431 3.6927212264 -2.5054994292

**1f** conf_4

energy (M062X/6-31g(d,p)) = -2585.2680866 Hartree

C -1.2821566017 -0.0324729344 0.7712020322
O -0.813075758 0.7086599111 1.5998661092
C -2.1444026762 0.4099674268 -0.4138430866
N -1.9363930572 1.8351422573 -0.6382058455
C -0.7079648446 2.3851021167 -0.8117082932
O 0.2990381514 1.7171776286 -1.0371133958
C -0.6455649263 3.9068755858 -0.6687194696
C -0.135550121 4.6348609021 -1.9187271229
C 1.3708050457 4.4897777825 -2.1206851648
C 2.1022172168 4.8174185786 -0.82307506
N 1.6206478245 4.0140327314 0.3056016045
N 0.2365453729 4.1853148748 0.4704793354
C -0.2872426579 4.3468169824 1.7122656283
O -1.5036535088 4.3843013638 1.9019081225
C 0.705201848 4.4958918725 2.8712981917

| | | | |
|---|---|---|---|
| N | 0.0994324842 | 3.9631397788 | 4.0834710429 |
| N | -0.9386015909 | 4.6826737121 | 4.694994164 |
| C | -0.5121822942 | 6.0468797156 | 4.9932685246 |
| C | -0.007749705 | 6.7462183077 | 3.7339999848 |
| C | 1.1271658134 | 5.9565499668 | 3.1025989448 |
| C | 0.3772644979 | 2.6953987557 | 4.4785882925 |
| O | 1.2163426595 | 2.0037153933 | 3.9062846105 |
| C | -0.3718755251 | 2.1428980313 | 5.6896624478 |
| C | 0.3579179218 | 2.5138212875 | 6.9827812144 |
| N | -0.4305705934 | 0.7076913793 | 5.4793724611 |
| C | -1.3325875345 | -0.079751732 | 6.0818551562 |
| O | -2.112874305 | 0.2956948282 | 6.9515849603 |
| C | -0.8361809903 | -2.4639816071 | 6.7576380234 |
| C | -1.3619823385 | -1.5555225964 | 5.6494048364 |
| N | -0.6487726176 | -1.8301767997 | 4.4064634788 |
| N | 0.652529164 | -2.2605068868 | 4.3551938912 |
| C | 1.2643068026 | -2.4838366859 | 5.4557034177 |
| C | 0.6881307992 | -2.3536754866 | 6.8447383865 |
| C | -1.2961000153 | -1.6392224063 | 3.2054771407 |
| O | -2.4661489539 | -1.3078914294 | 3.1639569182 |
| C | -0.4552441886 | -1.8573303094 | 1.9533047115 |
| O | -1.1567465107 | -1.3684724994 | 0.8168234623 |
| O | 1.2153522184 | -3.337272557 | 7.6988200622 |
| Cl | 0.5544584961 | 8.4174492341 | 4.1451749882 |
| C | -3.6115773254 | 0.2023807452 | -0.02238201 |
| C | -1.8254931004 | -0.3879567056 | -1.6969350429 |
| O | -2.6296734181 | 0.0328191164 | -2.7743832372 |
| O | -1.1979948402 | -3.81849135 | 6.5593718839 |
| H | 2.2895453591 | -2.8315004724 | 5.3624685009 |
| H | -2.6671740135 | 2.4482062015 | -0.3063415998 |
| H | -1.6258417121 | 4.2975010379 | -0.3959077115 |
| H | -0.6905093436 | 4.2774234526 | -2.7913602327 |
| H | -0.3832183144 | 5.6950283742 | -1.7939263373 |
| H | 1.7032740508 | 5.1607301748 | -2.9190228332 |
| H | 1.970907304 | 5.8719964338 | -0.558051112 |
| H | 3.175027197 | 4.625930514 | -0.9094757507 |
| H | 1.7603887154 | 3.0269315365 | 0.0828965453 |
| H | 1.5904181653 | 3.9015966673 | 2.661049574 |
| H | -1.7013857253 | 4.7019980397 | 4.0172351409 |
| H | 0.2818423281 | 6.011467234 | 5.7451393837 |
| H | -1.3682141839 | 6.5757088963 | 5.417545913 |
| H | -0.8298160051 | 6.8847608845 | 3.028917272 |
| H | 1.4427376936 | 6.404615546 | 2.1576480917 |
| H | 1.9864044113 | 5.958433087 | 3.7806615291 |
| H | -1.388417067 | 2.5351702211 | 5.7241567602 |
| H | 1.3927591854 | 2.1628003553 | 6.951902305 |
| H | 0.354450142 | 3.5969832128 | 7.1259382389 |
| H | -0.1503620757 | 2.048062392 | 7.8292129261 |
| H | 0.1876736071 | 0.3545789198 | 4.7587848803 |
| H | -1.292982179 | -2.1654291774 | 7.7014572186 |
| H | -2.4137859789 | -1.7886983285 | 5.476742381 |
| H | 0.9703977476 | -1.3794387126 | 7.2604352417 |
| H | -0.2999976187 | -2.9218279419 | 1.775559732 |
| H | 0.5137763361 | -1.3686573245 | 2.0461249333 |

```
H   0.6839060212   -4.1328148901  7.5243815711
H   -3.8730523893  0.8011595976   0.8542112892
H   -4.2482940143  0.4879292102   -0.8620728914
H   -3.7886541151  -0.8480288403  0.2132137204
H   -2.0548853579  -1.4400660725  -1.5246407107
H   -0.7601097765  -0.294389082   -1.92759198
H   -2.4242560877  0.9650497856   -2.9337980516
H   -1.0064902597  -4.0664325431  5.6421759052
H   1.6149416361   3.4681133307   -2.4270461426
```

**1f** conf_5

energy (M062X/6-31g(d,p)) = -2585.2669265 Hartree

```
C   -1.9528812233  -0.1342503513  1.2417315816
O   -2.6018050228  0.6754353648   1.8654746811
C   -1.1343060189  0.1946256041   -0.0067929335
N   -1.2608898287  1.645112057    -0.1490676446
C   -0.5761916037  2.4311126962   -0.9936345691
O   0.2613879654   2.028096682    -1.8110445937
C   -0.8422415976  3.9289283224   -0.8017624627
C   -0.6080096134  4.7848354414   -2.0476582839
C   0.8689564667   5.0508670175   -2.337290934
C   1.5829775569   5.5016588092   -1.0688140463
N   1.3992120618   4.5552361558   0.0368149279
N   0.0334961758   4.3665708689   0.2938792625
C   -0.4057824906  4.3172395423   1.5764061477
O   -1.5742630916  4.0444031258   1.8524243522
C   0.6330432655   4.5676201563   2.6746895262
N   0.1355245191   4.0190209561   3.9271987231
N   -0.8487711272  4.7271217148   4.6364443036
C   -0.4295067228  6.096620797    4.9008448313
C   -0.0723848257  6.8055183079   3.5992571698
C   1.0190212449   6.0430755386   2.8679704639
C   0.253703587    2.6820155488   4.1444679575
O   0.8114562053   1.9438495263   3.3359260441
C   -0.2421641716  2.137955581    5.4824554548
C   0.7792475955   2.4965763304   6.5681052681
N   -0.3897267189  0.7076329562   5.2934074539
C   -0.8419340471  -0.13942364    6.2227844056
O   -1.1208063799  0.1687845145   7.3852191948
C   0.5321734499   -2.1681044515  6.2554788766
C   -0.8455017547  -1.6203264965  5.8542422439
N   -1.137914514   -1.890019647   4.4491577094
N   -0.5234009055  -2.8770914108  3.72231795
C   0.3160056724   -3.6447585204  4.3019128273
C   0.6812029818   -3.596779094   5.7609816911
C   -2.3674546426  -1.4622495135  3.9870442423
O   -3.1095290453  -0.8235788629  4.7110309111
C   -2.7856227496  -1.8683764013  2.5791141164
O   -1.9000813858  -1.4330983803  1.5429735228
O   -0.2008254357  -4.4496131573  6.4655741382
Cl  0.4796709702   8.4929931204   3.946653381
C   -1.7648883834  -0.5280098108  -1.2056217653
```

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C   0.3379961607   -0.2617214147  0.2043218118
O   1.0541641472   -0.4161923463  -0.9893794124
O   0.6397437575   -2.1861689902  7.6599996848
H   0.7615873145   -4.4035746777  3.6662129622
H   -1.8611202064  2.0913783305   0.5397448292
H   -1.8635124759  4.0685302802   -0.44617951
H   -1.094012347   4.3056020378   -2.9018355499
H   -1.1196846963  5.7387940494   -1.8797582353
H   0.960072801    5.8199241438   -3.1107919983
H   1.2070429497   6.4734214367   -0.7315761648
H   2.6604005727   5.5962240167   -1.2266433296
H   1.7948310634   3.6530920079   -0.2312753084
H   1.5333720478   4.0143860374   2.4128846572
H   -1.6849195756  4.7230842804   4.0509732673
H   0.4370170986   6.078160957    5.5682835544
H   -1.2518851272  6.6012205974   5.4119048062
H   -0.9637452806  6.9176845585   2.9773340657
H   1.2362167693   6.4909726831   1.8972490323
H   1.9350771248   6.0763770146   3.4658647698
H   -1.2087158805  2.5755463546   5.7373297805
H   1.7683537735   2.1139071901   6.3021125635
H   0.8372021682   3.5810789041   6.6817302482
H   0.4709134335   2.0565143568   7.5166915152
H   -0.0984395864  0.3616300904   4.3860317231
H   1.3210314138   -1.5511438372  5.8043775028
H   -1.6019817171  -2.0981325399  6.4827600102
H   1.7229120207   -3.9183967721  5.8895240007
H   -3.7766942026  -1.4453686151  2.4199778364
H   -2.8142311405  -2.9527905519  2.4891268294
H   -0.1153625818  -4.174031596   7.3943872682
H   -2.8188917996  -0.2574534798  -1.3035280294
H   -1.2394369938  -0.239200189   -2.1158100013
H   -1.681182767   -1.6092205812  -1.0836351439
H   0.3243227014   -1.2383728895  0.6914121314
H   0.8138848163   0.4537431856   0.8903060892
H   0.9707114943   0.4402908035   -1.4573115031
H   0.156465939    -1.4140491142  8.0066486561
H   1.3453003924   4.1430272802   -2.717761536
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**1f** conf_6

energy (M062X/6-31g(d,p)) = -2585.2662571 Hartree

```
C   -1.1031531379  -0.4092640168  0.7952948385
O   -0.4050813011  0.141123095    1.6208163302
C   -1.7465024959  0.3087257951   -0.3901208475
N   -1.290293582   1.6874502437   -0.2410522084
C   -1.2846114257  2.6696607572   -1.1457335721
O   -1.7040843234  2.5819640952   -2.306883527
C   -0.7616329471  4.0236073478   -0.6552237326
C   0.1553814774   4.7049702883   -1.6839423261
C   1.5559135845   4.087626014    -1.7086819872
C   2.1272905142   3.962729453    -0.2979854288
N   1.1525477752   3.2289421546   0.5005728862
```

| | | | |
|---|---|---|---|
| N | -0.0518694367 | 3.9443426237 | 0.6146650722 |
| C | -0.3754801652 | 4.7872683753 | 1.6376296679 |
| O | -1.4488712925 | 5.390917018 | 1.6675923912 |
| C | 0.5932650058 | 4.8940957111 | 2.8155917561 |
| N | 0.0313435675 | 4.1634149485 | 3.9534464559 |
| N | -1.0351651118 | 4.7346230782 | 4.6585982601 |
| C | -0.697596985 | 6.0701222712 | 5.1429702958 |
| C | -0.2873860387 | 6.9720893956 | 3.9865755149 |
| C | 0.8673688285 | 6.3541090239 | 3.2159739986 |
| C | 0.382410248 | 2.8669872705 | 4.1677252948 |
| O | 1.1563538363 | 2.2748626787 | 3.4159457435 |
| C | -0.1449346804 | 2.2001186722 | 5.428003855 |
| C | 0.8535700458 | 2.4391271728 | 6.5671631038 |
| N | -0.3270027102 | 0.7843352575 | 5.1567920467 |
| C | -1.113167829 | 0.045917979 | 5.9574680747 |
| O | -1.6941731869 | 0.4962258341 | 6.9413211945 |
| C | -0.7578598363 | -2.2911639675 | 6.8073510538 |
| C | -1.2871354469 | -1.4474285617 | 5.6487385754 |
| N | -0.6999492532 | -1.9080697855 | 4.3956706603 |
| N | 0.5437640595 | -2.4818019879 | 4.3060069707 |
| C | 1.2199930752 | -2.6428664326 | 5.3787516026 |
| C | 0.771393536 | -2.308134324 | 6.7801821686 |
| C | -1.4535133365 | -1.8241477015 | 3.2465074971 |
| O | -2.5699829994 | -1.338169115 | 3.2597013372 |
| C | -0.829015852 | -2.3751583945 | 1.9714908949 |
| O | -1.4001178953 | -1.7067349391 | 0.8463342644 |
| O | 1.2822011386 | -3.2370235584 | 7.7028778699 |
| Cl | 0.2045463898 | 8.5944542147 | 4.6249441708 |
| C | -3.272772743 | 0.2183732783 | -0.2669892395 |
| C | -1.2621760773 | -0.3544965953 | -1.7098763548 |
| O | -2.0449902613 | -0.023168483 | -2.8203791771 |
| O | -1.2444785695 | -3.6197922882 | 6.7722552273 |
| H | 2.195979115 | -3.1041606435 | 5.2543970133 |
| H | -0.8100663059 | 1.8693209593 | 0.6330552139 |
| H | -1.6432625268 | 4.644959737 | -0.4805857431 |
| H | 0.2235357278 | 5.7628571941 | -1.4075324535 |
| H | -0.3154844986 | 4.6498466936 | -2.6675495674 |
| H | 2.2182162711 | 4.6963750454 | -2.3312761081 |
| H | 2.3452030083 | 4.958285564 | 0.1221262262 |
| H | 3.0539404401 | 3.383561325 | -0.3008552829 |
| H | 1.4521242635 | 2.9063412396 | 1.4169830735 |
| H | 1.5509189536 | 4.4320361806 | 2.5906336818 |
| H | -1.8263936771 | 4.7947718639 | 4.0178856013 |
| H | 0.119114582 | 5.9821685982 | 5.8652876341 |
| H | -1.5752916504 | 6.4645535262 | 5.6589255679 |
| H | -1.136281758 | 7.1590327482 | 3.3305937061 |
| H | 1.0979126175 | 6.9393546099 | 2.3224413136 |
| H | 1.7572401036 | 6.3553322095 | 3.8531920629 |
| H | -1.1095717312 | 2.6232480015 | 5.7036590142 |
| H | 0.4988976838 | 1.9301687217 | 7.4650297954 |
| H | 1.8391130637 | 2.0500151162 | 6.2988305342 |
| H | 0.9420588559 | 3.5064415503 | 6.7849055484 |
| H | 0.1318854602 | 0.394249797 | 4.3430424536 |
| H | -1.1183547861 | -1.8617390703 | 7.741472418 |

H -2.3648436269 -1.6042315219 5.5726297745
H 1.1635602083 -1.3238298441 7.0615057123
H -1.092447686 -3.4267986185 1.8543218387
H 0.2529451623 -2.2686957487 1.9691234751
H 0.6786081026 -3.9979294194 7.6557535674
H -3.6017504064 -0.8190311501 -0.3518451926
H -3.6044201169 0.6206438438 0.6928320121
H -3.7286540185 0.7944085382 -1.0728136597
H -1.328375251 -1.4370001927 -1.583854276
H -0.2033715554 -0.0926910287 -1.8518327544
H -2.0065711489 0.9568307333 -2.8758274242
H -1.1308707505 -3.9761117688 5.8782283124
H 1.5134137134 3.0876513142 -2.1549737614

**1f** conf_7

energy (M062X/6-31g(d,p)) = -2585.2658575 Hartree

C -2.2536625115 -0.03650844 1.2845224327
O -2.8682700011 0.8590662145 1.8174927852
C -1.3385295102 0.1314954718 0.0715008599
N -1.2165464593 1.5761597696 -0.1117428322
C -0.3524121505 2.1931409644 -0.9281570818
O 0.4374429332 1.6156116607 -1.6868076362
C -0.408840715 3.7286266714 -0.8607149788
C 0.3838754696 4.4069034595 -1.9785431371
C 1.8898386047 4.3946082287 -1.7234411036
C 2.186753708 4.9229260148 -0.3247118395
N 1.4352955236 4.2191082356 0.7145154976
N 0.0657293185 4.2135956842 0.4385151912
C -0.8079174816 4.3824647621 1.4657712115
O -2.0031261285 4.1239104019 1.3449677172
C -0.2611653389 5.1043517238 2.7036568218
N 0.1608117606 4.2184847398 3.7982329627
N 0.5890008755 4.8468103425 4.9731591894
C -0.4402030718 5.7152761553 5.525257583
C -0.9647356072 6.7299101799 4.5194278559
C -1.3553264343 6.0432748959 3.2225649663
C 0.2530516461 2.8697216697 3.7132003641
O -0.000045883 2.2525228424 2.6803993363
C 0.7008791169 2.118494803 4.9640859915
C 2.2262308648 1.9929164707 4.9962101807
N 0.0516164736 0.8219228057 4.920937085
C -0.2743947091 0.1625858152 6.042229056
O 0.0039348767 0.5524069048 7.1736338083
C -0.2081218536 -2.3018419986 6.5061675935
C -1.0307879378 -1.1638971599 5.8965846514
N -1.4491691744 -1.5043330851 4.5390885141
N -0.7768437777 -2.396601025 3.7425764124
C 0.3012807023 -2.9165773067 4.1856672663
C 0.9097866824 -2.7006516983 5.5481136503
C -2.7082322687 -1.1215141681 4.1267935505
O -3.435926841 -0.4631595231 4.8495513429
C -3.1913332203 -1.6036056059 2.760879668

| | | | |
|---|---|---|---|
| O | -2.3213061543 | -1.3132197695 | 1.6674121811 |
| O | 1.5697897631 | -3.859698472 | 5.9908807476 |
| Cl | 0.3225016533 | 7.9867994867 | 4.2049310015 |
| C | -2.0360378594 | -0.5128037594 | -1.1370334385 |
| C | 0.030439593 | -0.5556785876 | 0.3508053414 |
| O | 0.7405943732 | -0.8949687132 | -0.8087614187 |
| O | -0.9863896583 | -3.4713707869 | 6.6738254904 |
| H | 0.7946385945 | -3.6195622606 | 3.5195003225 |
| H | -1.774200547 | 2.1549598218 | 0.5155063715 |
| H | -1.4589370153 | 4.0231265663 | -0.9187837738 |
| H | 0.0339854231 | 5.4431375638 | -2.0436489809 |
| H | 0.1449417374 | 3.9201508309 | -2.9269388045 |
| H | 2.4008446829 | 5.0092671335 | -2.4715036913 |
| H | 1.9271727162 | 5.9848070089 | -0.2506033558 |
| H | 3.2455047457 | 4.8214008101 | -0.0723305312 |
| H | 1.747253364 | 3.2522710451 | 0.7982116877 |
| H | 0.6192754493 | 5.6746461576 | 2.3965287162 |
| H | 1.4291574827 | 5.3839424109 | 4.7635010482 |
| H | -0.026596093 | 6.2054103631 | 6.4084024807 |
| H | -1.279070256 | 5.0883301533 | 5.8452767807 |
| H | -1.8047394528 | 7.2890355122 | 4.9317691487 |
| H | -2.2587115222 | 5.4545647055 | 3.4096485414 |
| H | -1.5998586402 | 6.7807821773 | 2.4545995441 |
| H | 0.3636321256 | 2.6337418338 | 5.862078007 |
| H | 2.6923249814 | 2.978471093 | 5.0668762306 |
| H | 2.5208869998 | 1.4061617835 | 5.8690784719 |
| H | 2.5898453182 | 1.4925776926 | 4.0946467157 |
| H | -0.2145426525 | 0.4742187964 | 4.0093791245 |
| H | 0.2068522903 | -1.9552014278 | 7.4553857327 |
| H | -1.9426626349 | -1.0402266928 | 6.4847840611 |
| H | 1.6585354808 | -1.9022335242 | 5.4972194647 |
| H | -4.1627790289 | -1.1381066074 | 2.599572351 |
| H | -3.2878334561 | -2.6888943974 | 2.7645094289 |
| H | 0.8599941341 | -4.4430422018 | 6.3085231642 |
| H | -2.1420365185 | -1.5891222265 | -0.9881790624 |
| H | -3.0246465208 | -0.0715067534 | -1.2854210868 |
| H | -1.4353087839 | -0.3436775981 | -2.0306278573 |
| H | -0.1581415496 | -1.485865717 | 0.8876022873 |
| H | 0.6018093678 | 0.1101606885 | 1.0128442879 |
| H | 0.8262145044 | -0.0555567497 | -1.307094532 |
| H | -1.4430884019 | -3.4215972663 | 7.5238793118 |
| H | 2.2717544844 | 3.3737629998 | -1.818836446 |

**1f** conf_8

energy (M062X/6-31g(d,p)) = -2585.2658099 Hartree

| | | | |
|---|---|---|---|
| C | -0.9771447027 | -0.2946825477 | 0.7957417791 |
| O | -0.0846197218 | 0.2100376959 | 1.4403188291 |
| C | -1.6924941255 | 0.4041735402 | -0.3597792945 |
| N | -1.1891459332 | 1.7747384298 | -0.2925472736 |
| C | -1.254507486 | 2.7429969596 | -1.2143774804 |
| O | -1.7058894859 | 2.6135878679 | -2.3568634772 |
| C | -0.7556938265 | 4.1220548697 | -0.7507228755 |

| | | | |
|---|---|---|---|
| C | -0.0253821176 | 4.8744068936 | -1.8658694453 |
| C | 1.3993795313 | 4.3580016756 | -2.047385232 |
| C | 2.1266029094 | 4.3638067504 | -0.7071730844 |
| N | 1.4086738421 | 3.6157988089 | 0.3295462285 |
| N | 0.076753858 | 4.0436576805 | 0.4487933616 |
| C | -0.3786788371 | 4.5373369633 | 1.6381706077 |
| O | -1.5154808562 | 4.996515165 | 1.7419671292 |
| C | 0.561164371 | 4.4605057676 | 2.8443094656 |
| N | -0.2054159051 | 4.0316621301 | 4.0069604364 |
| N | -1.1341809073 | 4.9225531769 | 4.5639732835 |
| C | -0.4850534438 | 6.1811925509 | 4.9261860342 |
| C | 0.2324031909 | 6.7944304886 | 3.7270250978 |
| C | 1.2342900832 | 5.813426724 | 3.1389682005 |
| C | -0.0673847977 | 2.7684003444 | 4.510681674 |
| O | 0.7493142356 | 1.9794483885 | 4.0568207435 |
| C | -1.0102829592 | 2.3909168583 | 5.6651450691 |
| C | -0.4916799127 | 2.9010945247 | 7.0092028715 |
| N | -1.2695951017 | 0.9617642721 | 5.6394713229 |
| C | -0.4968535378 | -0.0178882856 | 6.150113832 |
| O | 0.5126973639 | 0.1359252279 | 6.8272581786 |
| C | -0.6941556285 | -2.4344748418 | 6.9437827174 |
| C | -1.0615307753 | -1.4284941521 | 5.8580692883 |
| N | -0.6150376807 | -1.9312380174 | 4.5503658385 |
| N | 0.445853675 | -2.782306465 | 4.3777198616 |
| C | 1.080812221 | -3.1896957768 | 5.4091691492 |
| C | 0.7742426706 | -2.8444446384 | 6.8404650586 |
| C | -1.2969762855 | -1.5628949691 | 3.4229337209 |
| O | -2.2425594213 | -0.7886803696 | 3.469134493 |
| C | -0.8251293735 | -2.1919351297 | 2.1173972463 |
| O | -1.4393645935 | -1.5259872073 | 1.0180129342 |
| O | 1.0546145722 | -3.9299700662 | 7.6910177894 |
| Cl | 1.080768417 | 8.3120663347 | 4.2372677403 |
| C | -3.2094608282 | 0.3684564351 | -0.1493807739 |
| C | -1.3002748968 | -0.3180151044 | -1.6797260055 |
| O | -2.1341739156 | -0.0069884913 | -2.757478054 |
| O | -1.5115517281 | -3.592832366 | 6.8783942616 |
| H | 1.9058390121 | -3.8694822612 | 5.213060724 |
| H | -0.7822980316 | 2.0196183027 | 0.6014843693 |
| H | -1.6520964985 | 4.6747352054 | -0.4561402753 |
| H | -0.6059551223 | 4.7764993533 | -2.7849293805 |
| H | -0.0025744473 | 5.9356947324 | -1.5969944464 |
| H | 1.9377003011 | 4.9790586484 | -2.769808952 |
| H | 2.2536997707 | 5.3899041544 | -0.3459942225 |
| H | 3.119320505 | 3.9131365458 | -0.7830557232 |
| H | 1.3987733176 | 2.6242778097 | 0.0949241796 |
| H | 1.325522502 | 3.7092438533 | 2.6649083513 |
| H | -1.8301940576 | 5.0977567945 | 3.8393978332 |
| H | 0.2318152064 | 5.9866283349 | 5.729710254 |
| H | -1.2559447214 | 6.8555023521 | 5.3055219033 |
| H | -0.4935059089 | 7.1100377376 | 2.9762611608 |
| H | 1.6894149912 | 6.2150166413 | 2.230034521 |
| H | 2.0342093673 | 5.6367658616 | 3.8649352363 |
| H | -1.9728123343 | 2.8702934436 | 5.4808069946 |
| H | 0.5242125483 | 2.5612827336 | 7.2040602317 |

H -0.5191786237 3.9921558219 7.0085387179
H -1.1388966812 2.5409050254 7.8128369947
H -1.9676459137 0.6504617933 4.972353949
H -0.8854633847 -1.9916304926 7.9217679007
H -2.1512001699 -1.3728173182 5.8066911603
H 1.3975062419 -2.0005397874 7.1491555036
H -1.1532737283 -3.2299230871 2.058300433
H 0.2590432694 -2.1552764202 2.032850226
H 0.2767844905 -4.5094130814 7.6265362348
H -3.4734055365 0.8050435772 0.8164475448
H -3.6940282005 0.9373063883 -0.9435908937
H -3.5749652013 -0.659187343 -0.1857963414
H -1.3894211253 -1.3929433936 -1.5075348622
H -0.2439875569 -0.0933834924 -1.8876962851
H -2.07121044 0.9672040511 -2.8586423343
H -1.533710358 -3.9119584627 5.9635959067
H 1.3830543621 3.337597882 -2.4510778617

**1f** conf_9

energy (M062X/6-31g(d,p)) = -2585.2647703 Hartree

C -1.5750688615 -1.0678248446 0.3761106119
O -2.2715822031 -1.9975940881 0.705546398
C -1.8143333142 -0.1939608777 -0.8643450803
N -1.7869040349 1.2210713661 -0.4792634427
C -0.8780778726 2.1797643951 -0.7340195916
O 0.1895253103 2.0023589589 -1.3341445702
C -1.2596107004 3.5776137135 -0.238121366
C -1.4605177722 4.5711995397 -1.3930389355
C -0.1414310151 5.0218998953 -2.0179878051
C 0.838064601 5.458031881 -0.9312842344
N 1.0318304572 4.4338403717 0.1032349859
N -0.2052251927 4.062101207 0.6509324115
C -0.4014536483 4.1038148269 1.9911250316
O -1.4752449019 3.7875352086 2.5020268921
C 0.7937232366 4.524387342 2.8615578614
N 0.533937645 4.0702031197 4.2220476582
N -0.4177092127 4.7687793145 4.9854467091
C -0.0696372246 6.1796247371 5.0819118855
C 0.0652719527 6.7913789425 3.6915743985
C 1.0954050417 6.0309011243 2.8734552879
C 0.7823258373 2.770017327 4.5283589692
O 1.4146307788 2.0374139734 3.7712964175
C 0.2730211661 2.2406017178 5.8689530436
C 1.2301460914 2.611764256 7.0025974661
N 0.1496056128 0.8080128961 5.6912188953
C -0.8735158415 0.0974589348 6.1727784674
O -1.676697237 0.5114750473 7.0163621361
C -0.3668620361 -2.1565173277 6.957923695
C -0.9627554158 -1.3704430074 5.7748126561
N -0.2953640137 -1.7059343492 4.5220342226
N 0.4724897859 -2.8267901007 4.3425812148
C 0.5327551232 -3.697862247 5.2735974987

| | | | |
|---|---|---|---|
| C | -0.2101060867 | -3.6187901067 | 6.5788680443 |
| C | -0.7247513868 | -1.0890727705 | 3.3632498232 |
| O | -1.5792382924 | -0.2240759408 | 3.3858499417 |
| C | -0.0427619554 | -1.5508615105 | 2.0843540294 |
| O | -0.4405207235 | -0.7214084433 | 1.0016501581 |
| O | -1.4818190514 | -4.2139617482 | 6.405034663 |
| Cl | 0.5457211666 | 8.5311836189 | 3.8263373414 |
| C | -3.1885979166 | -0.4897351717 | -1.455401636 |
| C | -0.7081553353 | -0.5788646869 | -1.8817262762 |
| O | -0.7741864627 | 0.1626594582 | -3.0675561006 |
| O | -1.2433511529 | -2.0866540124 | 8.055287354 |
| H | 1.1595813751 | -4.5584068533 | 5.0623742334 |
| H | -2.610999842 | 1.5195202528 | 0.0241435338 |
| H | -2.1634233712 | 3.5334648816 | 0.3691621451 |
| H | -1.9822363972 | 5.4399799429 | -0.9761008001 |
| H | -2.1233783633 | 4.127794582 | -2.1422907061 |
| H | -0.3254691399 | 5.8525373066 | -2.7066928462 |
| H | 0.4793006233 | 6.3656066507 | -0.4333272036 |
| H | 1.8249869119 | 5.6752117269 | -1.3480960771 |
| H | 1.4121082909 | 3.5951347496 | -0.3359694263 |
| H | 1.6766866665 | 3.9997680711 | 2.5007247861 |
| H | -1.3101744852 | 4.6575379352 | 4.5015060432 |
| H | 0.8736576981 | 6.2736006193 | 5.6278639757 |
| H | -0.8546623453 | 6.6769587043 | 5.6553123166 |
| H | -0.9065510535 | 6.8019229942 | 3.1924256653 |
| H | 1.1433456378 | 6.4044763364 | 1.8500882463 |
| H | 2.0814144125 | 6.1704041093 | 3.3278118503 |
| H | -0.7156699524 | 2.6432546218 | 6.0858581347 |
| H | 0.8710437445 | 2.1759262365 | 7.9376041819 |
| H | 2.2349183109 | 2.2310857854 | 6.8007530019 |
| H | 1.2789418083 | 3.6969298913 | 7.1182142944 |
| H | 0.7358575305 | 0.420380709 | 4.9609496907 |
| H | 0.6215729551 | -1.7462300762 | 7.2072587892 |
| H | -2.0256732779 | -1.6177755183 | 5.703412678 |
| H | 0.3616608086 | -4.1361744721 | 7.3601257513 |
| H | -0.2850227398 | -2.593706491 | 1.8765407093 |
| H | 1.038749439 | -1.4481160786 | 2.1684304611 |
| H | -2.0049442663 | -3.8983512183 | 7.1616280702 |
| H | -3.2893953816 | -1.5559471723 | -1.6644062649 |
| H | -3.9894398823 | -0.2037642704 | -0.7679103771 |
| H | -3.2988323788 | 0.0696149318 | -2.3859003601 |
| H | -0.8749222975 | -1.630505903 | -2.1340882079 |
| H | 0.2719063213 | -0.4910781007 | -1.4073266931 |
| H | -0.3218015326 | 0.9969436838 | -2.8458063754 |
| H | -1.6180042895 | -1.1836459987 | 8.0634615249 |
| H | 0.2998935176 | 4.2069054904 | -2.5989618761 |

Compound **1g**

**1g** conf_1

energy (M062X/6-31g(d,p)) = -2585.2752616 Hartree

| | | | |
|---|---|---|---|
| C | -0.4563100162 | -3.3410385142 | -0.0775140261 |
| O | -0.6217558204 | -2.3844183701 | 0.6421967759 |
| C | 0.8866228414 | -3.8188171901 | -0.6202183654 |
| N | 1.7979429372 | -2.681480708 | -0.4636282014 |
| C | 3.1349314249 | -2.7454066636 | -0.3491472567 |
| O | 3.7963869215 | -3.7796279699 | -0.2377866311 |
| C | 3.8970764398 | -1.4135060034 | -0.3665748882 |
| C | 5.0151339555 | -1.4231465912 | 0.6816442824 |
| C | 4.4427601097 | -1.2132512475 | 2.0812455604 |
| C | 3.5861257555 | 0.0494318237 | 2.1085203864 |
| N | 2.5487142414 | 0.0688686661 | 1.0751727792 |
| N | 3.0692993793 | -0.2310197064 | -0.1880363396 |
| C | 2.8873629058 | 0.6482620744 | -1.2210975179 |
| O | 3.2863425411 | 0.4150767415 | -2.348352988 |
| C | 2.3451770619 | 2.0364457754 | -0.8461488386 |
| N | 0.9109801014 | 2.1406867478 | -0.5716722675 |
| N | 0.4641985272 | 3.406478356 | -0.1768549395 |
| C | 0.7455673725 | 4.4004668882 | -1.2040096162 |
| C | 2.2093811669 | 4.4292211846 | -1.6286391852 |
| C | 2.7103690102 | 3.0292015402 | -1.9505553087 |
| C | 0.0080591027 | 1.1366605496 | -0.7165818062 |
| O | 0.3196143323 | 0.0330456365 | -1.1501257208 |
| C | -1.4164914682 | 1.4384594484 | -0.25961385 |
| C | -1.5016211601 | 1.3530899977 | 1.2698839252 |
| N | -2.2852456558 | 0.4594391813 | -0.8805080904 |
| C | -3.6061705776 | 0.647292806 | -0.9245979027 |
| O | -4.1291243298 | 1.7155913859 | -0.5834133907 |
| C | -5.9721613511 | -0.1591003917 | -1.3607966733 |
| C | -4.4777014572 | -0.5277084711 | -1.4503786468 |
| N | -4.1904532786 | -1.7984216278 | -0.7586015315 |
| N | -5.0981430792 | -2.4704426074 | 0.0445694562 |
| C | -6.3285095784 | -2.2844427463 | -0.2299805833 |
| C | -6.8333962201 | -1.4173835722 | -1.3536365396 |
| C | -3.0420620035 | -2.4764950501 | -1.031096099 |
| O | -2.2644571669 | -2.1063655466 | -1.9007438361 |
| C | -2.7590031212 | -3.705538214 | -0.173680559 |
| O | -1.4506236922 | -4.1605945861 | -0.4637319737 |
| O | -8.186857362 | -1.0961092831 | -1.2003472057 |
| Cl | 3.1980469965 | 5.1575757692 | -0.2847464094 |
| C | 0.7807937432 | -4.212818905 | -2.0952957265 |
| C | 1.2762779256 | -5.0588884355 | 0.2488689873 |
| O | 2.2156846473 | -5.9017686194 | -0.330974109 |
| O | -6.339589029 | 0.4831671182 | -0.1655291271 |
| H | -7.050611653 | -2.8044311298 | 0.3941191456 |
| H | 1.3909809522 | -1.769987132 | -0.6633633667 |
| H | 4.3222618254 | -1.3289407926 | -1.370700005 |
| H | 5.715636862 | -0.6151115998 | 0.4414390656 |
| H | 5.5509725624 | -2.3706714659 | 0.6089468547 |

| | | | |
|---|---|---|---|
| H | 5.2492865343 | -1.1349515569 | 2.8178488106 |
| H | 4.218512898 | 0.932253797 | 1.9551712097 |
| H | 3.0773327141 | 0.174304902 | 3.068963506 |
| H | 1.821162374 | -0.6140254154 | 1.2843845912 |
| H | 2.8471889524 | 2.3233420924 | 0.0853672591 |
| H | 0.936033497 | 3.6570827359 | 0.6907872893 |
| H | 0.4220056361 | 5.3741411744 | -0.8295361745 |
| H | 0.1360342164 | 4.1541604452 | -2.0808619351 |
| H | 2.3527250751 | 5.1009098662 | -2.4767281181 |
| H | 2.2522741635 | 2.6948732134 | -2.8871182895 |
| H | 3.7902634987 | 3.0328126938 | -2.10939209 |
| H | -1.7195697533 | 2.4360649549 | -0.5771232701 |
| H | -2.5305094724 | 1.5470670694 | 1.5795997785 |
| H | -1.2099083107 | 0.3549392087 | 1.6058254388 |
| H | -0.8551146055 | 2.098239165 | 1.7376712387 |
| H | -1.8608309496 | -0.3907588566 | -1.2473775187 |
| H | -6.2175567941 | 0.4639691137 | -2.2311173998 |
| H | -4.2163632794 | -0.6801733596 | -2.5042151433 |
| H | -6.7269485392 | -1.9650374551 | -2.2989892558 |
| H | -3.4272819661 | -4.530439429 | -0.4192147076 |
| H | -2.8757828771 | -3.4565596343 | 0.8824134579 |
| H | -8.1968758925 | -0.3749840225 | -0.5490859986 |
| H | 1.7690454002 | -4.5032461728 | -2.4535564819 |
| H | 0.1088284363 | -5.0629071707 | -2.2185215196 |
| H | 0.4051640078 | -3.3760410832 | -2.6885040192 |
| H | 0.3661687779 | -5.6500631235 | 0.3772630542 |
| H | 1.5843171962 | -4.6923982302 | 1.239637421 |
| H | 3.0322215062 | -5.3640927976 | -0.3690067227 |
| H | -5.736574374 | 1.2542412549 | -0.1018554975 |
| H | 3.8347383075 | -2.0811519292 | 2.3671433904 |

**1g** conf_2

energy (M062X/6-31g(d,p)) = -2585.2742168 Hartree

| | | | |
|---|---|---|---|
| C | -1.0036446005 | 0.0287759319 | 0.5016499 |
| O | -0.7630091858 | 0.7304810479 | 1.4511204717 |
| C | -1.7552137346 | 0.4724382344 | -0.7597373508 |
| N | -1.6664705187 | 1.9221740333 | -0.8499395876 |
| C | -0.4934596122 | 2.5950465294 | -0.8295537904 |
| O | 0.598989729 | 2.0390803927 | -0.9387907449 |
| C | -0.6055139891 | 4.1063967183 | -0.616907474 |
| C | -0.0766323764 | 4.9417042117 | -1.7908698223 |
| C | 1.4487114668 | 4.9578190654 | -1.8693386456 |
| C | 2.0375198498 | 5.2898783949 | -0.5009399722 |
| N | 1.5501741965 | 4.3895168257 | 0.5482767174 |
| N | 0.1471647669 | 4.4216070128 | 0.6011573066 |
| C | -0.4890183895 | 4.4847084437 | 1.7984145589 |
| O | -1.7157410012 | 4.4158652679 | 1.8855618464 |
| C | 0.3876395417 | 4.6481809956 | 3.0452354443 |
| N | -0.2613839655 | 3.9783391819 | 4.1647087687 |
| N | -1.4027705316 | 4.5619769572 | 4.736244501 |
| C | -1.124659784 | 5.9311743447 | 5.1580277468 |
| C | -0.5974120948 | 6.760666833 | 3.9907596158 |

| | | | |
|---|---|---|---|
| C | 0.6493903667 | 6.1202665546 | 3.4033614508 |
| C | 0.0627022738 | 2.6929196477 | 4.4540154671 |
| O | 0.9717194138 | 2.1046981197 | 3.8737532698 |
| C | -0.7159148713 | 1.9863875796 | 5.5626295407 |
| C | -0.0507802028 | 2.2540339567 | 6.9153807068 |
| N | -0.69494075 | 0.5807760273 | 5.1962634581 |
| C | -1.4557417935 | -0.346955551 | 5.7707753912 |
| O | -2.2358726401 | -0.1245118943 | 6.7090720975 |
| C | -0.9971692645 | -2.7981722043 | 6.2790988669 |
| C | -1.4094938419 | -1.7732953263 | 5.2099924646 |
| N | -0.5500556163 | -1.9262450418 | 4.0489676971 |
| N | 0.7922542648 | -2.1683829893 | 4.1501252894 |
| C | 1.2763182243 | -2.473993954 | 5.2928582142 |
| C | 0.5008571075 | -2.6697712236 | 6.5666472885 |
| C | -1.0737108867 | -1.7587053643 | 2.7859947533 |
| O | -2.2662288666 | -1.5960729548 | 2.6075778914 |
| C | -0.0678648831 | -1.7833549737 | 1.6409703759 |
| O | -0.684399953 | -1.2810901778 | 0.4589310577 |
| O | 0.7523618648 | -1.5699305335 | 7.4178236399 |
| Cl | -0.2241467616 | 8.4409467697 | 4.5522056377 |
| C | -3.2286148426 | 0.0959253655 | -0.5745676842 |
| C | -1.1960447102 | -0.1763584258 | -2.0507511849 |
| O | -1.4950791497 | -1.5457405277 | -2.1738754798 |
| O | -1.7250433595 | -2.6485512483 | 7.4731222234 |
| H | 2.3520268938 | -2.621078098 | 5.3127951304 |
| H | -2.504216015 | 2.4379256103 | -0.6234409638 |
| H | -1.6408211954 | 4.3797859314 | -0.4133408867 |
| H | -0.4422873199 | 5.9644879112 | -1.6451507652 |
| H | -0.5188515165 | 4.5727542507 | -2.7212001512 |
| H | 1.7731371047 | 5.6973591033 | -2.608210352 |
| H | 1.7806184061 | 6.3126381255 | -0.2050059184 |
| H | 3.1276290067 | 5.2074937228 | -0.5052601679 |
| H | 1.7995581742 | 3.4316438009 | 0.2953830113 |
| H | 1.3400244021 | 4.1530202062 | 2.8762289925 |
| H | -2.1116550157 | 4.5670414372 | 4.0018378983 |
| H | -0.3864368821 | 5.9085222608 | 5.9652023059 |
| H | -2.0534693301 | 6.3519929646 | 5.5488066909 |
| H | -1.3748710455 | 6.8764377386 | 3.2328728066 |
| H | 0.9921049817 | 6.6605029505 | 2.5178863746 |
| H | 1.4512850765 | 6.1505113775 | 4.1477627254 |
| H | -1.7491970837 | 2.3320180945 | 5.5899017753 |
| H | 0.9979607138 | 1.9472097383 | 6.8917175667 |
| H | -0.1051169162 | 3.3180438472 | 7.1578074913 |
| H | -0.5680954553 | 1.6902570836 | 7.6930864998 |
| H | -0.034339771 | 0.3385457205 | 4.467138252 |
| H | -1.1903229164 | -3.7944870887 | 5.8660087429 |
| H | -2.4283859141 | -1.9870628375 | 4.8813691123 |
| H | 0.8519392314 | -3.6023544395 | 7.0319656872 |
| H | 0.2297497231 | -2.8065034355 | 1.4104090883 |
| H | 0.8196585475 | -1.2017110313 | 1.8852429804 |
| H | 0.1153667036 | -1.6766219561 | 8.144040655 |
| H | -3.6324545008 | 0.5428686097 | 0.337774233 |
| H | -3.3321613871 | -0.9862781086 | -0.5120596698 |
| H | -3.8054862727 | 0.4509115736 | -1.433204253 |

| | | | |
|---|---|---|---|
| H | -0.1203067121 | 0.015036423 | -2.1124673168 |
| H | -1.6812178256 | 0.3282114639 | -2.8900263948 |
| H | -1.0353391191 | -1.9957909706 | -1.450260541 |
| H | -2.1280034337 | -1.7521440313 | 7.4486677584 |
| H | 1.8212057737 | 3.9821599986 | -2.1967303206 |

**1g** conf_3

energy (M062X/6-31g(d,p)) = -2585.2739813 Hartree

| | | | |
|---|---|---|---|
| C | -0.5224711749 | -0.2926307859 | 0.5806389592 |
| O | 0.255150168 | 0.270138088 | 1.3184717998 |
| C | -1.1992740802 | 0.3789637308 | -0.6135720741 |
| N | -0.8746667095 | 1.7939325959 | -0.4389658041 |
| C | -1.0183818191 | 2.7994541962 | -1.3105912849 |
| O | -1.3670106694 | 2.6782336749 | -2.4895631119 |
| C | -0.7660743728 | 4.2035791934 | -0.7369046596 |
| C | -0.0868088083 | 5.127843784 | -1.750428306 |
| C | 1.4097362427 | 4.8456335008 | -1.8472145294 |
| C | 2.0325334963 | 4.8780387114 | -0.4561386246 |
| N | 1.3728408991 | 3.9630091034 | 0.4811368522 |
| N | -0.0154890159 | 4.1714837847 | 0.5169278992 |
| C | -0.6250675689 | 4.4876073295 | 1.6972838798 |
| O | -1.8260884074 | 4.7472166145 | 1.7449318781 |
| C | 0.2391518836 | 4.4720049972 | 2.9621004305 |
| N | -0.5583327026 | 3.9702315341 | 4.0728093523 |
| N | -1.5815621768 | 4.780654216 | 4.5872181985 |
| C | -1.0552062464 | 6.0816441022 | 4.9934547408 |
| C | -0.3240666063 | 6.7604523947 | 3.8391104185 |
| C | 0.7860599796 | 5.8678595175 | 3.3091633296 |
| C | -0.4060092213 | 2.6852716786 | 4.5101983921 |
| O | 0.451955506 | 1.9461355241 | 4.0498126315 |
| C | -1.376198599 | 2.2185883449 | 5.6067890628 |
| C | -0.9231784861 | 2.676028734 | 6.9926315419 |
| N | -1.5816176643 | 0.7825246554 | 5.4976064263 |
| C | -0.773628487 | -0.194032832 | 5.9382319278 |
| O | 0.2565420347 | -0.0099939995 | 6.5932040695 |
| C | -1.0668562485 | -2.6637391149 | 6.6537926115 |
| C | -1.2642097822 | -1.6030048782 | 5.5569607574 |
| N | -0.5925549952 | -2.0457577661 | 4.3321807321 |
| N | 0.5935105672 | -2.7241540326 | 4.3339385105 |
| C | 1.052101845 | -3.1759866335 | 5.4374844711 |
| C | 0.3959380639 | -3.0988968305 | 6.789980674 |
| C | -1.0955865197 | -1.6624987118 | 3.117413066 |
| O | -2.0910707815 | -0.9592243215 | 3.0315912769 |
| C | -0.3642596009 | -2.1981454195 | 1.8915586811 |
| O | -0.8823809132 | -1.5693950329 | 0.7238674842 |
| O | 1.1079962731 | -2.2685702665 | 7.6855114506 |
| Cl | 0.3662932548 | 8.3385700612 | 4.3992096345 |
| C | -2.7143712473 | 0.1585806152 | -0.5620186532 |
| C | -0.5967095523 | -0.2195656323 | -1.9161057105 |
| O | -1.3552168746 | 0.0503451014 | -3.0588255516 |
| O | -1.5692922514 | -2.2111268554 | 7.8817987892 |
| H | 2.0140280491 | -3.6756829404 | 5.3656804312 |

| | | | |
|---|---|---|---|
| H | -0.5670506958 | 2.0351701132 | 0.494935295 |
| H | -1.754680097 | 4.5956876979 | -0.4819507124 |
| H | -0.2479126924 | 6.1609332649 | -1.4248534139 |
| H | -0.5806790427 | 5.0018493591 | -2.7155759328 |
| H | 1.8934947339 | 5.5855240632 | -2.4921390812 |
| H | 1.969444311 | 5.8863459035 | -0.033324092 |
| H | 3.0871105445 | 4.592234964 | -0.4773444972 |
| H | 1.5370296932 | 2.999783361 | 0.191719795 |
| H | 1.0713037957 | 3.7865869575 | 2.8245130141 |
| H | -2.2519506242 | 4.9060147557 | 3.8287990532 |
| H | -0.3702933476 | 5.9362962307 | 5.8343260984 |
| H | -1.8971990012 | 6.6885377591 | 5.3332366762 |
| H | -1.0302028444 | 7.0209941018 | 3.0485924436 |
| H | 1.2640767856 | 6.3129722232 | 2.4332871117 |
| H | 1.5504325215 | 5.7460425704 | 4.0830639034 |
| H | -2.3496921679 | 2.6698787729 | 5.4121913845 |
| H | 0.09534891 | 2.3575928835 | 7.2093373449 |
| H | -0.9819337871 | 3.7649653299 | 7.0400155825 |
| H | -1.5894065362 | 2.261071845 | 7.7531055755 |
| H | -2.2778399261 | 0.4915424564 | 4.8226560108 |
| H | -1.6509179765 | -3.5358251535 | 6.3414440577 |
| H | -2.328294742 | -1.5533757364 | 5.3229213321 |
| H | 0.420942512 | -4.0995643174 | 7.2318082104 |
| H | -0.5596798401 | -3.2638113126 | 1.769586328 |
| H | 0.709289969 | -2.0395443773 | 1.9763951646 |
| H | 1.0400398121 | -1.3585618398 | 7.3086066017 |
| H | -3.118674701 | 0.5010075371 | 0.3930245167 |
| H | -2.9499544553 | -0.8995546705 | -0.6870054229 |
| H | -3.1853334707 | 0.7165861591 | -1.3718906542 |
| H | -0.5692915005 | -1.3056735025 | -1.8009480537 |
| H | 0.438999837 | 0.1392484037 | -2.0052323199 |
| H | -1.4220406708 | 1.0286893986 | -3.0999896601 |
| H | -0.7858452408 | -1.9123348072 | 8.3774181357 |
| H | 1.5811632548 | 3.8620698752 | -2.3030918457 |

**1g** conf_4

energy (M062X/6-31g(d,p)) = -2585.2738904 Hartree

| | | | |
|---|---|---|---|
| C | -0.7497613306 | 1.3166295458 | -0.8891628878 |
| O | -0.4081382323 | 0.1800163464 | -0.6522708407 |
| C | 0.2201869809 | 2.4818819407 | -1.0661992508 |
| N | 1.5041100006 | 1.9211611051 | -0.6455179333 |
| C | 2.7337563277 | 2.4143666661 | -0.849755334 |
| O | 3.0048472389 | 3.4026705799 | -1.5321813019 |
| C | 3.8696993923 | 1.6697503754 | -0.1266364725 |
| C | 5.1376772948 | 1.6267612157 | -0.9816830635 |
| C | 5.0192927261 | 0.5786501143 | -2.0851879274 |
| C | 4.624163927 | -0.7664658448 | -1.4835294725 |
| N | 3.4119358163 | -0.6961501688 | -0.6661882414 |
| N | 3.4900741571 | 0.3224068568 | 0.2941643746 |
| C | 3.3446736178 | 0.0270584629 | 1.6214452585 |
| O | 3.4706720816 | 0.8950682104 | 2.4819355088 |
| C | 2.990566452 | -1.4135086827 | 1.9931946195 |

| | | | |
|---|---|---|---|
| N | 1.9291541809 | -1.3907608545 | 2.9923381303 |
| N | 2.221796888 | -0.9333110249 | 4.2842675436 |
| C | 3.328470621 | -1.6963215042 | 4.8562029342 |
| C | 4.5574371156 | -1.6679408244 | 3.9505485264 |
| C | 4.2039762882 | -2.1698497229 | 2.5584041027 |
| C | 0.646040415 | -1.6774810733 | 2.6321719172 |
| O | 0.3606518183 | -2.0258042543 | 1.493278146 |
| C | -0.433027586 | -1.5556928706 | 3.7062120794 |
| C | -0.3832254657 | -2.709828456 | 4.7084762113 |
| N | -1.7032779292 | -1.5368820158 | 2.9934253022 |
| C | -2.7369031003 | -0.7966604493 | 3.4875262969 |
| O | -2.7590457829 | -0.3387352781 | 4.615173532 |
| C | -4.7442134865 | -2.1054760335 | 2.8807484068 |
| C | -4.0152093425 | -0.7733674005 | 2.6401551284 |
| N | -3.8134783681 | -0.571080732 | 1.2061130449 |
| N | -4.644493737 | -1.0941274738 | 0.2489138259 |
| C | -5.6317713603 | -1.8139899671 | 0.6124906169 |
| C | -6.0037825584 | -2.1797368074 | 2.0272595717 |
| C | -2.9972111044 | 0.4512998767 | 0.7764856938 |
| O | -2.3390398661 | 1.1139165981 | 1.5530362541 |
| C | -2.9766244559 | 0.6809863124 | -0.7333752307 |
| O | -2.0242587956 | 1.6906858383 | -1.0366886734 |
| O | -6.5899474479 | -3.4527437123 | 2.0851396651 |
| Cl | 5.8626920125 | -2.6882038636 | 4.662867493 |
| C | -0.1844131069 | 3.6568482993 | -0.1717058487 |
| C | 0.2093018451 | 2.9048266123 | -2.5657804351 |
| O | 0.7446192585 | 4.1661241276 | -2.8019824559 |
| O | -3.9830892058 | -3.2205961952 | 2.4743430445 |
| H | -6.2488716572 | -2.2126463089 | -0.1888011885 |
| H | 1.4231483735 | 1.0924090331 | -0.0700853905 |
| H | 4.0554135585 | 2.227217135 | 0.7958132357 |
| H | 5.9840502972 | 1.3863647851 | -0.3284799415 |
| H | 5.3035083888 | 2.6224015313 | -1.3966901208 |
| H | 5.9660748599 | 0.4858183848 | -2.6270356529 |
| H | 5.4293193555 | -1.1465170949 | -0.8441281389 |
| H | 4.4367929997 | -1.5193262767 | -2.2543231345 |
| H | 2.5957838 | -0.5176316099 | -1.2492545009 |
| H | 2.6028114855 | -1.9349428886 | 1.1215470545 |
| H | 2.4998288581 | 0.0434172534 | 4.1858404426 |
| H | 3.0017052129 | -2.7309310951 | 5.0025083917 |
| H | 3.5573349554 | -1.2695430726 | 5.8355579493 |
| H | 4.9621228523 | -0.6555863879 | 3.9050736892 |
| H | 5.0581296392 | -2.076584322 | 1.8818616329 |
| H | 3.9429589906 | -3.231670198 | 2.6170106494 |
| H | -0.3186298137 | -0.6148298704 | 4.2494435593 |
| H | -0.4597366401 | -3.6727974236 | 4.1945659237 |
| H | 0.5434762717 | -2.6824679796 | 5.2836722566 |
| H | -1.2210815038 | -2.6091529614 | 5.4021821063 |
| H | -1.6065248672 | -1.6649680024 | 1.9885723476 |
| H | -4.9982176707 | -2.1603830378 | 3.9469461931 |
| H | -4.615005694 | 0.0450234421 | 3.0519764279 |
| H | -6.7507275165 | -1.470729979 | 2.4029326765 |
| H | -3.9369910257 | 1.0600155653 | -1.0810344021 |
| H | -2.7495618249 | -0.2458315262 | -1.2605513129 |

| | | | |
|---|---|---|---|
| H | -5.8506789252 | -4.07850312 | 2.0218012132 |
| H | -0.2705657724 | 3.336306281 | 0.8688382192 |
| H | -1.143989537 | 4.0630120945 | -0.4945052631 |
| H | 0.5665743341 | 4.4430303809 | -0.2549843777 |
| H | -0.8344095933 | 2.9400258213 | -2.8877125885 |
| H | 0.7138228902 | 2.1119532791 | -3.1409864742 |
| H | 1.669942994 | 4.1256968898 | -2.4860111563 |
| H | -3.0975641081 | -3.1511956529 | 2.8691019796 |
| H | 4.2642718388 | 0.8935530572 | -2.8169341641 |

**1g** conf_5

energy (M062X/6-31g(d,p)) = -2585.2720115 Hartree

| | | | |
|---|---|---|---|
| C | 0.0824346905 | -3.124228307 | -0.3763832456 |
| O | 0.1854660463 | -2.2614579099 | 0.4633649433 |
| C | 1.2303414177 | -3.631463728 | -1.2553111712 |
| N | 2.3322274212 | -2.6918121814 | -1.0986998704 |
| C | 3.299873779 | -2.6964464755 | -0.1589424628 |
| O | 3.6729353821 | -3.6818684227 | 0.4742316783 |
| C | 3.9537791467 | -1.3157486013 | 0.0462720916 |
| C | 5.1026505779 | -1.3598049259 | 1.0522408868 |
| C | 4.6000242112 | -1.4544011175 | 2.4911969144 |
| C | 3.578151771 | -0.3548278977 | 2.7565279602 |
| N | 2.4838569647 | -0.3471366627 | 1.7896702875 |
| N | 2.9557434445 | -0.3246579509 | 0.4710899359 |
| C | 2.2866086004 | 0.4185696913 | -0.4439651297 |
| O | 2.4651651177 | 0.2478440262 | -1.6554195709 |
| C | 1.3418424527 | 1.5010987583 | 0.0838487959 |
| N | 0.3809527465 | 1.8636142881 | -0.9397226615 |
| N | 0.8337488657 | 2.5488962122 | -2.074764083 |
| C | 1.5161038289 | 3.7797567842 | -1.6892506935 |
| C | 2.6440006771 | 3.502545774 | -0.6968069708 |
| C | 2.1162707453 | 2.7581361963 | 0.5210873293 |
| C | -0.8987922122 | 1.3809055042 | -0.8758209294 |
| O | -1.2720762076 | 0.695106244 | 0.0594259281 |
| C | -1.8335868022 | 1.7370700958 | -2.0480815343 |
| C | -2.2911175407 | 3.1948952054 | -2.0191710574 |
| N | -2.9236845309 | 0.7755539785 | -2.060634757 |
| C | -3.8819515311 | 0.7206934569 | -1.1162200468 |
| O | -4.1893901512 | 1.6583463754 | -0.3829611255 |
| C | -6.0983608932 | -0.3615045534 | -0.542529084 |
| C | -4.6882353258 | -0.614664889 | -1.1042197945 |
| N | -3.9966381375 | -1.6870720177 | -0.3619879102 |
| N | -4.5774750191 | -2.4077428572 | 0.6654384499 |
| C | -5.8489956287 | -2.4071756916 | 0.7403755708 |
| C | -6.7801458069 | -1.6787149005 | -0.1928086929 |
| C | -2.8324706217 | -2.2271043499 | -0.8297913358 |
| O | -2.3137103545 | -1.882538213 | -1.8827541711 |
| C | -2.2223834779 | -3.3349144198 | 0.0253492622 |
| O | -1.0476229124 | -3.805860913 | -0.6169050893 |
| O | -8.0301382552 | -1.4533546776 | 0.3978632022 |
| Cl | 3.4176756589 | 5.0525434157 | -0.1975095188 |
| C | 0.8433674681 | -3.6573350606 | -2.7343458024 |

| | | | |
|---|---|---|---|
| C | 1.5803065942 | -5.0689722559 | -0.7778325132 |
| O | 2.7658888865 | -5.5432758002 | -1.3381365764 |
| O | -6.1207097895 | 0.3425330566 | 0.6705843565 |
| H | -6.2818119447 | -2.981258516 | 1.5558399721 |
| H | 2.1886210438 | -1.7938113648 | -1.5542059342 |
| H | 4.3135001879 | -0.9720804722 | -0.9277359821 |
| H | 5.6974583716 | -0.4475450406 | 0.9266843964 |
| H | 5.742708945 | -2.2112916964 | 0.811463382 |
| H | 5.4384827094 | -1.3649010289 | 3.189835058 |
| H | 4.0581861595 | 0.630193969 | 2.7175990756 |
| H | 3.1206209369 | -0.455789229 | 3.7445951761 |
| H | 1.8873837827 | -1.1693261261 | 1.8872914976 |
| H | 0.7818054064 | 1.104646789 | 0.9281376725 |
| H | 1.4873590164 | 1.9201661983 | -2.5422315718 |
| H | 0.7865604953 | 4.458840674 | -1.2371253813 |
| H | 1.9042961748 | 4.2497150798 | -2.5962971008 |
| H | 3.4331358424 | 2.9275686226 | -1.188709595 |
| H | 2.9295376115 | 2.4852155723 | 1.1974136825 |
| H | 1.4285702489 | 3.4094537957 | 1.0697361345 |
| H | -1.2822864293 | 1.5810274905 | -2.9781827309 |
| H | -2.7369469556 | 3.4548969425 | -1.0605053417 |
| H | -1.4354521194 | 3.8413554151 | -2.2208831136 |
| H | -3.0378849135 | 3.3556075565 | -2.8010436362 |
| H | -2.6620213497 | -0.1467714078 | -2.4041255893 |
| H | -6.667741834 | 0.1675757294 | -1.3206897112 |
| H | -4.7930160211 | -0.9513726334 | -2.1431863471 |
| H | -6.9465176278 | -2.2870641424 | -1.090601872 |
| H | -2.8924517655 | -4.1894884084 | 0.1015863182 |
| H | -2.0047886617 | -2.9585795119 | 1.0259911711 |
| H | -7.888896529 | -0.6978345552 | 0.9926599513 |
| H | 1.6685871813 | -4.0986346653 | -3.2970118703 |
| H | 0.6453943846 | -2.6498981199 | -3.1119800934 |
| H | -0.0574058034 | -4.253441241 | -2.8826876932 |
| H | 0.7644356194 | -5.7177695237 | -1.1064768897 |
| H | 1.6151946602 | -5.0941796751 | 0.3170331367 |
| H | 3.4624488625 | -5.1360290297 | -0.7932429151 |
| H | -5.4997546505 | 1.0959081049 | 0.5500645943 |
| H | 4.143657668 | -2.4362298356 | 2.6512003557 |

**1g** conf_6

energy (M062X/6-31g(d,p)) = -2585.2719508 Hartree

| | | | |
|---|---|---|---|
| C | 0.4268613279 | -2.8197457469 | -0.9371525744 |
| O | 0.4038229608 | -1.8418815502 | -0.2335648105 |
| C | 1.6223234935 | -3.2812178644 | -1.7799583479 |
| N | 2.7900743476 | -2.528952556 | -1.3504772677 |
| C | 3.2000121789 | -2.5055653121 | -0.0512841709 |
| O | 2.905836178 | -3.3507569305 | 0.7806692427 |
| C | 4.031492372 | -1.2611240115 | 0.2895094944 |
| C | 4.9354646678 | -1.4364820467 | 1.5097308565 |
| C | 4.168580394 | -1.3977538666 | 2.8305348061 |
| C | 3.2579781788 | -0.1758252562 | 2.8642629791 |
| N | 2.3701433365 | -0.1012222687 | 1.706996514 |

| | | | |
|---|---|---|---|
| N | 3.094124663 | -0.1459827848 | 0.5080376507 |
| C | 2.6711165276 | 0.6037647871 | -0.5404391596 |
| O | 3.0953693839 | 0.4010591642 | -1.6847579972 |
| C | 1.6979509363 | 1.7448978388 | -0.2386394954 |
| N | 0.8608038082 | 2.0094678658 | -1.3942790437 |
| N | 1.4443844196 | 2.5773083013 | -2.5353014435 |
| C | 2.106694889 | 3.8341698847 | -2.1981565242 |
| C | 3.1204718001 | 3.6433084349 | -1.0716096565 |
| C | 2.452465718 | 3.0303006227 | 0.1500402455 |
| C | -0.4418897027 | 1.5856894722 | -1.4062873053 |
| O | -0.9380225705 | 1.0232894107 | -0.4466694671 |
| C | -1.2443221884 | 1.8497241102 | -2.6953146537 |
| C | -1.6807253215 | 3.3089306604 | -2.8208995456 |
| N | -2.341952886 | 0.8981065018 | -2.7461692953 |
| C | -3.396381961 | 0.9175997786 | -1.9103617196 |
| O | -3.7748917851 | 1.9108256235 | -1.2925898308 |
| C | -5.6475468481 | -0.1237508739 | -1.3964341474 |
| C | -4.2157950408 | -0.4114779894 | -1.882116546 |
| N | -3.5757310372 | -1.4696957694 | -1.0727237945 |
| N | -4.2067050046 | -2.1314301296 | -0.0335627779 |
| C | -5.4799497644 | -2.1103606682 | -0.0121552654 |
| C | -6.3587712168 | -1.4175884495 | -1.0203765689 |
| C | -2.416656026 | -2.0624948154 | -1.4773039367 |
| O | -1.8533513097 | -1.7806658124 | -2.5275102667 |
| C | -1.8650170235 | -3.1500604662 | -0.5573468004 |
| O | -0.6418810533 | -3.6314073637 | -1.1007409464 |
| O | -7.6326702988 | -1.1552802415 | -0.501207571 |
| Cl | 3.8689856142 | 5.228343792 | -0.6471711457 |
| C | 1.3424067489 | -2.9178531317 | -3.2416853833 |
| C | 1.872343992 | -4.80639146 | -1.6534874902 |
| O | 0.9267411736 | -5.587048158 | -2.3390770447 |
| O | -5.7165699368 | 0.6323883594 | -0.2163820041 |
| H | -5.9550964585 | -2.6371963471 | 0.8115823082 |
| H | 2.952952412 | -1.6597568697 | -1.8529636296 |
| H | 4.6285677644 | -0.9833014501 | -0.5817148644 |
| H | 5.675966108 | -0.6278702927 | 1.4927943776 |
| H | 5.4800587171 | -2.3790846305 | 1.4070571667 |
| H | 4.8711584811 | -1.3677826753 | 3.6701214077 |
| H | 3.8481985206 | 0.7478077869 | 2.8831342173 |
| H | 2.6177149319 | -0.173874723 | 3.7508581713 |
| H | 1.7172297398 | -0.8856924377 | 1.6971447078 |
| H | 1.0403639662 | 1.4465588763 | 0.574363991 |
| H | 2.1389876068 | 1.9038462656 | -2.8590926522 |
| H | 1.3472056845 | 4.5603073859 | -1.8917447594 |
| H | 2.5951804794 | 4.2107359106 | -3.1003527392 |
| H | 3.9428572872 | 3.0133211254 | -1.4190433328 |
| H | 3.1855365237 | 2.8178137404 | 0.9323924632 |
| H | 1.7262058676 | 3.7416103563 | 0.5563272774 |
| H | -0.6035639729 | 1.6192422599 | -3.549120287 |
| H | -2.2224479959 | 3.6394901413 | -1.9360620364 |
| H | -0.7992230995 | 3.9339400699 | -2.9743683352 |
| H | -2.3373549034 | 3.4183891168 | -3.6878554104 |
| H | -2.0750045632 | -0.0428406052 | -3.0295097423 |
| H | -6.1764518366 | 0.3757515646 | -2.2209777618 |

| | | | |
|---|---|---|---|
| H | -4.2745417685 | -0.7847607089 | -2.9122273529 |
| H | -6.4876051775 | -2.0657559741 | -1.8963542381 |
| H | -2.5340909554 | -4.0080069354 | -0.5135345458 |
| H | -1.7228656773 | -2.7555267619 | 0.4490637658 |
| H | -7.512871932 | -0.3705989591 | 0.0597977138 |
| H | 1.1612678084 | -1.8445667003 | -3.3458446887 |
| H | 0.4697492614 | -3.4558691828 | -3.6060999531 |
| H | 2.2072890079 | -3.1968960803 | -3.8499773816 |
| H | 1.9466824867 | -5.0748170062 | -0.5949904436 |
| H | 2.8407375753 | -5.0041000048 | -2.120083047 |
| H | 0.0720572641 | -5.4192493813 | -1.919055714 |
| H | -5.1084069141 | 1.3921613157 | -0.3582448447 |
| H | 3.5694396258 | -2.3068872745 | 2.9282924016 |

**1g** conf_7

energy (M062X/6-31g(d,p)) = -2585.271894 Hartree

| | | | |
|---|---|---|---|
| C | -0.9220552266 | -2.5475351072 | 0.4474302345 |
| O | -0.7565095323 | -1.5303295892 | 1.0821563038 |
| C | 0.1487234334 | -3.1779399214 | -0.4385508338 |
| N | 1.2502060953 | -2.2159300438 | -0.3702038499 |
| C | 2.4951994468 | -2.3585148582 | -0.8474878564 |
| O | 2.9608639243 | -3.3953842743 | -1.321468759 |
| C | 3.3631995239 | -1.0874027711 | -0.8080220559 |
| C | 4.8402312507 | -1.4304107255 | -0.6079466271 |
| C | 5.115250854 | -1.8243834528 | 0.8411488049 |
| C | 4.5825961424 | -0.750039502 | 1.7842349024 |
| N | 3.1703329246 | -0.4319909466 | 1.5582438859 |
| N | 2.9166470218 | -0.1401387999 | 0.2109816345 |
| C | 2.4111742064 | 1.0815987837 | -0.139390938 |
| O | 2.2716342322 | 1.3990736486 | -1.3173822618 |
| C | 1.991769593 | 2.0189310533 | 0.9956327322 |
| N | 0.7288443659 | 2.6510767679 | 0.638667116 |
| N | 0.7135017826 | 3.618571335 | -0.3756475084 |
| C | 1.6565522956 | 4.6903832195 | -0.0728409399 |
| C | 3.0624143888 | 4.1423949599 | 0.1616144638 |
| C | 3.0476333507 | 3.1014999103 | 1.2711569452 |
| C | -0.4359770869 | 2.1669769592 | 1.1600660435 |
| O | -0.4438149599 | 1.2706894714 | 1.9923422356 |
| C | -1.742928299 | 2.8020482799 | 0.6984727768 |
| C | -2.0820597031 | 3.9944837155 | 1.597070594 |
| N | -2.7398293242 | 1.7463745871 | 0.7738371393 |
| C | -3.9258487657 | 1.8614085969 | 0.1741204432 |
| O | -4.3067959696 | 2.8815813558 | -0.4049775564 |
| C | -6.2569676432 | 1.2253660718 | 0.7320753781 |
| C | -4.9062798945 | 0.6784472109 | 0.212441408 |
| N | -4.4404802851 | -0.5042461403 | 0.9352840549 |
| N | -4.881164476 | -0.8651742307 | 2.1973322474 |
| C | -6.0700057425 | -0.5054960423 | 2.4875350081 |
| C | -7.0128379528 | 0.1648955304 | 1.5249689353 |
| C | -3.5435816058 | -1.3399732181 | 0.3193588932 |
| O | -3.1265070548 | -1.1174884505 | -0.8016926128 |
| C | -3.1328564632 | -2.5732829541 | 1.1215261156 |

| | | | |
|---|---|---|---|
| O | -2.0686939886 | -3.2327298674 | 0.4462972493 |
| O | -8.1340737085 | 0.7081423039 | 2.1603651143 |
| Cl | 4.1828982571 | 5.4884759827 | 0.5897118126 |
| C | -0.3809236913 | -3.3095868731 | -1.8708172501 |
| C | 0.5337592318 | -4.5714444951 | 0.1357538818 |
| O | 1.2007471543 | -5.3905169384 | -0.770036992 |
| O | -6.1040218389 | 2.2998930989 | 1.6353633656 |
| H | -6.4310212672 | -0.7617116216 | 3.480037419 |
| H | 0.9829922882 | -1.3134249131 | 0.0065232565 |
| H | 3.216749138 | -0.5829500139 | -1.7676824261 |
| H | 5.435731469 | -0.5508484512 | -0.8772342632 |
| H | 5.1016230678 | -2.2393628093 | -1.2920895057 |
| H | 6.1888808047 | -1.966279177 | 1.0020033718 |
| H | 5.1497889885 | 0.1792904058 | 1.6578894603 |
| H | 4.6719235284 | -1.0467170096 | 2.8331397913 |
| H | 2.580799816 | -1.2196282888 | 1.8230100594 |
| H | 1.8176429057 | 1.4402159404 | 1.8993871327 |
| H | 1.0049918963 | 3.1408237447 | -1.2290283445 |
| H | 1.3108722308 | 5.2209358873 | 0.8199249925 |
| H | 1.6469284476 | 5.3911442334 | -0.9110169894 |
| H | 3.4513504855 | 3.7146416533 | -0.7645908508 |
| H | 4.0343403446 | 2.6461243927 | 1.3923262761 |
| H | 2.7928756926 | 3.5919154859 | 2.2164382948 |
| H | -1.669596556 | 3.1437560813 | -0.334119017 |
| H | -2.1380795397 | 3.6801746724 | 2.6424871505 |
| H | -1.3188213795 | 4.7706494572 | 1.4980441382 |
| H | -3.0419732587 | 4.4138494584 | 1.2922783278 |
| H | -2.4699539019 | 0.9135097691 | 1.2837686913 |
| H | -6.8563489506 | 1.5436353052 | -0.1267699043 |
| H | -5.0187114763 | 0.3758051505 | -0.832256859 |
| H | -7.3697194692 | -0.607920363 | 0.8298370034 |
| H | -3.9479701345 | -3.2963059936 | 1.1652143412 |
| H | -2.8468670479 | -2.2971708901 | 2.1366060757 |
| H | -7.8520603827 | 1.5884855051 | 2.4586476523 |
| H | -0.7427895717 | -2.3460629747 | -2.235756613 |
| H | -1.2018075568 | -4.0274201466 | -1.902082948 |
| H | 0.4192745014 | -3.6728772296 | -2.5161025307 |
| H | -0.3918409771 | -5.086572782 | 0.4037908515 |
| H | 1.107324227 | -4.404481157 | 1.062107035 |
| H | 1.9890946237 | -4.8898393407 | -1.0617391518 |
| H | -5.7327810545 | 3.0337202581 | 1.1174695002 |
| H | 4.6319918054 | -2.7849778795 | 1.0602149039 |

**1g** conf_8

energy (M062X/6-31g(d,p)) = -2585.2716893 Hartree

| | | | |
|---|---|---|---|
| C | -0.0059510582 | -3.8167021079 | -0.62605148 |
| O | -0.7769713315 | -4.7447858232 | -0.6238320829 |
| C | 1.2583958316 | -3.8075020564 | -1.4802546706 |
| N | 2.2361545233 | -2.8089952477 | -1.0693198213 |
| C | 2.7434394946 | -2.7211383296 | 0.1870363928 |
| O | 2.5461405514 | -3.5440420247 | 1.0697039939 |
| C | 3.5938922587 | -1.4602479701 | 0.401581434 |

| | | | |
|---|---|---|---|
| C | 4.6475347136 | -1.6110648063 | 1.5009099801 |
| C | 4.0636237443 | -1.5118996966 | 2.9084995411 |
| C | 3.1875816813 | -0.2701563529 | 3.0166423105 |
| N | 2.1492998084 | -0.2279706103 | 1.9864348331 |
| N | 2.7031799033 | -0.3306590448 | 0.702584979 |
| C | 2.2144264471 | 0.4342928755 | -0.3078096463 |
| O | 2.4804893496 | 0.1826398705 | -1.4875423315 |
| C | 1.3914067296 | 1.6612140138 | 0.0764470162 |
| N | 0.3220951118 | 1.8766404005 | -0.8869100243 |
| N | 0.6389697938 | 2.3176673705 | -2.1783035031 |
| C | 1.4311544553 | 3.5428624764 | -2.1287133856 |
| C | 2.6731606675 | 3.3722306725 | -1.2579225019 |
| C | 2.2793201491 | 2.91761851 | 0.1389159635 |
| C | -0.9473992157 | 1.5004928745 | -0.5814605569 |
| O | -1.2145108364 | 0.9860821878 | 0.5016323745 |
| C | -2.0527282888 | 1.7707293201 | -1.6098729034 |
| C | -2.4053827669 | 3.2560805971 | -1.6827517496 |
| N | -3.1803995094 | 0.9647821555 | -1.1707605728 |
| C | -3.8008047155 | 0.1092547575 | -2.0422439777 |
| O | -3.8848836414 | 0.289540729 | -3.2393169153 |
| C | -5.8499726393 | -0.5406177708 | -0.7489936848 |
| C | -4.5327411672 | -1.0516779639 | -1.3473806457 |
| N | -3.7037223782 | -1.6616868493 | -0.304842168 |
| N | -4.1811316162 | -2.1333805783 | 0.8878423031 |
| C | -5.4412797662 | -2.1223876894 | 1.0827764498 |
| C | -6.4873097662 | -1.6207038665 | 0.1181693177 |
| C | -2.3910237821 | -1.9503890833 | -0.5997131247 |
| O | -1.9374049148 | -1.7244571558 | -1.7060288783 |
| C | -1.538206231 | -2.5022487726 | 0.5350201947 |
| O | -0.2172592302 | -2.6650039197 | 0.0398488545 |
| O | -7.6162042888 | -1.1355549523 | 0.7948581112 |
| Cl | 3.5785255525 | 4.9281703024 | -1.1718341912 |
| C | 0.8170375282 | -3.4575758961 | -2.9068497525 |
| C | 1.8955604712 | -5.2135592383 | -1.4578532023 |
| O | 3.0145343114 | -5.2842865653 | -2.3085655553 |
| O | -5.672390008 | 0.5467327634 | 0.1358580193 |
| H | -5.7800276357 | -2.5002812224 | 2.0437874642 |
| H | 2.3042084289 | -1.9664876024 | -1.6322884763 |
| H | 4.0809767208 | -1.205741724 | -0.5419473779 |
| H | 5.3906580751 | -0.8176432093 | 1.357501518 |
| H | 5.1612372767 | -2.5663469682 | 1.3634579499 |
| H | 4.8716709862 | -1.4690259058 | 3.6462419007 |
| H | 3.7860232756 | 0.642157845 | 2.913943904 |
| H | 2.6737154321 | -0.2192794674 | 3.9806520682 |
| H | 1.5162328864 | -1.0190272488 | 2.1062066866 |
| H | 0.9281976135 | 1.4916919188 | 1.0455170511 |
| H | 1.1879478861 | 1.5727303778 | -2.6070738555 |
| H | 0.8081863568 | 4.3487074637 | -1.7275201079 |
| H | 1.7056307601 | 3.8035241963 | -3.1534806002 |
| H | 3.3553209047 | 2.6558257157 | -1.719811911 |
| H | 3.1639857945 | 2.7224895368 | 0.7509126774 |
| H | 1.707709856 | 3.7144409931 | 0.626212423 |
| H | -1.7425013464 | 1.4256212249 | -2.5982357331 |
| H | -1.5604681878 | 3.8387048559 | -2.0543700853 |

H -3.2441247433 3.3863597518 -2.3704297184
H -2.6981259782 3.6352758333 -0.6992085741
H -3.0323582674 0.616471404 -0.225238214
H -6.5160271194 -0.2706648687 -1.5779199588
H -4.748785243 -1.7800068796 -2.1347326702
H -6.8289344851 -2.4493011653 -0.5132431796
H -1.935207142 -3.4428232631 0.914914002
H -1.4880393539 -1.7710674442 1.3418086854
H -7.3596913173 -0.2614050039 1.1290361643
H 0.0647960818 -4.1729999765 -3.2426847275
H 0.376842512 -2.458322922 -2.9453057675
H 1.6812093151 -3.5211203637 -3.571870339
H 1.1639578541 -5.9307824811 -1.8294844034
H 2.1493519072 -5.4802658539 -0.4264819203
H 3.6644218485 -4.6572765873 -1.9644033247
H -5.1717976444 1.2449479741 -0.3157883211
H 3.4678607659 -2.4044164382 3.1197920281

**1g** conf_9

energy (M062X/6-31g(d,p)) = -2585.2704595 Hartree

C -0.5496063072 -0.554950757 0.791857345
O 0.17430095 -0.1265544849 1.6647817917
C -0.9274238044 0.1997479748 -0.4757123372
N -0.7057045586 1.6229467934 -0.1895450049
C -0.7307867914 2.5843302958 -1.1272338829
O -0.7731323872 2.3691699389 -2.3448453746
C -0.7618083828 4.0433293484 -0.6572400751
C 0.0443362649 4.9499676023 -1.5935608087
C 1.5414563036 4.8157190999 -1.3310128874
C 1.8285767874 5.0462841903 0.1483418204
N 1.0318483917 4.1842921367 1.0270101284
N -0.3318470586 4.2425019665 0.7172430692
C -1.2225454839 4.655435932 1.6683258483
O -2.4189820599 4.7535025752 1.4340551701
C -0.6273428005 5.1633173342 2.9876571304
N -0.0616838231 4.1456566869 3.8746197491
N 0.5686818033 4.628451222 5.0268391441
C -0.3594493504 5.4084343549 5.8388566497
C -1.0790518011 6.5058975617 5.0638236912
C -1.6644293637 5.97411837 3.7631524489
C -0.2600137164 2.8128681377 3.7360450344
O -0.9546673537 2.3499721241 2.8349908824
C 0.478511745 1.9079640962 4.7290788602
C 1.9692460755 1.8388892412 4.3901907933
N -0.1008153572 0.5846935127 4.6972243563
C -0.8400213951 0.0999220303 5.7022618398
O -1.1080750753 0.740342982 6.7257711796
C -1.2210269773 -2.1736816943 6.8114223221
C -1.4172614744 -1.3147505518 5.5471669929
N -0.8889758091 -2.0415274922 4.3994509786
N 0.2147152219 -2.8453141304 4.4691280784
C 0.7335201191 -3.0900932535 5.6107429496

| | | | |
|---|---|---|---|
| C | 0.2460801379 | -2.572344438 | 6.9424580239 |
| C | -1.4747605647 | -1.8708773898 | 3.1682391999 |
| O | -2.4764042162 | -1.1906454277 | 3.0309104512 |
| C | -0.7832827896 | -2.5347213271 | 1.9834283248 |
| O | -1.0799033178 | -1.7809898853 | 0.8113018836 |
| O | 0.9913204875 | -1.4345764207 | 7.3417890193 |
| Cl | 0.0968043525 | 7.8587859368 | 4.7077786323 |
| C | -2.3932918545 | -0.0489859677 | -0.8436575859 |
| C | 0.0272936784 | -0.3538897033 | -1.5864187138 |
| O | -0.4540946095 | -0.201616799 | -2.8870251568 |
| O | -1.7332888563 | -1.5568655569 | 7.9543952843 |
| H | 1.6182296468 | -3.7211206275 | 5.5826634452 |
| H | -0.7438432862 | 1.9027737309 | 0.7905903025 |
| H | -1.8173362088 | 4.3302213419 | -0.6829337376 |
| H | -0.2718286885 | 5.9831419613 | -1.4136407648 |
| H | -0.2042172843 | 4.6980034266 | -2.62545363 |
| H | 2.1000863127 | 5.5353104218 | -1.937773265 |
| H | 1.6054643078 | 6.084754786 | 0.4178386652 |
| H | 2.8775982369 | 4.8588396985 | 0.3919336899 |
| H | 1.3347614581 | 3.2162771408 | 0.9363144068 |
| H | 0.2116889527 | 5.8126882386 | 2.7130518723 |
| H | 1.3640596335 | 5.1976530314 | 4.7432991957 |
| H | 0.1954571322 | 5.8190094654 | 6.6843999358 |
| H | -1.1173429583 | 4.7230729457 | 6.2335542187 |
| H | -1.8511243482 | 6.9665737224 | 5.6803816341 |
| H | -2.5139086303 | 5.3285696826 | 4.0087197265 |
| H | -2.0449485987 | 6.7920003231 | 3.1487491503 |
| H | 0.347643002 | 2.2917773862 | 5.7394837866 |
| H | 2.4259594288 | 2.8274429399 | 4.4575743561 |
| H | 2.4705717625 | 1.1723171856 | 5.0959289891 |
| H | 2.1192114517 | 1.4506471901 | 3.3787254383 |
| H | -0.0018294906 | 0.0641097354 | 3.8342438545 |
| H | -1.7863049577 | -3.098481088 | 6.6515040867 |
| H | -2.4884759541 | -1.1840320011 | 5.3787913984 |
| H | 0.3295816469 | -3.3708593017 | 7.6898487936 |
| H | -1.1977037684 | -3.5281700124 | 1.8097575643 |
| H | 0.2912296324 | -2.6112584075 | 2.1322164735 |
| H | 1.900203806 | -1.7138989833 | 7.5184765903 |
| H | -2.6525160881 | 0.5567818804 | -1.7122552259 |
| H | -3.0455234458 | 0.2228666136 | -0.0104532429 |
| H | -2.5562608818 | -1.097841028 | -1.093638968 |
| H | 0.1400639426 | -1.4283061333 | -1.4210069685 |
| H | 1.0102523765 | 0.116431594 | -1.4397509789 |
| H | -0.6005179086 | 0.7641362901 | -2.9781650459 |
| H | -1.4817859269 | -0.6129040901 | 7.8742362867 |
| H | 1.8863907163 | 3.8153147757 | -1.6222992799 |

**1g** conf_10

energy (M062X/6-31g(d,p)) = -2585.2700633 Hartree

| | | | |
|---|---|---|---|
| C | -0.4228669055 | -2.9937069224 | 0.1734555526 |
| O | -0.2628458561 | -2.226598037 | 1.0933764057 |
| C | 0.7057784822 | -3.5196570235 | -0.7108030765 |

| | | | |
|---|---|---|---|
| N | 1.7926658097 | -2.565407982 | -0.4874018556 |
| C | 3.1130126389 | -2.7465271422 | -0.6369335144 |
| O | 3.6638639381 | -3.8006999441 | -0.9551648394 |
| C | 3.979921343 | -1.4976995529 | -0.4024493223 |
| C | 5.2767623156 | -1.8587592362 | 0.3268143685 |
| C | 5.0203012584 | -2.0968130047 | 1.8128782811 |
| C | 4.2777276103 | -0.9039890802 | 2.4091341345 |
| N | 3.0491407256 | -0.5707864224 | 1.6890064882 |
| N | 3.27305033 | -0.4375507187 | 0.3112105466 |
| C | 2.9502816289 | 0.7284230017 | -0.324482909 |
| O | 3.1907949279 | 0.8890156116 | -1.519540808 |
| C | 2.248052165 | 1.8100536297 | 0.495754009 |
| N | 1.1819129916 | 2.4007403378 | -0.3032653326 |
| N | 1.5320161207 | 3.2111323658 | -1.3956817825 |
| C | 2.3742480069 | 4.3178372136 | -0.9553615039 |
| C | 3.6143618165 | 3.8051755423 | -0.2270894769 |
| C | 3.2143716266 | 2.9192462893 | 0.9433339255 |
| C | -0.0718005647 | 1.846911091 | -0.236136362 |
| O | -0.3063389776 | 0.9094486766 | 0.5059920684 |
| C | -1.1563281353 | 2.4652843394 | -1.1372252949 |
| C | -1.4339976952 | 3.9396705996 | -0.8395042877 |
| N | -2.3524482495 | 1.6409597937 | -1.0769894711 |
| C | -3.1403869883 | 1.562692812 | 0.0134276186 |
| O | -3.055576036 | 2.3160690285 | 0.9809300254 |
| C | -5.5432041444 | 1.1146318767 | 0.6032017335 |
| C | -4.3053974665 | 0.5356982841 | -0.1049492984 |
| N | -3.9668556081 | -0.7911623938 | 0.4323535669 |
| N | -4.7909372033 | -1.5159777471 | 1.2670496493 |
| C | -5.9998783435 | -1.1384417086 | 1.4013827241 |
| C | -6.630869306 | 0.0551028293 | 0.7328343644 |
| C | -2.9761438505 | -1.5335967897 | -0.150310527 |
| O | -2.3471733378 | -1.1435539651 | -1.1212548267 |
| C | -2.7284783062 | -2.9077841452 | 0.4702429404 |
| O | -1.6121081985 | -3.5038432661 | -0.1724271309 |
| O | -7.7163715752 | 0.5421434097 | 1.473036718 |
| Cl | 4.6042270927 | 5.1951746395 | 0.356132902 |
| C | 0.3018135729 | -3.5440851248 | -2.1853615956 |
| C | 1.0420945415 | -4.958118166 | -0.2125486498 |
| O | 1.7881060256 | -5.7123669904 | -1.1103455773 |
| O | -5.3085698147 | 1.5064813 | 1.9290612732 |
| H | -6.6151911793 | -1.735437692 | 2.0698751729 |
| H | 1.4877849313 | -1.6357182502 | -0.2285997974 |
| H | 4.2044900419 | -1.0922994039 | -1.3928483922 |
| H | 5.9832731767 | -1.0308504668 | 0.1987481152 |
| H | 5.7030470092 | -2.7432164102 | -0.1497457006 |
| H | 5.9653019799 | -2.2552876196 | 2.3426476208 |
| H | 4.9195018166 | -0.015376439 | 2.3929487494 |
| H | 3.9910527453 | -1.080863706 | 3.4495288275 |
| H | 2.3374195027 | -1.2868006811 | 1.8293504271 |
| H | 1.7881651195 | 1.3570583472 | 1.3703810178 |
| H | 2.0689509978 | 2.6152956516 | -2.0283140017 |
| H | 1.7898484177 | 4.9606529132 | -0.2897056215 |
| H | 2.6548035821 | 4.8999998411 | -1.8365684996 |
| H | 4.252513987 | 3.2586440263 | -0.9245696023 |

| | | | |
|---|---|---|---|
| H | 4.0958986253 | 2.4829564023 | 1.421063832 |
| H | 2.700961088 | 3.5305898203 | 1.6925103044 |
| H | -0.7986313957 | 2.400183461 | -2.1689685321 |
| H | -1.6568906835 | 4.0988800576 | 0.2141144815 |
| H | -0.5666873528 | 4.5321263854 | -1.1302631208 |
| H | -2.2936345756 | 4.2693687591 | -1.4289891198 |
| H | -2.3180501777 | 0.7687037125 | -1.5964127669 |
| H | -5.9043490976 | 1.9563457095 | -0.0060750766 |
| H | -4.5449066282 | 0.4188840167 | -1.169293178 |
| H | -7.0143882817 | -0.2369593761 | -0.2524611592 |
| H | -3.5705407109 | -3.574377221 | 0.2894239176 |
| H | -2.5699076114 | -2.816355478 | 1.5449855278 |
| H | -7.313766372 | 1.044763516 | 2.2008797089 |
| H | -0.0271395087 | -2.5545428172 | -2.5103213449 |
| H | -0.511936905 | -4.2528206895 | -2.3444980614 |
| H | 1.1566367159 | -3.8637139158 | -2.7823018974 |
| H | 0.0903590028 | -5.4790139409 | -0.077253457 |
| H | 1.5213637959 | -4.8695131448 | 0.7747211571 |
| H | 2.6441336849 | -5.2441055976 | -1.1884200546 |
| H | -4.4671863557 | 2.0145067328 | 1.9129271261 |
| H | 4.4249722095 | -3.0092738119 | 1.9456215445 |

**1g** conf_11

energy (M062X/6-31g(d,p)) = -2585.2699553 Hartree

| | | | |
|---|---|---|---|
| C | 0.197272409 | -3.0715637007 | -0.475200318 |
| O | 0.2102037397 | -2.1029064475 | 0.2481028474 |
| C | 1.3475661221 | -3.4838032401 | -1.4045158713 |
| N | 2.4915815729 | -2.6330174936 | -1.1168758491 |
| C | 3.0755401334 | -2.5986851754 | 0.1125892418 |
| O | 2.9592413794 | -3.4729201229 | 0.9577397844 |
| C | 3.8875313998 | -1.3181893968 | 0.3547790077 |
| C | 4.9374807206 | -1.4601287877 | 1.4567377259 |
| C | 4.3307320831 | -1.4572730216 | 2.8587328908 |
| C | 3.3883345111 | -0.2689798273 | 3.0119883892 |
| N | 2.3735954813 | -0.2096816782 | 1.9636741049 |
| N | 2.9524552576 | -0.2315597484 | 0.6883130048 |
| C | 2.4151979887 | 0.531515787 | -0.2951452385 |
| O | 2.6836146161 | 0.3278222513 | -1.4860215229 |
| C | 1.5276877761 | 1.6998667749 | 0.1298398308 |
| N | 0.4238169468 | 1.8577012883 | -0.8033967438 |
| N | 0.6873627107 | 2.3195750331 | -2.0996182624 |
| C | 1.3946544996 | 3.5967506066 | -2.0558127229 |
| C | 2.6636808456 | 3.5048721949 | -1.2121811707 |
| C | 2.3357283241 | 3.0094980541 | 0.1880129794 |
| C | -0.8272194003 | 1.4483075378 | -0.4537396961 |
| O | -1.0652666736 | 0.9801461112 | 0.6525888908 |
| C | -1.9421476058 | 1.6094277624 | -1.4871231343 |
| C | -2.4193472162 | 3.0582101346 | -1.5868798638 |
| N | -3.0065497472 | 0.7236467675 | -1.0403413975 |
| C | -3.7899470694 | 0.0842135199 | -1.9538824775 |
| O | -3.9331196925 | 0.4508966781 | -3.1048636888 |
| C | -5.844014575 | -0.4173842399 | -0.6313803227 |

| | | | |
|---|---|---|---|
| C | -4.6592198772 | -1.0440213834 | -1.380331663 |
| N | -3.9280984777 | -1.9519389185 | -0.4944092039 |
| N | -4.4997771527 | -2.5954394221 | 0.5711317571 |
| C | -5.7359438006 | -2.3994473911 | 0.8156079432 |
| C | -6.6726409912 | -1.5039730463 | 0.0430602915 |
| C | -2.7035365168 | -2.434995106 | -0.8986909295 |
| O | -2.1771627393 | -2.0434613346 | -1.9224698657 |
| C | -2.0518269675 | -3.4694418809 | 0.0137160711 |
| O | -0.846871375 | -3.9007181837 | -0.5930201684 |
| O | -7.6571286535 | -0.9556538342 | 0.8784452462 |
| Cl | 3.4605299816 | 5.1209304797 | -1.1296019673 |
| C | 0.9113956667 | -3.2068137581 | -2.8467192782 |
| C | 1.7490940706 | -4.9792344274 | -1.2442859505 |
| O | 0.8588169071 | -5.8884675516 | -1.8370808347 |
| O | -5.4408477066 | 0.4193118488 | 0.4307217567 |
| H | -6.1391124717 | -2.9236870037 | 1.6782824583 |
| H | 2.5241618487 | -1.7501656244 | -1.620769299 |
| H | 4.365102763 | -1.0228805043 | -0.5821737507 |
| H | 5.6382905798 | -0.6224016898 | 1.3581066285 |
| H | 5.5019317197 | -2.3802451712 | 1.28317011 |
| H | 5.125690191 | -1.4060333362 | 3.6103378072 |
| H | 3.9464146784 | 0.6741642197 | 2.9789150423 |
| H | 2.8520904596 | -0.2990259145 | 3.9645901829 |
| H | 1.7329657888 | -1.0018044922 | 2.0206181924 |
| H | 1.0995728642 | 1.4859395242 | 1.1062869445 |
| H | 1.2853873901 | 1.6173314938 | -2.5349441216 |
| H | 0.7259183137 | 4.3542523802 | -1.6346963439 |
| H | 1.6298646186 | 3.8840811562 | -3.0833950855 |
| H | 3.3843065379 | 2.8433740863 | -1.6967019147 |
| H | 3.2467565001 | 2.8653353862 | 0.7750397824 |
| H | 1.7257555186 | 3.7613379473 | 0.6995957973 |
| H | -1.59880038 | 1.2819105596 | -2.4709532199 |
| H | -2.7344832622 | 3.4296254297 | -0.6072555023 |
| H | -1.6265832353 | 3.7000354476 | -1.9756627339 |
| H | -3.2674360298 | 3.1022984854 | -2.2736191135 |
| H | -2.7868823242 | 0.2527396398 | -0.1657323383 |
| H | -6.4521864609 | 0.1309067253 | -1.362065722 |
| H | -5.0327896433 | -1.591905258 | -2.2516084693 |
| H | -7.1971343593 | -2.0949837936 | -0.716889391 |
| H | -2.6791311908 | -4.3536696593 | 0.115693197 |
| H | -1.8717831419 | -3.0440361981 | 1.0025715658 |
| H | -7.2157096437 | -0.2342133924 | 1.3546616695 |
| H | 0.6680017499 | -2.1501278686 | -2.983889684 |
| H | 1.721193563 | -3.4712916686 | -3.5352358173 |
| H | 0.0144074791 | -3.7768106825 | -3.0864599068 |
| H | 1.8060422982 | -5.2332276872 | -0.1877478692 |
| H | 2.7622387758 | -5.0666370499 | -1.6621064085 |
| H | 0.9530276556 | -5.8218572768 | -2.7946455185 |
| H | -4.8179307713 | 1.0807358163 | 0.0875405421 |
| H | 3.7813927147 | -2.3890577384 | 3.0162486675 |

**1g** conf_12

energy (M062X/6-31g(d,p)) = -2585.2691954 Hartree

| | | | |
|---|---|---|---|
| C | -0.2327320808 | -2.935692837 | -1.518090215 |
| O | -0.3748947409 | -1.7342814951 | -1.5051270379 |
| C | 1.0870766831 | -3.6502008739 | -1.2489019733 |
| N | 2.0325875505 | -2.5603271991 | -1.0072029404 |
| C | 3.235110947 | -2.6319592041 | -0.414758283 |
| O | 3.756918937 | -3.6567769174 | 0.0253609641 |
| C | 3.9581459854 | -1.2712476968 | -0.3241172111 |
| C | 5.3152287604 | -1.3744589226 | 0.3701700784 |
| C | 5.1789239923 | -1.4899352837 | 1.8868404687 |
| C | 4.2790919077 | -0.3785764311 | 2.4147623296 |
| N | 2.9777517379 | -0.3399494576 | 1.7465014953 |
| N | 3.118432193 | -0.2781880945 | 0.3549372757 |
| C | 2.3573418145 | 0.5900018982 | -0.3623200213 |
| O | 2.3488598863 | 0.5544850433 | -1.594499842 |
| C | 1.5192487062 | 1.6088464382 | 0.4122968822 |
| N | 0.2991749047 | 1.8921479588 | -0.3269199862 |
| N | 0.3809563016 | 2.6336512957 | -1.5140701179 |
| C | 1.0381280404 | 3.9124801359 | -1.2753915137 |
| C | 2.4122493033 | 3.7167721165 | -0.6388385639 |
| C | 2.2879236715 | 2.92046608 | 0.6512732376 |
| C | -0.8387211449 | 1.1997535639 | -0.0347094875 |
| O | -0.891375615 | 0.4114161972 | 0.8995239945 |
| C | -2.0733670762 | 1.4839601666 | -0.8877741804 |
| C | -2.7738639419 | 2.7601107159 | -0.414276501 |
| N | -2.9146751919 | 0.3126669193 | -0.7413160246 |
| C | -3.9031609053 | 0.024502531 | -1.5829223357 |
| O | -4.2371936771 | 0.7375075829 | -2.5387664975 |
| C | -6.1536612679 | -1.1054345996 | -1.2302203387 |
| C | -4.6380534439 | -1.3120587119 | -1.4036483641 |
| N | -4.1346625005 | -2.136411827 | -0.3147434414 |
| N | -4.5454924567 | -1.9174342565 | 0.9759046831 |
| C | -5.5610727354 | -1.1733248808 | 1.1844839729 |
| C | -6.4372177435 | -0.5196579856 | 0.1523300444 |
| C | -3.0085661474 | -2.9458564689 | -0.436093186 |
| O | -2.4560343205 | -3.4644408255 | 0.5026223832 |
| C | -2.5062361832 | -3.1844457 | -1.8686835839 |
| O | -1.2270522058 | -3.7898553144 | -1.8004586039 |
| O | -6.1934095625 | 0.868699152 | 0.1644849672 |
| Cl | 3.1729149576 | 5.3173531852 | -0.3108737845 |
| C | 1.4942398519 | -4.470827527 | -2.4786740595 |
| C | 0.906718222 | -4.5831952993 | -0.010440529 |
| O | 1.8623376187 | -5.5936132823 | 0.0706438914 |
| O | -6.692733264 | -0.2796133213 | -2.2273772799 |
| H | -5.8034768556 | -1.0211823741 | 2.2328820126 |
| H | 1.7260457267 | -1.6536263016 | -1.348333115 |
| H | 4.081196357 | -0.8992033702 | -1.3446931718 |
| H | 5.8892775401 | -0.4751782185 | 0.118550231 |
| H | 5.8493378388 | -2.2364029031 | -0.0347064177 |
| H | 6.1649098189 | -1.4322925634 | 2.3594035382 |
| H | 4.7485934058 | 0.6007770765 | 2.2682879627 |
| H | 4.0786478587 | -0.4899462423 | 3.4840198462 |
| H | 2.4407275796 | -1.1769349186 | 1.973202047 |
| H | 1.2288254324 | 1.1800726477 | 1.3684936862 |

| | | | |
|---|---|---|---|
| H | 0.938306426 | 2.073296842 | -2.1598693013 |
| H | 0.4068258486 | 4.5152847947 | -0.6151147776 |
| H | 1.122670067 | 4.4305195114 | -2.2336162757 |
| H | 3.0771245302 | 3.2117094861 | -1.3435803016 |
| H | 3.2715503201 | 2.7075779319 | 1.0777662809 |
| H | 1.7300413084 | 3.5136715723 | 1.3830300531 |
| H | -1.8007715779 | 1.5924846102 | -1.9379114414 |
| H | -2.1266826093 | 3.6263453523 | -0.5695911807 |
| H | -3.6900709733 | 2.8989296801 | -0.9902843955 |
| H | -3.0315830009 | 2.6854715204 | 0.645103543 |
| H | -2.6855060331 | -0.2825348306 | 0.047907988 |
| H | -6.6226493203 | -2.0950328439 | -1.2952946845 |
| H | -4.5096869538 | -1.8422506302 | -2.349774962 |
| H | -7.4867499412 | -0.7278124699 | 0.4140881765 |
| H | -2.4417617383 | -2.2644863233 | -2.4505375532 |
| H | -3.1509669458 | -3.9028208611 | -2.380225497 |
| H | -6.637446486 | 1.1962132882 | -0.6354023373 |
| H | 0.7550158595 | -5.248515512 | -2.678607826 |
| H | 1.5894916044 | -3.8282405337 | -3.3581724704 |
| H | 2.4509684468 | -4.9541014571 | -2.2802317434 |
| H | -0.0669429059 | -5.0665025342 | -0.0963581649 |
| H | 0.8792525829 | -3.9472246964 | 0.8867508045 |
| H | 2.7212722029 | -5.1387060665 | 0.1655872137 |
| H | -5.9422085259 | 0.2234993013 | -2.617595014 |
| H | 4.7542373448 | -2.4668145317 | 2.1415064825 |

**1g** conf_13

energy (M062X/6-31g(d,p)) = -2585.2689887 Hartree

| | | | |
|---|---|---|---|
| C | -0.4434493428 | -0.1656687029 | 0.6495048559 |
| O | 0.2121030265 | 0.416768556 | 1.4863449276 |
| C | -1.1740496383 | 0.5377690801 | -0.4919809468 |
| N | -0.7220626831 | 1.9256239068 | -0.3947453559 |
| C | -1.0893208181 | 2.9456681641 | -1.1747228681 |
| O | -1.7727126263 | 2.8417177256 | -2.2009922409 |
| C | -0.5917858338 | 4.3449078009 | -0.7873993585 |
| C | 0.3182587076 | 4.8807396049 | -1.8955690116 |
| C | 1.650775489 | 4.1276320314 | -1.9328188856 |
| C | 2.2225158145 | 3.9643725901 | -0.5040810368 |
| N | 1.4959913243 | 4.7472936378 | 0.4957774609 |
| N | 0.1318113672 | 4.4099540273 | 0.4886809264 |
| C | -0.5568917044 | 4.3880760813 | 1.6630182942 |
| O | -1.7742240638 | 4.2140641028 | 1.677827785 |
| C | 0.2580364927 | 4.5777308879 | 2.9444423339 |
| N | -0.3842858968 | 3.8646596844 | 4.0389282871 |
| N | -1.5821367721 | 4.3714878888 | 4.5625619958 |
| C | -1.4194873784 | 5.7560472404 | 4.9959104498 |
| C | -0.885960788 | 6.6236379615 | 3.8603511644 |
| C | 0.4217345557 | 6.0603208856 | 3.3282971357 |
| C | 0.1155057674 | 2.6759197023 | 4.4658475509 |
| O | 1.1154720519 | 2.1699286816 | 3.9645278568 |
| C | -0.5786204041 | 1.9777855147 | 5.6306018024 |
| C | 0.1817186287 | 2.2701764548 | 6.9263396657 |

| | | | |
|---|---|---|---|
| N | -0.5756775972 | 0.5615291011 | 5.2969859206 |
| C | -1.3690785878 | -0.3143530731 | 5.9105497133 |
| O | -2.1340558823 | -0.0099995816 | 6.8386018938 |
| C | -1.1193469494 | -2.7857436004 | 6.5103283105 |
| C | -1.416226492 | -1.757887296 | 5.404659746 |
| N | -0.5630239978 | -2.033130871 | 4.2580805749 |
| N | 0.71425509 | -2.5092459359 | 4.3641911148 |
| C | 1.1588808032 | -2.8338282967 | 5.5171204634 |
| C | 0.3791808489 | -2.8115569387 | 6.8020788137 |
| C | -1.0523324615 | -1.7838593253 | 2.9968442237 |
| O | -2.1625493013 | -1.3105110794 | 2.8350140008 |
| C | -0.1453013241 | -2.1383294812 | 1.8248760532 |
| O | -0.6413209193 | -1.4841406174 | 0.6589960679 |
| O | 0.7618109346 | -1.6694709112 | 7.543476909 |
| Cl | -0.6357888933 | 8.3167381257 | 4.4492854761 |
| C | -2.6821960107 | 0.4311702122 | -0.2173031178 |
| C | -0.8093995308 | -0.1072338984 | -1.8534705341 |
| O | -1.7052182966 | 0.2184797508 | -2.8799393576 |
| O | -1.8300642998 | -2.5222412578 | 7.693861007 |
| H | 2.190902992 | -3.1707586463 | 5.5340359405 |
| H | -0.1735308823 | 2.1274916818 | 0.4334776743 |
| H | -1.4949454986 | 4.9573259205 | -0.7061097243 |
| H | 0.4816337273 | 5.9494145791 | -1.725725927 |
| H | -0.2122413587 | 4.7894188219 | -2.844606379 |
| H | 2.3527701444 | 4.6717155259 | -2.570013938 |
| H | 3.264454166 | 4.286506353 | -0.449452735 |
| H | 2.1890538671 | 2.9207312725 | -0.1810492833 |
| H | 1.5788874811 | 5.738013534 | 0.2736863194 |
| H | 1.2430838619 | 4.1387008352 | 2.8009632603 |
| H | -2.263424147 | 4.3199310788 | 3.805434502 |
| H | -0.7262820845 | 5.7802144345 | 5.8418913683 |
| H | -2.3938680654 | 6.1121735682 | 5.3367051781 |
| H | -1.6317426736 | 6.7029772692 | 3.0665874971 |
| H | 0.7751143495 | 6.6365203957 | 2.4703090888 |
| H | 1.1855979519 | 6.123717377 | 4.1095537528 |
| H | -1.6115053864 | 2.308814129 | 5.7258314119 |
| H | 0.1393895206 | 3.336872324 | 7.1616039544 |
| H | -0.2738730353 | 1.7140244094 | 7.747216561 |
| H | 1.2280383502 | 1.9709211233 | 6.827648658 |
| H | 0.0839334166 | 0.2670602045 | 4.5878288972 |
| H | -1.4156244193 | -3.7683978351 | 6.1252043269 |
| H | -2.4467486926 | -1.8923028363 | 5.0685011475 |
| H | 0.6152226061 | -3.7287031564 | 7.3597310437 |
| H | -0.2025096155 | -3.2068986963 | 1.6154955774 |
| H | 0.8894204271 | -1.8629867111 | 2.0162117936 |
| H | 0.1478602031 | -1.6489912232 | 8.2960521384 |
| H | -2.915702905 | 0.8296345829 | 0.7720633285 |
| H | -3.2263251493 | 0.9999897247 | -0.9707637277 |
| H | -3.0010915035 | -0.6111474805 | -0.2648909562 |
| H | -0.8396683835 | -1.1924124324 | -1.7368545447 |
| H | 0.2246289398 | 0.1795323485 | -2.0960126015 |
| H | -1.7954069759 | 1.1951387843 | -2.8615213256 |
| H | -2.1565241315 | -1.5970099814 | 7.6308159945 |
| H | 1.5085404946 | 3.1437701868 | -2.3907383402 |

**1g** conf_14

energy (M062X/6-31g(d,p)) = -2585.2686654 Hartree

| | | | |
|---|---|---|---|
| C | -0.6746235295 | -0.8329720674 | 0.2175863124 |
| O | -0.8601807281 | -1.886797989 | -0.3395602582 |
| C | 0.4920049686 | 0.125828827 | -0.0501037936 |
| N | 0.045575558 | 1.5044368223 | 0.1083234234 |
| C | -1.0301877141 | 1.969021201 | -0.5677062463 |
| O | -1.6325732429 | 1.300442719 | -1.402470153 |
| C | -1.5203648194 | 3.3842387138 | -0.2317082127 |
| C | -1.8438763821 | 4.1920287504 | -1.4912097689 |
| C | -0.5748295794 | 4.7295435275 | -2.1476512656 |
| C | 0.2782358456 | 5.462332297 | -1.1165481216 |
| N | 0.5887175788 | 4.6290468415 | 0.0514687647 |
| N | -0.5862440224 | 4.1088506444 | 0.6184396967 |
| C | -0.8800030641 | 4.345201984 | 1.9247944628 |
| O | -1.9639371353 | 4.033895978 | 2.417760471 |
| C | 0.2437022327 | 4.894301298 | 2.8012513194 |
| N | 0.3032838919 | 4.0292917336 | 3.9854496424 |
| N | -0.6385348756 | 4.2070881906 | 5.0117546864 |
| C | -0.6709332053 | 5.590215289 | 5.4691016951 |
| C | -0.9714823377 | 6.5275818931 | 4.305511517 |
| C | 0.0773710569 | 6.3616063221 | 3.2189186358 |
| C | 0.8876270484 | 2.8168244167 | 3.8526742839 |
| O | 1.3953750942 | 2.4804528822 | 2.7743425109 |
| C | 0.904536367 | 1.876310872 | 5.0504228799 |
| C | 2.2996346872 | 1.292598829 | 5.2510457781 |
| N | -0.0913687095 | 0.8423410235 | 4.7974775247 |
| C | -0.7561822949 | 0.2361627383 | 5.7943785846 |
| O | -0.6791172377 | 0.5849374429 | 6.9747606992 |
| C | -1.3466176575 | -2.1861775186 | 6.2671373969 |
| C | -1.6790187802 | -0.9339692403 | 5.4307630273 |
| N | -1.6533398104 | -1.296009313 | 4.0218109644 |
| N | -0.696239064 | -2.1305309554 | 3.5020519818 |
| C | 0.0588979904 | -2.772913228 | 4.3099607918 |
| C | 0.0016899719 | -2.747980336 | 5.819794031 |
| C | -2.6611119654 | -0.8736010894 | 3.1772117658 |
| O | -3.6139999845 | -0.2394296333 | 3.5928644233 |
| C | -2.4881826746 | -1.2045818471 | 1.7041316307 |
| O | -1.4140908923 | -0.3827931777 | 1.2462520912 |
| O | 1.0296567587 | -1.931724774 | 6.3536958838 |
| Cl | -0.9912556992 | 8.2405014918 | 4.884858165 |
| C | 1.0914527397 | -0.1091024585 | -1.4323601224 |
| C | 1.5520194061 | -0.1875302552 | 1.0403133327 |
| O | 2.6290774037 | 0.7092075858 | 1.0261979633 |
| O | -1.4200622846 | -1.9446135046 | 7.6399658527 |
| H | 0.8105260028 | -3.394486591 | 3.8295698529 |
| H | 0.3802078864 | 2.0221197011 | 0.9140461419 |
| H | -2.4276608737 | 3.2476989052 | 0.3622250782 |
| H | -2.4902221535 | 5.0267386719 | -1.2001892031 |
| H | -2.4088094051 | 3.5543713851 | -2.1739193515 |
| H | -0.8314384839 | 5.4045779925 | -2.9698922995 |

| | | | |
|---|---|---|---|
| H | -0.2393935109 | 6.3560073228 | -0.7528719098 |
| H | 1.2363800937 | 5.7788029155 | -1.5365882936 |
| H | 1.1658080735 | 3.8414230247 | -0.2421011321 |
| H | 1.1875357092 | 4.7920557208 | 2.2724957422 |
| H | -1.5436896581 | 3.9595316024 | 4.6091609031 |
| H | 0.2955779353 | 5.8373451955 | 5.9177570254 |
| H | -1.4397935009 | 5.660506999 | 6.2408263477 |
| H | -1.9744632276 | 6.3379433013 | 3.9197549973 |
| H | -0.1656350723 | 6.9616277185 | 2.3387478095 |
| H | 1.0406109263 | 6.7115857455 | 3.6031077295 |
| H | 0.5773891856 | 2.4111879453 | 5.9397169872 |
| H | 2.2692227067 | 0.5684289805 | 6.0666882 |
| H | 2.6503510096 | 0.7928010072 | 4.345557728 |
| H | 3.0092818551 | 2.0839048432 | 5.5081257957 |
| H | -0.1623563884 | 0.4593432924 | 3.8653004707 |
| H | -2.1056693287 | -2.936550132 | 6.021647908 |
| H | -2.696281062 | -0.6127896829 | 5.6613335466 |
| H | 0.0976446451 | -3.7768046943 | 6.1887587866 |
| H | -3.4052732785 | -0.9170219332 | 1.1897003237 |
| H | -2.2669112021 | -2.2559110043 | 1.524869416 |
| H | 1.8815410976 | -2.3391243655 | 6.1453352251 |
| H | 0.3865577496 | 0.1778184693 | -2.212485688 |
| H | 2.0013622351 | 0.4870976769 | -1.5263590285 |
| H | 1.3422193473 | -1.1643052425 | -1.5570172613 |
| H | 1.931941208 | -1.1935894937 | 0.839327857 |
| H | 1.068134953 | -0.2073588754 | 2.0217908726 |
| H | 2.4327179677 | 1.3936998006 | 1.6888563119 |
| H | -1.0101879803 | -1.0676899899 | 7.7789193134 |
| H | 0.0062736289 | 3.9054508606 | -2.5813504508 |

**1g** conf_15

energy (M062X/6-31g(d,p)) = -2585.2683561 Hartree

| | | | |
|---|---|---|---|
| C | 0.3866306087 | -3.7110345842 | -1.115003534 |
| O | -0.3532523031 | -4.6624731513 | -1.1552960239 |
| C | 1.737450843 | -3.6844017852 | -1.8263063504 |
| N | 2.6706839951 | -2.7199369648 | -1.2568210639 |
| C | 2.9745740933 | -2.6695496103 | 0.066277354 |
| O | 2.6236753452 | -3.5090631021 | 0.8827692231 |
| C | 3.7970749021 | -1.4290108734 | 0.447445693 |
| C | 4.62410025 | -1.6124616148 | 1.7216756273 |
| C | 3.7917921172 | -1.5015894386 | 2.9973903895 |
| C | 2.9420898396 | -0.2375798435 | 2.9512256602 |
| N | 2.110827472 | -0.1705575159 | 1.7492286739 |
| N | 2.8889281461 | -0.2819064423 | 0.5884153583 |
| C | 2.599843579 | 0.4917145793 | -0.4892007892 |
| O | 3.080330296 | 0.2422273818 | -1.6004177841 |
| C | 1.7079242751 | 1.7119902584 | -0.2629504657 |
| N | 0.9248243209 | 1.9880617462 | -1.4552089785 |
| N | 1.5753892846 | 2.4848323361 | -2.5938700014 |
| C | 2.3008178285 | 3.710173159 | -2.2760970035 |
| C | 3.2760521691 | 3.4894752676 | -1.1216614513 |
| C | 2.5408642059 | 2.9562466612 | 0.0989058039 |

| | | | |
|---|---|---|---|
| C | -0.3627884966 | 1.5344071608 | -1.5340700294 |
| O | -0.8777313446 | 0.9392468241 | -0.6001890388 |
| C | -1.1255485692 | 1.8094615533 | -2.8460638993 |
| C | -1.516086255 | 3.2788852545 | -2.9977522496 |
| N | -2.2424267333 | 0.8810138702 | -2.9142333536 |
| C | -3.3026833263 | 0.9340157982 | -2.0802185311 |
| O | -3.7065160782 | 1.9622726614 | -1.5414929865 |
| C | -5.4913536066 | -0.2420013089 | -1.4565636473 |
| C | -4.0265934886 | -0.4317529522 | -1.8920155076 |
| N | -3.2755111207 | -1.2674808915 | -0.9355977046 |
| N | -3.7830994788 | -1.6948258058 | 0.2765950986 |
| C | -5.0503175091 | -1.8099364257 | 0.346096597 |
| C | -6.0054087115 | -1.5108844529 | -0.7800919164 |
| C | -2.044170653 | -1.7614363962 | -1.2512253582 |
| O | -1.5817844908 | -1.7029977892 | -2.3851732248 |
| C | -1.2660139684 | -2.3947334513 | -0.1068817646 |
| O | 0.0826884981 | -2.540123828 | -0.5252822418 |
| O | -7.3151482036 | -1.3328693864 | -0.3175277506 |
| Cl | 4.1119112747 | 5.034268031 | -0.7186437958 |
| C | 1.4663718002 | -3.2650704282 | -3.2753642521 |
| C | 2.3570221216 | -5.0968249041 | -1.791942715 |
| O | 3.5689808753 | -5.1412155062 | -2.5068053181 |
| O | -5.6999783155 | 0.7448631991 | -0.4802027878 |
| H | -5.4551564513 | -2.1489104852 | 1.296042815 |
| H | 2.8491048065 | -1.8695574323 | -1.7831966195 |
| H | 4.4550445368 | -1.1805522625 | -0.387979992 |
| H | 5.4027703363 | -0.8404172004 | 1.7254391441 |
| H | 5.1270976201 | -2.5819293689 | 1.673832264 |
| H | 4.4493461582 | -1.4844789963 | 3.8727780628 |
| H | 3.5718637291 | 0.6591088462 | 2.9624765281 |
| H | 2.2629723536 | -0.1734830637 | 3.8059464762 |
| H | 1.4511294886 | -0.9489279349 | 1.7470799725 |
| H | 1.0102748943 | 1.4976046606 | 0.5430631461 |
| H | 2.2379370816 | 1.7623498221 | -2.8778135785 |
| H | 1.5783961603 | 4.4871557932 | -2.0076685671 |
| H | 2.8299497499 | 4.0314101077 | -3.1765439253 |
| H | 4.0638665592 | 2.7988021699 | -1.4313977563 |
| H | 3.2402503412 | 2.7209717328 | 0.9053755676 |
| H | 1.8554830982 | 3.7265354087 | 0.4666578075 |
| H | -0.4660483737 | 1.553673261 | -3.6782515657 |
| H | -2.0755164451 | 3.6351295666 | -2.1343320142 |
| H | -0.6127194583 | 3.8769039165 | -3.1305887939 |
| H | -2.1434489761 | 3.3956846848 | -3.8848199284 |
| H | -1.9591660483 | -0.0743488036 | -3.1261433582 |
| H | -6.0786173961 | -0.0282321639 | -2.3614984255 |
| H | -4.0245401597 | -0.9600264933 | -2.8521396933 |
| H | -6.0147732033 | -2.3550543884 | -1.48122836 |
| H | -1.686082206 | -3.3603266318 | 0.1766349892 |
| H | -1.2722851374 | -1.7259461883 | 0.752255834 |
| H | -7.3246309371 | -0.4382342093 | 0.0614459903 |
| H | 2.3985021102 | -3.3174718566 | -3.8425535938 |
| H | 0.7449342877 | -3.94840484 | -3.7265700047 |
| H | 1.0511893649 | -2.255349807 | -3.3166186878 |
| H | 1.6722996478 | -5.7921368269 | -2.2771883208 |

| | | | |
|---|---|---|---|
| H | 2.484425039 | -5.4093628969 | -0.7499848295 |
| H | 4.1748512799 | -4.534692652 | -2.0603558228 |
| H | -5.097357988 | 1.4895307053 | -0.7042049464 |
| H | 3.1439186485 | -2.3784534625 | 3.0856962262 |

Compound **1h**

**1h** conf_1

energy (M062X/6-31g(d,p)) = -2585.2815114 Hartree

| | | | |
|---|---|---|---|
| C | 0.7074163716 | 2.9001341837 | 0.2025650602 |
| O | 0.703962895 | 1.9416722495 | 0.9398588918 |
| C | -0.5428774748 | 3.573099239 | -0.353186929 |
| N | -1.6106499302 | 2.5736590436 | -0.236545067 |
| C | -2.9237703481 | 2.834157957 | -0.3225019608 |
| O | -3.4145556568 | 3.9682099992 | -0.3779351804 |
| C | -3.8758342189 | 1.635562089 | -0.3907017661 |
| C | -5.1420579835 | 1.8844383588 | 0.4366424529 |
| C | -4.8714342465 | 1.6857254914 | 1.9252592599 |
| C | -4.2504553983 | 0.3127666356 | 2.1567647769 |
| N | -3.0537278883 | 0.080026126 | 1.3423582559 |
| N | -3.2761756263 | 0.364768087 | -0.0103798555 |
| C | -3.1135507922 | -0.6241116621 | -0.940404254 |
| O | -3.3021537608 | -0.4275221133 | -2.1324935006 |
| C | -2.8684417572 | -2.0391310266 | -0.3976789713 |
| N | -1.5140940151 | -2.3280046536 | 0.0820285119 |
| N | -1.3240963598 | -3.5995268935 | 0.6349409149 |
| C | -1.6510286533 | -4.645536424 | -0.3273814694 |
| C | -3.0322403391 | -4.4902409375 | -0.950244858 |
| C | -3.2481618205 | -3.0726766984 | -1.4581670787 |
| C | -0.4424921914 | -1.5236036046 | -0.0956901716 |
| O | -0.5193134064 | -0.4429644062 | -0.6793186091 |
| C | 0.878220668 | -1.9961080492 | 0.5110063265 |
| C | 0.8737939205 | -1.7953164518 | 2.0309749235 |
| N | 1.9259243694 | -1.215755714 | -0.1157364637 |
| C | 3.1999712347 | -1.6139013842 | -0.1363324128 |
| O | 3.5767819648 | -2.7089656793 | 0.3014605693 |
| C | 5.6506479345 | -1.1058388535 | -0.6560092958 |
| C | 4.2019472084 | -0.6152459843 | -0.7562894292 |
| N | 4.1010783011 | 0.7067182036 | -0.1238969515 |
| N | 4.8910694002 | 1.1186368029 | 0.9161136335 |
| C | 5.81503329 | 0.3435488916 | 1.3339148556 |
| C | 6.1331640638 | -1.0128759015 | 0.7876840706 |
| C | 3.1613560792 | 1.5913773527 | -0.5671203359 |
| O | 2.4305554602 | 1.32248104 | -1.5114054489 |
| C | 3.0339703061 | 2.9009172619 | 0.2006058515 |
| O | 1.8222036566 | 3.5322823673 | -0.1897424612 |
| O | 7.5256184645 | -1.2113643627 | 0.8833485607 |
| Cl | -4.3034956107 | -4.9082730044 | 0.2931008365 |
| C | -0.3525045382 | 3.9838587577 | -1.8151159034 |
| C | -0.7758048488 | 4.8260114883 | 0.5512554285 |
| O | -1.5583252873 | 5.8232813805 | -0.033184325 |
| O | 5.8171199568 | -2.4016147791 | -1.1719334405 |
| H | 6.4162192836 | 0.7224886662 | 2.1557760858 |
| H | -1.3185505807 | 1.5998155796 | -0.2869813725 |
| H | -4.1385999562 | 1.5359006367 | -1.4477328335 |
| H | -5.9069825867 | 1.1754120511 | 0.1021033103 |
| H | -5.5042087102 | 2.8919225268 | 0.2262736344 |

| | | | |
|---|---|---|---|
| H | -5.800800035 | 1.7771895918 | 2.4960249664 |
| H | -4.9736913603 | -0.4726974883 | 1.9098905089 |
| H | -3.9521540113 | 0.1728828662 | 3.1989826902 |
| H | -2.2875527222 | 0.6673209065 | 1.6666055412 |
| H | -3.5208192446 | -2.1530499664 | 0.4743666675 |
| H | -1.9089970444 | -3.6789669736 | 1.4646502234 |
| H | -1.5474513317 | -5.6085628847 | 0.1757730481 |
| H | -0.9106100425 | -4.6041511128 | -1.1336029911 |
| H | -3.1768214098 | -5.2174224706 | -1.7494516079 |
| H | -4.2843370275 | -2.9286322779 | -1.769773575 |
| H | -2.6189886591 | -2.9269961514 | -2.341957661 |
| H | 1.0411649635 | -3.0503614532 | 0.286270219 |
| H | 0.1039656756 | -2.4097962383 | 2.50059035 |
| H | 1.8456220369 | -2.08931464 | 2.4335034789 |
| H | 0.6952264015 | -0.7447383708 | 2.272717407 |
| H | 1.6446176631 | -0.3426787868 | -0.5547035787 |
| H | 6.2780907511 | -0.4414972782 | -1.2578684253 |
| H | 3.9366538226 | -0.4792822348 | -1.8075356476 |
| H | 5.5908655623 | -1.7649440128 | 1.3824735555 |
| H | 3.8348781805 | 3.5906826459 | -0.0656976387 |
| H | 3.056244599 | 2.7253334231 | 1.2751605411 |
| H | 7.6998880758 | -2.0633627491 | 0.4562587696 |
| H | 0.4201417268 | 4.7486311596 | -1.9032963227 |
| H | -0.0662056703 | 3.1199659258 | -2.4190512605 |
| H | -1.2886215589 | 4.3927510105 | -2.1968359114 |
| H | 0.2016785276 | 5.2731610758 | 0.748136379 |
| H | -1.1853711955 | 4.4738592959 | 1.5088767734 |
| H | -2.4122044945 | 5.378227623 | -0.220779501 |
| H | 5.1664236659 | -2.9426029759 | -0.6817145481 |
| H | -4.1916569663 | 2.4650815218 | 2.2929096317 |

**1h** conf_2

energy (M062X/6-31g(d,p)) = -2585.2748786 Hartree

| | | | |
|---|---|---|---|
| C | -1.1456659491 | -0.4534718169 | 0.8347665295 |
| O | -0.7338331029 | 0.1694597015 | 1.7911745294 |
| C | -1.5245913399 | 0.1876662505 | -0.4945423352 |
| N | -1.5716826846 | 1.6169456838 | -0.214149799 |
| C | -1.5575970547 | 2.585389154 | -1.1557228702 |
| O | -1.8604778059 | 2.4177340532 | -2.3323919945 |
| C | -1.1270998666 | 3.968667543 | -0.650205253 |
| C | -0.3489500333 | 4.7490475181 | -1.7195034671 |
| C | 1.0657407123 | 4.1953363595 | -1.916680581 |
| C | 1.7842464984 | 4.0051024399 | -0.5828066452 |
| N | 0.9171142965 | 3.1874561338 | 0.2688716059 |
| N | -0.2919768007 | 3.8613510731 | 0.5412113353 |
| C | -0.512303329 | 4.6923140974 | 1.6042870628 |
| O | -1.5779974587 | 5.2927583562 | 1.7372671449 |
| C | 0.5518359633 | 4.7846658148 | 2.6967014576 |
| N | 0.0895416226 | 4.0195790532 | 3.8561732971 |
| N | -0.9317246392 | 4.556921652 | 4.6476057134 |
| C | -0.5750638516 | 5.8820896119 | 5.1454127581 |
| C | -0.2591099087 | 6.8221117621 | 3.9892620205 |

| | | | |
|---|---|---|---|
| C | 0.8375750186 | 6.2392030719 | 3.1121157434 |
| C | 0.4960365765 | 2.7312212985 | 4.0208539342 |
| O | 1.21447252 | 2.1727376133 | 3.1935978898 |
| C | 0.1188667692 | 2.0384497421 | 5.3215242417 |
| C | 1.3459439166 | 2.042904544 | 6.2396421619 |
| N | -0.3247435404 | 0.6837066998 | 5.0220360611 |
| C | -1.0411423114 | -0.0021018967 | 5.9192477969 |
| O | -1.371398807 | 0.4714119762 | 7.0157924826 |
| C | -1.1711210079 | -2.3809130671 | 6.7673577748 |
| C | -1.4749523972 | -1.4359003893 | 5.5925107699 |
| N | -0.8483324034 | -1.9751341028 | 4.3959925796 |
| N | 0.3773761999 | -2.5916521927 | 4.4198285758 |
| C | 0.928270728 | -2.8139704487 | 5.5502081668 |
| C | 0.3433345164 | -2.4980895592 | 6.8969209874 |
| C | -1.5344607929 | -1.9656762774 | 3.2025771989 |
| O | -2.6902563574 | -1.5903189237 | 3.1308782499 |
| C | -0.7499329601 | -2.4274742287 | 1.9819597066 |
| O | -1.2537500122 | -1.7803041427 | 0.8136192418 |
| O | 0.7148715874 | -3.5238091224 | 7.7876882971 |
| Cl | 0.2701510242 | 8.4281337372 | 4.6382761113 |
| C | -2.8442859058 | -0.3462291214 | -1.0461377182 |
| C | -0.3428220434 | -0.1002981306 | -1.4543128318 |
| O | 0.8801849854 | 0.3479101958 | -0.9230264554 |
| O | -1.7694168914 | -1.9968259898 | 7.9748572509 |
| H | 1.8988334324 | -3.3011091267 | 5.5151328757 |
| H | -1.2278946606 | 1.8684834102 | 0.7055468909 |
| H | -2.0225512108 | 4.5213206563 | -0.3578368379 |
| H | -0.2976565133 | 5.7929887441 | -1.3918806222 |
| H | -0.9087390272 | 4.7207550518 | -2.6561727037 |
| H | 1.6426806182 | 4.8679919722 | -2.5577179904 |
| H | 2.0133259295 | 4.9759304035 | -0.1179384416 |
| H | 2.7214349202 | 3.4592404578 | -0.7156117021 |
| H | 1.3232293847 | 2.8606083772 | 1.1440676561 |
| H | 1.4933989053 | 4.339689975 | 2.3852571445 |
| H | -1.7672775027 | 4.6209843587 | 4.0663972744 |
| H | 0.2916800521 | 5.7818662776 | 5.8049746469 |
| H | -1.4176009414 | 6.2508640039 | 5.7338849085 |
| H | -1.1573607954 | 7.0221018208 | 3.4069868174 |
| H | 1.7760237735 | 6.2369452775 | 3.6751768038 |
| H | 0.9881865671 | 6.850520715 | 2.2190513927 |
| H | -0.7021762302 | 2.5651304745 | 5.8036517059 |
| H | 1.6468121482 | 3.0686083916 | 6.4692151807 |
| H | 1.1001435509 | 1.5377320432 | 7.1752878276 |
| H | 2.1817210762 | 1.52874422 | 5.7592903122 |
| H | -0.0787006889 | 0.2791952573 | 4.125789416 |
| H | -1.5618964486 | -3.3705815699 | 6.50859723 |
| H | -2.5516125608 | -1.4109401726 | 5.4104492007 |
| H | 0.7441734473 | -1.5297103392 | 7.2420883439 |
| H | -0.8986568416 | -3.4944886509 | 1.8147293205 |
| H | 0.3136142598 | -2.2249954048 | 2.0902049936 |
| H | 0.2435289741 | -3.3352566861 | 8.6133707453 |
| H | -3.0747739371 | 0.1730174196 | -1.977427441 |
| H | -2.775719416 | -1.4181508139 | -1.2403327067 |
| H | -3.6554516423 | -0.168691701 | -0.336131785 |

| | | | |
|---|---|---|---|
| H | -0.5740275805 | 0.3652980478 | -2.4188627862 |
| H | -0.2576008001 | -1.1791736217 | -1.6020742218 |
| H | 0.781019553 | 1.2831512897 | -0.6493835315 |
| H | -1.6976747242 | -1.0189873539 | 8.0003871033 |
| H | 1.0146912495 | 3.2258110689 | -2.4249057469 |

**1h** conf_3

energy (M062X/6-31g(d,p)) = -2585.273408 Hartree

| | | | |
|---|---|---|---|
| C | 0.0011959305 | -0.6672637412 | 0.7364472608 |
| O | 0.6927685993 | -0.4509005121 | 1.715705646 |
| C | 0.206997789 | 0.0668781377 | -0.5956287872 |
| N | -0.372347561 | 1.389811354 | -0.4072022134 |
| C | -1.580957006 | 1.8885386546 | -0.7464477351 |
| O | -2.4416852715 | 1.3112425007 | -1.3969283819 |
| C | -1.8579519634 | 3.3123511673 | -0.2186915972 |
| C | -2.3473675332 | 4.2551767576 | -1.3228214334 |
| C | -1.1892785303 | 4.842909954 | -2.1243039056 |
| C | -0.1707271075 | 5.4640689749 | -1.1754398798 |
| N | 0.3257101935 | 4.5060105246 | -0.1834805667 |
| N | -0.7333866565 | 3.8957477737 | 0.510977271 |
| C | -0.7409614593 | 3.9059073664 | 1.874333097 |
| O | -1.6992747924 | 3.4749913844 | 2.5129599457 |
| C | 0.521130155 | 4.4065093791 | 2.5843652936 |
| N | 0.7282616629 | 3.5844707355 | 3.7732985549 |
| N | -0.1268811068 | 3.7626463256 | 4.8697663924 |
| C | -0.132659372 | 5.1546437518 | 5.3048569105 |
| C | -0.5105763043 | 6.0816036928 | 4.1537875703 |
| C | 0.4401263919 | 5.8884210984 | 2.9840342131 |
| C | 1.5316122883 | 2.4876493335 | 3.709213531 |
| O | 2.1946750618 | 2.2361798548 | 2.7060075274 |
| C | 1.5530706369 | 1.5592453171 | 4.9273260886 |
| C | 2.8946318074 | 0.8532184394 | 5.0515205094 |
| N | 0.457477953 | 0.6100009012 | 4.7614652415 |
| C | -0.4131069647 | 0.3387304305 | 5.7431629829 |
| O | -0.3619252361 | 0.8632254522 | 6.8615693986 |
| C | -1.9763160588 | -1.4557288565 | 6.6539700438 |
| C | -1.5605868135 | -0.6353266025 | 5.4242663457 |
| N | -1.249071119 | -1.5592001282 | 4.3392650315 |
| N | -0.6446109334 | -2.7720606608 | 4.5537021246 |
| C | -0.4416586977 | -3.1539143137 | 5.7549985048 |
| C | -0.8418671008 | -2.413460641 | 6.9970715503 |
| C | -1.6052736405 | -1.2403923671 | 3.0503147617 |
| O | -2.1979978506 | -0.2079512112 | 2.7896353163 |
| C | -1.1936517444 | -2.2292266247 | 1.9695294273 |
| O | -1.0071522767 | -1.5327405429 | 0.7359617186 |
| O | -1.2311465745 | -3.3595975652 | 7.9654605449 |
| Cl | -0.4633121252 | 7.8033075058 | 4.7114717844 |
| C | -0.3310695558 | -0.6963774263 | -1.7956678691 |
| C | 1.7309678062 | 0.3004184661 | -0.7677302199 |
| O | 2.2344467823 | 1.3282755551 | 0.0480025222 |
| O | -2.3498232561 | -0.6718510893 | 7.7544963975 |
| H | 0.0431988659 | -4.1197851978 | 5.8674144527 |

| | | | |
|---|---|---|---|
| H | 0.2190686534 | 1.967862942 | 0.175651199 |
| H | -2.6511385483 | 3.1796065226 | 0.5204728312 |
| H | -2.9102856815 | 5.067133131 | -0.8502405695 |
| H | -3.0400897395 | 3.7006399438 | -1.959477461 |
| H | -1.560980349 | 5.5974338336 | -2.8243576467 |
| H | -0.6153343351 | 6.3043023102 | -0.6314872206 |
| H | 0.705568991 | 5.8386874822 | -1.7103410413 |
| H | 0.8611494819 | 3.7789469644 | -0.6571488684 |
| H | 1.3810024304 | 4.2639907082 | 1.935479439 |
| H | -1.0582377524 | 3.4928485592 | 4.5536092714 |
| H | 0.8626268852 | 5.4095129744 | 5.6811559165 |
| H | -0.8465854798 | 5.2401823722 | 6.1266965864 |
| H | -1.5448793079 | 5.9035628985 | 3.8535735729 |
| H | 1.442563988 | 6.2133857631 | 3.2799139161 |
| H | 0.1346730509 | 6.4864945997 | 2.1222394593 |
| H | 1.3224306321 | 2.1281937556 | 5.8260013676 |
| H | 3.6956073877 | 1.5831992139 | 5.1957088271 |
| H | 2.8770814169 | 0.1827108821 | 5.9137747886 |
| H | 3.1175735443 | 0.2743506108 | 4.153016938 |
| H | 0.4098566351 | 0.0990798536 | 3.886334614 |
| H | -2.8469564126 | -2.0582526208 | 6.3752671898 |
| H | -2.4029828286 | -0.0238787203 | 5.0904209215 |
| H | 0.0192202008 | -1.8267144172 | 7.3586746224 |
| H | -1.9982604421 | -2.9415434133 | 1.7852436507 |
| H | -0.2875287262 | -2.7671497487 | 2.2378992345 |
| H | -1.5873464855 | -2.8436702989 | 8.7046771892 |
| H | 0.2368898546 | -1.6234942061 | -1.9138189983 |
| H | -1.3853455346 | -0.9369731876 | -1.6863383087 |
| H | -0.2034747946 | -0.0941285189 | -2.6975645881 |
| H | 1.8997742541 | 0.6192065671 | -1.798938793 |
| H | 2.257782831 | -0.6488724252 | -0.6106082216 |
| H | 2.1785672092 | 1.0641763221 | 0.9831588036 |
| H | -1.6648712634 | 0.0280372912 | 7.8052533893 |
| H | -0.7017870773 | 4.0627287469 | -2.7229173823 |

**1h** conf_4

energy (M062X/6-31g(d,p)) = -2585.2730414 Hartree

| | | | |
|---|---|---|---|
| C | -1.0566504223 | -0.2101980607 | 0.6725559379 |
| O | -0.6882070505 | 0.5405082824 | 1.5424805927 |
| C | -1.8426278685 | 0.2079063572 | -0.5728585381 |
| N | -1.7038963069 | 1.647086459 | -0.7551623421 |
| C | -0.5043491958 | 2.2770289534 | -0.8212126321 |
| O | 0.5595030019 | 1.6788746525 | -0.9680567677 |
| C | -0.554518864 | 3.79950626 | -0.6727439722 |
| C | -0.0554102519 | 4.5611803108 | -1.9077432816 |
| C | 1.4634311782 | 4.5199885433 | -2.057391693 |
| C | 2.1252126487 | 4.9012851793 | -0.7370897038 |
| N | 1.6632013107 | 4.0684319497 | 0.3782268855 |
| N | 0.2652721591 | 4.1419493501 | 0.4940466754 |
| C | -0.310537737 | 4.2709192708 | 1.7162099915 |
| O | -1.5322580888 | 4.2282061396 | 1.8655218368 |
| C | 0.629229926 | 4.4801635871 | 2.9093956541 |

| | | | |
|---|---|---|---|
| N | 0.008599782 | 3.9129373791 | 4.0994560717 |
| N | -1.0810070544 | 4.5802034962 | 4.6806291694 |
| C | -0.7312472569 | 5.9615465149 | 4.9959984468 |
| C | -0.2300459436 | 6.6886447512 | 3.7519324992 |
| C | 0.9628890462 | 5.9609577579 | 3.1545542669 |
| C | 0.2887957483 | 2.6336678595 | 4.4534750967 |
| O | 1.1406072403 | 1.9678846035 | 3.8701680783 |
| C | -0.4653308734 | 2.0327123949 | 5.638254297 |
| C | 0.2890074816 | 2.3274129044 | 6.9372092933 |
| N | -0.5457275182 | 0.6100715362 | 5.3490736719 |
| C | -1.3406431478 | -0.2345847087 | 6.0043181618 |
| O | -2.0303044218 | 0.0796191744 | 6.9844961739 |
| C | -0.9633153429 | -2.6535697227 | 6.6358106276 |
| C | -1.3954178022 | -1.6883499702 | 5.5212054242 |
| N | -0.592729969 | -1.944973822 | 4.3325290944 |
| N | 0.7089024168 | -2.3749283731 | 4.3807219606 |
| C | 1.2311567649 | -2.6163326017 | 5.5211094343 |
| C | 0.5384764959 | -2.4969651987 | 6.847714055 |
| C | -1.1702400474 | -1.8120235887 | 3.0894621199 |
| O | -2.3489780115 | -1.5353246801 | 2.9641423615 |
| C | -0.2416295509 | -2.0131511874 | 1.8979666521 |
| O | -0.8746450198 | -1.5396577487 | 0.7150637647 |
| O | 1.0525785648 | -3.4887418345 | 7.7042732925 |
| Cl | 0.2304436841 | 8.3869214567 | 4.1777624409 |
| C | -3.3224683398 | -0.093429421 | -0.3115309281 |
| C | -1.368464683 | -0.5427464905 | -1.8368709803 |
| O | -2.1025587625 | -0.1479438514 | -2.9724495321 |
| O | -1.6778920133 | -2.4786616194 | 7.8296523608 |
| H | 2.2640039119 | -2.9529571641 | 5.5082647632 |
| H | -2.5001839265 | 2.2072537645 | -0.4874396446 |
| H | -1.5690343272 | 4.1193618904 | -0.4349402409 |
| H | -0.3800733269 | 5.6016759249 | -1.7945407622 |
| H | -0.5541136843 | 4.1649147371 | -2.7974381576 |
| H | 1.7763233562 | 5.2093149595 | -2.8479126985 |
| H | 1.9108512641 | 5.9446363868 | -0.4821035299 |
| H | 3.2111619234 | 4.7858488918 | -0.7863732635 |
| H | 1.8772400069 | 3.0928689711 | 0.163657167 |
| H | 1.5534374051 | 3.9367144046 | 2.7318759342 |
| H | -1.8233921369 | 4.5652475011 | 3.980242408 |
| H | 0.0434507237 | 5.9616815637 | 5.7685765142 |
| H | -1.6237784644 | 6.4446962004 | 5.3989659528 |
| H | -1.038262716 | 6.783739436 | 3.0237964253 |
| H | 1.7999364731 | 6.0084295141 | 3.8582015582 |
| H | 1.2823719653 | 6.4267051603 | 2.2196340193 |
| H | -1.4740783933 | 2.440330126 | 5.7027391709 |
| H | 0.3061979524 | 3.4033366171 | 7.1269809737 |
| H | -0.2142167929 | 1.8336210205 | 7.769889488 |
| H | 1.3172071935 | 1.9622067335 | 6.872360098 |
| H | 0.0243306998 | 0.2934679158 | 4.5732763033 |
| H | -1.144525186 | -3.6765282377 | 6.2884120722 |
| H | -2.4372485587 | -1.8811613961 | 5.2588127189 |
| H | 0.7353868679 | -1.4929833588 | 7.2618422301 |
| H | -0.0536621075 | -3.0743696988 | 1.7327061369 |
| H | 0.7092654127 | -1.505418665 | 2.0544627147 |

| | | | |
|---|---|---|---|
| H | 0.5238567971 | -3.435455171 | 8.5146860806 |
| H | -3.9027243515 | 0.1771450408 | -1.195844489 |
| H | -3.4568416414 | -1.1579265599 | -0.1143953592 |
| H | -3.6910034355 | 0.4664674296 | 0.5522254964 |
| H | -1.5472589805 | -1.6098613843 | -1.7011836114 |
| H | -0.2949374433 | -0.3819467693 | -1.9744053414 |
| H | -1.9340816819 | 0.7957735202 | -3.1050594733 |
| H | -1.908040292 | -1.527357785 | 7.8799944659 |
| H | 1.7882295876 | 3.5164962357 | -2.3492721383 |

**1h** conf_5

energy (M062X/6-31g(d,p)) = -2585.2730379 Hartree

| | | | |
|---|---|---|---|
| C | -2.1924671693 | -0.5428905496 | 0.9174146607 |
| O | -3.0943830982 | 0.1493944588 | 1.3293783369 |
| C | -1.070084391 | -0.0759666766 | -0.0064820627 |
| N | -1.3104359747 | 1.3372854258 | -0.25721473 |
| C | -0.4210844303 | 2.1297120116 | -0.8962010389 |
| O | 0.5226892343 | 1.70790733 | -1.5637521779 |
| C | -0.6220610184 | 3.6290720362 | -0.6582159788 |
| C | -0.2353841223 | 4.5190702522 | -1.8413450289 |
| C | 1.2752887292 | 4.6610993616 | -2.0261804189 |
| C | 1.9412705367 | 4.9927166218 | -0.6954162391 |
| N | 1.589452626 | 4.0399375817 | 0.3626434104 |
| N | 0.1970339468 | 3.9727052294 | 0.5134218544 |
| C | -0.3389669084 | 3.9174262236 | 1.7576727624 |
| O | -1.5363051798 | 3.6836385975 | 1.9296018409 |
| C | 0.6063429009 | 4.2015494357 | 2.9351235011 |
| N | -0.0376930392 | 3.7906015717 | 4.1691290125 |
| N | -1.1454770585 | 4.5312871003 | 4.6060022571 |
| C | -0.7928121067 | 5.9381178278 | 4.7731307907 |
| C | -0.1970833769 | 6.5101625865 | 3.4898930085 |
| C | 0.9972892444 | 5.6871562881 | 3.0353329853 |
| C | 0.3567869498 | 2.6691101878 | 4.8376833194 |
| O | 1.3602983268 | 2.0415508501 | 4.5255655249 |
| C | -0.5171014817 | 2.2543312786 | 6.0282054283 |
| C | 0.0564502215 | 2.8145335561 | 7.3245105918 |
| N | -0.5861926782 | 0.8081495628 | 6.1070718179 |
| C | -1.0022298208 | 0.0688422353 | 5.0746131806 |
| O | -1.2727883186 | 0.5419588379 | 3.9689099674 |
| C | -0.0823918979 | -2.1594242369 | 6.0648114464 |
| C | -1.2287421757 | -1.4309506959 | 5.3677537864 |
| N | -1.5045932235 | -2.1133019771 | 4.1137987124 |
| N | -0.5248947867 | -2.6940993412 | 3.3612657362 |
| C | 0.6714505586 | -2.7062815833 | 3.8116447967 |
| C | 1.1205825162 | -2.1525725477 | 5.1407930617 |
| C | -2.7658366653 | -1.9976578168 | 3.5742379698 |
| O | -3.7032735028 | -1.5964435127 | 4.2412231035 |
| C | -2.9613609749 | -2.4259451127 | 2.1237340102 |
| O | -2.0355630003 | -1.8371918135 | 1.212563226 |
| O | 2.1147550204 | -2.9522823267 | 5.7473101691 |
| Cl | 0.298573216 | 8.2316663364 | 3.7594415052 |
| C | -1.1134970167 | -0.9011326172 | -1.299488738 |

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C   0.2968218731   -0.2764249317  0.7055710084
O   0.5474111149   0.6684970026   1.7114701892
O   0.1902272922   -1.5562124451  7.3075742447
H   1.4088693881   -3.1975618857  3.1824622674
H   -1.9536947359  1.7818258526   0.3884451527
H   -1.656238462   3.8225622669   -0.3719491309
H   -0.6715477719  5.5073184519   -1.6565316888
H   -0.7042436424  4.1264403913   -2.7482777679
H   1.48708283     5.4501893623   -2.7549818026
H   1.6430420761   5.9886224978   -0.3495945316
H   3.0312161634   4.982740278    -0.7795945921
H   1.9101327964   3.1084534601   0.0943530992
H   1.5059024046   3.5994758383   2.8208750051
H   -1.8601662921  4.4240978762   3.8862629308
H   -0.0683648379  6.0243035386   5.5886266643
H   -1.6991849129  6.4772949138   5.0573235062
H   -0.961649791   6.5547110994   2.7106762429
H   1.8000063153   5.7781777122   3.7738172417
H   1.3783225157   6.040121348    2.0759623614
H   -1.5234978737  2.6456537475   5.8756009704
H   0.0473967063   3.9057431395   7.2969435961
H   -0.5443451922  2.4908257502   8.1787780696
H   1.0870269679   2.4781713008   7.4682405716
H   -0.2732438324  0.3211233926   6.9408312822
H   -0.3892478466  -3.204109581   6.2115326954
H   -2.129582423   -1.5050986837  5.9817654665
H   1.4756490074   -1.1188334796  5.0192951072
H   -3.982027145   -2.1550997492  1.8562488919
H   -2.8172257503  -3.5012073781  2.0207155014
H   2.9796904517   -2.6692350935  5.4229514218
H   -0.903281585   -1.9513521327  -1.0878928897
H   -2.0974530377  -0.8284047399  -1.7697180424
H   -0.36344375    -0.5154736189  -1.9901674964
H   1.0761545242   -0.1411888147  -0.0451214006
H   0.3430830132   -1.3064529771  1.0756300278
H   -0.0533624132  0.5330362283   2.4667598106
H   1.0659892561   -1.8756186108  7.5770335752
H   1.6902159873   3.7280466954   -2.4155029202
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**1h** conf_6

energy (M062X/6-31g(d,p)) = -2585.2712264 Hartree

```
C   -0.8230106155  -0.5276974048  0.7222696989
O   -0.1857986111  0.0544601049   1.5754269414
C   -1.4375280256  0.1578045486   -0.4964824348
N   -1.0472906671  1.5547171045   -0.3352910353
C   -1.0992056194  2.5429388788   -1.2313797499
O   -1.4994424221  2.4350151558   -2.3978424555
C   -0.6718100646  3.9257876178   -0.7282949256
C   0.2438518885   4.6528385706   -1.7270395496
C   1.6787658189   4.1221544265   -1.6892859586
C   2.1980719489   4.0493477948   -0.2552319186
N   1.2410877526   3.2608564314   0.5118221284
```

| | | | |
|---|---|---|---|
| N | -0.0116163004 | 3.8952006654 | 0.5694997556 |
| C | -0.4535393538 | 4.6849434585 | 1.5892289466 |
| O | -1.5763271167 | 5.1923455762 | 1.5803973283 |
| C | 0.4541198209 | 4.8613373176 | 2.8064365166 |
| N | -0.0774801134 | 4.0702783707 | 3.9180605368 |
| N | -1.2195314192 | 4.5334393382 | 4.583111204 |
| C | -1.0247195929 | 5.8872632372 | 5.0931945815 |
| C | -0.6518153091 | 6.8391575615 | 3.9638938283 |
| C | 0.5802318999 | 6.3354402234 | 3.2299900252 |
| C | 0.3980109267 | 2.8167817811 | 4.1444583177 |
| O | 1.2325562794 | 2.2985109036 | 3.4030869841 |
| C | -0.0537145262 | 2.1074356712 | 5.4111899897 |
| C | 1.051150672 | 2.2522489183 | 6.4636358312 |
| N | -0.3151282468 | 0.7110060705 | 5.0909595556 |
| C | -1.0536095828 | -0.0400611519 | 5.913784331 |
| O | -1.5404486259 | 0.3998696582 | 6.9651609767 |
| C | -0.9715363809 | -2.4353908467 | 6.7319733356 |
| C | -1.3311343207 | -1.5034662343 | 5.5610597895 |
| N | -0.6510759121 | -1.9815664495 | 4.3636352941 |
| N | 0.569599801 | -2.6092000904 | 4.3905807848 |
| C | 1.1273397013 | -2.8175276191 | 5.5199674498 |
| C | 0.5467805059 | -2.4731822147 | 6.8601969609 |
| C | -1.3069788882 | -1.9096910662 | 3.1573347763 |
| O | -2.4182245679 | -1.418374475 | 3.0684139083 |
| C | -0.5731071035 | -2.4684906934 | 1.9454036949 |
| O | -1.0772531022 | -1.8338139766 | 0.7701863677 |
| O | 0.9662223139 | -3.4446202724 | 7.7879415057 |
| Cl | -0.3281769565 | 8.4878829469 | 4.6403164105 |
| C | -2.9629923048 | 0.0038085507 | -0.4411741816 |
| C | -0.866748603 | -0.4867439584 | -1.7903431426 |
| O | -1.6158412091 | -0.1925170645 | -2.9343896478 |
| O | -1.5883918923 | -2.0910018174 | 7.9415814068 |
| H | 2.09483464 | -3.3107089269 | 5.4870158409 |
| H | -0.591584455 | 1.7574187947 | 0.5471790241 |
| H | -1.5938374595 | 4.4962997856 | -0.5940561268 |
| H | 0.2370670488 | 5.7155904495 | -1.4613027134 |
| H | -0.1838771496 | 4.5593657941 | -2.7272876768 |
| H | 2.3272400679 | 4.7627518954 | -2.2941939988 |
| H | 2.3333342173 | 5.061322673 | 0.160384831 |
| H | 3.1594020565 | 3.5315830817 | -0.2124533826 |
| H | 1.5241361695 | 2.9667621135 | 1.4432044238 |
| H | 1.4580195208 | 4.4923275468 | 2.612852289 |
| H | -1.9849544654 | 4.527351738 | 3.9094281713 |
| H | -0.2337929408 | 5.8618533039 | 5.8481234465 |
| H | -1.9546657952 | 6.1937906834 | 5.5762856584 |
| H | -1.4893434128 | 6.9615129458 | 3.2786340369 |
| H | 1.4436402331 | 6.4086909288 | 3.8986852435 |
| H | 0.7890461412 | 6.9493325154 | 2.3504468907 |
| H | -0.9760797183 | 2.5483728919 | 5.7840073947 |
| H | 0.7533357261 | 1.7285339467 | 7.3735158383 |
| H | 1.9873577501 | 1.828620309 | 6.0923288343 |
| H | 1.2119931174 | 3.3058290475 | 6.7066756982 |
| H | 0.0943208715 | 0.3253041001 | 4.2487165292 |
| H | -1.3063715987 | -3.4445024732 | 6.4685243976 |

| | | | |
|---|---|---|---|
| H | -2.404502359 | -1.5667726347 | 5.3689519511 |
| H | 0.9054208917 | -1.473700855 | 7.1615358042 |
| H | -0.7959005084 | -3.5292968161 | 1.8275339916 |
| H | 0.5026563607 | -2.3303122014 | 2.0231666235 |
| H | 0.472139249 | -3.2573316701 | 8.6007732214 |
| H | -3.2444464558 | -1.0453626773 | -0.5481395034 |
| H | -3.3515245702 | 0.3819864658 | 0.5069450869 |
| H | -3.4075280837 | 0.5687290246 | -1.2609687703 |
| H | -0.8888725131 | -1.5711996538 | -1.6643524129 |
| H | 0.1843078711 | -0.1771250968 | -1.8872758244 |
| H | -1.6412659852 | 0.7882189701 | -2.9814015213 |
| H | -1.646431302 | -1.1117553382 | 7.9461300204 |
| H | 1.7144149638 | 3.1159937906 | -2.1220574795 |