

## Intramolecular hydrogen bonding in conformationally semi-rigid $\alpha$ -acylmethane derivatives: a theoretical NMR study

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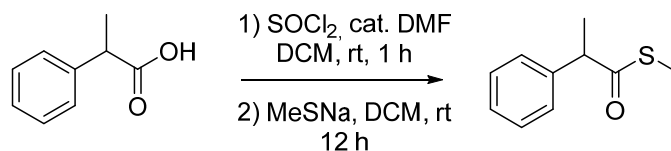
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### **A. General information**

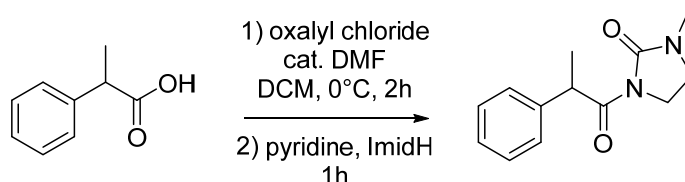
Unless otherwise stated, all glassware was flame-dried before use and all reactions were performed under an atmosphere of argon. All reagents and dry solvents were used as received from commercial suppliers unless otherwise stated. Reaction progress was monitored by thin layer chromatography (TLC) performed on aluminum plates coated with silica gel F<sub>254</sub> with 0.2 mm thickness. Chromatograms were visualized by fluorescence quenching with UV light at 254 nm or by staining using potassium permanganate. Flash column chromatography was performed using silica gel 60 (230-400 mesh, Merck and co.). Neat infra-red spectra were recorded using a Perkin-Elmer Spectrum 100 FT-IR spectrometer or a Shimadzu IRAffinity-1 FTIR spectrometer, using KBr platelets. Wavenumbers ( $\nu = 1/\lambda$ ) are reported in  $\text{cm}^{-1}$ . Mass spectra were obtained using a Finnigan MAT 8200 or (70 eV) or an Agilent 5973 (70 eV) spectrometer, using electrospray ionization (ESI). All <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra were recorded using a Bruker AV-400, AV-600 or AMX 300 spectrometer at 300K. Chemical shifts were given in parts per million (ppm,  $\delta$ ), referenced to the solvent peak of CDCl<sub>3</sub>, defined at  $\delta = 7.26$  ppm (<sup>1</sup>H NMR) and  $\delta = 77.16$  (<sup>13</sup>C NMR). References to the solvent peak for DMSO-*d*<sub>6</sub> and CD<sub>3</sub>OD was defined at  $\delta = 2.50$  and 3.31 ppm (<sup>1</sup>H NMR), respectively. Coupling constants are quoted in Hz (*J*). <sup>1</sup>H NMR splitting patterns were designated as singlet (s), doublet (d), triplet (t), quartet (q). Splitting patterns that could not be interpreted or easily visualized were designated as multiplet (m).

## B. Synthesis of $\alpha$ -acylmethane derivatives 5-Me and 7-Me



**Synthesis of 5-Me:** To a solution of carboxylic acid (1 mmol) in dry DCM (1 mL) were added thionyl chloride (1.5 mmol) and dry DMF (0.1 mmol) and the mixture was stirred 1 hour at room temperature. The volatiles were evaporated under high vacuum, and the residue was diluted in 2 mL of dry DCM. Sodium methanethiolate (2 mmol) was added in one portion and the mixture was stirred 12 hours at room temperature. The mixture was filtered, washed with DCM, dried with sodium sulfate and concentrated under reduced pressure to yield the crude product, which was purified by column chromatography on silica gel using 98:2 heptane:diethyl ether as the eluent. With this procedure, the product was obtained as a colorless liquid (110 mg, 61%).  $R_f$ (hept : ether 98:2) = 0.3.

$^1\text{H NMR}$  (600 MHz,  $\text{CDCl}_3$ )  $\delta$  7.38 – 7.31 (m, 4H), 7.31 – 7.26 (m, 1H), 3.91 (q,  $J = 7.1$  Hz, 1H), 2.26 (s, 3H), 1.55 (d,  $J = 7.1$  Hz, 3H).  $^{13}\text{C NMR}$  (151 MHz,  $\text{CDCl}_3$ )  $\delta$  201.7, 140.0, 128.8, 128.0, 127.6, 54.2, 18.5, 11.9. **HRMS** (EI): calc. for [M]: 180.0603, found: 180.0601. **IR** (ATR): 3062 (w), 3029 (w), 2977 (m), 2930 (m), 1682 (vs), 1494 (m), 1452 (s), 1310 (w), 1101 (w), 998 (s), 937 (vs), 732 (s), 698 (vs), 557 (m).

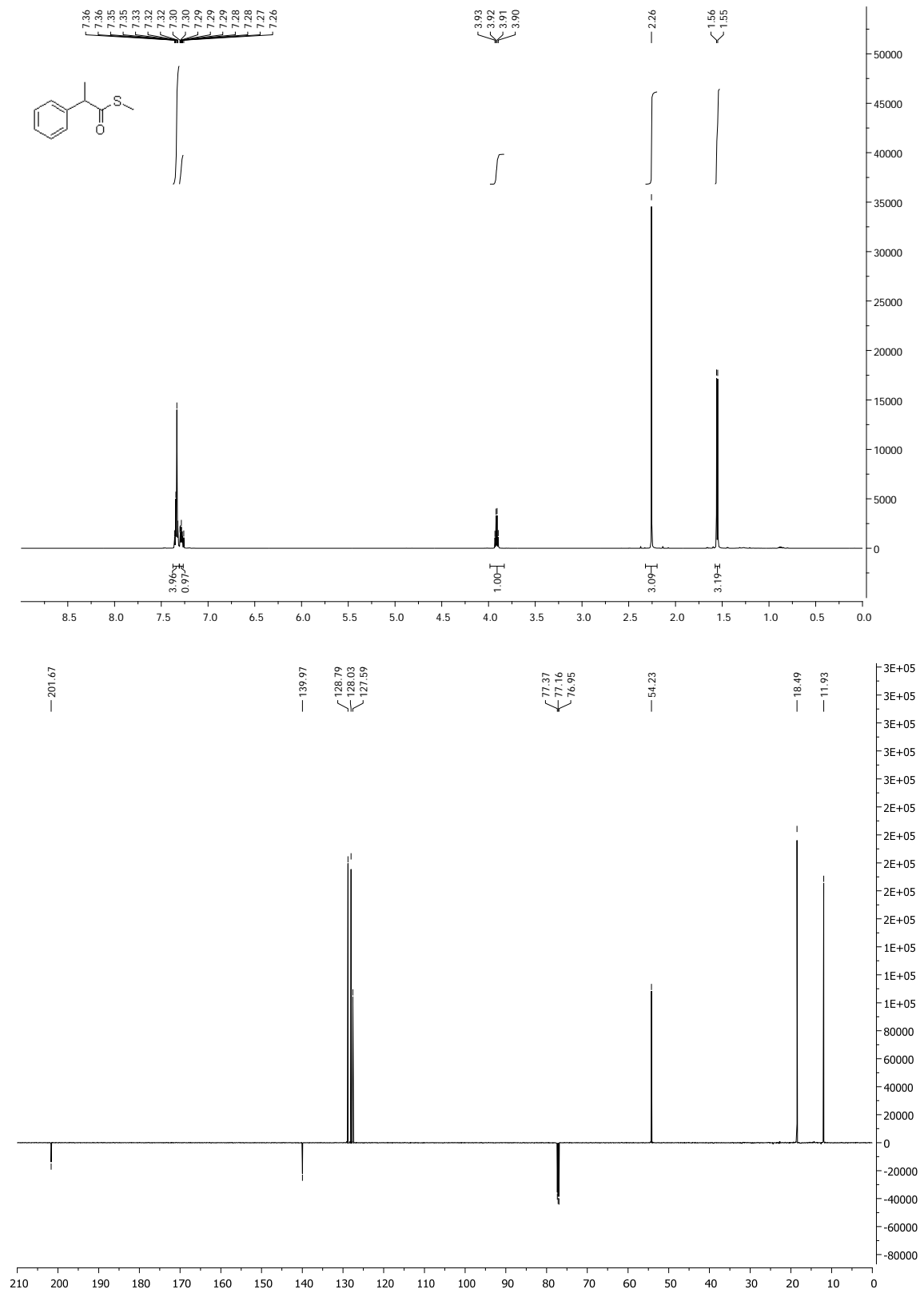


**Synthesis of 7-Me:** To a solution of carboxylic acid (1 mmol) in DCM (1ml) was added one drop of dry DMF and the mixture was cooled to 0 °C. At that temperature, oxalyl chloride (1.2 mmol) was added dropwise and the mixture was stirred 2 additional hours. Then, pyridine (2.2 mmol) and 1-methyl-2-imidazolidinone (2 mmol) were added and the reaction was continued for 1 hour. The reaction was quenched with water and extracted with DCM. The organic layer was dried with magnesium sulfate, filtered and concentrated under reduced pressure to give the desired product (163 mg, 70%).

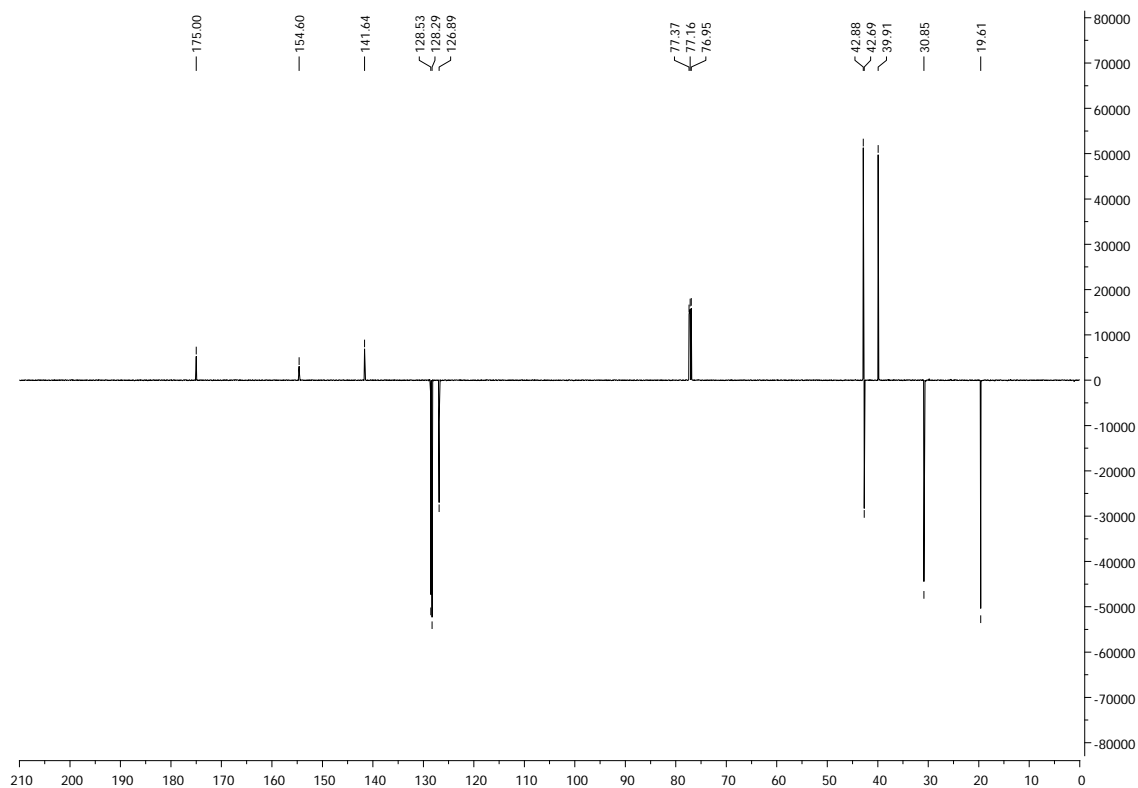
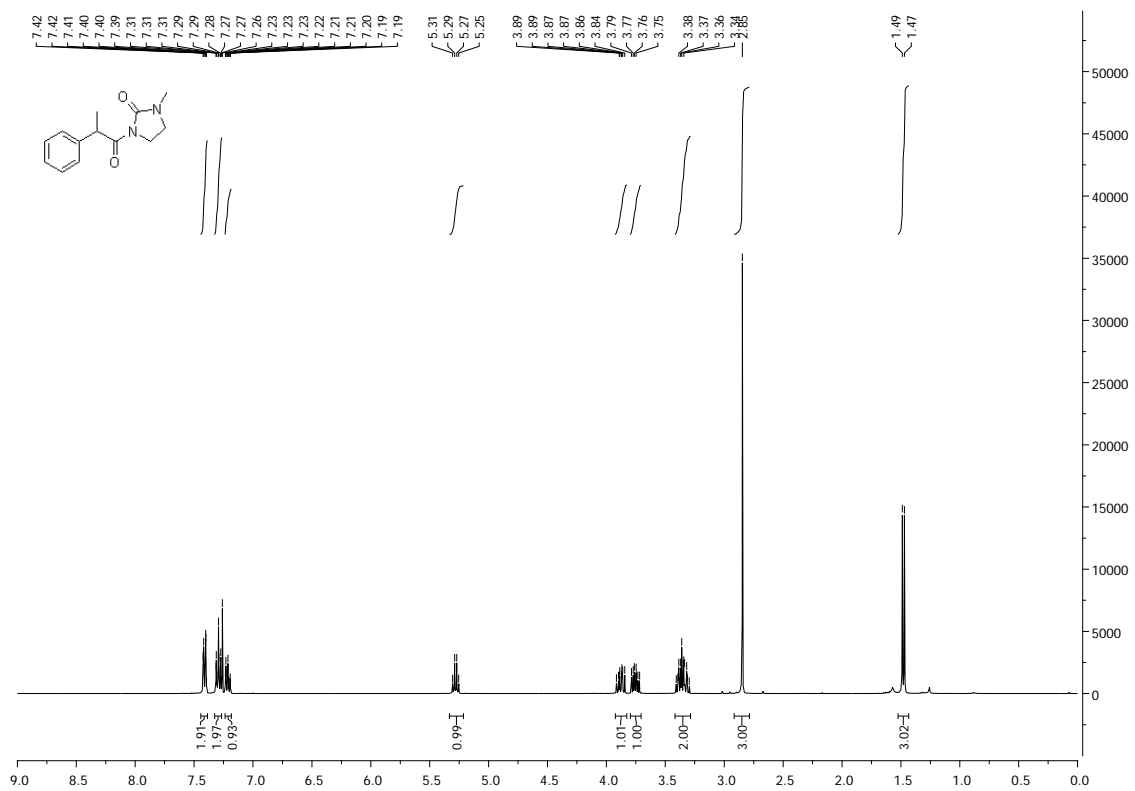
$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.41 (dt,  $J = 3.0, 1.8$  Hz, 2H), 7.32 – 7.27 (m, 2H), 7.24 – 7.18 (m, 1H), 5.28 (q,  $J = 7.0$  Hz, 1H), 3.88 (ddd,  $J = 11.6, 9.8, 6.9$  Hz, 1H), 3.75 (ddd,  $J = 11.6, 9.8, 5.9$  Hz, 1H), 3.46 – 3.27 (m, 2H), 2.85 (s, 3H), 1.48 (d,  $J = 7.0$  Hz, 3H).  $^{13}\text{C NMR}$  (151 MHz,  $\text{CDCl}_3$ )  $\delta$  175.0, 154.6, 141.6, 128.5, 128.3, 126.9, 42.9, 42.7, 39.9, 30.9, 19.6. **HRMS** (ESI+): calc. for [M-H] $^+$ : 233.1285, found: 233.1286. calc. for [M-Na] $^+$ : 255.1104, found: 255.1106. **IR** (ATR): 1720 (vs), 1667 (vs), 1483 (w), 1434 (w), 1377 (vs), 1240 (vs), 1061 (w), 908 (w), 745 (s), 724 (vs), 698 (vs), 570 (vs), 539 (m), 503 (m).

### C. NMR spectroscopic data for compounds 5-Me and 7-Me

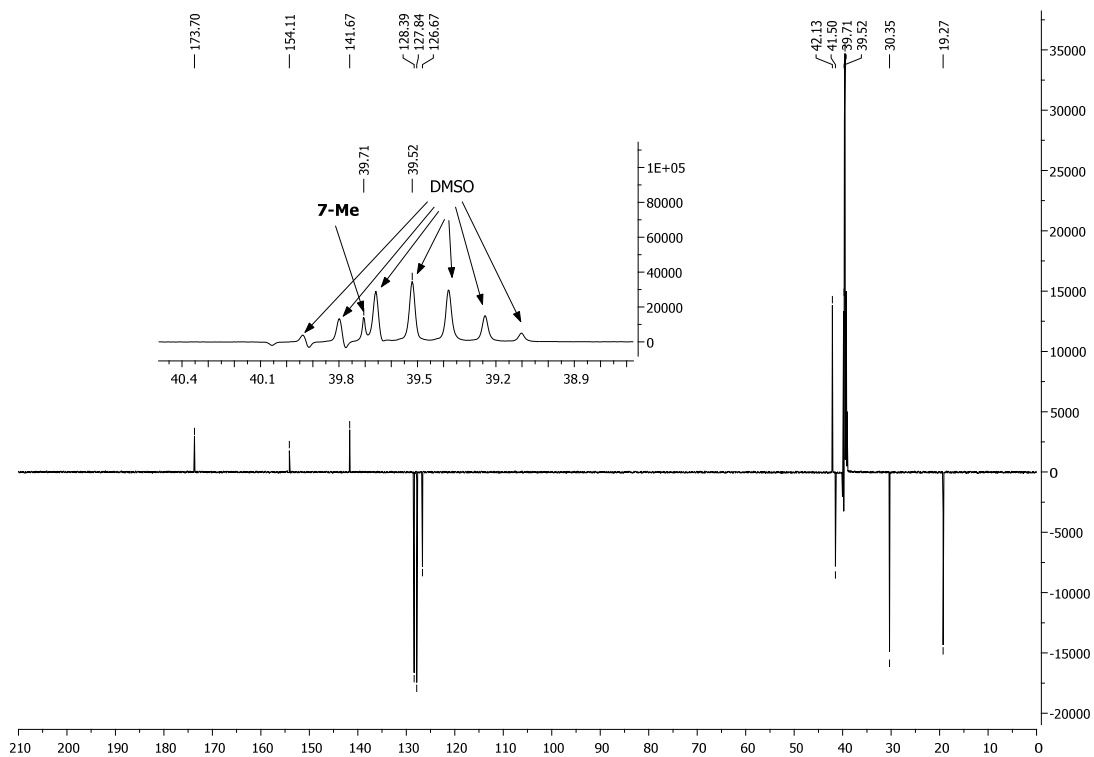
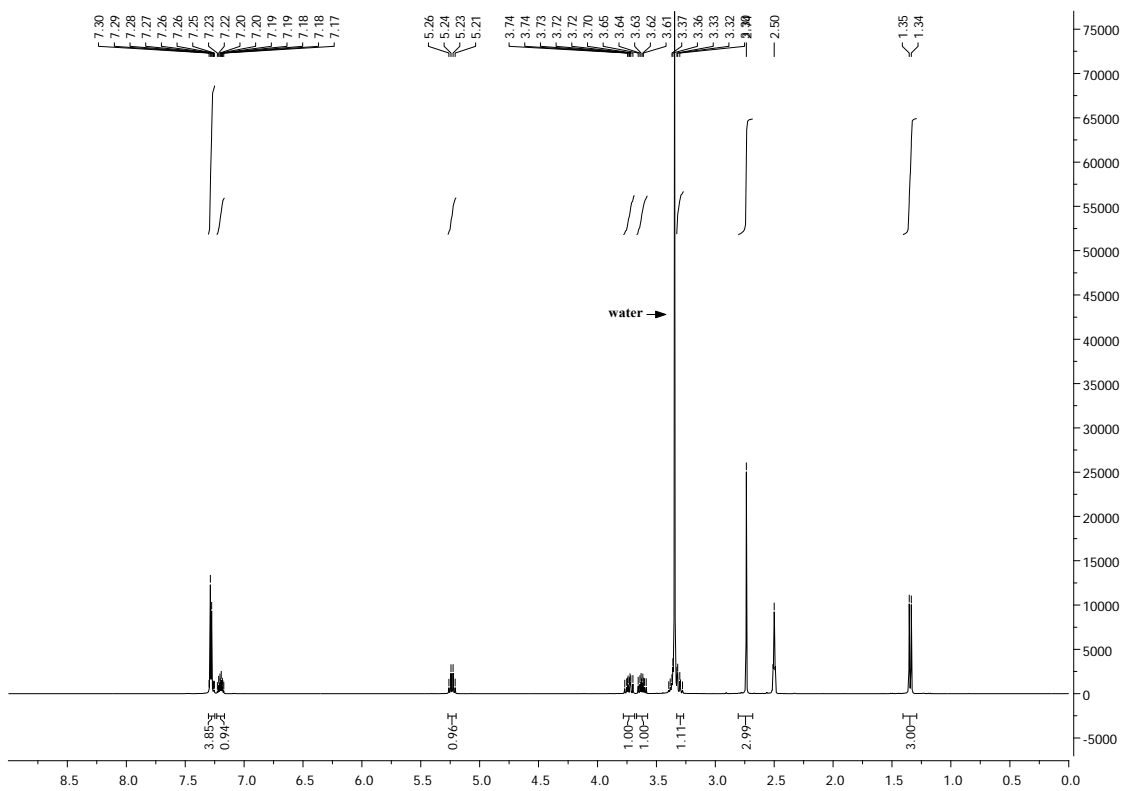
5-Me in CDCl<sub>3</sub> (<sup>1</sup>H and <sup>13</sup>C NMR)



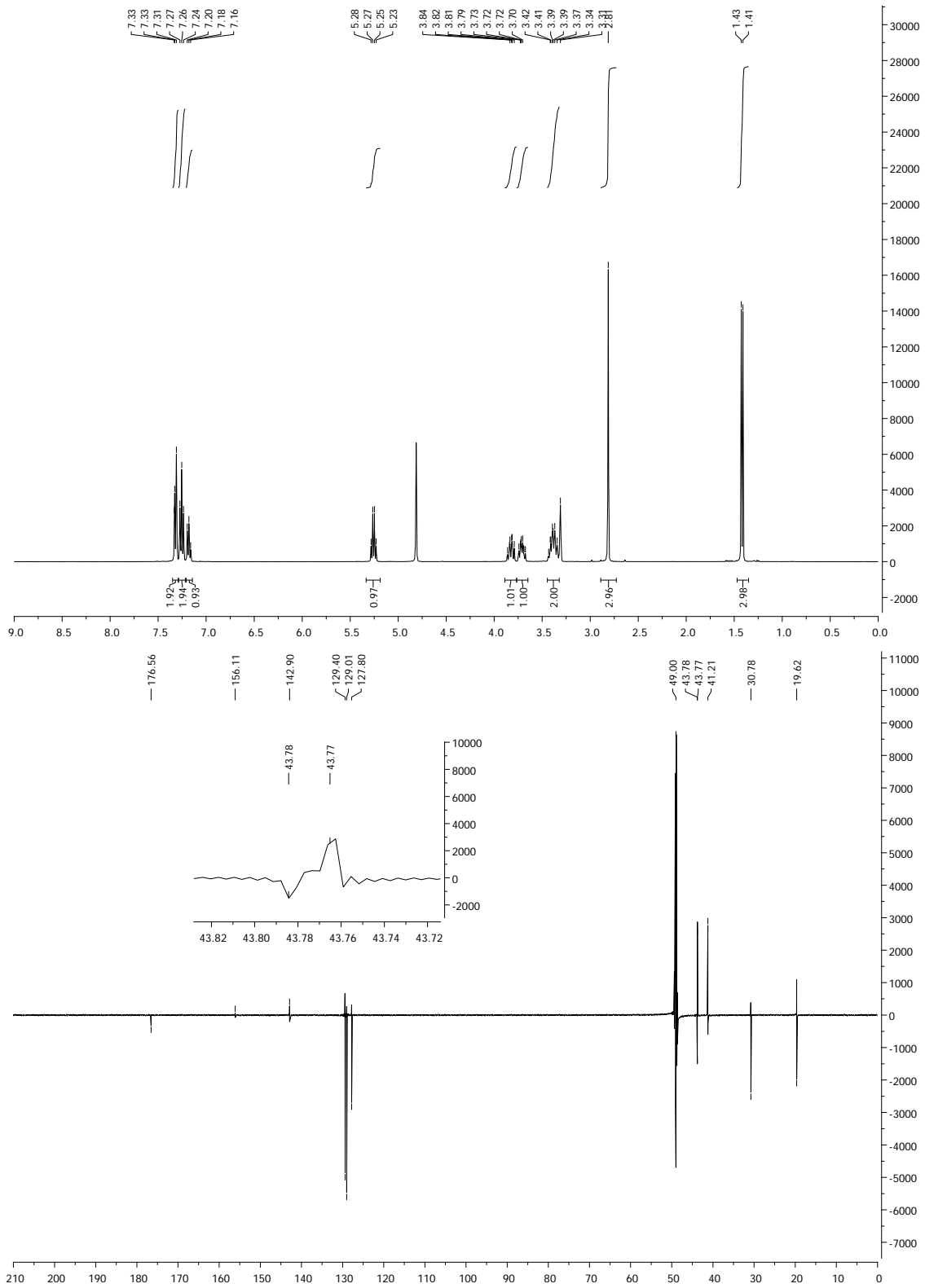
7-Me in CDCl<sub>3</sub> (<sup>1</sup>H and <sup>13</sup>C NMR)



# 7-Me in DMSO-*d*<sub>6</sub> (<sup>1</sup>H and <sup>13</sup>C NMR)



7-Me in CD<sub>3</sub>OD (<sup>1</sup>H and <sup>13</sup>C NMR)



NB: Difficulties were encountered in phasing of the <sup>13</sup>C spectrum.

**D. Cartesian coordinates for the calculated structures 2-Me-10-Me at the LC- $\omega$ PBE/6-311+G(d,p) level of theory in deuterated chloroform (PCM) except if otherwise is indicated**

**Cartesian coordinates [LC- $\omega$ PBE/6-311+G(d,p)]**

**2-Me**

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -1.465058000 | 0.256207000  | 0.260259000  |
| C | -1.948894000 | 0.456840000  | -1.028797000 |
| C | -1.958051000 | -0.807497000 | 1.004260000  |
| C | -2.904893000 | -0.391088000 | -1.562931000 |
| C | -2.918886000 | -1.654426000 | 0.472881000  |
| C | -3.394077000 | -1.449414000 | -0.812021000 |
| H | -1.573814000 | 1.285725000  | -1.622180000 |
| H | -1.578307000 | -0.978112000 | 2.005868000  |
| H | -3.271396000 | -0.223136000 | -2.570110000 |
| H | -3.295105000 | -2.480504000 | 1.066957000  |
| H | -4.144006000 | -2.112987000 | -1.229073000 |
| C | -0.446940000 | 1.211277000  | 0.859856000  |
| H | -0.107902000 | 0.785449000  | 1.803633000  |
| C | -1.041963000 | 2.592438000  | 1.099955000  |
| H | -0.305979000 | 3.263013000  | 1.546671000  |
| H | -1.387572000 | 3.041570000  | 0.168722000  |
| H | -1.891219000 | 2.507171000  | 1.779416000  |
| C | 0.742525000  | 1.300029000  | -0.071328000 |
| O | 0.927011000  | 2.233032000  | -0.820790000 |
| N | 1.631029000  | 0.231231000  | -0.125708000 |
| C | 1.786270000  | -0.827056000 | 0.763629000  |
| C | 2.706327000  | 0.235467000  | -1.105837000 |
| C | 3.204075000  | -1.194053000 | -0.983869000 |
| O | 2.779387000  | -1.609946000 | 0.322082000  |
| O | 1.188406000  | -1.045225000 | 1.778143000  |
| H | 2.325497000  | 0.468456000  | -2.097857000 |
| H | 3.465211000  | 0.972113000  | -0.834813000 |
| H | 4.285986000  | -1.285870000 | -1.033599000 |
| H | 2.740366000  | -1.856739000 | -1.715496000 |

**2b-Me**

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 1.538381000 | 0.315199000  | -0.242934000 |
| C | 1.672841000 | 0.200449000  | 1.136086000  |
| C | 2.372221000 | -0.434768000 | -1.063308000 |
| C | 2.617008000 | -0.654040000 | 1.682649000  |
| C | 3.320277000 | -1.286328000 | -0.519018000 |
| C | 3.443237000 | -1.399913000 | 0.856799000  |
| H | 1.035663000 | 0.785028000  | 1.793853000  |
| H | 2.278629000 | -0.351353000 | -2.142296000 |
| H | 2.707736000 | -0.735596000 | 2.760439000  |
| H | 3.963969000 | -1.864916000 | -1.172982000 |
| H | 4.182175000 | -2.068349000 | 1.285112000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.540114000  | 1.283386000  | -0.847470000 |
| H | 0.347041000  | 0.973313000  | -1.878860000 |
| C | 1.092829000  | 2.702346000  | -0.864848000 |
| H | 0.385321000  | 3.393097000  | -1.324916000 |
| H | 1.295778000  | 3.049921000  | 0.148488000  |
| H | 2.024895000  | 2.723836000  | -1.431427000 |
| C | -0.783576000 | 1.239461000  | -0.097986000 |
| O | -1.197834000 | 2.172223000  | 0.542391000  |
| N | -1.492695000 | 0.042997000  | -0.201514000 |
| C | -2.629488000 | -0.254783000 | 0.555723000  |
| C | -1.102277000 | -1.121368000 | -0.988259000 |
| C | -2.406320000 | -1.898825000 | -1.006410000 |
| O | -3.096608000 | -1.454913000 | 0.163938000  |
| O | -3.136994000 | 0.382704000  | 1.426857000  |
| H | -0.784644000 | -0.848682000 | -1.992613000 |
| H | -0.301099000 | -1.670788000 | -0.491014000 |
| H | -2.269058000 | -2.974928000 | -0.937341000 |
| H | -3.017514000 | -1.656572000 | -1.877471000 |

### 3-Me

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.169573000 | -0.293856000 | -0.011972000 |
| C | -0.565885000 | 0.985733000  | 0.365437000  |
| C | -1.142191000 | -1.209792000 | -0.391347000 |
| C | -1.904896000 | 1.339050000  | 0.366738000  |
| C | -2.484044000 | -0.860024000 | -0.388203000 |
| C | -2.868655000 | 0.415501000  | -0.009096000 |
| H | 0.180564000  | 1.716854000  | 0.663016000  |
| H | -0.847320000 | -2.211232000 | -0.689971000 |
| H | -2.197367000 | 2.341069000  | 0.661825000  |
| H | -3.231300000 | -1.588458000 | -0.684359000 |
| H | -3.917661000 | 0.691141000  | -0.007463000 |
| C | 1.297160000  | -0.671908000 | 0.001074000  |
| H | 1.381666000  | -1.665923000 | -0.455623000 |
| C | 1.900265000  | -0.698703000 | 1.396270000  |
| H | 2.950275000  | -0.991370000 | 1.358288000  |
| H | 1.846280000  | 0.285178000  | 1.865135000  |
| H | 1.361139000  | -1.408195000 | 2.025389000  |
| C | 2.044804000  | 0.244257000  | -0.936464000 |
| O | 3.025846000  | 0.877688000  | -0.641498000 |
| H | 1.625042000  | 0.307891000  | -1.958874000 |

### 4-Me

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 1.085781000 | 0.283909000  | -0.320558000 |
| C | 1.563686000 | 0.349080000  | 0.984388000  |
| C | 1.712881000 | -0.565328000 | -1.222105000 |
| C | 2.646806000 | -0.419166000 | 1.377038000  |
| C | 2.800308000 | -1.332736000 | -0.832258000 |
| C | 3.270031000 | -1.261899000 | 0.468659000  |
| H | 1.079961000 | 1.004064000  | 1.702684000  |
| H | 1.347285000 | -0.627425000 | -2.242471000 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 3.006620000  | -0.359554000 | 2.398737000  |
| H | 3.280534000  | -1.989660000 | -1.549685000 |
| H | 4.119471000  | -1.862409000 | 0.775890000  |
| C | -0.086502000 | 1.142441000  | -0.757709000 |
| H | -0.339435000 | 0.864500000  | -1.782887000 |
| C | 0.231988000  | 2.629533000  | -0.688676000 |
| H | -0.612004000 | 3.226165000  | -1.039273000 |
| H | 0.457248000  | 2.933150000  | 0.333997000  |
| H | 1.097869000  | 2.851804000  | -1.314005000 |
| C | -1.287678000 | 0.799654000  | 0.096870000  |
| O | -1.650418000 | 1.421293000  | 1.065024000  |
| O | -1.894996000 | -0.304663000 | -0.334598000 |
| C | -3.011145000 | -0.770100000 | 0.442788000  |
| H | -2.670603000 | -0.951960000 | 1.463961000  |
| H | -3.766412000 | 0.017594000  | 0.473432000  |
| C | -3.531354000 | -2.024086000 | -0.208443000 |
| H | -2.762119000 | -2.797152000 | -0.234326000 |
| H | -4.381856000 | -2.404822000 | 0.359460000  |
| H | -3.862072000 | -1.825143000 | -1.228881000 |

#### 5-Me

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1.015380000  | 0.320043000  | -0.284951000 |
| C | 1.467626000  | 0.383997000  | 1.028999000  |
| C | 1.760368000  | -0.389242000 | -1.217509000 |
| C | 2.642833000  | -0.247639000 | 1.399245000  |
| C | 2.939131000  | -1.019941000 | -0.849175000 |
| C | 3.383543000  | -0.950598000 | 0.460589000  |
| H | 0.891015000  | 0.927372000  | 1.770841000  |
| H | 1.416150000  | -0.448921000 | -2.245497000 |
| H | 2.982400000  | -0.191421000 | 2.428010000  |
| H | 3.510673000  | -1.568285000 | -1.590396000 |
| H | 4.304587000  | -1.444169000 | 0.751345000  |
| C | -0.258990000 | 1.030215000  | -0.701950000 |
| H | -0.446583000 | 0.789522000  | -1.751873000 |
| C | -0.162664000 | 2.541893000  | -0.536966000 |
| H | -1.077207000 | 3.029828000  | -0.879137000 |
| H | -0.006834000 | 2.808933000  | 0.508418000  |
| H | 0.675025000  | 2.924645000  | -1.121437000 |
| C | -1.415909000 | 0.473305000  | 0.110338000  |
| O | -1.762018000 | 0.915351000  | 1.176443000  |
| S | -2.198204000 | -0.917513000 | -0.637291000 |
| C | -3.386516000 | -1.337029000 | 0.636344000  |
| H | -2.877343000 | -1.614433000 | 1.557165000  |
| H | -4.055273000 | -0.499362000 | 0.822856000  |
| H | -3.958008000 | -2.186340000 | 0.265029000  |

#### 5-Me (CCl<sub>4</sub>)

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 1.019115000 | 0.315234000  | -0.284549000 |
| C | 1.468549000 | 0.374163000  | 1.030389000  |
| C | 1.769168000 | -0.384835000 | -1.219538000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.646483000  | -0.252866000 | 1.398559000  |
| C | 2.950678000  | -1.010878000 | -0.853112000 |
| C | 3.392621000  | -0.946073000 | 0.457336000  |
| H | 0.885863000  | 0.908737000  | 1.773822000  |
| H | 1.426285000  | -0.441623000 | -2.248175000 |
| H | 2.983929000  | -0.201007000 | 2.428234000  |
| H | 3.526116000  | -1.552423000 | -1.596286000 |
| H | 4.315904000  | -1.436152000 | 0.746824000  |
| C | -0.257221000 | 1.022243000  | -0.699856000 |
| H | -0.446111000 | 0.780884000  | -1.749542000 |
| C | -0.162971000 | 2.534208000  | -0.534328000 |
| H | -1.076308000 | 3.021909000  | -0.880307000 |
| H | -0.014306000 | 2.799551000  | 0.512467000  |
| H | 0.678074000  | 2.918446000  | -1.113022000 |
| C | -1.412736000 | 0.466053000  | 0.115242000  |
| O | -1.744182000 | 0.896712000  | 1.189578000  |
| S | -2.217977000 | -0.905766000 | -0.645029000 |
| C | -3.399327000 | -1.322148000 | 0.636217000  |
| H | -2.884398000 | -1.617074000 | 1.548395000  |
| H | -4.051170000 | -0.475471000 | 0.841240000  |
| H | -3.988938000 | -2.157804000 | 0.262039000  |

#### 6-Me

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.739103000  | 0.325834000  | -0.272350000 |
| C | 1.128814000  | 0.218889000  | 1.059587000  |
| C | 1.603518000  | -0.128786000 | -1.259585000 |
| C | 2.354568000  | -0.331515000 | 1.392951000  |
| C | 2.833638000  | -0.678335000 | -0.928192000 |
| C | 3.212436000  | -0.781372000 | 0.399545000  |
| H | 0.460167000  | 0.564743000  | 1.841771000  |
| H | 1.314336000  | -0.048890000 | -2.303519000 |
| H | 2.642855000  | -0.410208000 | 2.435884000  |
| H | 3.497179000  | -1.026335000 | -1.712809000 |
| H | 4.173207000  | -1.211148000 | 0.661723000  |
| C | -0.594011000 | 0.947680000  | -0.639807000 |
| H | -0.731145000 | 0.827253000  | -1.718489000 |
| C | -0.641962000 | 2.430696000  | -0.298793000 |
| H | -1.591904000 | 2.871022000  | -0.607024000 |
| H | -0.534747000 | 2.581868000  | 0.775474000  |
| H | 0.167572000  | 2.957018000  | -0.807285000 |
| C | -1.716116000 | 0.189689000  | 0.061251000  |
| O | -2.198263000 | 0.559656000  | 1.122289000  |
| N | -2.124208000 | -0.934113000 | -0.558864000 |
| H | -1.660019000 | -1.216937000 | -1.405878000 |
| C | -3.113542000 | -1.810699000 | 0.027279000  |
| H | -3.350264000 | -2.599579000 | -0.684509000 |
| H | -2.745942000 | -2.263396000 | 0.950799000  |
| H | -4.024409000 | -1.256359000 | 0.256278000  |

#### 7-Me

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1.752127000  | 0.056221000  | -0.302778000 |
| C | 2.382391000  | 0.373174000  | 0.896585000  |
| C | 1.974941000  | -1.193191000 | -0.866759000 |
| C | 3.217517000  | -0.540630000 | 1.517930000  |
| C | 2.814536000  | -2.107698000 | -0.248786000 |
| C | 3.437865000  | -1.784557000 | 0.945413000  |
| H | 2.215844000  | 1.345939000  | 1.349741000  |
| H | 1.476414000  | -1.452838000 | -1.794371000 |
| H | 3.700590000  | -0.279165000 | 2.453577000  |
| H | 2.979684000  | -3.078980000 | -0.703288000 |
| H | 4.093469000  | -2.499878000 | 1.430503000  |
| C | 0.869788000  | 1.072363000  | -1.006955000 |
| H | 0.389911000  | 0.567794000  | -1.843878000 |
| C | 1.676343000  | 2.263201000  | -1.509229000 |
| H | 1.036267000  | 2.975192000  | -2.033588000 |
| H | 2.160954000  | 2.788030000  | -0.685824000 |
| H | 2.445872000  | 1.915576000  | -2.200420000 |
| C | -0.210419000 | 1.528859000  | -0.047569000 |
| O | -0.120509000 | 2.562559000  | 0.586534000  |
| N | -1.304227000 | 0.717201000  | 0.167456000  |
| C | -1.753880000 | -0.399427000 | -0.563848000 |
| C | -2.291915000 | 1.108267000  | 1.166246000  |
| C | -3.180965000 | -0.125735000 | 1.261268000  |
| N | -2.908587000 | -0.804564000 | 0.013527000  |
| O | -1.222225000 | -0.893907000 | -1.536440000 |
| H | -1.804510000 | 1.356633000  | 2.106561000  |
| H | -2.843792000 | 1.984747000  | 0.819918000  |
| H | -4.237260000 | 0.133298000  | 1.344410000  |
| H | -2.909337000 | -0.761650000 | 2.110999000  |
| C | -3.566544000 | -2.032214000 | -0.351840000 |
| H | -3.194671000 | -2.348351000 | -1.324452000 |
| H | -3.363925000 | -2.820373000 | 0.379854000  |
| H | -4.644642000 | -1.875447000 | -0.415430000 |

### 7-Me (MeOD)

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 1.748046000 | 0.067115000  | -0.291689000 |
| C | 2.317752000 | 0.355133000  | 0.944719000  |
| C | 2.036676000 | -1.150920000 | -0.894053000 |
| C | 3.155405000 | -0.557051000 | 1.566199000  |
| C | 2.878983000 | -2.063401000 | -0.276645000 |
| C | 3.439974000 | -1.769781000 | 0.956043000  |
| H | 2.103002000 | 1.303826000  | 1.427760000  |
| H | 1.589290000 | -1.387799000 | -1.853410000 |
| H | 3.589497000 | -0.318650000 | 2.531515000  |
| H | 3.095251000 | -3.009793000 | -0.761178000 |
| H | 4.096763000 | -2.483815000 | 1.441362000  |
| C | 0.868289000 | 1.083491000  | -0.998245000 |
| H | 0.400078000 | 0.582139000  | -1.843658000 |
| C | 1.680226000 | 2.276499000  | -1.487012000 |
| H | 1.044803000 | 2.994793000  | -2.008289000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 2.165730000  | 2.791148000  | -0.657399000 |
| H | 2.450563000  | 1.931977000  | -2.178919000 |
| C | -0.227284000 | 1.534836000  | -0.053815000 |
| O | -0.155860000 | 2.579154000  | 0.568370000  |
| N | -1.311267000 | 0.714252000  | 0.159923000  |
| C | -1.737195000 | -0.419104000 | -0.561510000 |
| C | -2.318450000 | 1.105784000  | 1.140280000  |
| C | -3.198781000 | -0.134448000 | 1.234062000  |
| N | -2.890753000 | -0.832066000 | 0.004119000  |
| O | -1.181859000 | -0.917969000 | -1.520996000 |
| H | -1.848549000 | 1.364894000  | 2.086506000  |
| H | -2.872329000 | 1.973553000  | 0.776419000  |
| H | -4.258668000 | 0.116171000  | 1.286395000  |
| H | -2.942665000 | -0.754834000 | 2.099153000  |
| C | -3.540025000 | -2.065273000 | -0.360286000 |
| H | -3.155715000 | -2.389945000 | -1.325119000 |
| H | -3.345657000 | -2.844945000 | 0.382104000  |
| H | -4.617197000 | -1.910792000 | -0.438827000 |

#### 7-Me (DMSO-*d*<sub>6</sub>)

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1.747501000  | 0.068297000  | -0.290536000 |
| C | 2.310804000  | 0.352637000  | 0.949642000  |
| C | 2.042717000  | -1.146184000 | -0.896941000 |
| C | 3.148399000  | -0.559763000 | 1.570978000  |
| C | 2.885013000  | -2.058806000 | -0.279746000 |
| C | 3.439438000  | -1.768934000 | 0.956840000  |
| H | 2.091205000  | 1.298604000  | 1.435850000  |
| H | 1.600672000  | -1.380150000 | -1.859500000 |
| H | 3.577333000  | -0.324286000 | 2.539312000  |
| H | 3.106431000  | -3.002373000 | -0.767452000 |
| H | 4.096133000  | -2.483126000 | 1.442048000  |
| C | 0.868302000  | 1.085108000  | -0.997104000 |
| H | 0.401335000  | 0.584471000  | -1.843645000 |
| C | 1.680996000  | 2.278449000  | -1.483833000 |
| H | 1.046263000  | 2.997561000  | -2.004807000 |
| H | 2.166176000  | 2.791837000  | -0.653225000 |
| H | 2.451719000  | 1.934442000  | -2.175569000 |
| C | -0.228872000 | 1.535729000  | -0.054181000 |
| O | -0.159528000 | 2.580893000  | 0.567013000  |
| N | -1.311879000 | 0.714026000  | 0.159175000  |
| C | -1.735290000 | -0.420761000 | -0.561561000 |
| C | -2.320995000 | 1.105261000  | 1.137742000  |
| C | -3.200172000 | -0.135813000 | 1.231253000  |
| N | -2.888874000 | -0.834704000 | 0.002798000  |
| O | -1.177658000 | -0.919814000 | -1.519761000 |
| H | -1.852833000 | 1.365509000  | 2.084515000  |
| H | -2.875254000 | 1.972103000  | 0.772295000  |
| H | -4.260415000 | 0.113714000  | 1.281033000  |
| H | -2.945189000 | -0.754890000 | 2.097571000  |
| C | -3.536711000 | -2.068694000 | -0.361636000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -3.150705000 | -2.394011000 | -1.325571000 |
| H | -3.343057000 | -2.847497000 | 0.381824000  |
| H | -4.613839000 | -1.914945000 | -0.442010000 |

### 7b-Me

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1.548422000  | 0.301354000  | -0.245290000 |
| C | 1.686133000  | 0.209654000  | 1.135162000  |
| C | 2.381912000  | -0.462020000 | -1.053807000 |
| C | 2.632524000  | -0.634180000 | 1.694412000  |
| C | 3.332139000  | -1.303166000 | -0.497187000 |
| C | 3.458391000  | -1.393073000 | 0.880123000  |
| H | 1.048463000  | 0.804123000  | 1.783366000  |
| H | 2.285808000  | -0.397582000 | -2.133918000 |
| H | 2.725199000  | -0.697298000 | 2.773346000  |
| H | 3.975034000  | -1.892260000 | -1.142614000 |
| H | 4.199118000  | -2.053161000 | 1.318294000  |
| C | 0.549199000  | 1.259481000  | -0.863904000 |
| H | 0.352201000  | 0.930627000  | -1.888228000 |
| C | 1.110475000  | 2.674489000  | -0.912620000 |
| H | 0.404558000  | 3.359927000  | -1.383182000 |
| H | 1.318927000  | 3.041370000  | 0.092630000  |
| H | 2.040278000  | 2.679846000  | -1.483705000 |
| C | -0.771820000 | 1.237271000  | -0.102697000 |
| O | -1.150693000 | 2.185362000  | 0.543404000  |
| N | -1.501794000 | 0.064078000  | -0.201006000 |
| C | -2.657666000 | -0.223798000 | 0.560147000  |
| C | -1.114906000 | -1.113109000 | -0.979712000 |
| C | -2.402587000 | -1.928077000 | -1.017728000 |
| N | -3.061410000 | -1.469270000 | 0.184005000  |
| O | -3.179235000 | 0.474533000  | 1.394168000  |
| H | -0.779479000 | -0.844292000 | -1.979117000 |
| H | -0.317588000 | -1.656838000 | -0.469094000 |
| H | -2.203064000 | -2.998337000 | -0.987292000 |
| H | -2.994180000 | -1.700157000 | -1.909856000 |
| H | -3.986717000 | -1.767738000 | 0.446401000  |

### 8-Me

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -2.183759000 | 0.238522000  | 0.173408000  |
| C | -2.427880000 | 0.021012000  | -1.179500000 |
| C | -2.623373000 | -0.703881000 | 1.093538000  |
| C | -3.096512000 | -1.115402000 | -1.602453000 |
| C | -3.296885000 | -1.841060000 | 0.672263000  |
| C | -3.534321000 | -2.050508000 | -0.676049000 |
| H | -2.091119000 | 0.749624000  | -1.911611000 |
| H | -2.429731000 | -0.547844000 | 2.149611000  |
| H | -3.278937000 | -1.271117000 | -2.660546000 |
| H | -3.635629000 | -2.567092000 | 1.403761000  |
| H | -4.059877000 | -2.940161000 | -1.006170000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -1.469253000 | 1.496994000  | 0.632308000  |
| H | -1.286399000 | 1.405411000  | 1.702030000  |
| C | -2.283550000 | 2.752895000  | 0.356981000  |
| H | -1.755724000 | 3.642705000  | 0.703562000  |
| H | -2.482791000 | 2.873677000  | -0.708078000 |
| H | -3.237617000 | 2.688806000  | 0.882422000  |
| C | -0.124926000 | 1.564277000  | -0.067165000 |
| O | 0.113678000  | 2.367778000  | -0.939144000 |
| N | 0.822102000  | 0.589781000  | 0.251318000  |
| C | 0.941047000  | -0.071439000 | 1.469444000  |
| C | 2.023828000  | 0.327559000  | -0.574093000 |
| C | 2.397143000  | -1.057865000 | 0.012872000  |
| O | 1.967454000  | -0.921948000 | 1.394454000  |
| O | 0.293476000  | 0.079371000  | 2.469278000  |
| C | 1.593412000  | -2.202680000 | -0.581478000 |
| H | 0.525054000  | -1.977161000 | -0.600298000 |
| H | 1.921564000  | -2.423417000 | -1.597547000 |
| H | 1.746893000  | -3.093010000 | 0.029621000  |
| C | 1.733723000  | 0.254828000  | -2.064111000 |
| H | 2.575295000  | -0.230196000 | -2.563950000 |
| H | 0.830799000  | -0.318276000 | -2.274962000 |
| H | 1.616717000  | 1.251985000  | -2.481484000 |
| C | 3.874108000  | -1.373845000 | 0.016722000  |
| H | 4.256231000  | -1.383481000 | -1.006077000 |
| H | 4.439562000  | -0.646460000 | 0.596977000  |
| H | 4.036192000  | -2.362575000 | 0.447725000  |
| C | 3.072220000  | 1.395866000  | -0.283567000 |
| H | 3.342668000  | 1.417173000  | 0.774303000  |
| H | 3.975183000  | 1.219420000  | -0.870064000 |
| H | 2.669960000  | 2.370287000  | -0.559878000 |

### 9-Me

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -2.229810000 | 0.212698000  | 0.180117000  |
| C | -2.394149000 | 0.088411000  | -1.195409000 |
| C | -2.811734000 | -0.729759000 | 1.017459000  |
| C | -3.124462000 | -0.963036000 | -1.723831000 |
| C | -3.548463000 | -1.778467000 | 0.489832000  |
| C | -3.704878000 | -1.898597000 | -0.881509000 |
| H | -1.950958000 | 0.820561000  | -1.864678000 |
| H | -2.683119000 | -0.643949000 | 2.091249000  |
| H | -3.242128000 | -1.050028000 | -2.798505000 |
| H | -3.999553000 | -2.506735000 | 1.155128000  |
| H | -4.278251000 | -2.721374000 | -1.294527000 |
| C | -1.471711000 | 1.394528000  | 0.761541000  |
| H | -1.279845000 | 1.188064000  | 1.815143000  |
| C | -2.253575000 | 2.694400000  | 0.626186000  |
| H | -1.700847000 | 3.531583000  | 1.054805000  |
| H | -2.461409000 | 2.921767000  | -0.419600000 |
| H | -3.203125000 | 2.597078000  | 1.153327000  |
| C | -0.143088000 | 1.513240000  | 0.059329000  |

|   |             |              |              |
|---|-------------|--------------|--------------|
| O | 0.142904000 | 2.365702000  | -0.730908000 |
| N | 0.825051000 | 0.484078000  | 0.296814000  |
| C | 0.867817000 | -0.436086000 | 1.338268000  |
| C | 1.973890000 | 0.372327000  | -0.532835000 |
| C | 2.635276000 | -0.932385000 | 0.007786000  |
| O | 1.962394000 | -1.239238000 | 1.163764000  |
| O | 0.140177000 | -0.559143000 | 2.262162000  |
| F | 1.665353000 | 0.257145000  | -1.827716000 |
| F | 2.814343000 | 1.408805000  | -0.399212000 |
| F | 3.927755000 | -0.766441000 | 0.271771000  |
| F | 2.513593000 | -1.931478000 | -0.868374000 |

### 10-Me

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1.430647000  | 0.126863000  | -0.310195000 |
| C | 1.947444000  | 0.338699000  | 0.963838000  |
| C | 1.766292000  | -1.041153000 | -0.982491000 |
| C | 2.778505000  | -0.599264000 | 1.554560000  |
| C | 2.602492000  | -1.978558000 | -0.396342000 |
| C | 3.109856000  | -1.761216000 | 0.874693000  |
| H | 1.700381000  | 1.249985000  | 1.501427000  |
| H | 1.360092000  | -1.219937000 | -1.972395000 |
| H | 3.171191000  | -0.419941000 | 2.549859000  |
| H | 2.855984000  | -2.885306000 | -0.935475000 |
| H | 3.761922000  | -2.495564000 | 1.335378000  |
| C | 0.566550000  | 1.180831000  | -0.978688000 |
| H | 0.097823000  | 0.727154000  | -1.849146000 |
| C | 1.401525000  | 2.377417000  | -1.417236000 |
| H | 0.780972000  | 3.129388000  | -1.906928000 |
| H | 1.897876000  | 2.848675000  | -0.568643000 |
| H | 2.164466000  | 2.043086000  | -2.122322000 |
| C | -0.525878000 | 1.621924000  | -0.019931000 |
| O | -0.499629000 | 2.719302000  | 0.490906000  |
| N | -1.534824000 | 0.720320000  | 0.353323000  |
| C | -1.813573000 | -0.463066000 | -0.316850000 |
| C | -2.376802000 | 1.081411000  | 1.495522000  |
| C | -3.092935000 | -2.415237000 | -0.234617000 |
| O | -2.695772000 | -1.184423000 | 0.373944000  |
| O | -1.363129000 | -0.811122000 | -1.379612000 |
| H | -2.055820000 | 2.056463000  | 1.846148000  |
| H | -3.422819000 | 1.132576000  | 1.196632000  |
| H | -3.814059000 | -2.857541000 | 0.447593000  |
| H | -3.551718000 | -2.227792000 | -1.204920000 |
| H | -2.266864000 | 0.346299000  | 2.291025000  |
| H | -2.232157000 | -3.071742000 | -0.356976000 |