Supporting Information

Linear Free Energy Relationships Reveal Structural Changes in Hydrogen-Bonded Host-Guest Interactions

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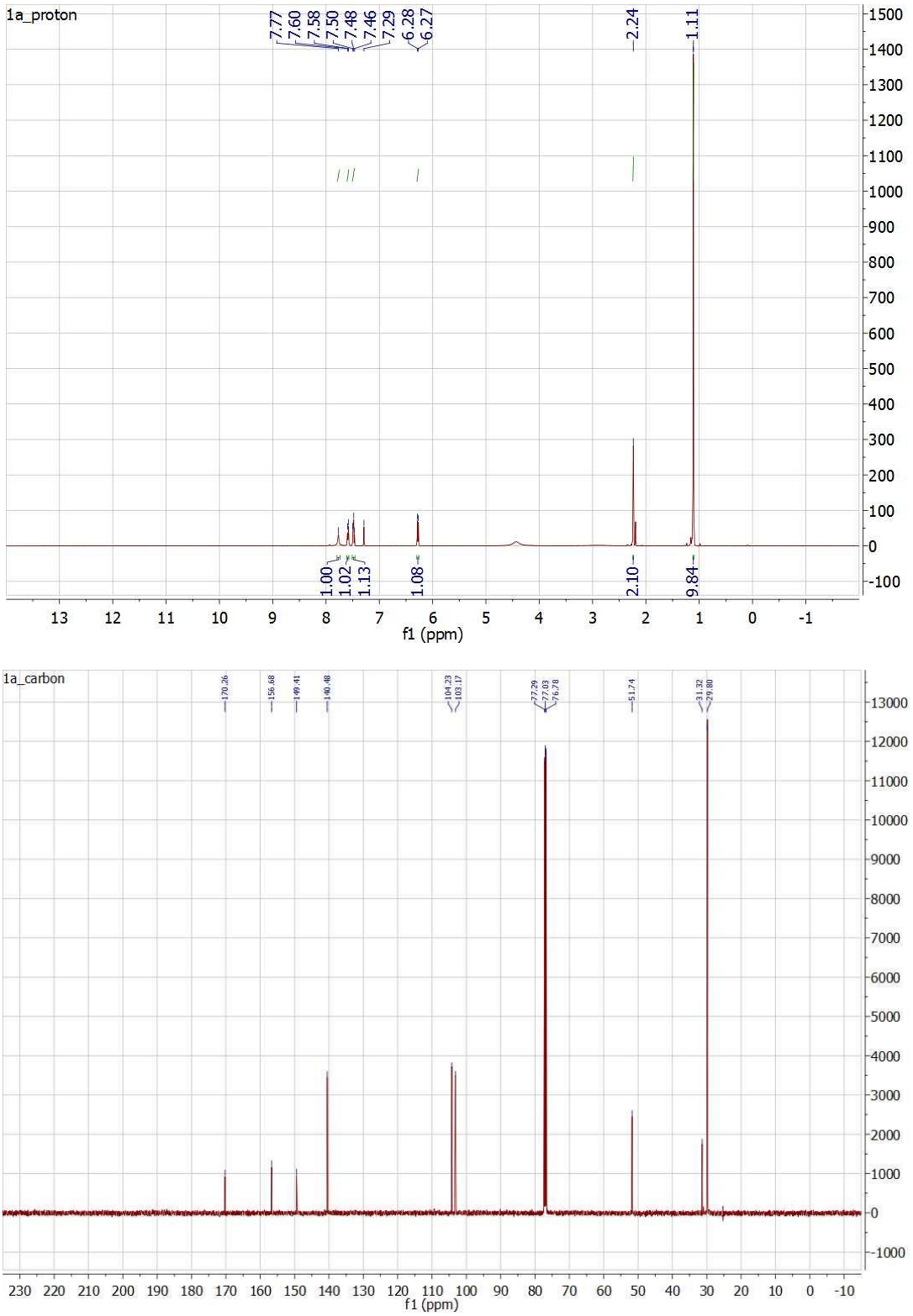

Figure S1. ^{1}H (500 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (125 MHz, $CDCl_3$) NMR spectra of **1a**.

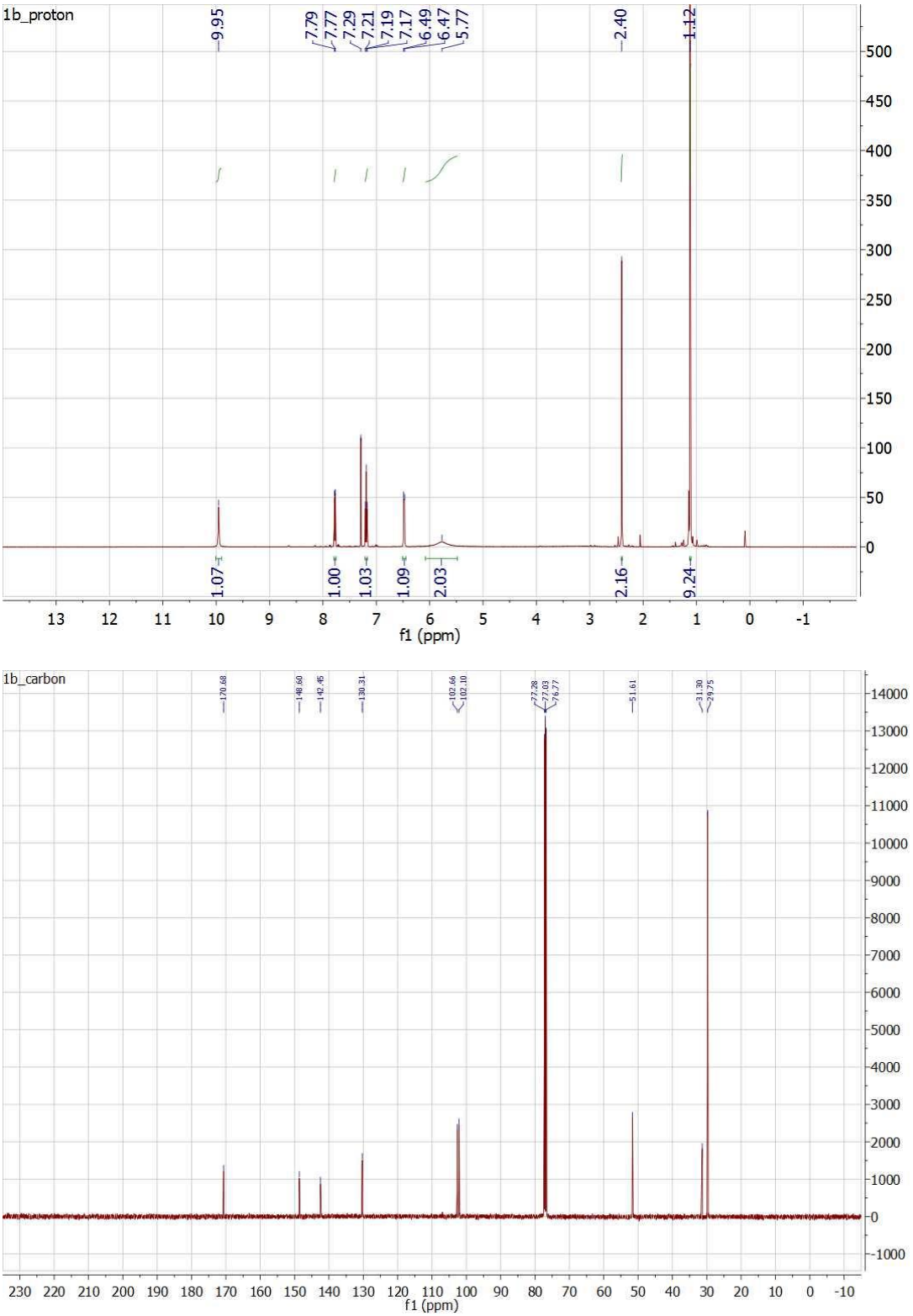

Figure S2. ^{1}H (500 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (125 MHz, $CDCl_3$) NMR spectra of **1b**.

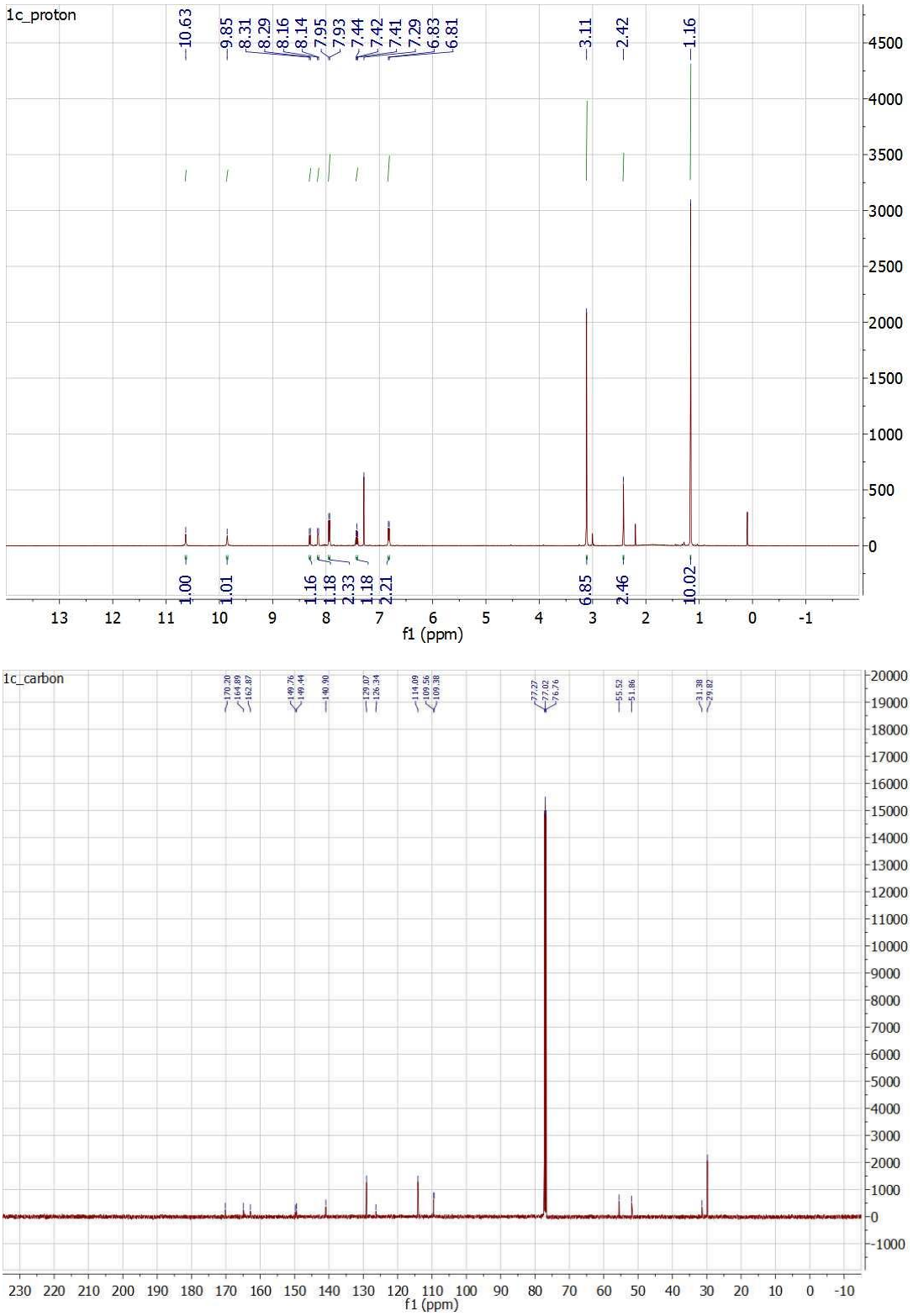

Figure S3. ^{1}H (500 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (125 MHz, $CDCl_3$) NMR spectra of **1c**.

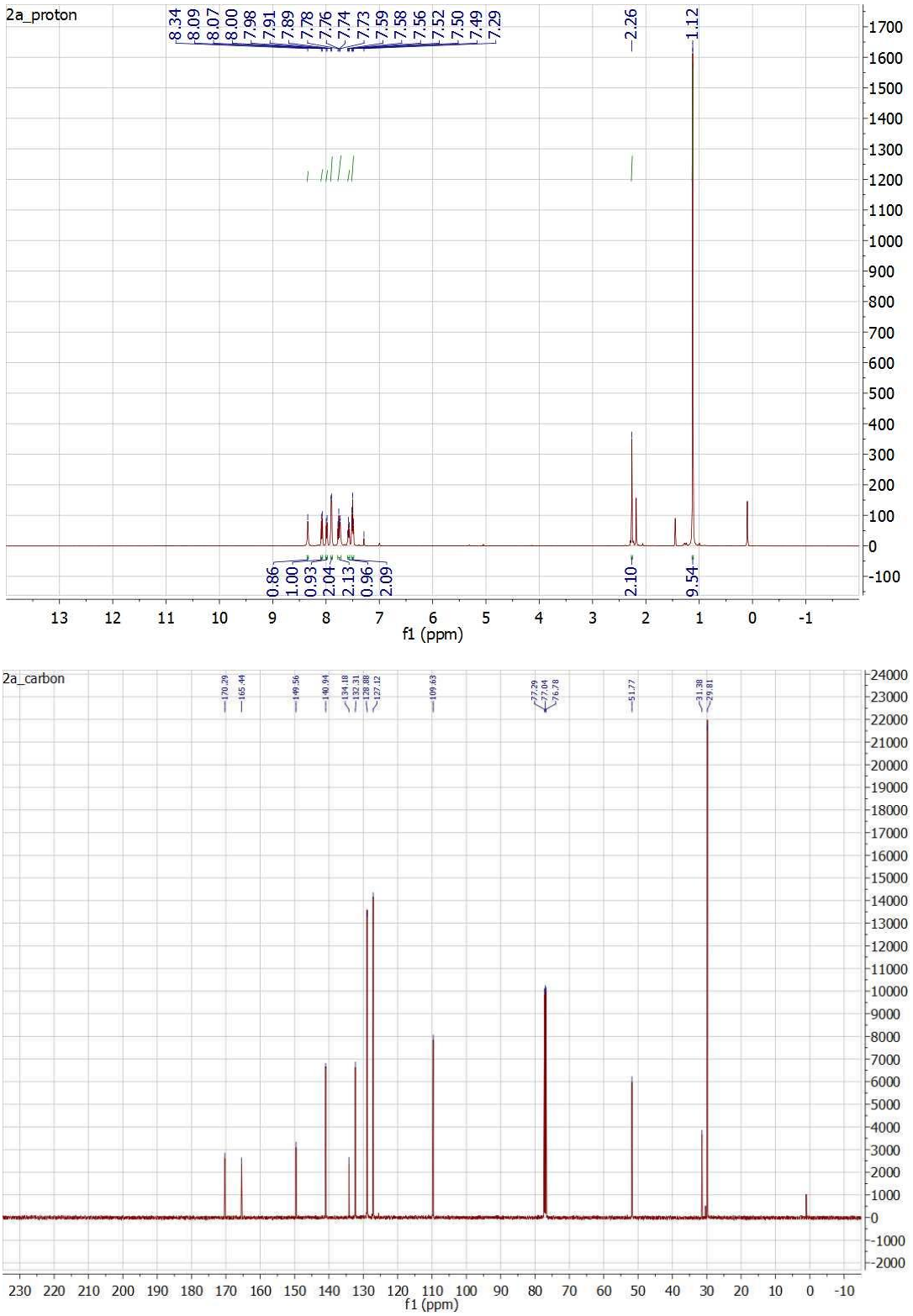

Figure S4. ^{1}H (500 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (125 MHz, $CDCl_3$) NMR spectra of **2a**.

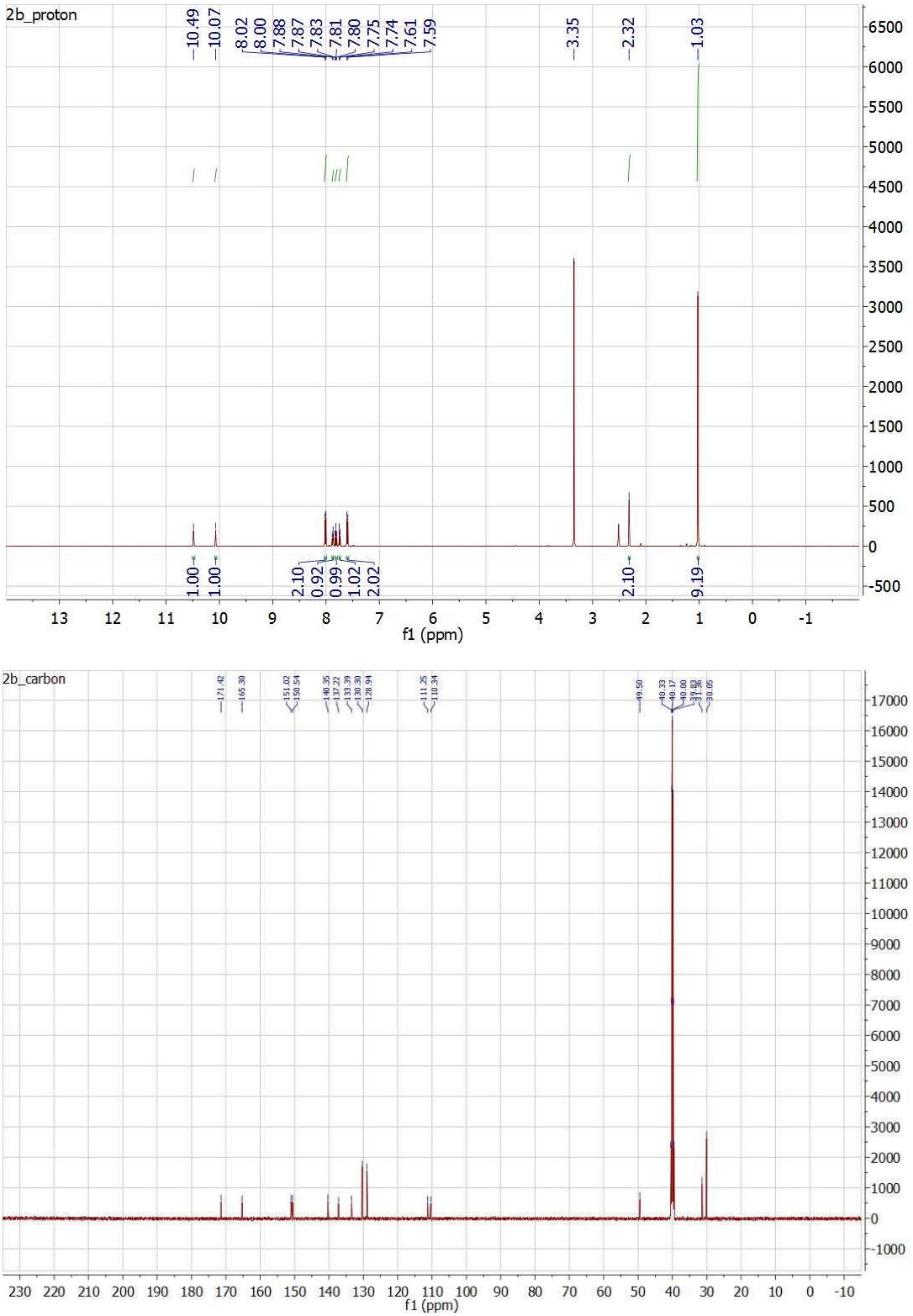

Figure S5. ^{1}H (500 MHz, DMSO) and $^{13}C\{^{1}H\}$ (125 MHz, DMSO) NMR spectra of **2b**.

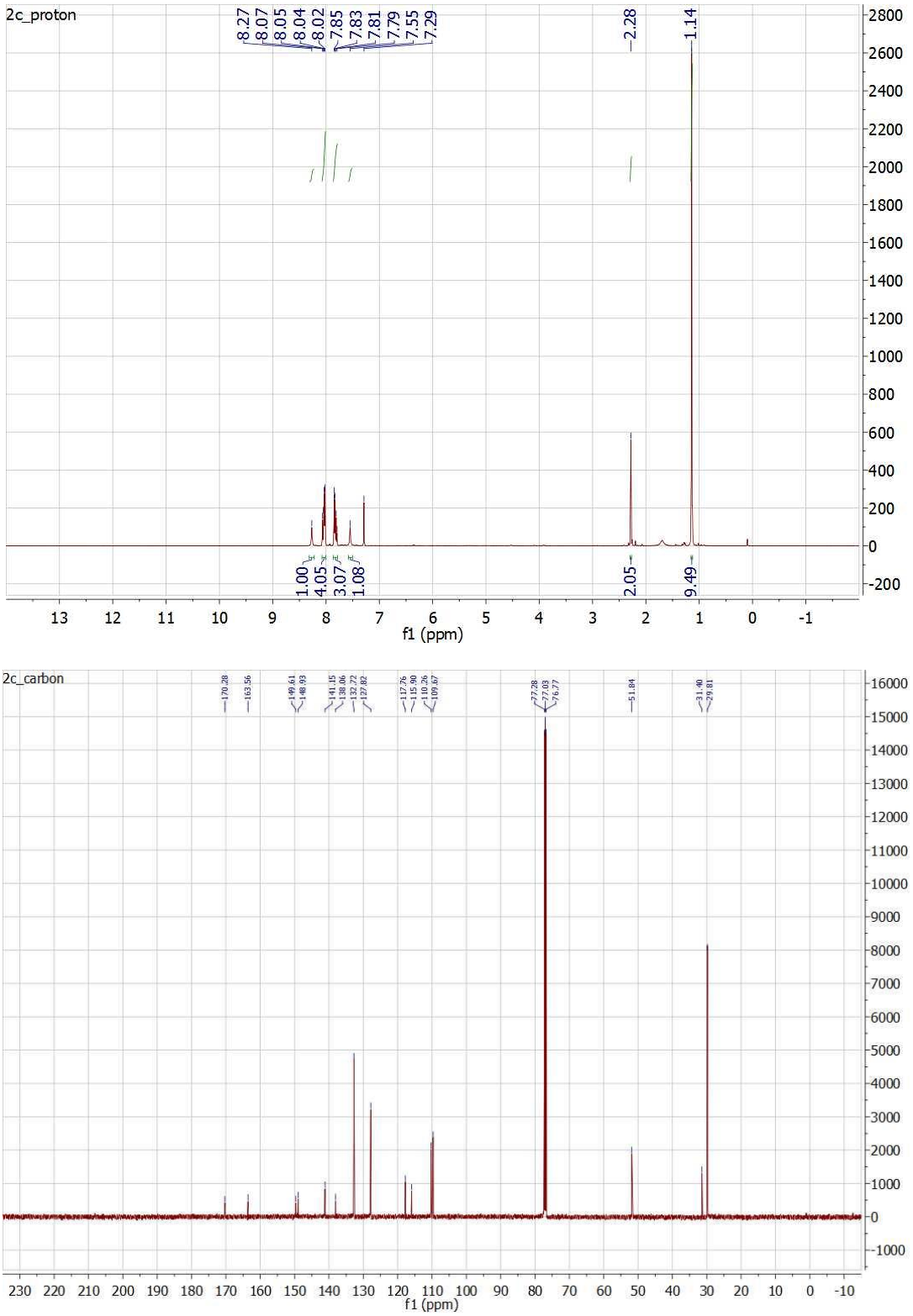

Figure S6. ^{1}H (500 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (125 MHz, $CDCl_3$) NMR spectra of **2c**.

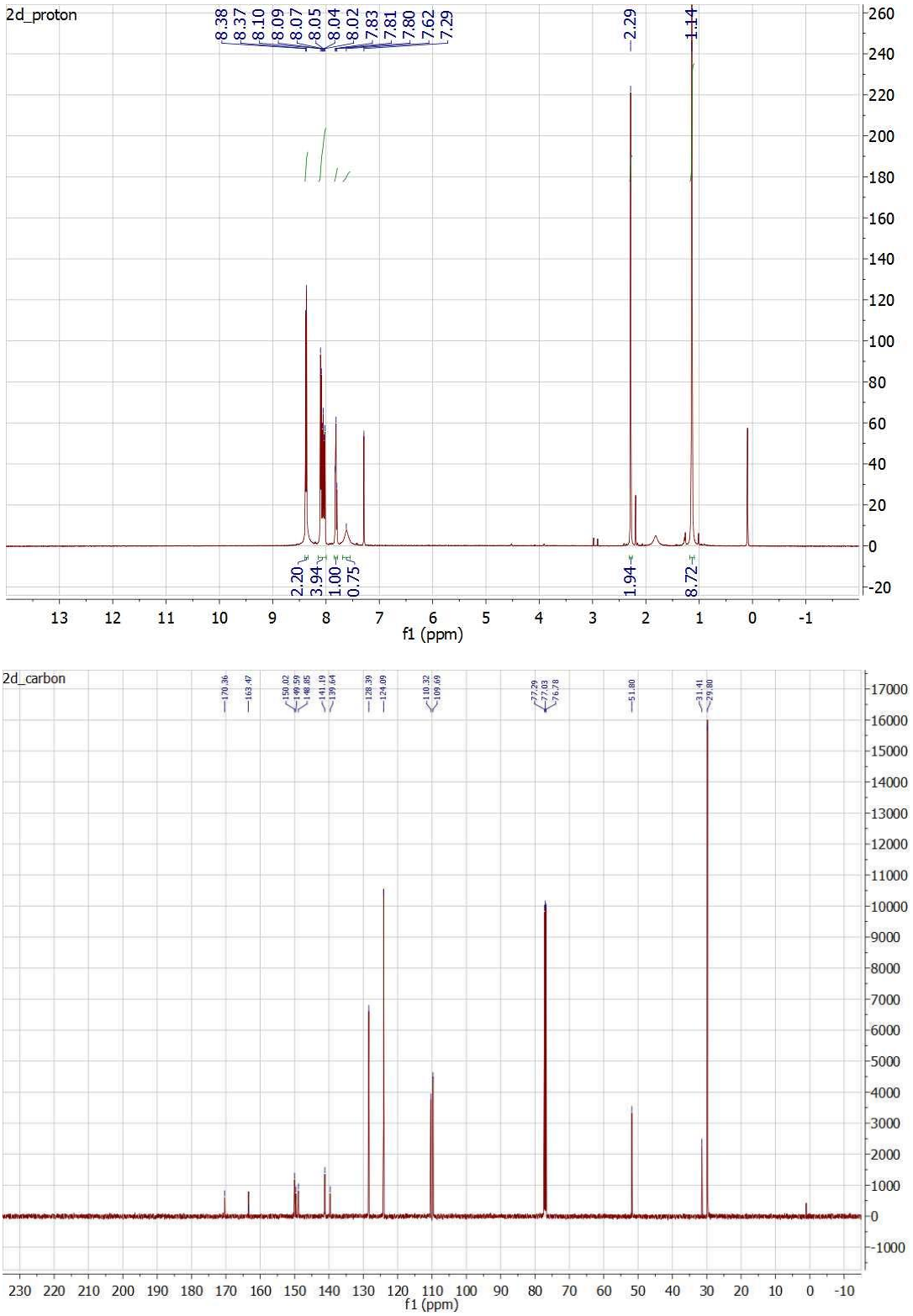

Figure S7. ^{1}H (500 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (125 MHz, $CDCl_3$) NMR spectra of **2d**.

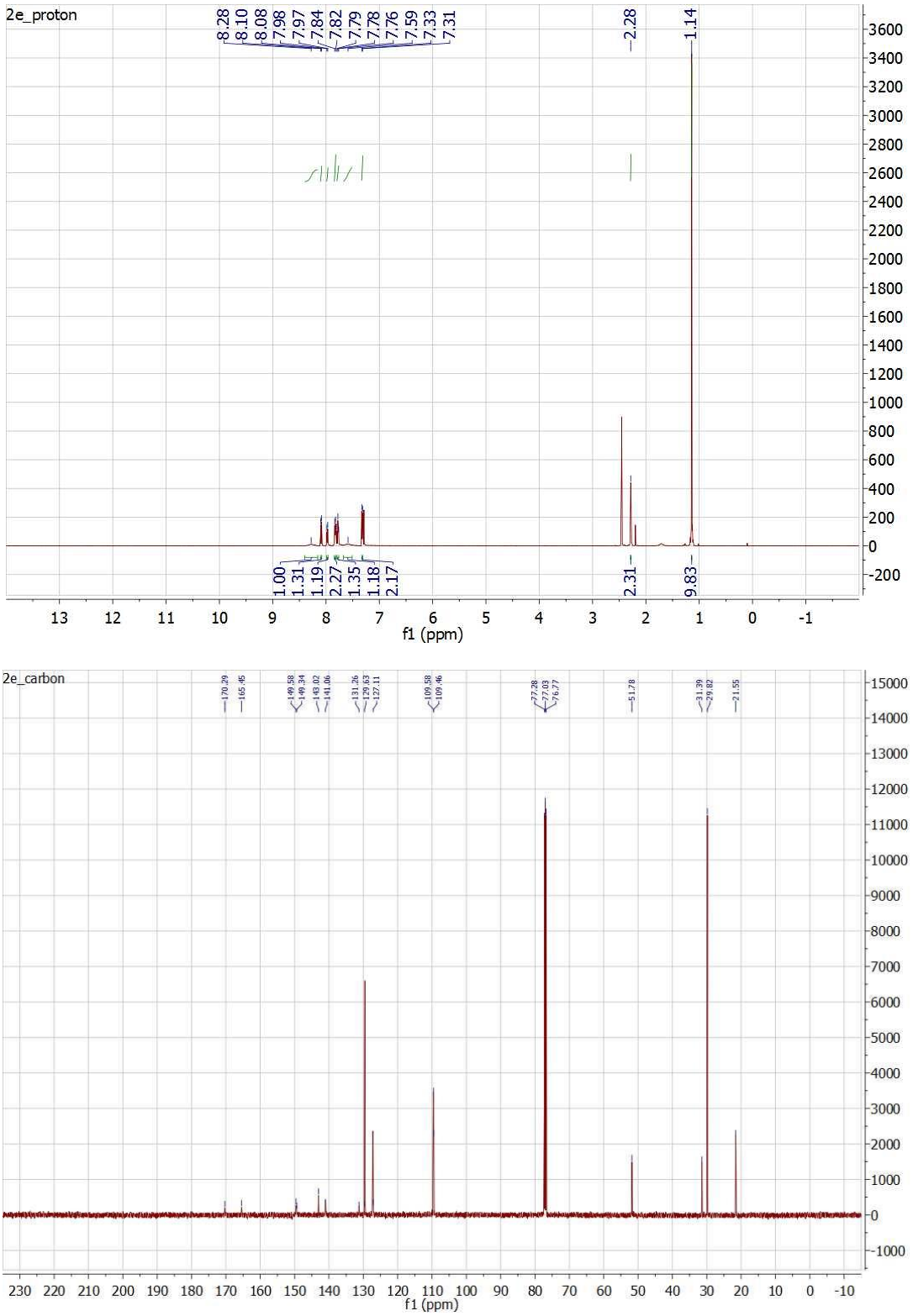

Figure S8. ^{1}H (500 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (125 MHz, $CDCl_3$) NMR spectra of **2e**.

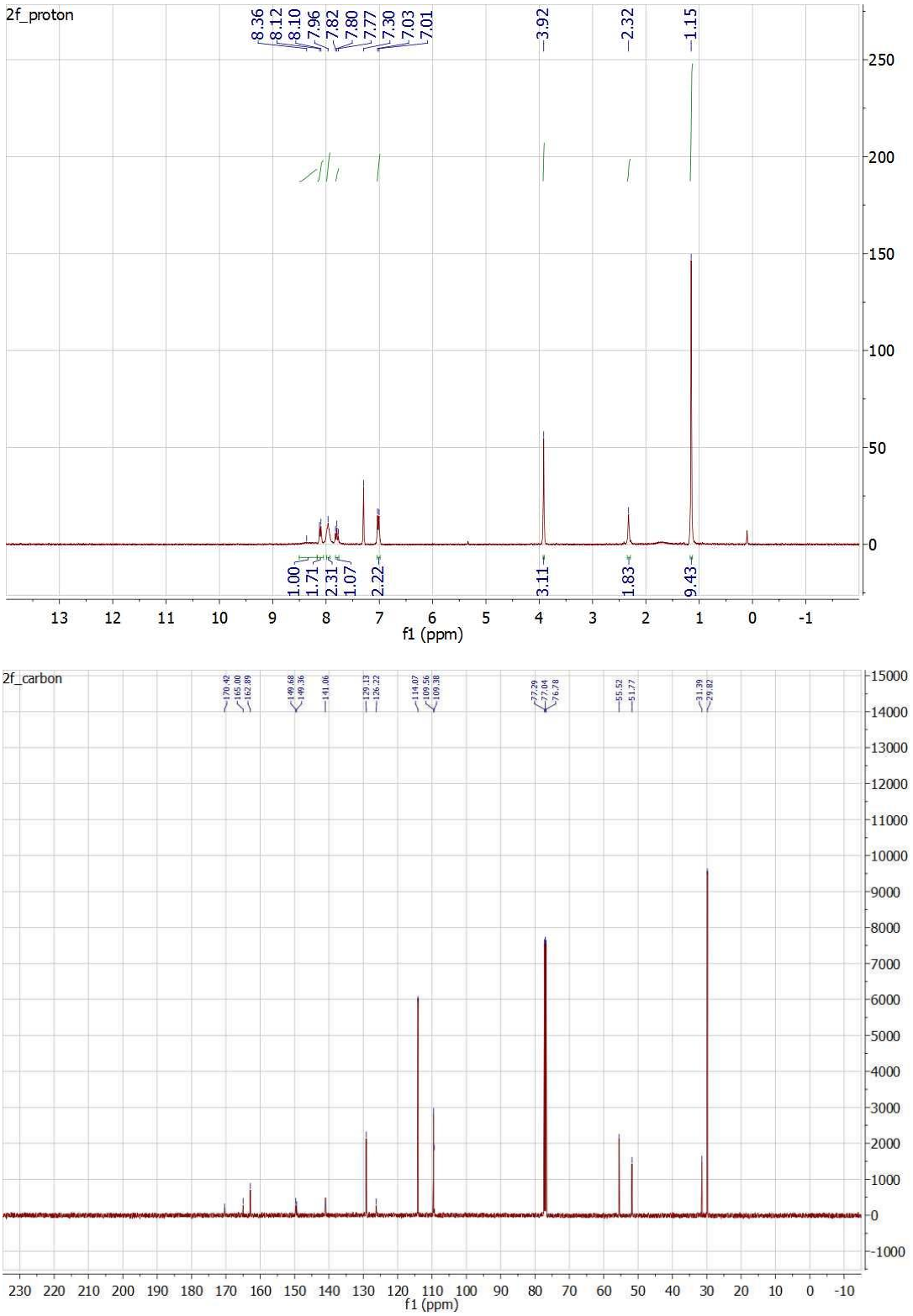

Figure S9. ^{1}H (500 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (125 MHz, $CDCl_3$) NMR spectra of **2f**.

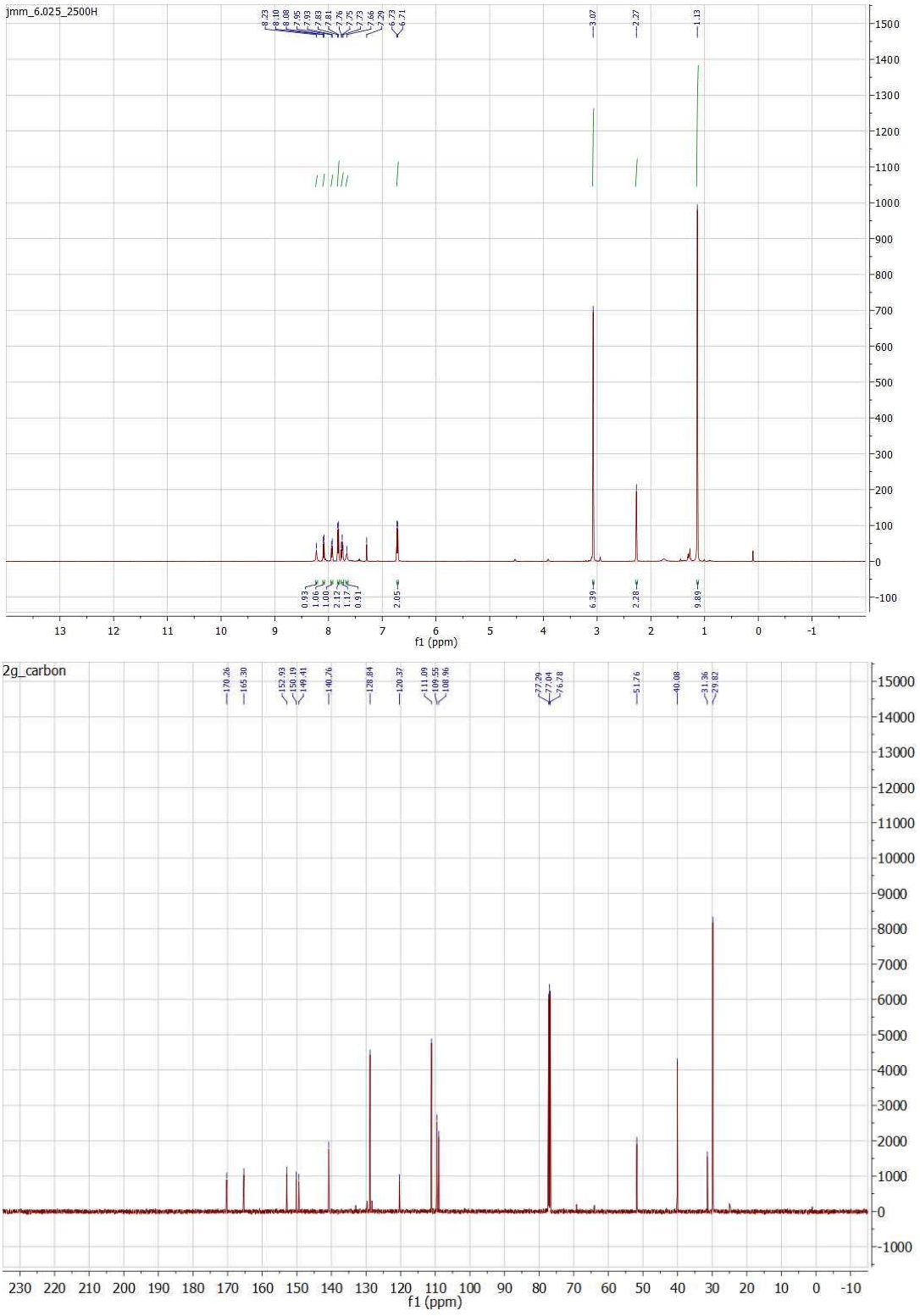

Figure S10. ^{1}H (500 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (125 MHz, $CDCl_3$) NMR spectra of **2g**.

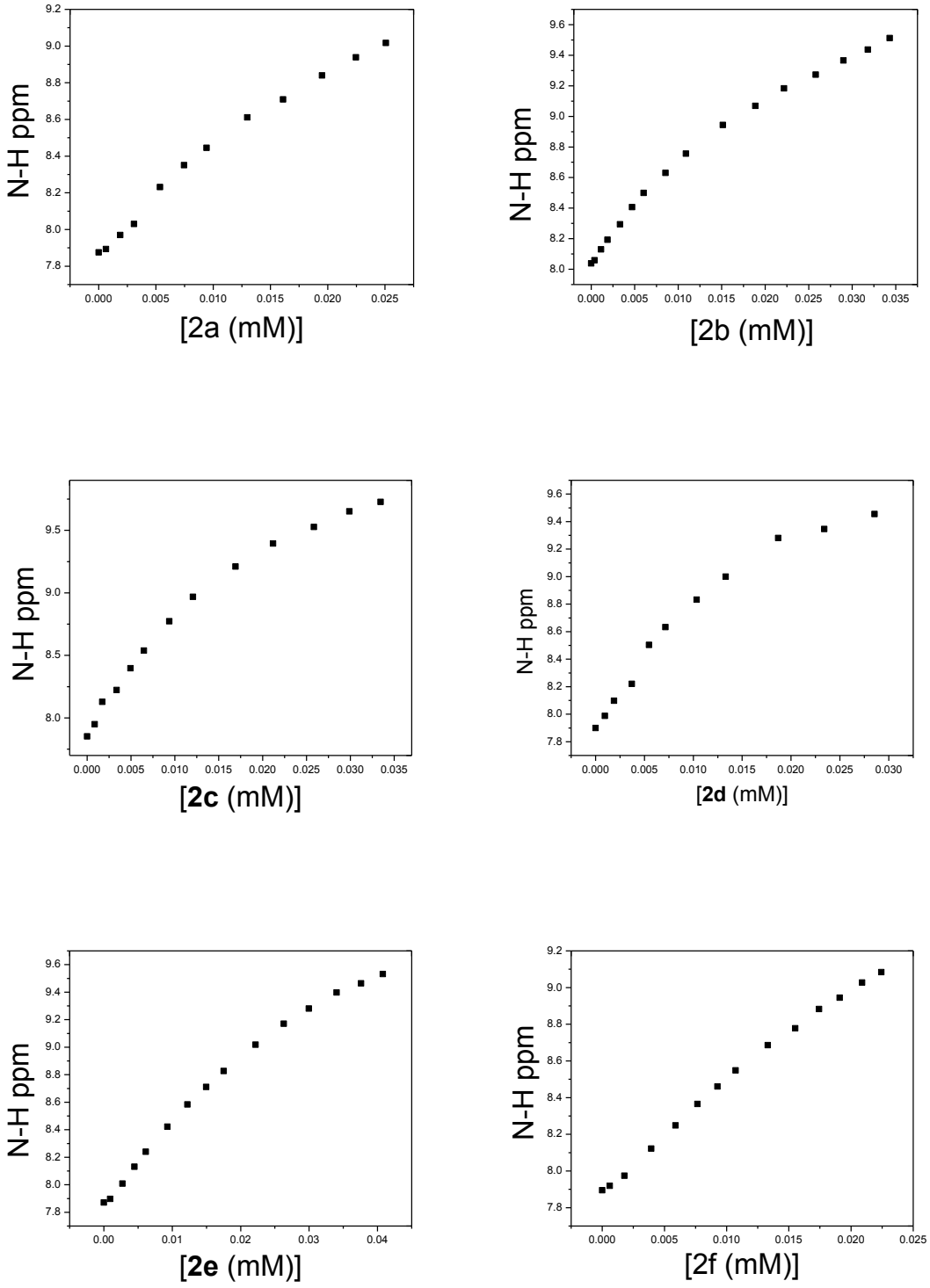

Figure S11. ^{1}H NMR (500 MHz, $CDCl_3$) titration data. Representative binding curves for hosts **2a-f** with **5**.

Calculated Geometries

Diethyl barbital

Sum of electronic and zero point energies: -646.9674167 Hartree
Lowest Frequency: 34.7 cm^{-1}
Coordinates: B3LYP/6-31+G(d,p) IEF-PCM $CHCl_3$

Atom	x	y	z
H	-1.89457700	-0.00259900	2.03104700
N	-1.35841700	-0.00201400	1.16878100
C	0.02232300	0.00064400	1.28614000
C	-2.10319000	-0.00487900	-0.00003300
C	0.85119500	0.00210000	-0.00003900
O	0.53956400	0.00187000	2.39282700
N	-1.35862900	-0.00469900	-1.16871700
O	-3.32340900	-0.00755700	0.00019500
C	0.02233300	-0.00203200	-1.28621000
C	1.75570700	1.27587500	-0.00135800
C	1.76530700	-1.26462000	0.00120400
H	-1.89473100	-0.00704800	-2.03094200
O	0.53928700	-0.00241500	-2.39292900
H	2.39809200	1.20683800	0.88129000
H	2.39754800	1.20545700	-0.88428700
H	2.40713700	-1.19093600	-0.88147500
H	2.40675900	-1.18942600	0.88403600
C	1.00972200	2.61449100	-0.00214600
H	1.72948100	3.43846400	-0.00266000
H	0.37831000	2.73235400	-0.88964500
H	0.37836200	2.73336000	0.88524600
C	1.02934200	-2.60881600	0.00222700
H	0.39910900	-2.73268500	-0.88527600
H	1.75519700	-3.42742700	0.00312200
H	0.39867000	-2.73112200	0.88963900

2a

Sum of electronic and zero point energies: -1013.047193 Hartree
Lowest Frequency: 20.7 cm^{-1}
Coordinates: B3LYP/6-31+G(d,p) IEF-PCM $CHCl_3$

Atom	x	y	z
N	0.045100	0.412300	-0.263000
C	-1.053800	1.152000	-0.060000
C	1.237000	1.023200	-0.312200
C	-1.019500	2.543700	0.106900
N	-2.226300	0.378800	-0.041700
C	1.392300	2.408800	-0.160600
N	2.295500	0.126600	-0.532200
C	0.232900	3.153800	0.050000
H	-1.929100	3.100400	0.273300
C	-3.528600	0.773500	0.161300
H	-2.042100	-0.609500	-0.156300
H	2.371700	2.860000	-0.208600

C	3.645100	0.374300	-0.662600
H	1.985300	-0.834000	-0.607400
H	0.306600	4.230100	0.173100
O	-3.845800	1.934200	0.427900
C	-4.555600	-0.317200	0.051100
O	4.125800	1.505900	-0.601100
C	4.497200	-0.865600	-0.892400
C	-5.765300	-0.138600	0.740600
C	-4.372000	-1.474400	-0.723600
H	3.866700	-1.701500	-1.216500
H	5.174700	-0.628300	-1.719700
C	-6.764000	-1.109900	0.676800
H	-5.906500	0.764200	1.324900
C	-5.377900	-2.440700	-0.794800
H	-3.465800	-1.619800	-1.304300
C	-6.572200	-2.264100	-0.090400
H	-7.691300	-0.966700	1.223100
H	-5.230500	-3.325500	-1.406500
H	-7.351600	-3.018300	-0.144100
C	5.347400	-1.331200	0.332700
C	4.440900	-1.591900	1.551600
H	3.949700	-0.675300	1.896300
H	3.662300	-2.328900	1.321100
H	5.031500	-1.983800	2.387100
C	6.044300	-2.645800	-0.073000
H	6.683200	-2.501000	-0.951900
H	6.675800	-3.012400	0.744200
H	5.313700	-3.428100	-0.310100
C	6.417500	-0.283100	0.693500
H	7.089000	-0.098900	-0.152900
H	5.968600	0.672600	0.975900
H	7.024300	-0.640800	1.533400

2b

Sum of electronic and zero point energies: -1472.650801 Hartree

Lowest Frequency: 14.0 cm^{-1}

Coordinates: B3LYP/6-31+G(d,p) IEF-PCM $CHCl_3$

Atom	x	y	z
N	0.829900	0.634000	-0.285200
C	-0.173800	1.497100	-0.077900
C	2.084200	1.102300	-0.342800
C	0.021600	2.875700	0.083900
N	-1.428800	0.864800	-0.051800
C	2.399300	2.461600	-0.198800
N	3.031700	0.089300	-0.561700
C	1.335900	3.336700	0.016000
H	-0.815700	3.534800	0.255900
C	-2.669400	1.404200	0.193000
H	-1.360900	-0.136900	-0.178300
H	3.424000	2.796300	-0.255200

C	4.401500	0.180300	-0.688800
H	2.614100	-0.830200	-0.629300
H	1.534500	4.397600	0.134000
O	-2.846300	2.587400	0.487400
C	-3.819500	0.443800	0.092100
O	5.007700	1.250300	-0.634100
C	5.109900	-1.149200	-0.904300
C	-4.980300	0.745600	0.819900
C	-3.799100	-0.706500	-0.711800
H	4.405000	-1.894600	-1.290700
H	5.861100	-0.974900	-1.681700
C	-6.092600	-0.091500	0.770700
H	-5.001200	1.642800	1.428700
C	-4.910100	-1.547900	-0.779800
H	-2.935300	-0.947400	-1.323700
C	-6.044600	-1.233900	-0.030900
H	-6.983600	0.139300	1.343800
H	-4.895600	-2.428600	-1.411900
C	5.822400	-1.744500	0.352700
C	4.810000	-1.978000	1.491000
H	4.373400	-1.038700	1.847100
H	3.991900	-2.633800	1.169100
H	5.302300	-2.457100	2.344400
C	6.429500	-3.097700	-0.070700
H	7.142800	-2.972700	-0.893500
H	6.963200	-3.557000	0.769000
H	5.653000	-3.798700	-0.398800
C	6.950200	-0.815500	0.840800
H	7.691600	-0.646700	0.051600
H	6.567200	0.160500	1.150600
H	7.464500	-1.269300	1.695800
Cl	-7.445200	-2.294000	-0.105200

2c

Sum of electronic and zero point energies: -1105.294665 Hartree

Lowest Frequency: 17.0 cm^{-1}

Coordinates: B3LYP/6-31+G(d,p) IEF-PCM $CHCl_3$

Atom	x	y	z
N	0.669300	0.600100	-0.287200
C	-0.342000	1.453400	-0.079800
C	1.918600	1.081400	-0.347200
C	-0.162600	2.833700	0.080100
N	-1.591900	0.807800	-0.053500
C	2.218600	2.444800	-0.205700
N	2.877000	0.079200	-0.564600
C	1.146800	3.308900	0.009700
H	-1.006400	3.484500	0.252000
C	-2.833700	1.334700	0.197700
H	-1.515000	-0.193300	-0.182700
H	3.239600	2.790300	-0.264400

C	4.245900	0.186600	-0.695000
H	2.470900	-0.845900	-0.627200
H	1.334300	4.372000	0.125900
O	-3.029500	2.512500	0.497200
C	-3.976100	0.359300	0.094200
O	4.837800	1.264800	-0.649700
C	4.970300	-1.135600	-0.900800
C	-3.961900	-0.746300	-0.770400
C	-5.112800	0.610200	0.877400
H	4.272700	-1.894700	-1.273400
H	5.713800	-0.960900	-1.685500
C	-5.060000	-1.599700	-0.842100
H	-3.113600	-0.934900	-1.420600
C	-6.210300	-0.241800	0.823900
H	-5.123500	1.477300	1.528100
C	-6.185600	-1.353200	-0.038000
H	-5.051600	-2.446800	-1.519000
H	-7.082500	-0.053100	1.440100
C	5.698600	-1.706900	0.358300
C	4.698200	-1.930700	1.509100
H	4.257800	-0.989200	1.854900
H	3.882000	-2.597100	1.204900
H	5.202000	-2.392900	2.365100
C	6.312100	-3.061600	-0.050800
H	7.015800	-2.943500	-0.882900
H	6.858300	-3.503600	0.790100
H	5.537900	-3.773700	-0.359800
C	6.823900	-0.762700	0.822700
H	7.556800	-0.599900	0.024300
H	6.436300	0.214800	1.122100
H	7.349000	-1.200600	1.679200
C	-7.315400	-2.235800	-0.101700
N	-8.231000	-2.952900	-0.151800

2d

Sum of electronic and zero point energies: -1217.554891 Hartree

Lowest Frequency: 14.9 cm^{-1}

Coordinates: B3LYP/6-31+G(d,p) IEF-PCM $CHCl_3$

Atom	x	y	z
N	1.089300	0.666300	-0.287500
C	0.114500	1.565000	-0.099600
C	2.357600	1.094100	-0.354900
C	0.349900	2.939600	0.032700
N	-1.161700	0.972100	-0.062700
C	2.713200	2.446700	-0.239800
N	3.274300	0.049500	-0.550900
C	1.678100	3.358600	-0.044100
H	-0.466600	3.628000	0.189100
C	-2.379900	1.556700	0.170100
H	-1.126200	-0.034000	-0.171000

H	3.747500	2.748800	-0.303000
C	4.646000	0.100500	-0.688300
H	2.831200	-0.859600	-0.596000
H	1.909500	4.415100	0.051100
O	-2.530300	2.748600	0.437300
C	-3.563200	0.627400	0.088500
O	5.279800	1.155200	-0.665400
C	5.317900	-1.252100	-0.872400
C	-4.682000	0.937800	0.876700
C	-3.601300	-0.487400	-0.764000
H	4.588100	-1.993400	-1.218200
H	6.056300	-1.122900	-1.670700
C	-5.817600	0.135400	0.840400
H	-4.650400	1.812000	1.516700
C	-4.735700	-1.294300	-0.819700
H	-2.766100	-0.720000	-1.416400
C	-5.824100	-0.972200	-0.009400
H	-6.682700	0.357000	1.452100
H	-4.783000	-2.150500	-1.480200
C	6.041900	-1.821000	0.390200
C	5.047300	-1.987200	1.555600
H	4.641800	-1.024600	1.885600
H	4.206000	-2.632000	1.274000
H	5.544600	-2.447800	2.416200
C	6.606000	-3.203300	0.002700
H	7.308700	-3.123600	-0.834800
H	7.141900	-3.648500	0.848500
H	5.806600	-3.894200	-0.289800
C	7.203100	-0.906000	0.823200
H	7.930800	-0.782600	0.013200
H	6.851500	0.089000	1.108700
H	7.724100	-1.345400	1.681500
N	-7.021900	-1.824600	-0.058700
O	-7.008100	-2.801600	-0.811600
O	-7.979300	-1.520100	0.656400

2e

Sum of electronic and zero point energies: -1052.34178 Hartree

Lowest Frequency: 15.5 cm^{-1}

Coordinates: B3LYP/6-31+G(d,p) IEF-PCM $CHCl_3$

Atom	x	y	z
N	0.457100	0.549600	-0.284800
C	-0.588400	1.361000	-0.072800
C	1.687000	1.079000	-0.340300
C	-0.458500	2.747200	0.095500
N	-1.810000	0.669800	-0.047700
C	1.936600	2.450700	-0.189400
N	2.682100	0.113100	-0.563900
C	0.831400	3.271800	0.030000
H	-1.327300	3.363400	0.270700

C	-3.079200	1.147800	0.191900
H	-1.695600	-0.327100	-0.177100
H	2.944000	2.834500	-0.243700
C	4.045900	0.268200	-0.688300
H	2.308400	-0.824800	-0.635700
H	0.978100	4.340600	0.153500
O	-3.308400	2.322400	0.488700
C	-4.178000	0.134000	0.082000
O	4.601800	1.365200	-0.631400
C	4.814800	-1.027500	-0.903100
C	-5.368200	0.380600	0.786000
C	-4.090300	-1.023900	-0.705200
H	4.141200	-1.809400	-1.272400
H	5.546400	-0.826100	-1.692600
C	-6.428600	-0.517900	0.720600
H	-5.444900	1.280800	1.386300
C	-5.162900	-1.915300	-0.774600
H	-3.205100	-1.230000	-1.300000
C	-6.347200	-1.683600	-0.061200
H	-7.336000	-0.313700	1.283300
H	-5.078300	-2.799900	-1.399900
C	5.570500	-1.576200	0.349700
C	4.588300	-1.820700	1.511900
H	4.127200	-0.889200	1.858000
H	3.786100	-2.509200	1.219700
H	5.113000	-2.265500	2.364600
C	6.213400	-2.916500	-0.061400
H	6.903600	-2.784200	-0.902600
H	6.780800	-3.341200	0.774400
H	5.453600	-3.649100	-0.358200
C	6.676700	-0.602400	0.799000
H	7.396900	-0.424600	-0.007700
H	6.267500	0.365900	1.098900
H	7.221400	-1.023900	1.651600
C	-7.509600	-2.643800	-0.136000
H	-7.817700	-2.969300	0.863800
H	-8.380700	-2.169000	-0.602600
H	-7.257600	-3.532400	-0.720600

2f

Sum of electronic and zero point energies: -1127.547005 Hartree

Lowest Frequency: 12.4 cm^{-1}

Coordinates: B3LYP/6-31+G(d,p) IEF-PCM $CHCl_3$

Atom	x	y	z
N	0.860900	0.609600	-0.281000
C	-0.156000	1.457000	-0.068900
C	2.110300	1.093000	-0.318400
C	0.025000	2.835400	0.118600
N	-1.402400	0.812300	-0.066600
C	2.410000	2.452200	-0.147800

N	3.070800	0.093400	-0.546500
C	1.334200	3.311500	0.071800
H	-0.821500	3.481700	0.293600
C	-2.656400	1.336000	0.165900
H	-1.322000	-0.185600	-0.210800
H	3.431500	2.798600	-0.188500
C	4.439800	0.200500	-0.663600
H	2.663100	-0.828900	-0.633700
H	1.519800	4.372400	0.210400
O	-2.837500	2.515700	0.479100
C	-3.793200	0.374500	0.028300
O	5.035300	1.275400	-0.585800
C	5.162400	-1.118000	-0.900000
C	-3.732400	-0.816900	-0.720900
C	-4.999000	0.697700	0.665200
H	4.462700	-1.867800	-1.287000
H	5.903900	-0.927500	-1.683000
C	-4.834700	-1.655400	-0.816300
H	-2.835600	-1.089400	-1.269200
C	-6.111700	-0.138800	0.586400
H	-5.057900	1.619500	1.233700
C	-6.032300	-1.326000	-0.158000
H	-4.793500	-2.566100	-1.404600
H	-7.023000	0.140000	1.100700
C	5.893700	-1.717500	0.343900
C	4.897900	-1.955800	1.495800
H	4.466400	-1.017700	1.861600
H	4.074900	-2.609900	1.183400
H	5.402600	-2.438100	2.340200
C	6.495700	-3.068600	-0.093500
H	7.195100	-2.940000	-0.927600
H	7.043800	-3.529800	0.735800
H	5.714800	-3.769600	-0.411200
C	7.028100	-0.789800	0.819100
H	7.759100	-0.620000	0.020300
H	6.649000	0.185700	1.135300
H	7.553400	-1.245400	1.666300
O	-7.052900	-2.211600	-0.306700
C	-8.307400	-1.931800	0.322600
H	-8.958900	-2.765300	0.061600
H	-8.198600	-1.878200	1.411300
H	-8.737600	-0.997600	-0.054800

2a-Barbital

Sum of electronic and zero point energies: -1660.226464 Hartree

Lowest Frequency: 8.7 cm^{-1}

Coordinates: B3LYP/6-31+G(d,p) IEF-PCM $CHCl_3$

Atom	x	y	z
N	-0.595500	1.673200	-0.307100
C	0.378700	2.601900	-0.311000

C	-1.873000	2.075800	-0.478600
C	0.124500	3.967800	-0.488100
N	1.690000	2.106500	-0.175500
C	-2.223400	3.419100	-0.669300
N	-2.822800	1.044000	-0.410300
C	-1.197100	4.360000	-0.670400
H	0.935100	4.681300	-0.481000
C	2.746200	2.785800	0.399200
H	1.834200	1.130300	-0.438300
H	-3.256900	3.695200	-0.810300
C	-4.144200	1.078800	-0.811800
H	-2.496300	0.170700	0.002400
H	-1.431900	5.410100	-0.815300
O	2.615300	3.871900	0.966800
C	4.087400	2.122000	0.301600
O	-4.658100	2.059300	-1.351800
C	-4.924900	-0.198400	-0.542300
C	4.473000	1.350300	-0.804700
C	5.006700	2.350900	1.338100
H	-5.481200	-0.420500	-1.459600
H	-4.237200	-1.029000	-0.357800
C	5.759700	0.809500	-0.867400
H	3.784000	1.183200	-1.625200
C	6.284100	1.795100	1.281300
H	4.706700	2.965500	2.180300
C	6.663900	1.024100	0.176300
H	6.054900	0.224500	-1.733300
H	6.984700	1.967000	2.092900
H	7.662000	0.598700	0.127100
C	-5.938200	-0.121900	0.645800
C	-7.069500	0.880700	0.349400
H	-6.686300	1.896000	0.218500
H	-7.609300	0.607600	-0.564800
H	-7.789000	0.887900	1.176500
C	-6.545100	-1.530200	0.812100
H	-5.774600	-2.269800	1.058900
H	-7.286900	-1.534300	1.619000
H	-7.047300	-1.855900	-0.106400
C	-5.216500	0.276200	1.948400
H	-4.394100	-0.411800	2.174200
H	-4.804700	1.289900	1.890100
H	-5.916300	0.253200	2.791400
H	-0.166000	-0.228000	-0.123700
N	0.065700	-1.237900	-0.033300
C	1.324400	-1.638600	-0.422200
C	-0.928000	-2.050400	0.467900
C	1.703200	-3.113400	-0.296000
O	2.116800	-0.808500	-0.857700
N	-0.608400	-3.386300	0.609700
O	-2.035100	-1.613500	0.767100
C	0.593500	-3.995600	0.277900

C	2.080300	-3.652800	-1.713000
C	2.953100	-3.224000	0.635200
H	-1.342700	-3.981700	0.980500
O	0.733900	-5.196100	0.445800
H	2.930700	-3.058600	-2.059500
H	2.428500	-4.680400	-1.575100
C	0.955400	-3.615900	-2.753000
H	3.246900	-4.277600	0.642100
H	3.755700	-2.658800	0.153300
C	2.751500	-2.726300	2.070600
H	1.319200	-4.014100	-3.704800
H	0.097200	-4.226300	-2.451300
H	0.601900	-2.596000	-2.940100
H	3.680600	-2.845500	2.635700
H	2.484500	-1.664500	2.103700
H	1.974800	-3.291700	2.597100

2b-barbital

Sum of electronic and zero point energies: -2119.83084 Hartree

Lowest Frequency: 6.8 cm^{-1}

Coordinates: B3LYP/6-31+G(d,p) IEF-PCM $CHCl_3$

Atom	x	y	z
N	-1.051700	-1.670500	0.309300
C	-0.065800	-2.586700	0.313500
C	-2.324400	-2.090400	0.475700
C	-0.301500	-3.956100	0.485800
N	1.239400	-2.072000	0.183700
C	-2.657100	-3.439300	0.660700
N	-3.287500	-1.071500	0.409300
C	-1.618700	-4.366400	0.662200
H	0.518300	-4.658900	0.479400
C	2.307700	-2.736500	-0.382500
H	1.366200	-1.091900	0.442300
H	-3.687300	-3.729600	0.797300
C	-4.610700	-1.127000	0.803800
H	-2.971200	-0.190700	0.004800
H	-1.840000	-5.419900	0.802800
O	2.201200	-3.826600	-0.946900
C	3.638500	-2.052100	-0.280500
O	-5.113700	-2.118200	1.334100
C	-5.407100	0.141500	0.539400
C	4.006200	-1.257300	0.814300
C	4.572000	-2.285200	-1.302300
H	-5.971200	0.349400	1.455300
H	-4.729700	0.982500	0.364600
C	5.281900	-0.695400	0.886900
H	3.312100	-1.081100	1.628000
C	5.842300	-1.716100	-1.251300
H	4.293200	-2.917300	-2.138400
C	6.183700	-0.925300	-0.151600

H	5.569400	-0.091300	1.740000
H	6.558000	-1.887100	-2.047600
C	-6.413200	0.059700	-0.654600
C	-7.533700	-0.958200	-0.369600
H	-7.138900	-1.969400	-0.242200
H	-8.081600	-0.696600	0.543100
H	-8.248800	-0.969600	-1.200600
C	-7.036100	1.461600	-0.815900
H	-6.273500	2.211500	-1.055400
H	-7.774300	1.461200	-1.626000
H	-7.546200	1.776300	0.102100
C	-5.679800	-0.321900	-1.955600
H	-4.864800	0.377400	-2.173000
H	-5.256000	-1.330900	-1.901100
H	-6.375400	-0.302600	-2.802100
Cl	7.789900	-0.210900	-0.071200
H	-0.645700	0.239400	0.128700
N	-0.425400	1.251800	0.040100
C	0.831800	1.664600	0.419300
C	-1.431800	2.055300	-0.451600
C	1.193800	3.143400	0.296100
O	1.637200	0.840700	0.844100
N	-1.128300	3.395000	-0.589500
O	-2.535100	1.606200	-0.745800
C	0.069100	4.016200	-0.263000
C	1.580300	3.680700	1.711400
C	2.432700	3.271600	-0.647800
H	-1.872000	3.984000	-0.951800
O	0.194500	5.219100	-0.424800
H	2.442900	3.096700	2.044600
H	1.912700	4.713600	1.574700
C	0.468700	3.623000	2.764800
H	2.714500	4.328400	-0.653400
H	3.246900	2.714000	-0.176300
C	2.221900	2.777400	-2.083000
H	0.838900	4.021400	3.714100
H	-0.401500	4.223100	2.477100
H	0.131600	2.597500	2.951100
H	3.144000	2.908700	-2.656800
H	1.965400	1.713000	-2.118000
H	1.434200	3.336800	-2.599500

2c-barbital

Sum of electronic and zero point energies: -1752.474457 Hartree

Lowest Frequency: 7.0 cm^{-1}

Coordinates: B3LYP/6-31+G(d,p) IEF-PCM $CHCl_3$

Atom	x	y	z
N	-0.973200	-1.674800	0.307200
C	-0.001500	-2.605600	0.320800
C	-2.252000	-2.074800	0.473900

C	-0.255700	-3.969800	0.502600
N	1.311500	-2.107900	0.188400
C	-2.604000	-3.418100	0.668000
N	-3.200600	-1.043500	0.399600
C	-1.579600	-4.359800	0.678900
H	0.554000	-4.684200	0.503500
C	2.373400	-2.792400	-0.357500
H	1.448600	-1.125100	0.433600
H	-3.638500	-3.692600	0.804400
C	-4.525800	-1.079500	0.791800
H	-2.870600	-0.167300	-0.004000
H	-1.816300	-5.409000	0.826500
O	2.272900	-3.899200	-0.887600
C	3.709800	-2.106300	-0.278400
O	-5.042700	-2.061900	1.324700
C	-5.304900	0.198000	0.520600
C	4.095000	-1.324200	0.819700
C	4.619000	-2.332500	-1.323600
H	-5.868100	0.416600	1.434400
H	-4.616300	1.029500	0.343800
C	5.369500	-0.764400	0.871300
H	3.413300	-1.158600	1.645500
C	5.887100	-1.764100	-1.291700
H	4.320500	-2.958000	-2.157500
C	6.266400	-0.976500	-0.189000
H	5.671200	-0.168600	1.725700
H	6.584400	-1.928400	-2.105900
C	-6.309400	0.124100	-0.675300
C	-7.442500	-0.879600	-0.389700
H	-7.059900	-1.895100	-0.258100
H	-7.989400	-0.608600	0.520800
H	-8.155500	-0.885400	-1.222300
C	-6.915300	1.532700	-0.842300
H	-6.143400	2.273100	-1.081800
H	-7.651500	1.538700	-1.654300
H	-7.424100	1.856000	0.073500
C	-5.577700	-0.270200	-1.973500
H	-4.753200	0.418100	-2.190500
H	-5.167000	-1.284500	-1.915400
H	-6.270700	-0.244100	-2.821800
C	7.576000	-0.391400	-0.144700
N	8.637400	0.085800	-0.110400
H	-0.538100	0.234100	0.115400
N	-0.303400	1.243100	0.033800
C	0.961300	1.634200	0.409500
C	-1.301800	2.065500	-0.444000
C	1.338900	3.110700	0.311900
O	1.760100	0.793400	0.814300
N	-0.981300	3.402300	-0.567500
O	-2.411500	1.633200	-0.738700
C	0.225400	4.004000	-0.237500

C	1.720400	3.620200	1.739300
C	2.584300	3.243100	-0.621900
H	-1.718000	4.005200	-0.921200
O	0.366700	5.206500	-0.387000
H	2.577600	3.025100	2.067300
H	2.060200	4.653200	1.622400
C	0.602500	3.551100	2.785300
H	2.876200	4.297100	-0.608500
H	3.390700	2.670400	-0.155500
C	2.376300	2.774800	-2.066300
H	0.969700	3.931500	3.743100
H	-0.262900	4.160800	2.503500
H	0.258600	2.524600	2.952700
H	3.302400	2.906700	-2.633500
H	2.109200	1.713700	-2.120300
H	1.596700	3.350400	-2.577100

2d-barbital

Sum of electronic and zero point energies: -1864.735918 Hartree

Lowest Frequency: 3.7 cm^{-1}

Coordinates: B3LYP/6-31+G(d,p) IEF-PCM $CHCl_3$

Atom	x	y	z
N	-1.234000	-1.681600	0.299200
C	-0.258500	-2.608900	0.302500
C	-2.511500	-2.089400	0.455800
C	-0.507300	-3.976800	0.462100
N	1.052300	-2.101300	0.183500
C	-2.858500	-3.437300	0.627500
N	-3.464800	-1.061600	0.396700
C	-1.830500	-4.374700	0.627200
H	0.305100	-4.687800	0.454900
C	2.128900	-2.777900	-0.340000
H	1.178400	-1.116000	0.426100
H	-3.892300	-3.718100	0.756200
C	-4.788900	-1.109100	0.792000
H	-3.139600	-0.177700	0.006300
H	-2.063400	-5.427000	0.757200
O	2.055100	-3.891600	-0.859100
C	3.455600	-2.071900	-0.248900
O	-5.300500	-2.102000	1.310100
C	-5.573100	0.170100	0.544600
C	3.823800	-1.301100	0.863200
C	4.371200	-2.270200	-1.294700
H	-6.132700	0.372400	1.464500
H	-4.887900	1.006400	0.378200
C	5.089200	-0.721500	0.929400
H	3.136000	-1.158300	1.688000
C	5.631400	-1.683700	-1.250900
H	4.086100	-2.887700	-2.138800
C	5.969700	-0.915900	-0.134200

H	5.391400	-0.132000	1.785500
H	6.342900	-1.817300	-2.055700
C	-6.583100	0.112400	-0.647500
C	-7.712400	-0.898500	-0.372200
H	-7.326900	-1.915000	-0.258400
H	-8.255500	-0.643200	0.545100
H	-8.429600	-0.893000	-1.201300
C	-7.193200	1.521900	-0.789500
H	-6.424100	2.267700	-1.021200
H	-7.933300	1.538800	-1.597700
H	-7.698100	1.829700	0.133700
C	-5.856700	-0.259600	-1.955200
H	-5.034500	0.433800	-2.164700
H	-5.444000	-1.273900	-1.915400
H	-6.553700	-0.221000	-2.799800
N	7.301200	-0.295200	-0.074900
O	8.071000	-0.480600	-1.020900
O	7.582700	0.382900	0.916900
H	-0.809100	0.235700	0.113400
N	-0.578400	1.245000	0.028000
C	0.690700	1.639400	0.384400
C	-1.584600	2.063900	-0.439400
C	1.062900	3.116800	0.280800
O	1.497100	0.800800	0.778800
N	-1.268200	3.400600	-0.572400
O	-2.697100	1.628200	-0.718100
C	-0.057300	4.005100	-0.263200
C	1.449100	3.630400	1.706000
C	2.303000	3.252600	-0.658900
H	-2.010000	4.000700	-0.920000
O	0.081400	5.206500	-0.423400
H	2.308200	3.037100	2.032000
H	1.787300	4.663400	1.585100
C	0.335000	3.563000	2.756200
H	2.590100	4.307900	-0.649500
H	3.114500	2.684900	-0.195000
C	2.089800	2.780100	-2.101200
H	0.706400	3.944000	3.712000
H	-0.530900	4.173200	2.477200
H	-0.009100	2.536900	2.926200
H	3.012000	2.915200	-2.673800
H	1.827300	1.717600	-2.151400
H	1.304600	3.350900	-2.608900

2e-barbital

Sum of electronic and zero point energies: -1699.521137 Hartree

Lowest Frequency: 8.1 cm^{-1}

Coordinates: B3LYP/6-31+G(d,p) IEF-PCM $CHCl_3$

Atom	x	y	z
N	-0.824500	-1.664100	0.325300

C	0.160200	-2.581600	0.336900
C	-2.097800	-2.079500	0.498700
C	-0.079400	-3.948800	0.525400
N	1.466000	-2.074500	0.196600
C	-2.433400	-3.424800	0.700800
N	-3.058500	-1.058500	0.418400
C	-1.396500	-4.354200	0.710400
H	0.739200	-4.653200	0.524500
C	2.524100	-2.743900	-0.389500
H	1.603000	-1.098000	0.461000
H	-3.463900	-3.711300	0.843100
C	-4.382700	-1.105500	0.808600
H	-2.739100	-0.185400	-0.000100
H	-1.619700	-5.405500	0.864200
O	2.391800	-3.827100	-0.963500
C	3.859900	-2.075000	-0.296800
O	-4.889900	-2.087100	1.353100
C	-5.176200	0.159600	0.519600
C	4.245500	-1.281100	0.791500
C	4.789100	-2.315600	-1.323200
H	-5.744400	0.383700	1.429000
H	-4.496600	0.996600	0.333700
C	5.530500	-0.735600	0.845300
H	3.558800	-1.096800	1.610400
C	6.060700	-1.753600	-1.270700
H	4.498600	-2.944800	-2.158000
C	6.456800	-0.954400	-0.183100
H	5.815800	-0.133600	1.703900
H	6.761200	-1.940200	-2.081000
C	-6.176100	0.059300	-0.678000
C	-7.299900	-0.951900	-0.381800
H	-6.907100	-1.961300	-0.234700
H	-7.852300	-0.673900	0.523300
H	-8.010300	-0.976700	-1.216400
C	-6.796000	1.459100	-0.866700
H	-6.030800	2.203800	-1.114400
H	-7.529600	1.446200	-1.680900
H	-7.310800	1.790100	0.042900
C	-5.436600	-0.346000	-1.968500
H	-4.620100	0.348800	-2.194400
H	-5.013600	-1.353900	-1.893600
H	-6.128000	-0.341500	-2.818700
C	7.845500	-0.363800	-0.129100
H	8.607200	-1.151700	-0.101100
H	8.048800	0.248100	-1.015300
H	7.978700	0.265100	0.755200
H	-0.415000	0.237100	0.142200
N	-0.192900	1.249200	0.048500
C	1.057900	1.665100	0.446900
C	-1.189800	2.048800	-0.466600
C	1.425500	3.141700	0.308800

O	1.853300	0.846400	0.898200
N	-0.882200	3.387000	-0.614000
O	-2.290000	1.599400	-0.772900
C	0.311100	4.009900	-0.276900
C	1.795500	3.697300	1.721200
C	2.677000	3.252600	-0.620700
H	-1.619400	3.972800	-0.994300
O	0.441100	5.210800	-0.450800
H	2.648900	3.112400	2.075700
H	2.136800	4.726000	1.574400
C	0.667900	3.662400	2.758400
H	2.962300	4.308400	-0.637800
H	3.482800	2.698800	-0.130800
C	2.483400	2.738300	-2.051300
H	1.025300	4.074200	3.706800
H	-0.194400	4.262000	2.447100
H	0.322500	2.641600	2.955500
H	3.413100	2.859200	-2.615100
H	2.225200	1.674200	-2.074100
H	1.703700	3.291900	-2.585900

2f-barbital

Sum of electronic and zero point energies: -1774.72628 Hartree

Lowest Frequency: 8.3 cm^{-1}

Coordinates: B3LYP/6-31+G(d,p) IEF-PCM $CHCl_3$

Atom	x	y	z
N	-1.039100	-1.654200	0.348500
C	-0.036500	-2.551300	0.391200
C	-2.307400	-2.092500	0.501300
C	-0.253800	-3.920700	0.591500
N	1.261400	-2.020300	0.271700
C	-2.620900	-3.441300	0.712300
N	-3.285500	-1.091100	0.388200
C	-1.566100	-4.349900	0.754300
H	0.578300	-4.608900	0.616300
C	2.340400	-2.672900	-0.298900
H	1.373400	-1.040800	0.534900
H	-3.648300	-3.746800	0.836800
C	-4.613700	-1.155700	0.761000
H	-2.975700	-0.219900	-0.041500
H	-1.771800	-5.403600	0.916300
O	2.227300	-3.756400	-0.878200
C	3.662200	-1.987600	-0.185900
O	-5.110000	-2.136600	1.316900
C	-5.426200	0.088900	0.437500
C	4.007100	-1.133400	0.878000
C	4.628400	-2.262400	-1.163600
H	-6.007700	0.322300	1.336100
H	-4.759300	0.933600	0.240600
C	5.273900	-0.568700	0.951500

H	3.295000	-0.918100	1.666400
C	5.898200	-1.688900	-1.111900
H	4.374200	-2.934800	-1.976100
C	6.226200	-0.835300	-0.046500
H	5.548200	0.079100	1.777800
H	6.615400	-1.913400	-1.891900
C	-6.411000	-0.054300	-0.768200
C	-7.521200	-1.077400	-0.461700
H	-7.113000	-2.076300	-0.287600
H	-8.088300	-0.788700	0.430900
H	-8.221600	-1.132800	-1.303200
C	-7.051400	1.330400	-0.995100
H	-6.295600	2.082300	-1.249500
H	-7.774300	1.287600	-1.817900
H	-7.583300	1.672400	-0.099500
C	-5.649900	-0.476200	-2.040700
H	-4.844900	0.229100	-2.275400
H	-5.207600	-1.473100	-1.936100
H	-6.332000	-0.506600	-2.897800
O	7.433700	-0.226600	0.107600
C	8.455800	-0.467000	-0.863800
H	8.143700	-0.126200	-1.857200
H	9.317600	0.112500	-0.533600
H	8.721000	-1.529200	-0.902400
H	-0.666300	0.244400	0.158200
N	-0.462100	1.260500	0.060700
C	0.762100	1.708300	0.504000
C	-1.456200	2.033200	-0.498900
C	1.103400	3.190900	0.363400
O	1.556500	0.911600	0.995000
N	-1.171200	3.376000	-0.651000
O	-2.534900	1.557200	-0.839600
C	-0.005500	4.028300	-0.275200
C	1.405700	3.770200	1.782300
C	2.386900	3.317100	-0.519500
H	-1.905900	3.941700	-1.065000
O	0.105600	5.229800	-0.458000
H	2.251800	3.203300	2.180900
H	1.737800	4.801900	1.636100
C	0.235700	3.731800	2.771200
H	2.652500	4.378000	-0.538000
H	3.184400	2.784100	0.005800
C	2.254900	2.784100	-1.950100
H	0.546500	4.161000	3.728300
H	-0.621000	4.314600	2.415700
H	-0.103600	2.708800	2.967700
H	3.202600	2.914300	-2.481000
H	2.014700	1.715700	-1.970300
H	1.486400	3.318800	-2.518900