ELECTRONIC SUPPLEMENTARY INFORMATION

Perlin- and Bohlmann-Type Effects in Cyclohexylamine and 1-Aminopiperidine Derivatives

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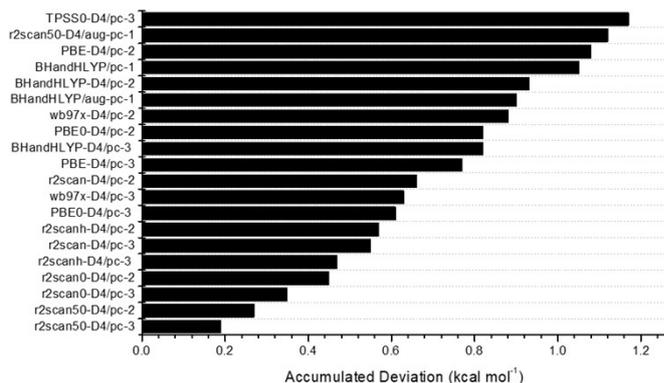
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Summary

Energy deviations from DLPNO-CCSD(T)/CBS for the 20 levels with lowest deviations:

Boltzmann weighted $^1J_{C28H29}$ coupling constants (considering the 6 conformers) for the 20 levels:

Boltzmann weighted $^1J_{C18H19}/ ^1J_{C18H20}$ coupling constants (considering the 6 conformers) for the 20 levels:
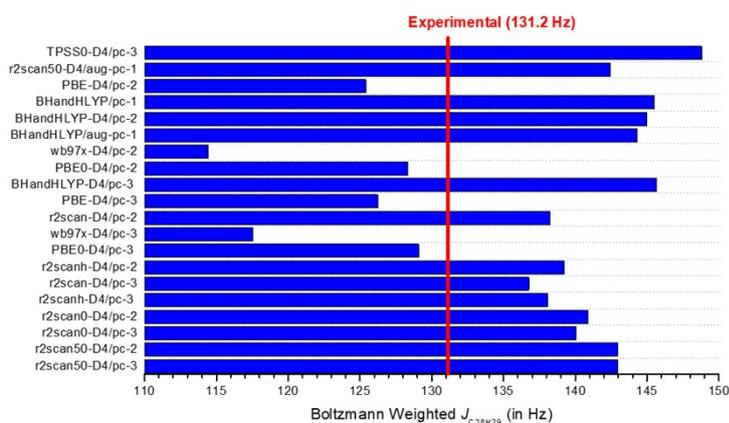

Figure S1. Benchmark study for **3** comparing DLPNO-CCSD(T)/CBS obtained energies and several DFT levels. $^1J_{CH}$ spin-spin coupling constants calculated at the 20 theoretical levels with lowest deviations from both DLPNO-CCSD(T)/CBS reference and $^1J_{CH}$ experimental values.

Table S1. Total NSA energy, in kcal mol^{-1}, obtained at the PBE0-D4/pc-3 theoretical level for conformers of compounds **1-4**.

	ax-1	ax-2	eq-1	eq-2	
1	170.8	171.32	167.03	166.9	
	ax-2	**eq-2**			
2	191.6	186.5			
	ax-1	**eq-1**	**eq-2**	**eq-2a**	**eq-3**
3	330.1	324.0	322.0	322.0	327.2
	ax-2	**eq-2a**	**eq-2b**	**eq-3**	**eq-3a**
4	344.1	335.1	336.8	342.8	344.0

ax-1

eq-1

eq-2

eq-2a

eq-3
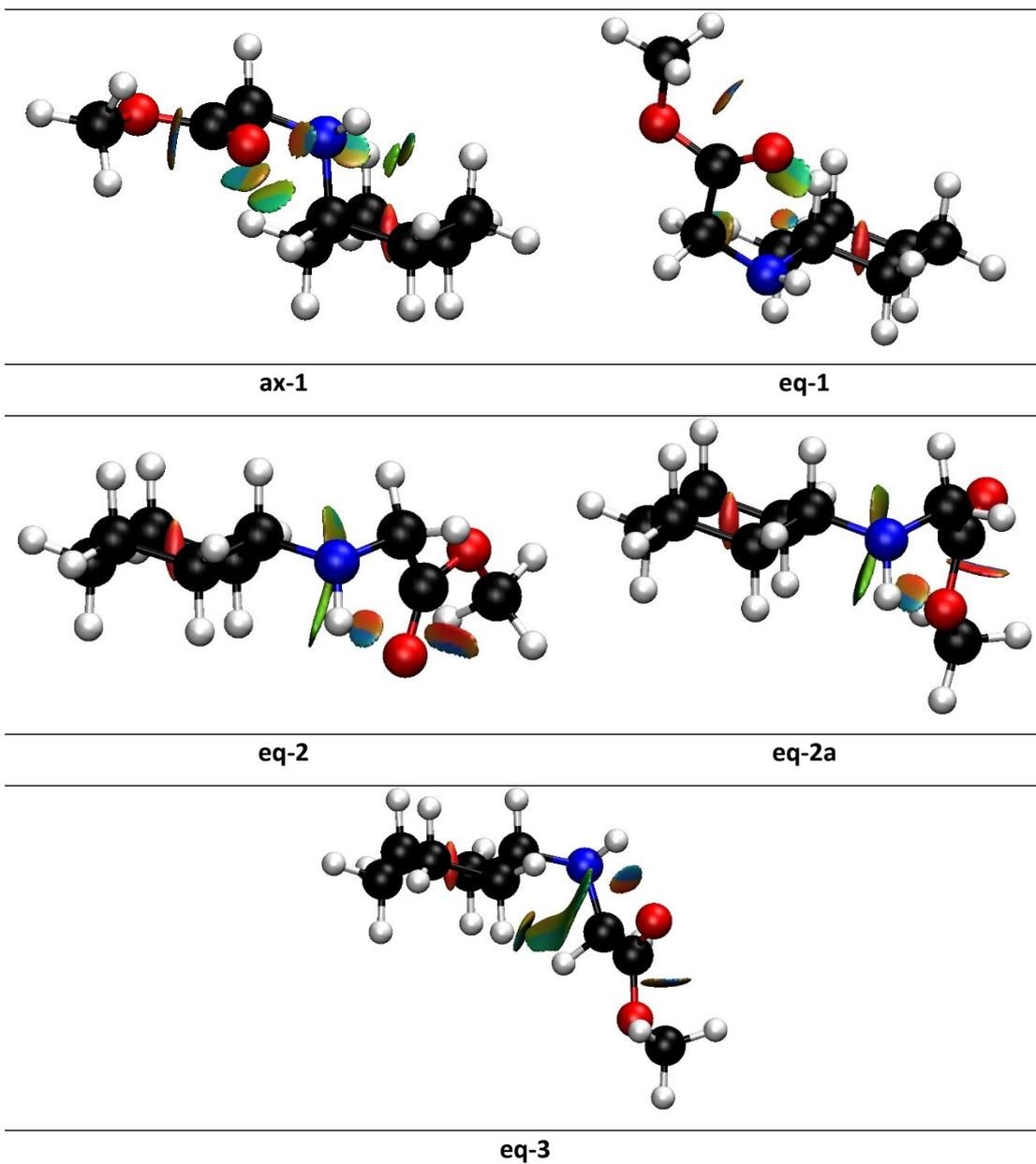
Figure S2. Isosurfaces from NCI for conformers of 3, using reduced density gradient (RDG) = 0.5 and blue-green-red color scale ranging from −0.02 < sign(λ2)ρ(r) < +0.02 au.

ax-1

eq-1

eq-2

eq-2a

eq-3
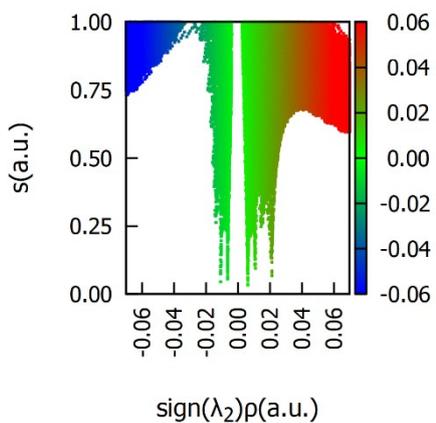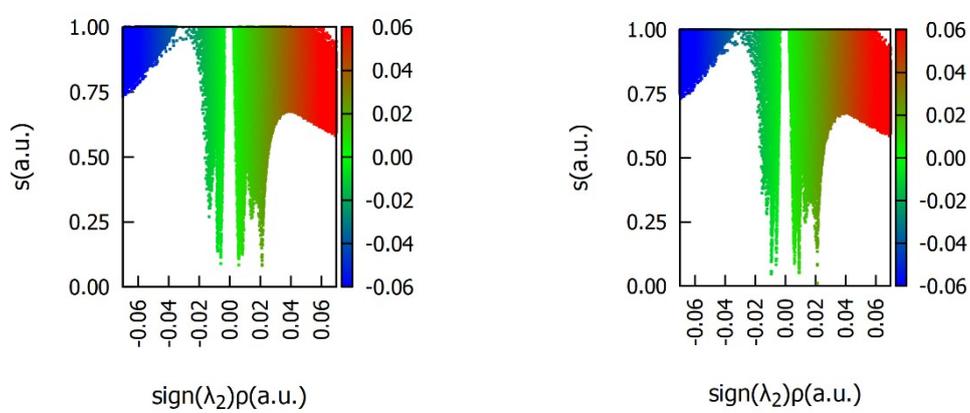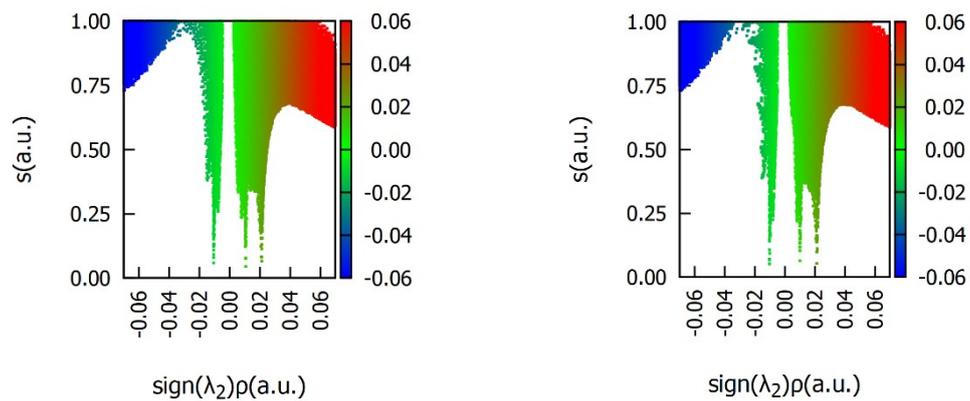
Figure S3. Reduced density gradient (RDG) *versus* sign($\lambda 2$)ρ plots for conformers of **3**.

ax-2
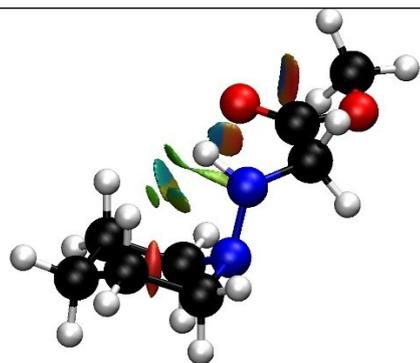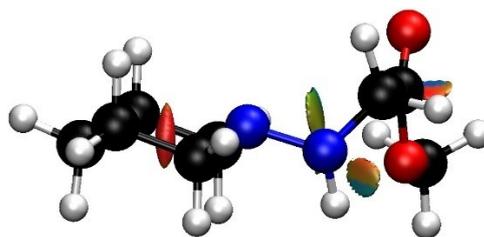
eq-2a
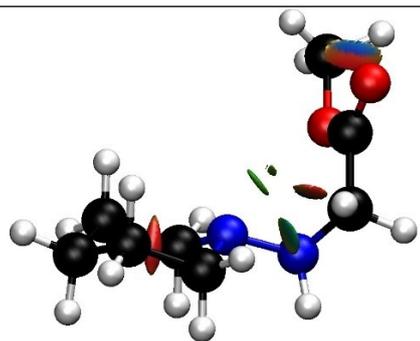
eq-2b
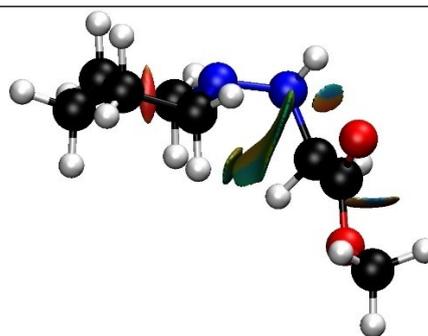
eq-3
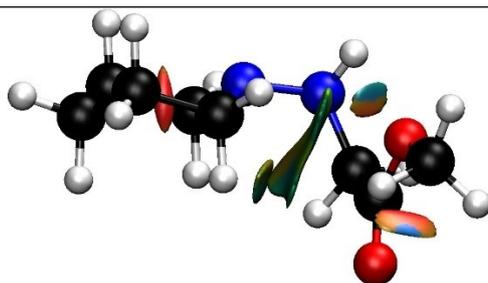
eq-3a

Figure S4. Isosurfaces from NCI for conformers of **4**, using reduced density gradient (RDG) = 0.5 and blue-green-red color scale ranging from −0.02 < sign(λ2)ρ(r) < +0.02 au.

ax-2

eq-2a

eq-2b

eq-3

eq-3a
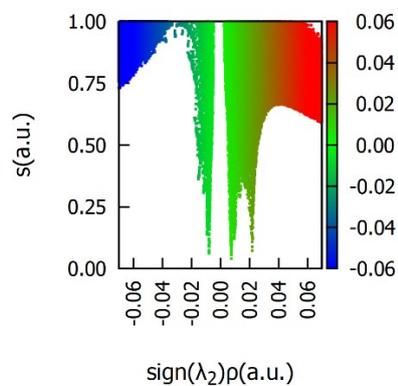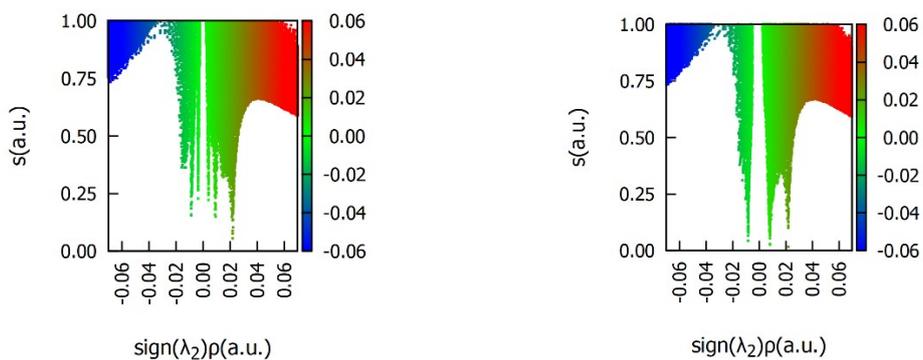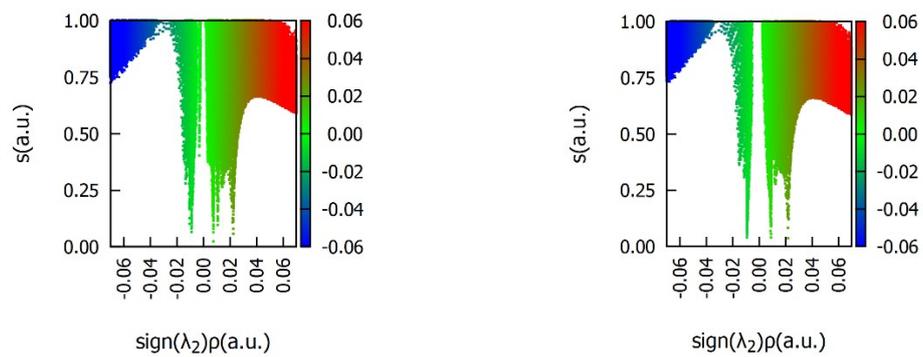
Figure S5. Reduced density gradient (RDG) *versus* sign(λ2)ρ plots for conformers of **4**.

ax-1

eq-1

eq-2

eq-2a

eq-3
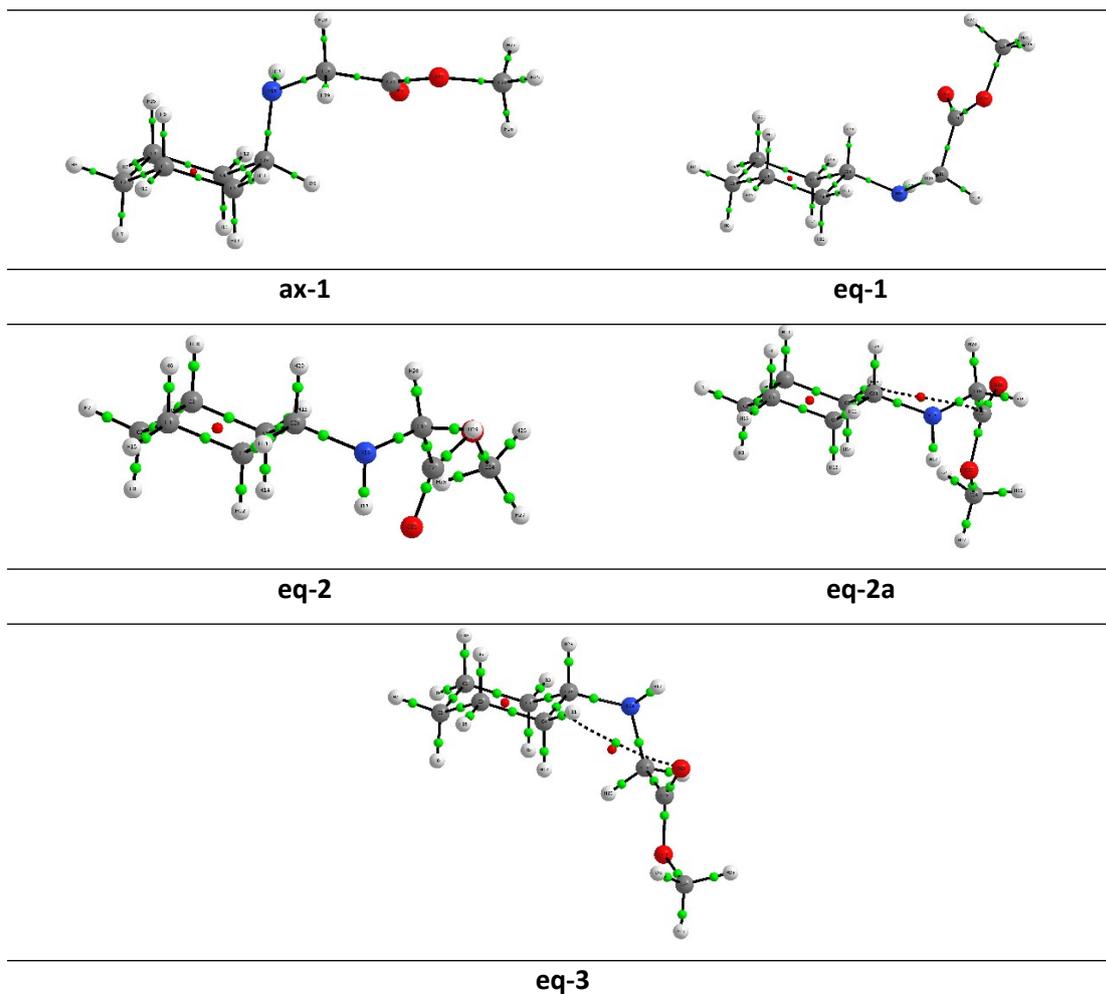
Figure S6. QTAIM molecular graphs for conformers of **3**. Bond critical points (green spheres) and ring critical points (red spheres).

ax-2

eq-2a

eq-2b

eq-3

eq-3a
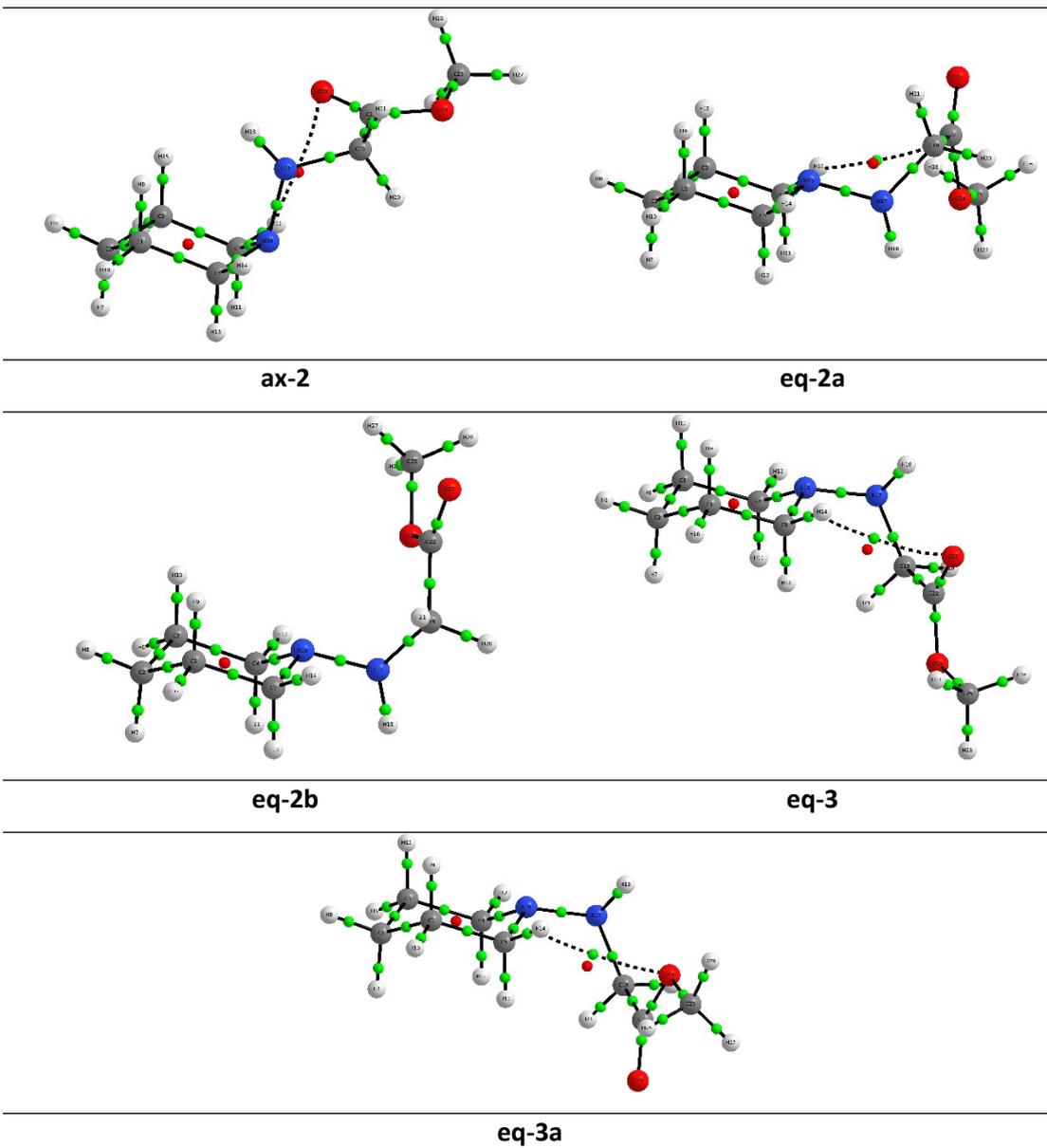
Figure S7. QTAIM molecular graphs for conformers of **4**. Bond critical points (green spheres) and ring critical points (red spheres).
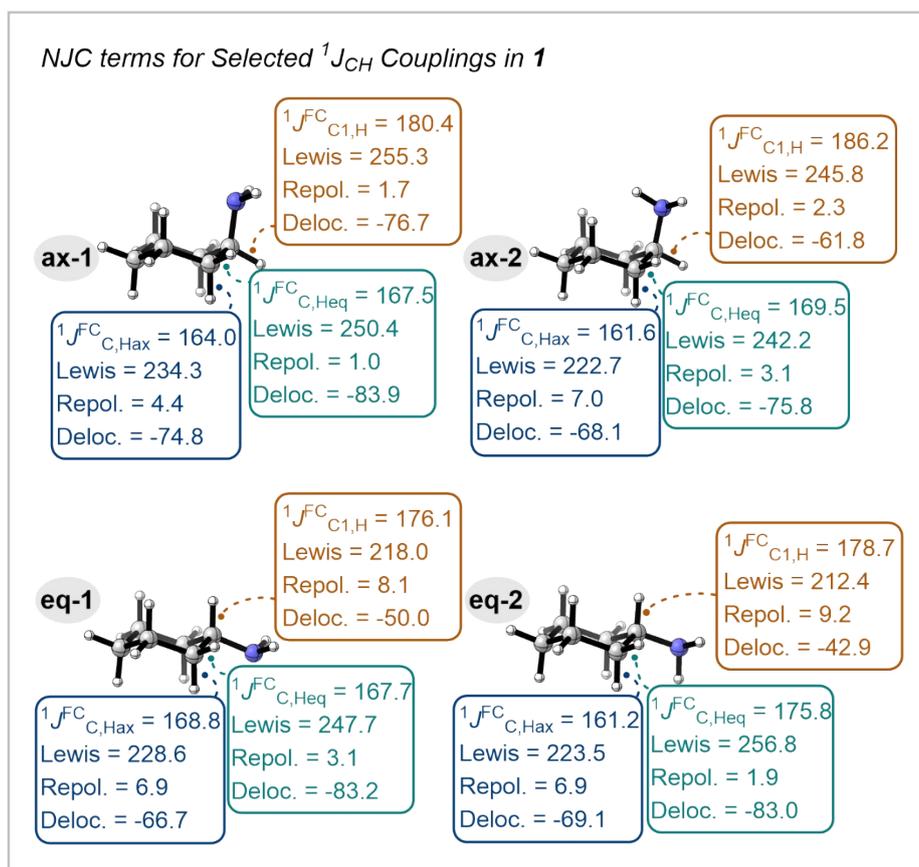
Figure S8. Decomposition of selected $^1J_{CH}$ couplings for compound **1** into NJC terms: Lewis, Repolarization and Delocalization, obtained at the PBE0-D3BJ/pcJ-3 theoretical level.
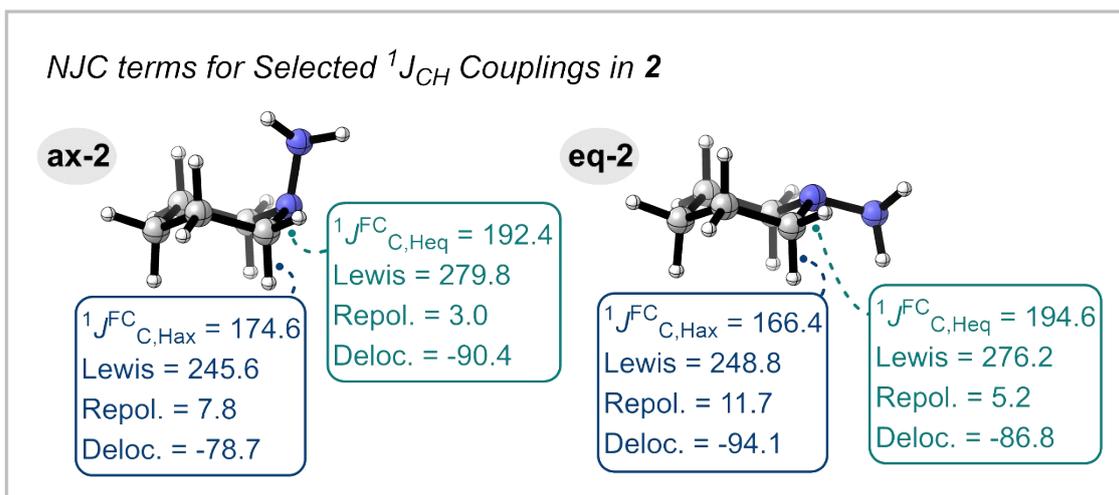
Figure S9. Decomposition of selected $^1J_{CH}$ couplings for compound **2** into NJC terms: Lewis, Repolarization and Delocalization, obtained at the PBE0-D3BJ/pcJ-3 theoretical level.

Figure S10. Decomposition of selected $^1J_{CH}$ couplings for compound **3** into NJC terms: Lewis, Repolarization and Delocalization, obtained at the PBE0-D3BJ/pcJ-3 theoretical level.

NJC terms for Selected $^1J_{CH}$ Couplings in **4**

ax-2

$^1J^{FC}_{C,Hax} = 175.5$
Lewis = 230.4
Repol. = 19.5
Deloc. = -74.3

$^1J^{FC}_{C,Heq} = 186.6$
Lewis = 290.6
Repol. = -4.9
Deloc. = -99.0

eq-2a

$^1J^{FC}_{C,Hax} = 150.8$
Lewis = 196.1
Repol. = 5.2
Deloc. = -50.6

$^1J^{FC}_{C,Heq} = 179.9$
Lewis = 274.0
Repol. = -0.9
Deloc. = -93.1

eq-2b

$^1J^{FC}_{C,Hax} = 168.2$
Lewis = 241.0
Repol. = 15.2
Deloc. = -88.0

$^1J^{FC}_{C,Heq} = 195.9$
Lewis = 281.9
Repol. = 4.3
Deloc. = -90.3

eq-3

$^1J^{FC}_{C,Hax} = 164.8$
Lewis = 260.6
Repol. = 9.1
Deloc. = -104.9

$^1J^{FC}_{C,Heq} = 192.7$
Lewis = 279.4
Repol. = 3.9
Deloc. = -90.6

eq-3a

$^1J^{FC}_{C,Hax} = 166.1$
Lewis = 262.6
Repol. = 8.7
Deloc. = -105.2

$^1J^{FC}_{C,Heq} = 192.4$
Lewis = 280.3
Repol. = 4.2
Deloc. = -92.1

Figure S11. Decomposition of selected $^1J_{CH}$ couplings for compound **4** into NJC terms: Lewis, Repolarization and Delocalization, obtained at the PBE0-D3BJ/pcJ-3 theoretical level.
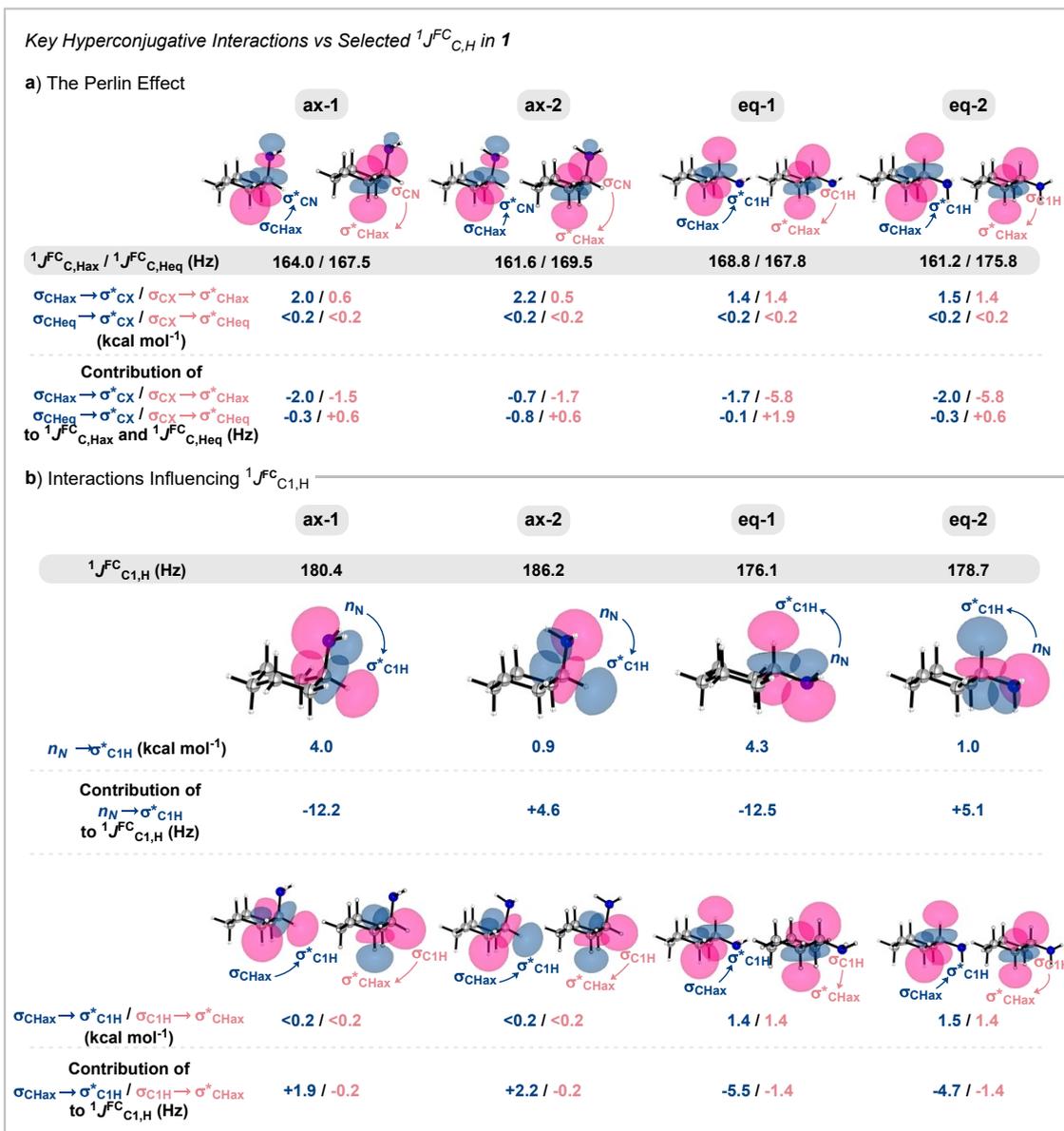
Figure S12. Contribution of hyperconjugative interactions to selected $^{1}J_{CH}$ couplings in **1** according to NJC analysis, obtained at the PBE0-D3BJ/pcJ-3 theoretical level.

Figure S13. Contribution of hyperconjugative interactions to selected $^1J_{CH}$ couplings in **2** according to NJC analysis, obtained at the PBE0-D3BJ/pcJ-3 theoretical level.
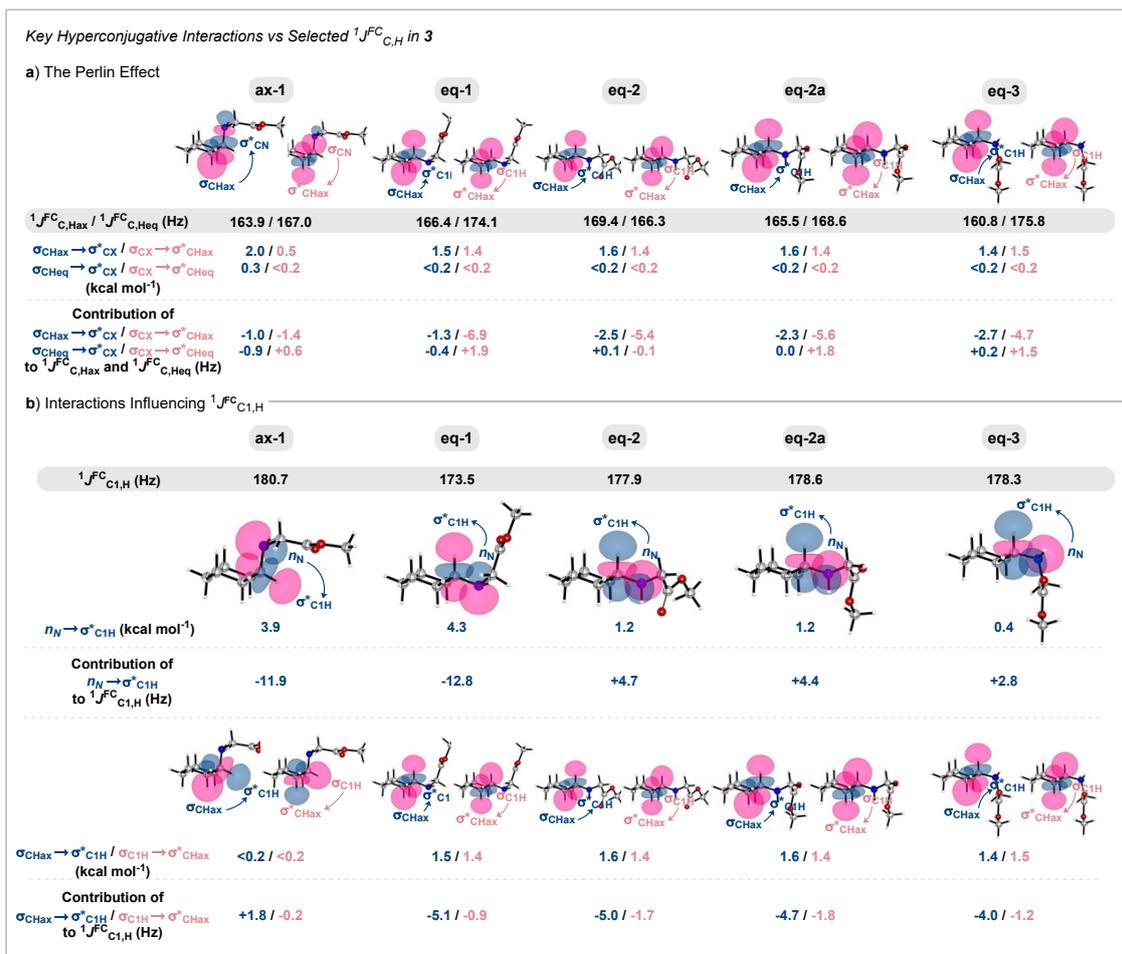
Figure S14. Contribution of hyperconjugative interactions to selected $^1J_{CH}$ couplings in **3** according to NJC analysis, obtained at the PBE0-D3BJ/pcJ-3 theoretical level.

Key Hyperconjugative Interactions and the Perlin Effect in **4**

	ax-2		eq-2a	eq-2b	eq-3	eq-3a
$^1J^{FC}_{C,Hax}$ / $^1J^{FC}_{C,Heq}$ (Hz)	175.5 / 186.6		150.8 / 179.9	168.2 / 195.9	164.8 / 192.7	166.1 / 192.4
$\sigma_{CHax} \rightarrow \sigma^*_{NN}$ / $\sigma_{NN} \rightarrow \sigma^*_{CHax}$	2.1 / 0.5	$n_N \rightarrow \sigma^*_{CHax}$	3.7	3.9	4.4	4.4
$\sigma_{CHeq} \rightarrow \sigma^*_{NN}$ / $\sigma_{NN} \rightarrow \sigma^*_{CHeq}$ (kcal mol^{-1})	<0.2 / <0.2	$n_N \rightarrow \sigma^*_{CHeq}$ (kcal mol^{-1})	0.8	0.9	0.8	0.8
Contribution of $\sigma_{CHax} \rightarrow \sigma^*_{NN}$ / $\sigma_{NN} \rightarrow \sigma^*_{CHax}$	+39.0 / -14.4	Contribution of $n_N \rightarrow \sigma^*_{CHax}$	-5.2	-13.4	-13.1	-12.9
$\sigma_{CHeq} \rightarrow \sigma^*_{NN}$ / $\sigma_{NN} \rightarrow \sigma^*_{CHeq}$ to $^1J^{FC}_{C,Hax}$ and $^1J^{FC}_{C,Heq}$ (Hz)	+0.4 / +0.8	$n_N \rightarrow \sigma^*_{CHeq}$ to $^1J^{FC}_{C,Hax}$ and $^1J^{FC}_{C,Heq}$ (Hz)	+3.6	+3.5	+3.5	+3.4
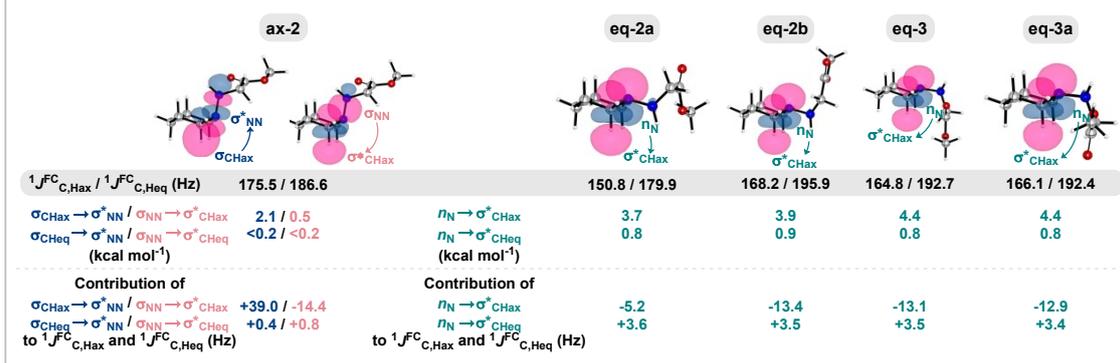
Figure S15. Contribution of hyperconjugative interactions to selected $^1J_{CH}$ couplings in **4** according to NJC analysis, obtained at the PBE0-D3BJ/pcJ-3 theoretical level.
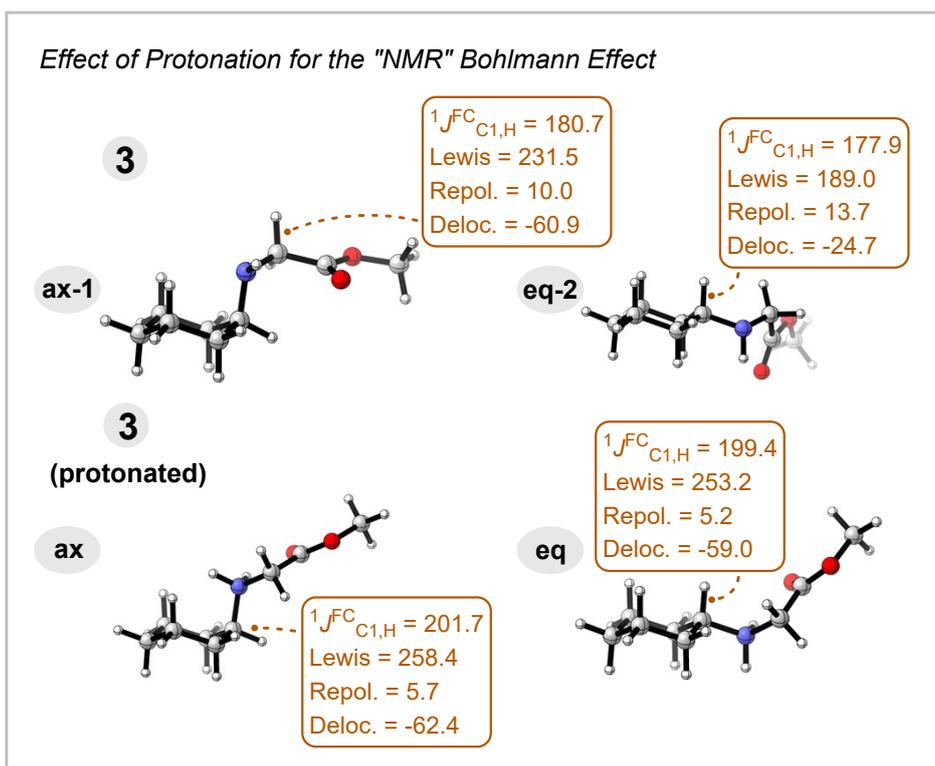
Figure S16. Decomposition of $^1J_{C1H}$ coupling for the most stable axial and equatorial conformers of **3** and its protonated derivative into NJC terms: Lewis, Repolarization and Delocalization, obtained at the PBE0-D3BJ/pcJ-3 theoretical level.

Table S2. Steric interactions (in kcal mol^{-1}) according to NSA analysis that govern the differences in $^1J_{C1H}$ coupling for the most stable axial and equatorial conformers of **3** and its protonated derivative, obtained at the PBE0-D3BJ/pcJ-3 theoretical level.

	ax-1	eq-2a
3		
σ_{C1H} / σ_{CC} (each)	4.3	1.2

	ax	eq
3 (protonated)		
σ_{C1H} / σ_{CC} (each)	4.4	0.8
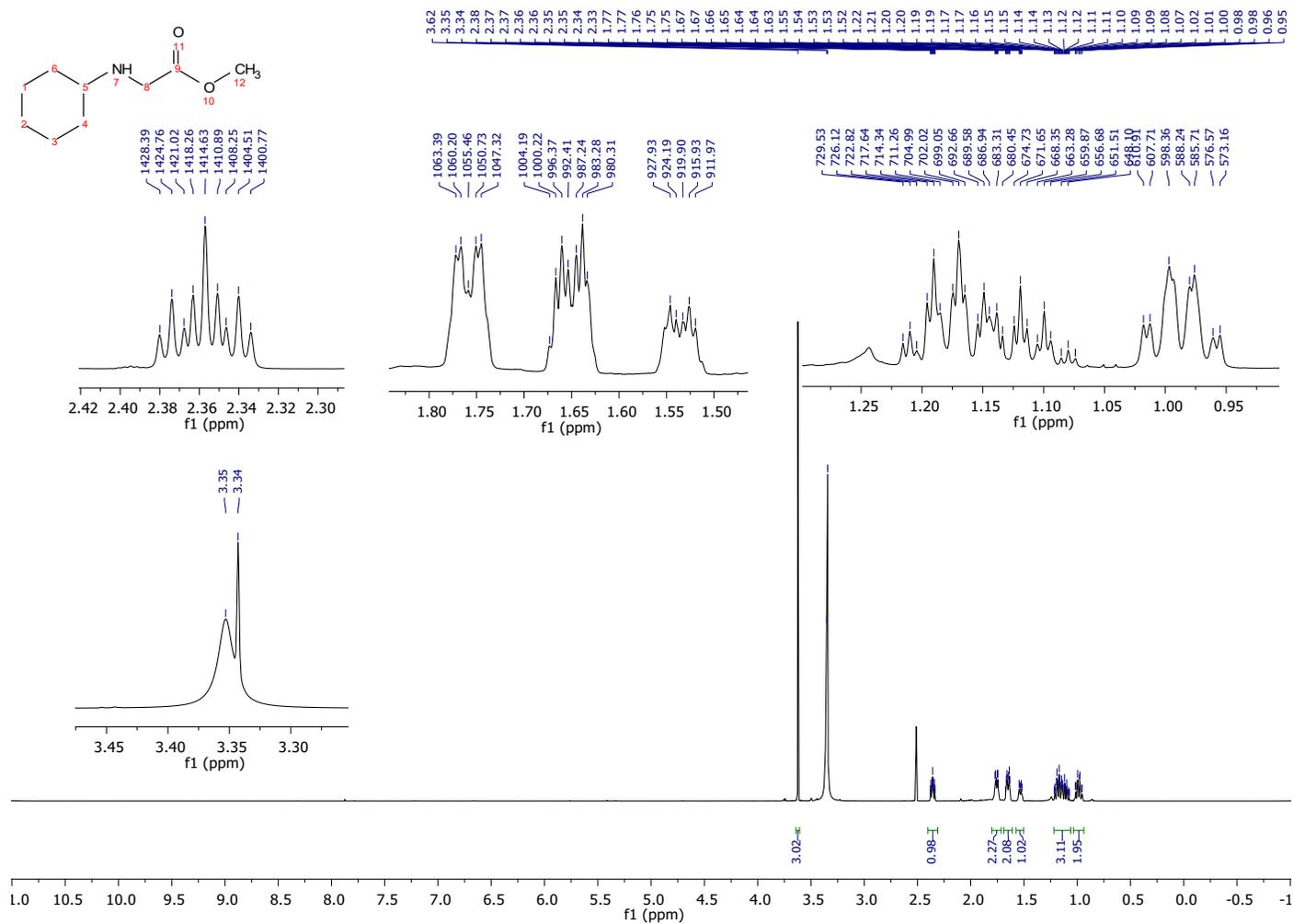
Figure S17. ^{1}H-NMR (600 MHz, DMSO-d$_6$) of free **3**.
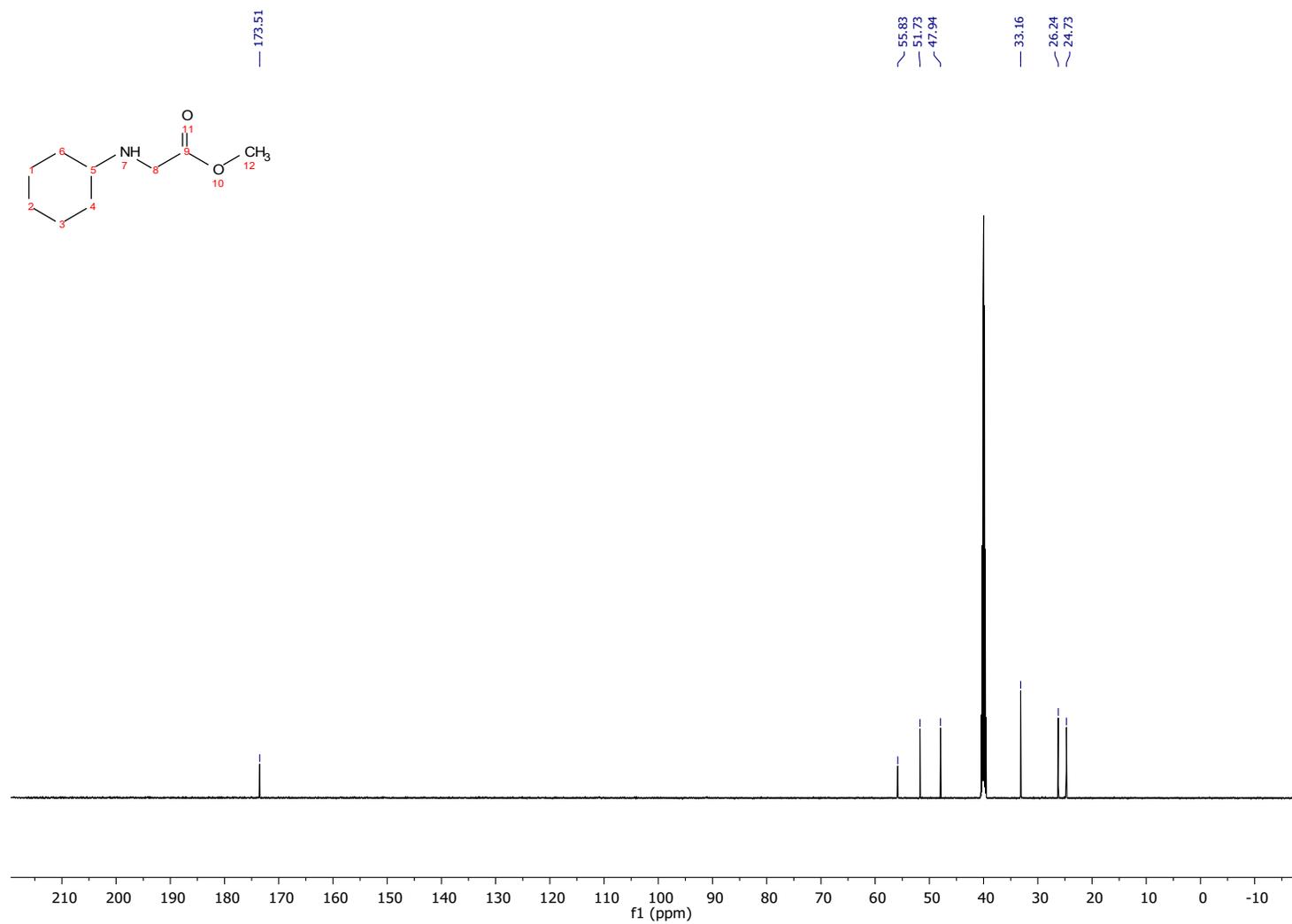
Figure S18. $^{13}C\{^1H\}$-NMR (151 MHz, DMSO-d$_6$) of free **3**.
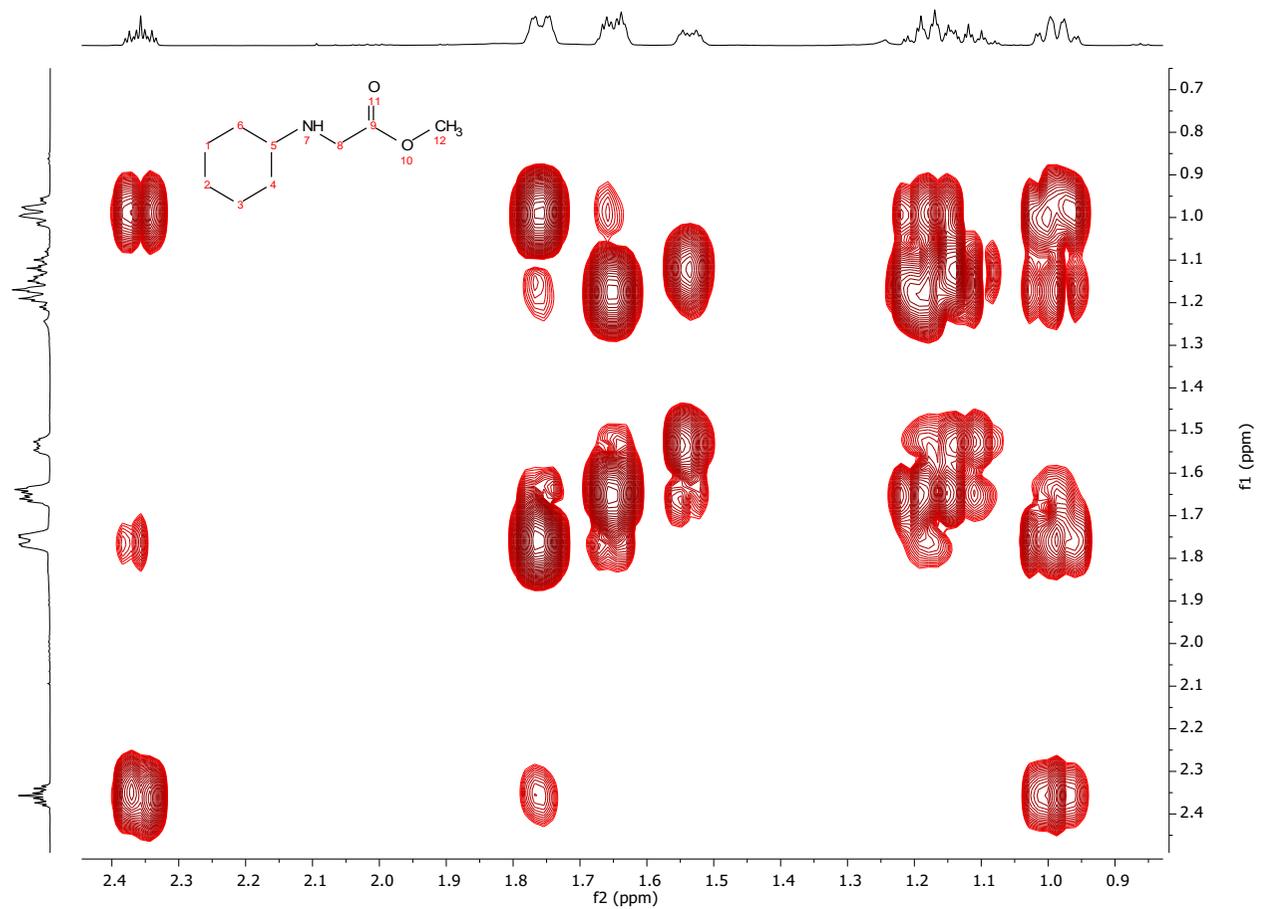
Figure S19. ^{1}H-^{1}H-DQF-COSY (600 MHz for ^{1}H, DMSO-d$_6$) of free **3**.
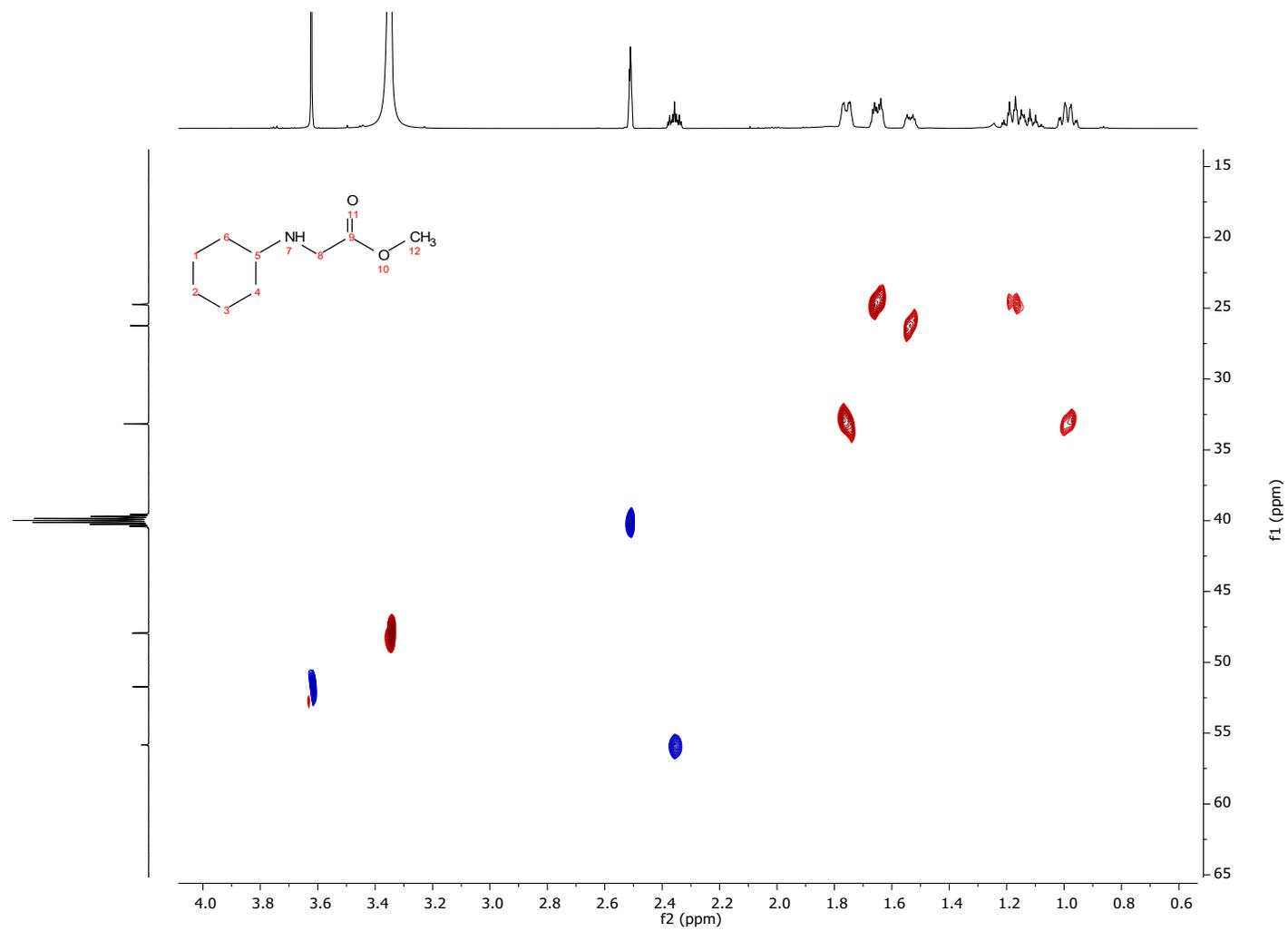
Figure S20. ^{1}H-^{13}C-HSQC (600 MHz for ^{1}H, DMSO-d$_6$) of free **3**.
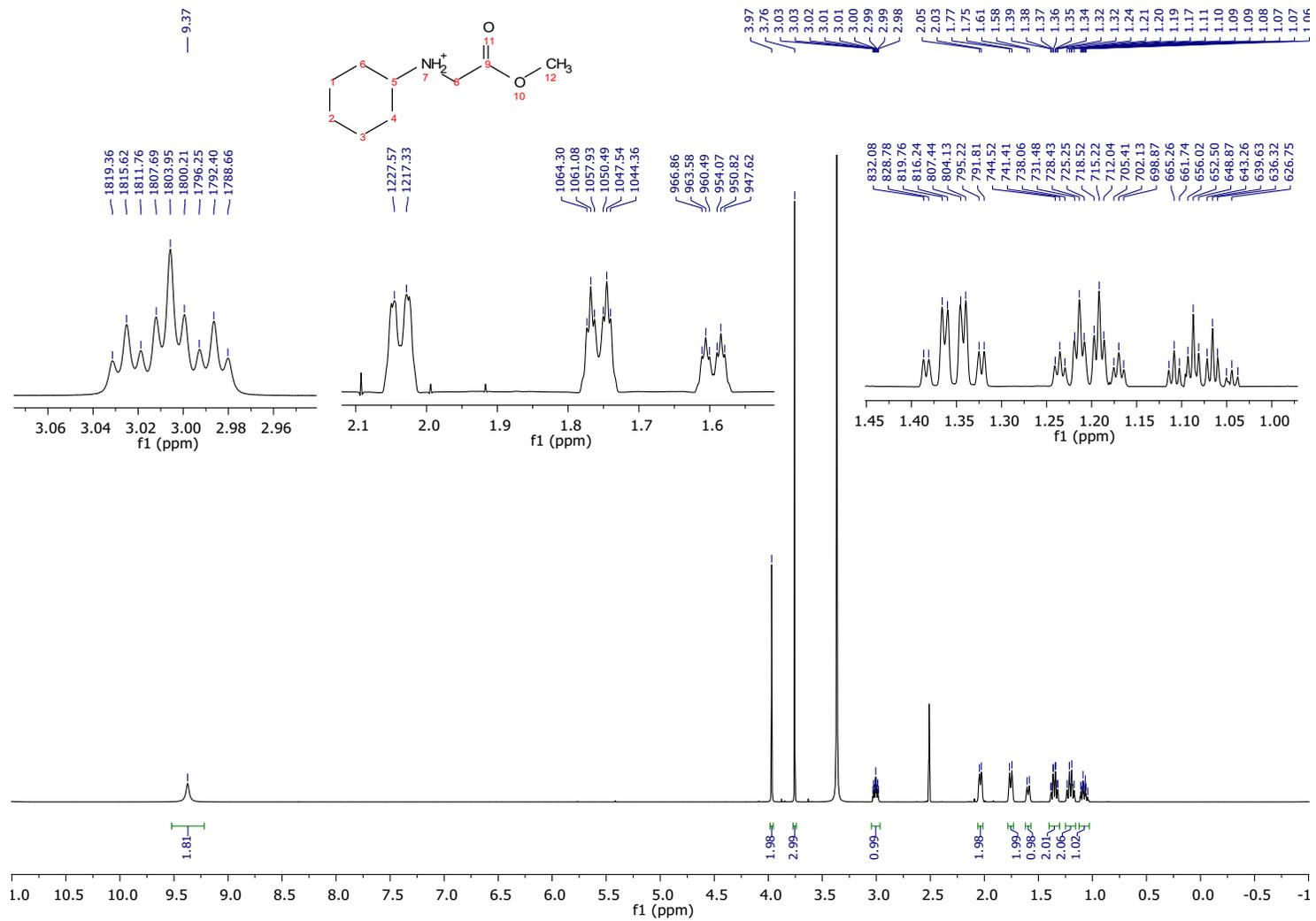
Figure S21. ^{1}H-NMR (600 MHz, DMSO-d$_6$) of protonated **3** (Hydrochloride).
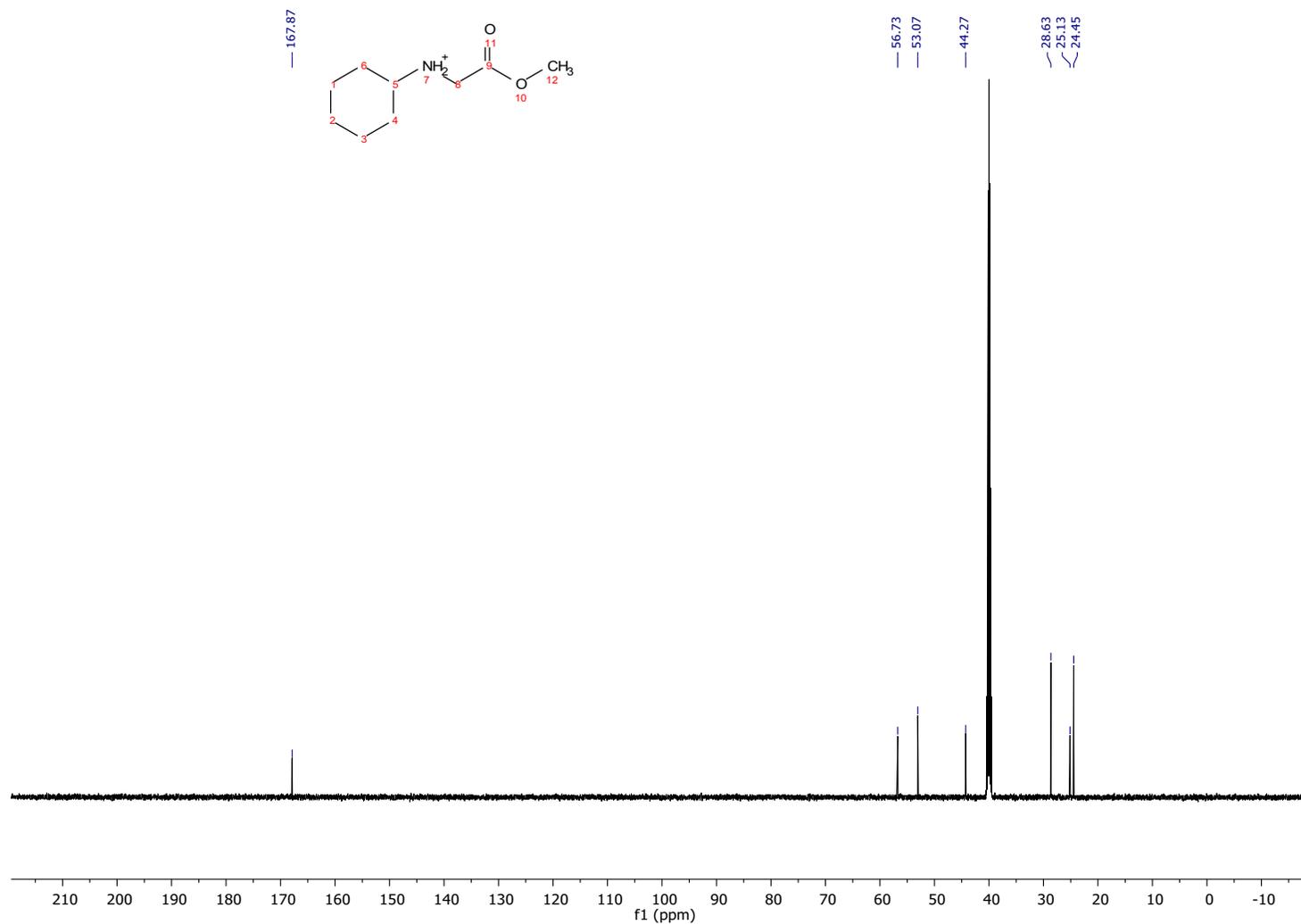
Figure S22. $^{13}C\{^1H\}$-NMR (151 MHz, DMSO-d$_6$) of protonated **3** (Hydrochloride).
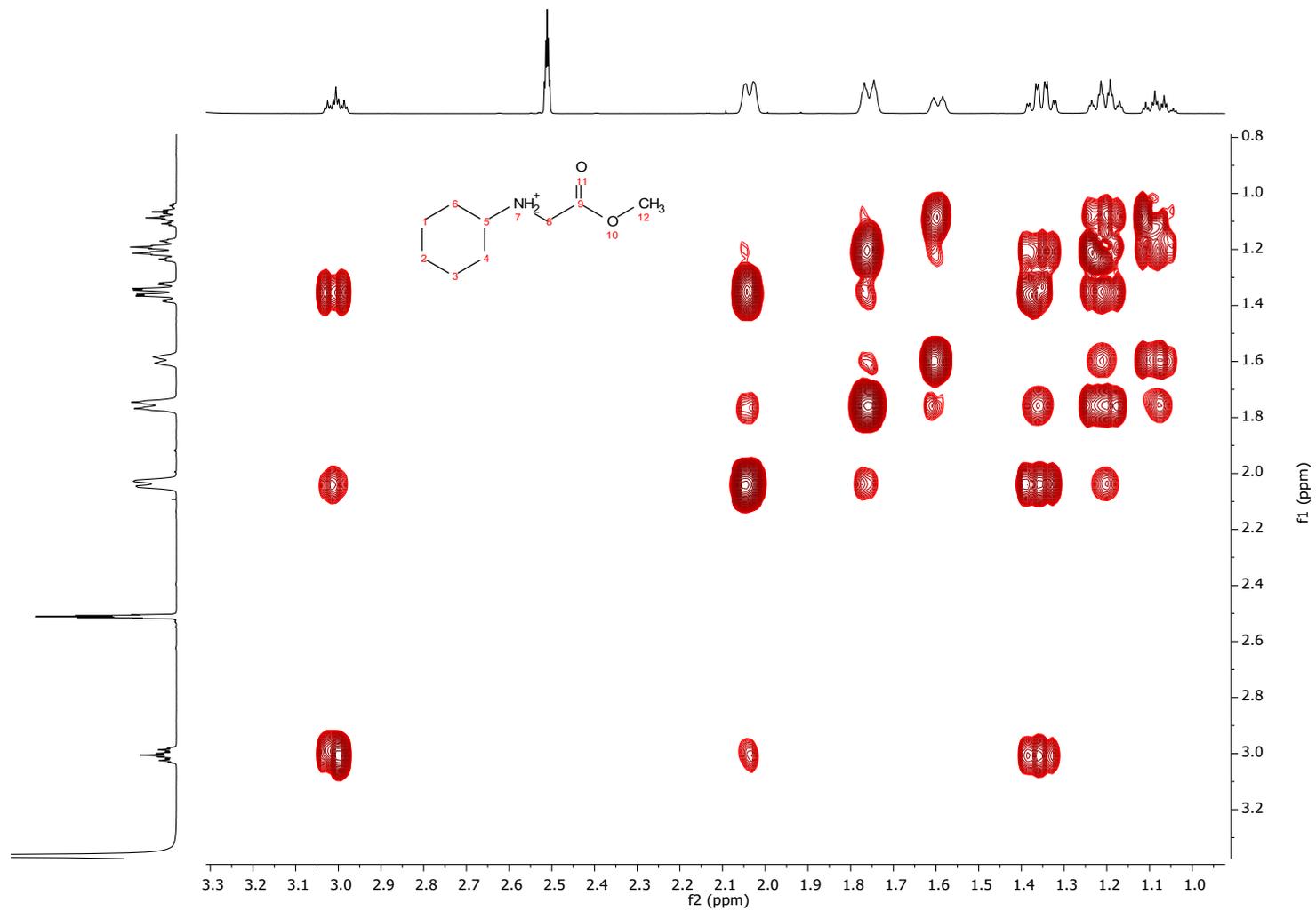
Figure S23. ^1H-^1H-DQF-COSY (600 MHz, DMSO-d_6) of protonated **3** (Hydrochloride).
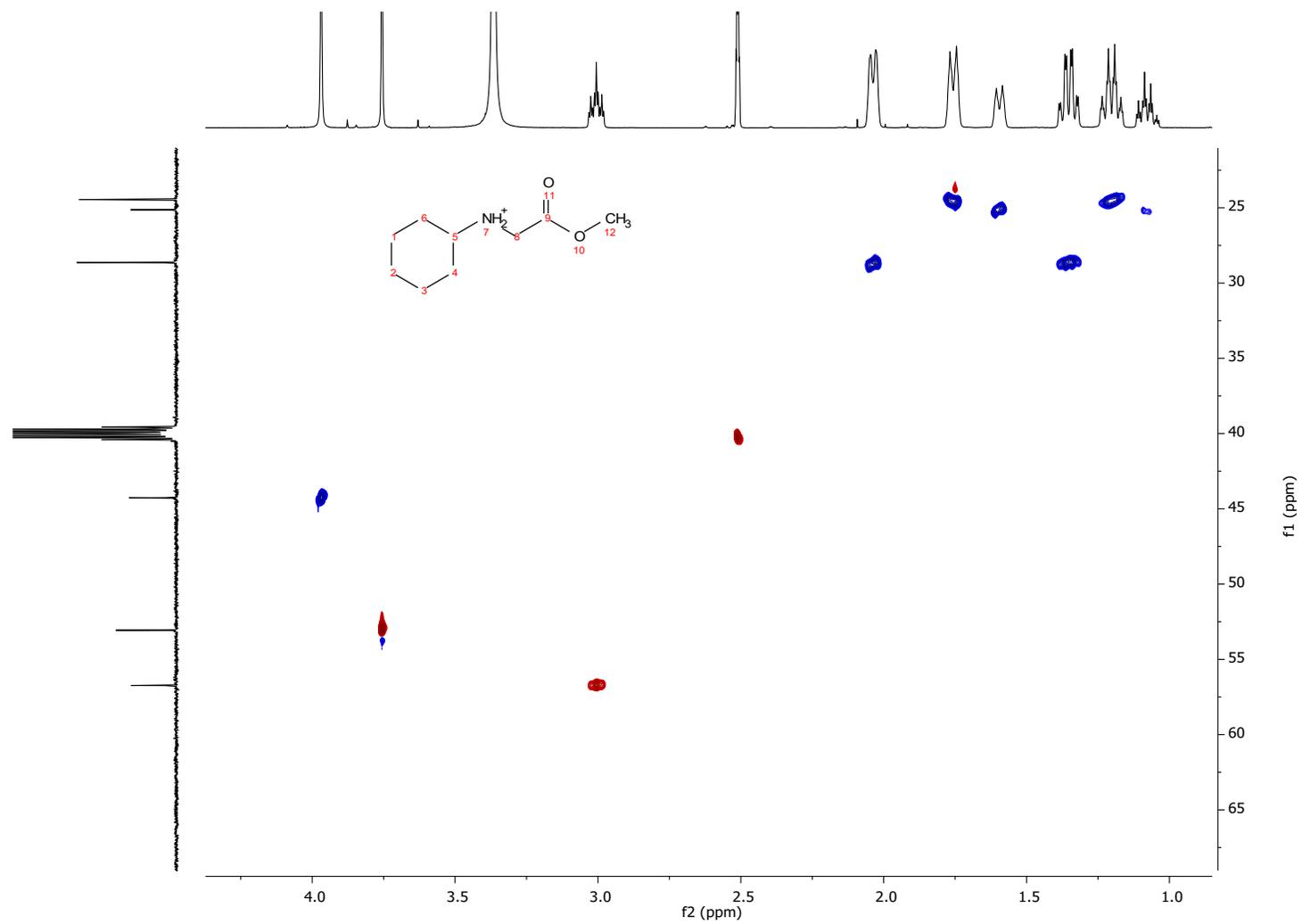
Figure S24. ^1H-^{13}C-HSQC (600 MHz for ^1H, DMSO-d_6) of protonated **3** (Hydrochloride).

Table S3. Cartesian coordinates, electronic energy, enthalpy, Gibbs free energy, and lowest harmonic vibrational frequency (LHVF) for the optimized conformers of compounds **1-4** at the PBE0-D4/pc-3 theoretical level.

1 ax-1 Electronic Energy (Hartree) = -291.01981120 Enthalpy (Hartree) = -290.82426191 Gibbs Free Energy (Hartree) = -290.86266657 LHVF (cm⁻¹) = 161.8				1 ax-2 Electronic Energy (Hartree) = -291.01952759 Enthalpy (Hartree) = -290.82398319 Gibbs Free Energy (Hartree) = -290.86244548 LHVF (cm⁻¹) = 162.5			
C	-3.185931000	-0.937426000	-0.294650000	C	-3.180387000	-0.839586000	-0.335371000
C	-1.686009000	-1.045174000	-0.057467000	C	-1.692677000	-0.990861000	-0.048587000
C	-1.078033000	0.323917000	0.213865000	C	-1.067161000	0.342851000	0.337148000
C	-1.771294000	1.007003000	1.384863000	C	-1.802285000	0.979606000	1.510168000
C	-3.281045000	1.116448000	1.190940000	C	-3.295338000	1.144676000	1.241396000
C	-3.876871000	-0.253109000	0.876846000	C	-3.905601000	-0.203989000	0.842983000
H	-0.008429000	0.233165000	0.418874000	H	-0.012653000	0.209492000	0.589986000
H	-1.501175000	-1.700642000	0.802378000	H	-1.558743000	-1.699113000	0.777278000
H	-1.198727000	-1.513944000	-0.915967000	H	-1.178740000	-1.419133000	-0.912598000
H	-3.364798000	-0.360775000	-1.205580000	H	-3.315533000	-0.221663000	-1.230439000
H	-3.619719000	-1.927961000	-0.452886000	H	-3.625150000	-1.809418000	-0.570239000
H	-1.585743000	0.438044000	2.301896000	H	-1.678147000	0.341775000	2.391205000
H	-1.350804000	2.004034000	1.551026000	H	-1.374182000	1.954181000	1.751708000
H	-3.784181000	-0.877989000	1.771258000	H	-3.852582000	-0.881995000	1.702507000
H	-4.949311000	-0.149874000	0.682806000	H	-4.967536000	-0.071970000	0.615401000
H	-1.181237000	0.945757000	-0.678863000	H	-1.082083000	1.018355000	-0.525724000
N	-3.565806000	2.035236000	0.094286000	N	-3.507517000	2.216803000	0.275522000
H	-4.562966000	2.136521000	-0.038032000	H	-3.101577000	1.986225000	-0.621127000
H	-3.195630000	2.954885000	0.292560000	H	-4.495934000	2.360568000	0.117260000
H	-3.717145000	1.462342000	2.140475000	H	-3.771030000	1.473653000	2.170155000

1 eq-1 Electronic Energy (Hartree) = -291.01727237 Enthalpy (Hartree) = -290.82154342 Gibbs Free Energy (Hartree) = -290.85986777 LHVF (cm⁻¹) = 159.8				1 eq-2 Electronic Energy (Hartree) = -291.01813568 Enthalpy (Hartree) = -290.82240732 Gibbs Free Energy (Hartree) = -290.86067083 LHVF (cm⁻¹) = 157.8			
C	-3.097584000	-1.265293000	0.151545000	C	-3.084743000	-1.277010000	0.103769000
C	-1.650603000	-1.034296000	-0.261115000	C	-1.642977000	-0.985555000	-0.287144000
C	-0.984994000	0.007229000	0.627500000	C	-1.007893000	0.013133000	0.669503000
C	-1.779721000	1.304905000	0.645848000	C	-1.834976000	1.288352000	0.759072000
C	-3.221032000	1.074290000	1.072832000	C	-3.282394000	1.006834000	1.158333000
C	-3.879463000	0.040071000	0.172805000	C	-3.906567000	-0.000007000	0.204092000
H	-0.907813000	-0.386550000	1.647307000	H	-0.934380000	-0.439378000	1.664991000
H	-1.092222000	-1.973131000	-0.230153000	H	-1.061631000	-1.910376000	-0.313827000
H	-1.625063000	-0.688567000	-1.300514000	H	-1.622067000	-0.573700000	-1.302601000
H	-3.577229000	-1.978072000	-0.523351000	H	-3.543208000	-1.962463000	-0.612936000
H	-3.119826000	-1.720469000	1.148273000	H	-3.097996000	-1.788753000	1.072710000
H	-1.307541000	2.031380000	1.314883000	H	-1.387586000	1.987835000	1.471841000
H	-1.789028000	1.756236000	-0.351899000	H	-1.837571000	1.792568000	-0.215620000
H	-4.907982000	-0.136775000	0.503081000	H	-4.927260000	-0.213433000	0.527243000
H	-3.940195000	0.459104000	-0.837094000	H	-3.980721000	0.462841000	-0.788730000
H	0.036937000	0.198176000	0.291856000	H	0.013864000	0.245015000	0.359428000
N	-3.958844000	2.325917000	1.001997000	N	-4.129184000	2.186704000	1.239850000
H	-4.916355000	2.197454000	1.300990000	H	-3.735227000	2.867436000	1.876100000
H	-3.546965000	3.021931000	1.609185000	H	-4.189657000	2.635380000	0.333909000
H	-3.199330000	0.656919000	2.094655000	H	-3.272675000	0.555034000	2.158646000

2 ax-2 Electronic Energy (Hartree) = -307.01517422 Enthalpy (Hartree) = -306.83158010 Gibbs Free Energy (Hartree) = -306.86950612 LHVF (cm⁻¹) = 164.0				2 eq-2 Electronic Energy (Hartree) = -307.01042687 Enthalpy (Hartree) = -306.82668826 Gibbs Free Energy (Hartree) = -306.86445441 LHVF (cm⁻¹) = 164.6			
C	-3.375782000	-0.978255000	0.528614000	C	-3.279166000	-1.202114000	0.426388000
C	-1.932945000	-1.206878000	0.096256000	C	-1.767382000	-1.311752000	0.311236000
C	-1.318480000	0.088407000	-0.418631000	C	-1.216285000	-0.119432000	-0.454403000
C	-1.480409000	1.200553000	0.611413000	C	-1.685089000	1.184117000	0.164588000
C	-3.454767000	0.180061000	1.518794000	C	-3.678816000	0.142426000	1.006725000
H	-0.259526000	-0.049825000	-0.650430000	H	-0.124408000	-0.138507000	-0.471304000
H	-1.354911000	-1.559911000	0.958388000	H	-1.328103000	-1.331255000	1.314891000
H	-1.876477000	-1.993056000	-0.660101000	H	-1.485036000	-2.248586000	-0.173965000
H	-3.994551000	-0.767595000	-0.351567000	H	-3.731689000	-1.304430000	-0.564033000
H	-3.796986000	-1.878661000	0.982470000	H	-3.683895000	-2.001287000	1.051385000
H	-0.908124000	0.946887000	1.510764000	H	-1.247721000	1.286420000	1.176826000

H	-1.100043000	2.148145000	0.231926000
H	-2.920254000	-0.096433000	2.434082000
H	-4.488203000	0.389902000	1.803236000
H	-1.805448000	0.386474000	-1.352952000
N	-3.592341000	2.037920000	-0.003864000
H	-4.026111000	1.365035000	-0.630486000
H	-4.328332000	2.584418000	0.420937000
N	-2.857504000	1.415401000	1.028415000

H	-1.351513000	2.042705000	-0.417191000
H	-3.334392000	0.210980000	2.058380000
H	-4.766428000	0.245246000	1.018173000
H	-1.557445000	-0.158857000	-1.492909000
N	-3.525773000	2.499369000	0.710295000
H	-4.485044000	2.660217000	0.434477000
H	-3.491042000	2.521387000	1.731009000
N	-3.131969000	1.235950000	0.226700000

3 ax-1
Electronic Energy (Hartree) = -558.03564023
Enthalpy (Hartree) = -557.76288758
Gibbs Free Energy (Hartree) = -557.81444698
LHVF (cm^{-1}) = 28.6

3 eq-1
Electronic Energy (Hartree) = -558.03375164
Enthalpy (Hartree) = -557.76093148
Gibbs Free Energy (Hartree) = -557.81239840

LHVF (cm^{-1}) = 29.9

C	2.635267000	-1.579955000	0.073141000
C	3.694430000	-0.490109000	-0.013587000
C	3.094387000	0.816509000	-0.513020000
C	1.919912000	1.243848000	0.357513000
C	1.464748000	-1.144185000	0.942307000
H	3.851085000	1.604839000	-0.523929000
H	4.130201000	-0.329263000	0.979856000
H	4.512902000	-0.806558000	-0.664759000
H	2.267470000	-1.804988000	-0.931421000
H	3.069113000	-2.501752000	0.468475000
H	2.280727000	1.464159000	1.366902000
H	1.470757000	2.168498000	-0.017512000
H	1.802542000	-1.001636000	1.974200000
H	0.706585000	-1.931085000	0.979392000
H	2.759158000	0.687201000	-1.545840000
N	0.204609000	-0.006110000	-0.837296000
H	0.108052000	0.898462000	-1.279303000
C	-1.083228000	-0.632560000	-0.784063000
H	-1.042313000	-1.559307000	-0.210511000
H	-1.407382000	-0.923116000	-1.789200000
C	-2.183858000	0.245459000	-0.218012000
O	-2.114902000	1.438661000	-0.101456000
O	-3.267112000	-0.470732000	0.096919000
C	-4.382589000	0.279644000	0.566748000
H	-5.166140000	-0.444759000	0.769521000
H	-4.122764000	0.823784000	1.474068000
H	-4.709570000	0.993188000	-0.188981000
C	0.845041000	0.168517000	0.464564000
H	0.112215000	0.501931000	1.215160000

C	2.823975000	-1.255862000	-1.030383000
C	3.648936000	-0.799139000	0.164142000
C	2.753246000	-0.391666000	1.324982000
C	1.748148000	0.668882000	0.898553000
C	1.806511000	-0.201243000	-1.439425000
H	2.216706000	-1.273554000	1.692721000
H	4.337895000	-1.589164000	0.473041000
H	4.267066000	0.056584000	-0.129934000
H	3.474819000	-1.493827000	-1.874920000
H	2.299205000	-2.182498000	-0.773119000
H	1.108186000	0.936929000	1.743197000
H	2.269624000	1.582970000	0.596756000
H	1.191255000	-0.568922000	-2.266182000
H	2.322818000	0.696545000	-1.797135000
H	3.353723000	-0.024241000	2.160147000
N	-0.010481000	1.238526000	-0.720643000
H	-0.303017000	1.038126000	-1.668026000
C	-1.176335000	1.395627000	0.099982000
H	-1.711174000	2.310710000	-0.175363000
H	-0.900840000	1.521651000	1.147487000
C	-2.180639000	0.263653000	-0.009560000
O	-2.207706000	-0.544772000	-0.897220000
O	-3.067341000	0.299984000	0.989628000
C	-4.095678000	-0.683515000	0.933429000
H	-4.726105000	-0.506643000	1.800114000
H	-4.672802000	-0.581964000	0.014927000
H	-3.668989000	-1.685223000	0.971020000
C	0.907454000	0.195410000	-0.280206000
H	0.356897000	-0.708741000	0.032560000

3 eq-2
Electronic Energy (Hartree) = -558.03690618
Enthalpy (Hartree) = -557.76402303
Gibbs Free Energy (Hartree) = -557.81568225
LHVF (cm^{-1}) = 31.2

3 eq-2a
Electronic Energy (Hartree) = -558.03391411
Enthalpy (Hartree) = -557.76098770
Gibbs Free Energy (Hartree) = -557.81246144
LHVF (cm^{-1}) = 39.6

C	2.098932000	-1.684892000	0.411676000
C	3.354601000	-1.166251000	-0.272490000
C	3.578082000	0.304903000	0.044395000
C	2.357395000	1.142283000	-0.306688000
C	0.881078000	-0.848646000	0.043001000
H	3.794157000	0.414035000	1.113189000
H	4.223832000	-1.756840000	0.027023000
H	3.250736000	-1.289775000	-1.356340000
H	1.926924000	-2.732483000	0.153241000
H	2.243696000	-1.654450000	1.497928000
H	2.506048000	2.188745000	-0.033399000
H	2.202250000	1.118256000	-1.392739000
H	0.000448000	-1.229894000	0.567898000
H	0.670386000	-0.944912000	-1.027288000
H	4.455035000	0.681736000	-0.487216000
N	-0.007616000	1.517807000	0.034108000
H	-0.126364000	1.556860000	-0.970860000
C	-1.267556000	1.210101000	0.649296000
H	-1.866825000	2.121596000	0.768150000
H	-1.116276000	0.822327000	1.658019000
C	-2.143502000	0.251672000	-0.127998000
O	-2.022816000	0.011583000	-1.298674000
O	-3.113801000	-0.256172000	0.637664000

C	1.955864000	-1.609073000	0.659668000
C	3.157013000	-1.295381000	-0.218934000
C	3.450885000	0.197287000	-0.225095000
C	2.227703000	1.006008000	-0.630106000
C	0.733255000	-0.806010000	0.236669000
H	3.769834000	0.504457000	0.777245000
H	4.032962000	-1.854184000	0.119329000
H	2.951139000	-1.627754000	-1.242807000
H	1.730015000	-2.677719000	0.634121000
H	2.200075000	-1.370787000	1.701219000
H	2.432381000	2.077368000	-0.585308000
H	1.971964000	0.776950000	-1.672730000
H	-0.103471000	-1.036536000	0.901428000
H	0.427427000	-1.101405000	-0.773475000
H	4.284497000	0.420453000	-0.895094000
N	-0.081733000	1.552779000	-0.173688000
H	-0.289656000	1.417757000	-1.153459000
C	-1.281311000	1.477963000	0.615326000
H	-1.886229000	2.375924000	0.442598000
H	-1.028623000	1.479113000	1.676008000
C	-2.224611000	0.311704000	0.390311000
O	-2.912196000	-0.188630000	1.238272000
O	-2.249696000	-0.062955000	-0.894812000

C	-4.043060000	-1.102729000	-0.031122000
H	-3.533886000	-1.963304000	-0.463612000
H	-4.753982000	-1.422470000	0.725317000
H	-4.551956000	-0.560192000	-0.827329000
C	1.095415000	0.629528000	0.370223000
H	1.240999000	0.713517000	1.456285000

C	-3.130408000	-1.137273000	-1.199924000
H	-2.852676000	-2.029119000	-0.638706000
H	-4.158032000	-0.874125000	-0.951717000
H	-3.029778000	-1.313810000	-2.267108000
C	1.018305000	0.697048000	0.239951000
H	1.263578000	0.986856000	1.270992000

3 eq-3
Electronic Energy (Hartree) = -558.03550070
Enthalpy (Hartree) = -557.76249257
Gibbs Free Energy (Hartree) = -557.81398970
LHVF (cm^{-1}) = 29.2

C	3.218789000	-0.383057000	1.070708000
C	3.060877000	-1.425554000	-0.026315000
C	2.365903000	-0.834035000	-1.243395000
C	1.025866000	-0.214098000	-0.871039000
C	1.882027000	0.243593000	1.442344000
H	3.008043000	-0.062473000	-1.683441000
H	4.034812000	-1.835537000	-0.304606000
H	2.467025000	-2.263992000	0.355486000
H	3.683388000	-0.825815000	1.954979000
H	3.900162000	0.402077000	0.723790000
H	0.547883000	0.232371000	-1.745428000
H	0.356002000	-1.007887000	-0.517879000
H	2.009499000	1.023999000	2.195115000
H	1.244330000	-0.526901000	1.890583000
H	2.227019000	-1.596106000	-2.014015000
N	-0.041787000	1.533264000	0.618198000
H	-0.330042000	2.157597000	-0.123143000
C	-1.160759000	0.707692000	0.982676000
H	-1.803809000	1.233086000	1.699642000
H	-0.833338000	-0.196537000	1.494789000
C	-2.065273000	0.322482000	-0.167708000
O	-2.093956000	0.878526000	-1.232149000
O	-2.875368000	-0.686781000	0.164082000
C	-3.820548000	-1.067228000	-0.830523000
H	-4.475694000	-0.232019000	-1.076322000
H	-3.311259000	-1.392258000	-1.737096000
H	-4.392438000	-1.885247000	-0.401904000
C	1.182724000	0.839652000	0.226578000
H	1.839385000	1.625035000	-0.165988000

3 (protonated) ax
Electronic Energy (Hartree) = -558.41757308
Enthalpy (Hartree) = -558.12972925
Gibbs Free Energy (Hartree) = -558.18178448
LHVF (cm^{-1}) = 10.7

C	2.697972000	-1.577412000	-0.204186000
C	3.709373000	-0.451807000	-0.366909000
C	3.017969000	0.891854000	-0.546076000
C	2.050298000	1.176765000	0.597606000
C	1.734744000	-1.302207000	0.945061000
H	3.749340000	1.698104000	-0.603174000
H	4.349087000	-0.413474000	0.520255000
H	4.366319000	-0.654761000	-1.213235000
H	2.149711000	-1.718108000	-1.146762000
H	3.200927000	-2.528687000	-0.028395000
H	2.611093000	1.282994000	1.529094000
H	1.524436000	2.124346000	0.451067000
H	2.287451000	-1.284941000	1.887115000
H	1.000019000	-2.105149000	1.045817000
H	2.494894000	0.912415000	-1.511484000
N	0.093851000	0.028652000	-0.350773000
H	-0.265697000	0.987483000	-0.514943000
C	-1.135387000	-0.777755000	-0.175789000
H	-1.104621000	-1.311211000	0.772168000
H	-1.240910000	-1.509611000	-0.974456000
C	-2.295134000	0.204233000	-0.196707000
O	-2.098229000	1.382005000	-0.365038000
O	-3.438697000	-0.388653000	-0.017402000
C	-4.612459000	0.451890000	-0.025610000
H	-5.447785000	-0.221987000	0.126583000
H	-4.546966000	1.180071000	0.779562000
H	-4.691443000	0.961663000	-0.983019000
C	1.053497000	0.050231000	0.816649000
H	0.425714000	0.260232000	1.684692000
H	0.606222000	-0.258786000	-1.181743000

3 (protonated) eq
Electronic Energy (Hartree) = -558.41866152
Enthalpy (Hartree) = -558.13075899
Gibbs Free Energy (Hartree) = -558.18279459
LHVF (cm^{-1}) = 17.3

C	2.952694000	-1.276175000	-0.991278000
C	3.859188000	-0.607451000	0.030567000
C	3.077862000	-0.174472000	1.261461000
C	1.907838000	0.731079000	0.888911000
C	1.780223000	-0.376744000	-1.367023000
H	2.696261000	-1.056117000	1.786108000
H	4.661339000	-1.287454000	0.319142000
H	4.340730000	0.265454000	-0.422142000
H	3.508461000	-1.534761000	-1.892732000
H	2.567449000	-2.216322000	-0.584314000
H	1.349541000	1.011203000	1.785414000
H	2.293527000	1.657226000	0.445052000
H	1.113314000	-0.888772000	-2.066293000
H	2.157948000	0.520873000	-1.871475000
H	3.723553000	0.349088000	1.966859000
N	-0.121000000	0.935939000	-0.532967000
H	-0.621048000	0.483567000	-1.320051000
C	-1.182198000	1.150953000	0.477991000
H	-1.472024000	2.200119000	0.513137000
H	-0.832948000	0.859778000	1.465639000
C	-2.363202000	0.301628000	0.039181000
O	-2.341928000	-0.278540000	-1.017479000
O	-3.323740000	0.313842000	0.916337000
C	-4.510000000	-0.440832000	0.588660000
H	-5.182811000	-0.293815000	1.425784000

4 ax-2
Electronic Energy (Hartree) = -574.02963007
Enthalpy (Hartree) = -573.76893926
Gibbs Free Energy (Hartree) = -573.82043807
LHVF (cm^{-1}) = 16.6

C	-1.845859000	-0.599061000	1.257304000
C	-0.815032000	-0.192933000	0.211758000
C	-1.353433000	0.928283000	-0.667713000
C	-1.857264000	2.083578000	0.189348000
C	-2.326841000	0.620731000	2.033537000
H	-0.584099000	1.290925000	-1.353623000
H	0.090008000	0.158679000	0.721112000
H	-0.517552000	-1.051589000	-0.394527000
H	-2.703276000	-1.077294000	0.772788000
H	-1.428179000	-1.335689000	1.948221000
H	-1.016980000	2.518148000	0.740716000
H	-2.279054000	2.872609000	-0.431678000
H	-1.489534000	1.046057000	2.597567000
H	-3.106563000	0.352945000	2.745869000
H	-2.165761000	0.554857000	-1.300373000
N	-2.849364000	1.683099000	1.185241000
N	-4.097562000	1.300451000	0.647436000
H	-3.996566000	0.834745000	-0.249329000
C	-5.012143000	2.401227000	0.522566000
H	-4.831847000	3.106179000	1.332838000
H	-6.043213000	2.046097000	0.638235000
C	-4.975244000	3.126628000	-0.804451000
O	-4.433458000	2.718891000	-1.797224000
O	-5.672735000	4.263293000	-0.754755000
C	-5.763000000	4.983258000	-1.980191000

H	-4.944178000	-0.059873000	-0.332809000	H	-6.236225000	4.373368000	-2.748962000
H	-4.254718000	-1.491700000	0.473206000	H	-6.365714000	5.861204000	-1.766628000
C	1.018598000	0.035776000	-0.122277000	H	-4.772241000	5.276790000	-2.325159000
H	0.538041000	-0.839210000	0.324636000				
H	0.263361000	1.819253000	-0.860910000				

<table>
<tr><td colspan="4" align="center">4 eq-2a
Electronic Energy (Hartree) = -574.03037435
Enthalpy (Hartree) = -573.76967112
Gibbs Free Energy (Hartree) = -573.82074213
LHVF (cm⁻¹) = 25.8</td><td colspan="4" align="center">4 eq-2b
Electronic Energy (Hartree) = -574.02837569
Enthalpy (Hartree) = -573.76757962
Gibbs Free Energy (Hartree) = -573.81857619
LHVF (cm⁻¹) = 30.8</td></tr>
</table>

C	-1.525218000	-0.471739000	1.287685000	C	-2.077009000	-0.553772000	0.538135000
C	-0.597331000	0.136676000	0.248797000	C	-0.749824000	-0.010367000	0.033026000
C	-1.413708000	0.802604000	-0.846026000	C	-0.966621000	1.308036000	-0.693175000
C	-2.410664000	1.787875000	-0.261918000	C	-1.724340000	2.289160000	0.181495000
C	-2.506237000	0.562730000	1.805944000	C	-2.806146000	0.490683000	1.363811000
H	-0.767083000	1.324190000	-1.555333000	H	-0.012944000	1.749883000	-0.989922000
H	0.043740000	0.883778000	0.730005000	H	-0.079011000	0.152297000	0.884041000
H	0.065131000	-0.622335000	-0.172767000	H	-0.260408000	-0.736763000	-0.619254000
H	-2.087036000	-1.297617000	0.841866000	H	-1.927689000	-1.452448000	1.140802000
H	-0.957250000	-0.881363000	2.125920000	H	-1.101614000	2.563014000	1.053393000
H	-1.870683000	2.637922000	0.198136000	H	-1.952949000	3.209290000	-0.354599000
H	-3.031476000	2.195270000	-1.060122000	H	-2.236275000	0.691263000	2.292409000
H	-1.954562000	1.346931000	2.357813000	H	-3.789499000	0.119859000	1.660338000
H	-3.217340000	0.119850000	2.502273000	H	-1.542469000	1.134184000	-1.606787000
H	-1.963691000	0.043251000	-1.408999000	N	-2.985469000	1.717705000	0.611368000
N	-3.269899000	1.144090000	0.717187000	N	-3.732872000	2.679161000	1.312885000
N	-4.255130000	1.993760000	1.250480000	H	-3.517238000	2.659544000	2.306876000
H	-3.887714000	2.928450000	1.416084000	C	-5.141878000	2.516819000	1.089763000
C	-5.457655000	2.044638000	0.456870000	H	-5.678087000	3.194357000	1.761505000
H	-6.262760000	2.448493000	1.080451000	H	-5.527132000	1.507047000	1.279140000
H	-5.732151000	1.031791000	0.172296000	C	-5.578042000	2.859098000	-0.317126000
C	-5.442888000	2.888024000	-0.802868000	O	-6.563897000	2.392728000	-0.823256000
O	-5.930252000	2.573966000	-1.853611000	O	-4.793829000	3.754572000	-0.911019000
O	-4.852482000	4.072947000	-0.588618000	C	-5.182582000	4.113665000	-2.230526000
C	-4.804286000	4.944321000	-1.711466000	H	-4.446958000	4.837334000	-2.570522000
H	-5.809621000	5.171435000	-2.064456000	H	-5.185193000	3.238836000	-2.880217000
H	-4.307626000	5.847772000	-1.369057000	H	-6.179481000	4.553713000	-2.233087000
H	-4.242868000	4.487764000	-2.526640000				

<table>
<tr><td colspan="4" align="center">4 eq-3
Electronic Energy (Hartree) = -574.03072685
Enthalpy (Hartree) = -573.77009597
Gibbs Free Energy (Hartree) = -573.82156017
LHVF (cm⁻¹) = 30.2</td><td colspan="4" align="center">4 eq-3a
Electronic Energy (Hartree) = -574.03113625
Enthalpy (Hartree) = -573.77052549
Gibbs Free Energy (Hartree) = -573.82166279
LHVF (cm⁻¹) = 43.7</td></tr>
</table>

C	-1.645896000	0.993484000	1.711336000	C	-2.481157000	-0.342431000	-0.310612000
C	-0.511130000	0.612110000	0.775587000	C	-1.514783000	-0.539338000	0.845495000
C	-1.004682000	-0.388870000	-0.256264000	C	-0.504190000	0.595757000	0.878022000
C	-2.230309000	0.139698000	-0.979840000	C	-1.203960000	1.942837000	0.898156000
C	-2.850963000	1.485055000	0.928967000	C	-3.123499000	1.032531000	-0.249913000
H	-0.223911000	-0.613956000	-0.986397000	H	0.145437000	0.513750000	1.752304000
H	-0.147096000	1.510029000	0.263289000	H	-2.074985000	-0.554194000	1.787257000
H	0.333162000	0.205622000	1.336613000	H	-1.010016000	-1.504549000	0.765487000
H	-1.943533000	0.123084000	2.302904000	H	-1.943855000	-0.436886000	-1.258499000
H	-1.331136000	1.769850000	2.412429000	H	-3.262060000	-1.106201000	-0.300716000
H	-1.930408000	1.009185000	-1.595886000	H	-1.738690000	2.049289000	1.860282000
H	-2.640702000	-0.608811000	-1.657257000	H	-0.486374000	2.760235000	0.832500000
H	-2.586774000	2.441768000	0.439055000	H	-3.775930000	1.080825000	0.640647000
H	-3.687592000	1.683900000	1.599516000	H	-3.751983000	1.194007000	-1.127371000
H	-1.267563000	-1.327847000	0.239156000	H	0.134588000	0.545155000	-0.008403000
N	-3.271595000	0.484146000	-0.035227000	N	-2.102889000	2.066296000	-0.230951000
N	-4.483430000	0.749229000	-0.703440000	N	-2.567313000	3.387654000	-0.357869000
H	-5.242621000	0.550837000	-0.065982000	H	-2.782818000	3.560604000	-1.328420000
C	-4.642359000	2.070966000	-1.268113000	C	-3.654951000	3.801300000	0.504384000
H	-5.359862000	2.017599000	-2.094659000	H	-3.667896000	4.896420000	0.522918000
H	-3.706755000	2.414245000	-1.707853000	H	-3.465684000	3.480484000	1.527365000
C	-5.181181000	3.121512000	-0.322713000	C	-5.070148000	3.384425000	0.159013000
O	-5.817305000	2.884744000	0.668522000	O	-5.930913000	3.154291000	0.963525000
O	-4.909862000	4.356014000	-0.753781000	O	-5.272837000	3.365147000	-1.164590000
C	-5.444985000	5.412870000	0.037250000	C	-6.591142000	3.019025000	-1.573835000
H	-6.531309000	5.344656000	0.083551000	H	-6.851164000	2.022256000	-1.218527000
H	-5.046944000	5.369963000	1.050467000	H	-7.314689000	3.730714000	-1.177996000
H	-5.141991000	6.334392000	-0.451308000	H	-6.584837000	3.046068000	-2.659729000

		Cyclohexane	
	Electronic Energy (Hartree) = -235.69923943		
	Enthalpy (Hartree) = -235.52222111		
	Gibbs Free Energy (Hartree) = -235.55766853		
	LHVF (cm^{-1}) = 231.0		
C	2.631561000	-1.581198000	0.081757000
C	3.689524000	-0.490494000	-0.018227000
C	3.088477000	0.821576000	-0.504130000
C	1.923948000	1.256686000	0.375226000
C	1.466876000	-1.146333000	0.961026000
H	3.853256000	1.601701000	-0.534683000
H	4.138149000	-0.334615000	0.969747000
H	4.499404000	-0.806465000	-0.680489000
H	2.256234000	-1.809292000	-0.922601000
H	3.072949000	-2.504810000	0.464639000
H	2.299407000	1.485442000	1.379358000
H	1.482203000	2.179780000	-0.008510000
H	1.821781000	-1.019770000	1.990378000
H	0.701783000	-1.926200000	0.990350000
H	2.733288000	0.694050000	-1.533286000
C	0.866108000	0.166007000	0.475768000
H	0.056493000	0.482044000	1.138507000
H	0.416580000	0.010687000	-0.511772000