SUPPLEMENTARY MATERIALS

Catalytic activity of halohydrin dehalogenases towards spiroepoxides

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Content.

1. GC analyses

GC analyses for compounds were carried with β-DEX 225 column. Details are given in Table S1.

Table S1. GC analyses

Conditions	Retention time (min)		
	Epoxide	Azido alcohols	
100 °C 2 min, 10 °C/min to 150 °C, 10 min at 180 °C	3.7 (**1a**)	9.9 (**2a**)	9.6 (**2a'**)
110 °C 2 min, 10 °C/min to 180 °C, 10 min at 180 °C	4.4 (**1b**)	10.2 (**2b**)	10.7 (**2b'**)
120 °C 2 min, 10 °C/min to 200 °C, 10 min at 200 °C	5.2 (**1c**)	10.8 (**2c**)	11.4 (**2c'**)
110 °C 5 min, 15 °C/min to 150 °C, 10 min at 150 °C	5.0 (**1d**)	13.1 (**2d**)	
110 °C 5 min, 15 °C/min to 150 °C, 10 min at 150 °C	4.5 (**1e**)	13.1, 13.3 (**2e**)	
110 °C 5 min, 15 °C/min to 150 °C, 10 min at 150 °C	5.4 (**1f**)	13.8 (**2f**)	

Determination of enantiomeric excesses was performed using different chiral columns, Table S2.

Table S2. Chiral GC analyses

Comp.	Column	Conditions	Retention time (min)
1d	β-DEX 225	80 °C	11.3 (3*R*,4*S*)/11.5 (3*S*,4*R*)
2d	Lipodex E	60 °C 0 min, 2 °C/min to 150 °C	37.2 (3*S*,4*R*)/37.6(3*R*,4*S*)
1e	CP Chirasil DEX	130 °C	5.1 (3*R*,5*R*)/5.3 (3*S*,5*S*)
2e	β-DEX 225	110 °C 5 min, 15 °C/min to 150 °C, 10 min at 150 °C	13.1 (3*R*,5*R*)/13.3 (3*S*,5*S*)
1f	Chiraldex G-TA	60 °C	32.9 (*S*)/35.8 (*R*)
2f	CP Chirasil DEX	140 °C 0 min, 5 °C/min to 170 °C	9.3(*S*)/9.5 (*R*)

2. Reaction profiles for the non-enzyme ring opening of spiroepoxides

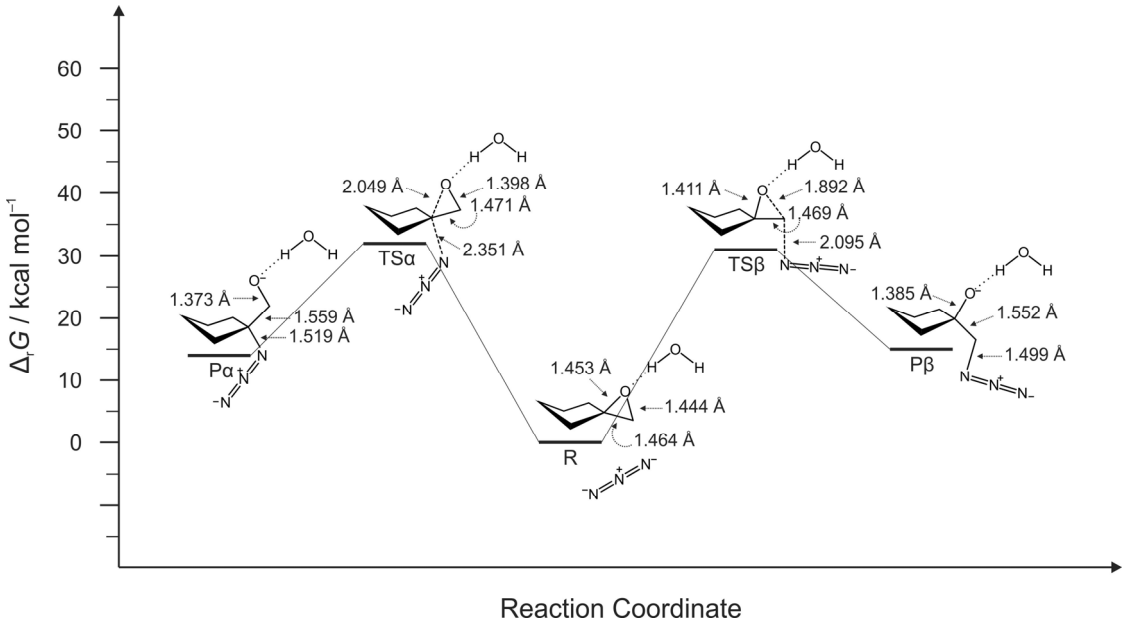


Figure S1. Calculated reaction profile for nucleophilic attack of azide on **1a**. R stands for reactants, TSα is the transition state for the attack on the Cα and TSβ for the attack on the Cβ carbon atom. Pα and Pβ are products, respectively. Calculations were carried out at the B3LYP/6-311++g(d,p) level with the polarizable continuum model using the integral equation formalism variant in H_2O (ε = 78.3553). Gibbs energies were calculated at 298.15 K and 1 atm.

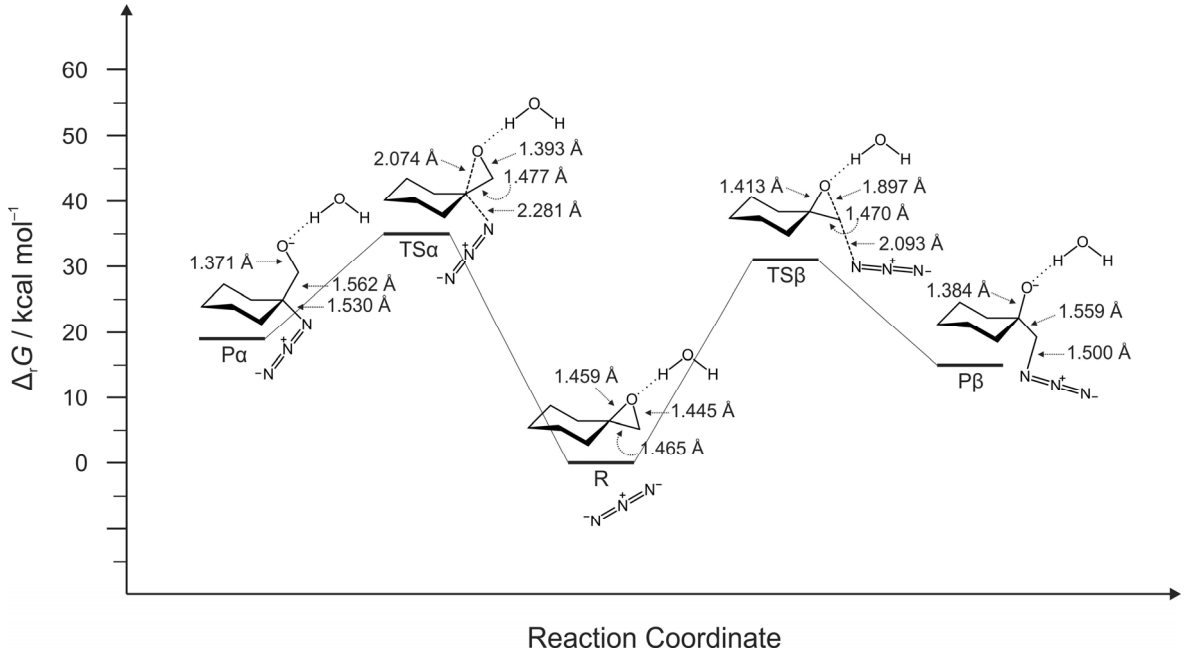


Figure S2. Calculated reaction profile for nucleophilic attack of azide on **1b**. R stands for reactants, TSα is the transition state for the attack on the Cα and TSβ for the attack on the Cβ carbon atom. Pα and Pβ are products, respectively. Calculations were carried out at the B3LYP/6-311++g(d,p) level with the polarizable continuum model using the integral equation formalism variant in H_2O (ε = 78.3553). Gibbs energies were calculated at 298.15 K and 1 atm.

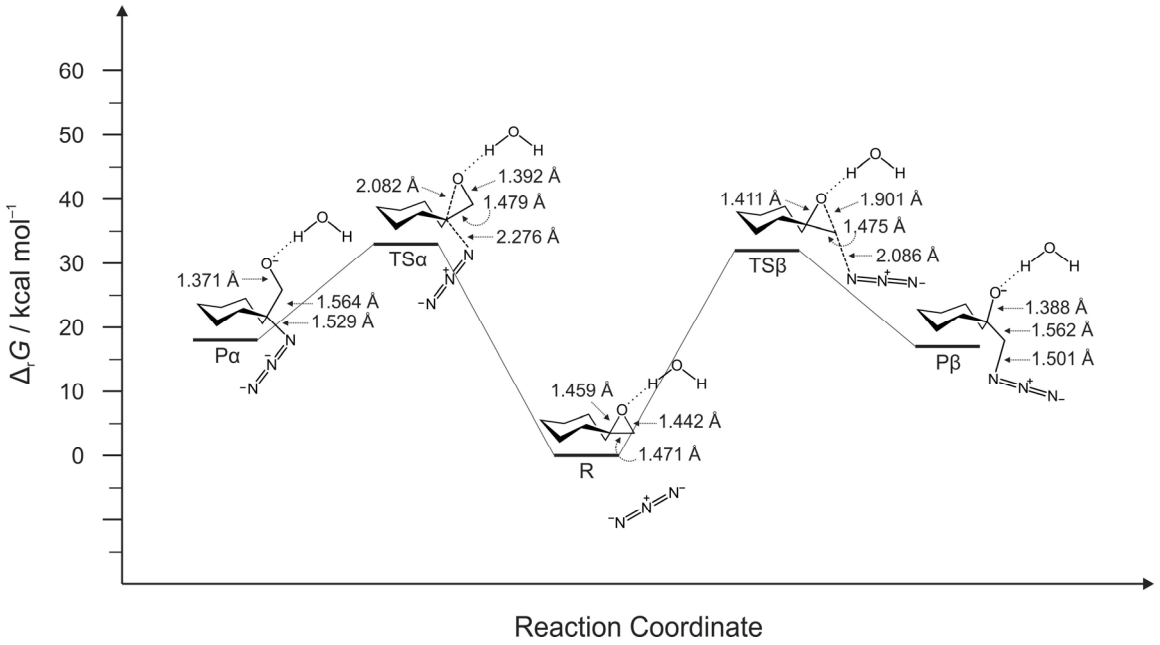


Figure S3. Calculated reaction profile for nucleophilic attack of azide on **1c**. R stands for reactants, TSα is the transition state for the attack on the Cα and TSβ for the attack on the Cβ carbon atom. Pα and Pβ are products, respectively. Calculations were carried out at the B3LYP/6-311++g(d,p) level with the polarizable continuum model using the integral equation formalism variant in H_2O (ε = 78.3553). Gibbs energies were calculated at 298.15 K and 1 atm.

3. Docking studies of 1-oxaspiro[2.5]octane compounds 1b and 1d–1f in the active site of HheA and HheC

3.1. Estimated lowest Gibbs energies of binding

Table S3. Estimated lowest Gibbs energy of binding for distinct conformational clusters of ligands (enzyme 1ZMO-**HheA**, rms tolerance for clustering was 0.5 Å) by the docking studies with the AutoDock 4.2 suite of programs. ***O-ax*** and ***O-eq*** stands for the *O*-axial and *O*-equatorial conformer respectively.

Comp. (*3R*)-enantiomers	ΔG / kcal mol^{-1}	Contribution in cluster / %	Comp. (*3S*)-enantiomers	ΔG / kcal mol^{-1}	Contribution in cluster / %
1a	−4.71	100			
1b$_{O\text{-}ax}$	−5.39	100			
1b$_{O\text{-}eq}$	−5.36	100			
1c	−6.06	100			
(*3R,4S*)-**1d**$_{O\text{-}ax}$	−5.78	100	(*3S,4R*)-**1d**$_{O\text{-}ax}$	−5.63 −5.58	97 3
(*3R,4S*)-**1d**$_{O\text{-}eq}$	−5.70	100	(*3S,4R*)-**1d**$_{O\text{-}eq}$	−5.75	100
(*3R,5R*)-**1e**$_{O\text{-}ax}$	−5.90	100	(*3S,5S*)-**1e**$_{O\text{-}ax}$	−5.71 −5.70	1 99
(*3R*)-**1f**$_{O\text{-}ax}$	−6.38	100	(*3S*)-**1f**$_{O\text{-}ax}$	−6.04	100
(*3R*)-**1f**$_{O\text{-}eq}$	−5.87	100	(*3S*)-**1f**$_{O\text{-}eq}$	−6.12	100

Table S4. Estimated lowest Gibbs energy of binding for distinct conformational clusters of ligands (enzyme 1ZMT-**HheC**, rms tolerance for clustering was 0.5 Å) by the docking studies with the AutoDock 4.2 suite of programs. ***O-ax*** and ***O-eq*** stands for the *O*-axial and *O*-equatorial conformer respectively.

Comp. (*3R*)-enantiomers	ΔG / kcal mol^{-1}	Contribution in cluster / %	Comp. (*3S*)-enantiomers	ΔG / kcal mol^{-1}	Contribution in cluster / %
1a	−5.44	100			
1b$_{O\text{-}ax}$	−5.90	100			
1b$_{O\text{-}eq}$	−5.65	100			
1c	−5.64	100			
(*3R,4S*)-**1d**$_{O\text{-}ax}$	−5.48	100	(*3S,4R*)-**1d**$_{O\text{-}ax}$	−5.62	100
(*3R,4S*)-**1d**$_{O\text{-}eq}$	−5.68	100	(*3S,4R*)-**1d**$_{O\text{-}eq}$	−5.54	100
(*3R,5R*)-**1e**$_{O\text{-}ax}$	−6.61	100	(*3S,5S*)-**1e**$_{O\text{-}ax}$	−5.69	100
(*3R*)-**1f**$_{O\text{-}ax}$	−6.78	100	(*3S*)-**1f**$_{O\text{-}ax}$	−5.81	100
(*3R*)-**1f**$_{O\text{-}eq}$	−5.95	100	(*3S*)-**1f**$_{O\text{-}eq}$	−6.36	100

3.2. Overlay of equatorial and axial lowest energy conformers in the active site of HheA for 1d and 1f enantiomers

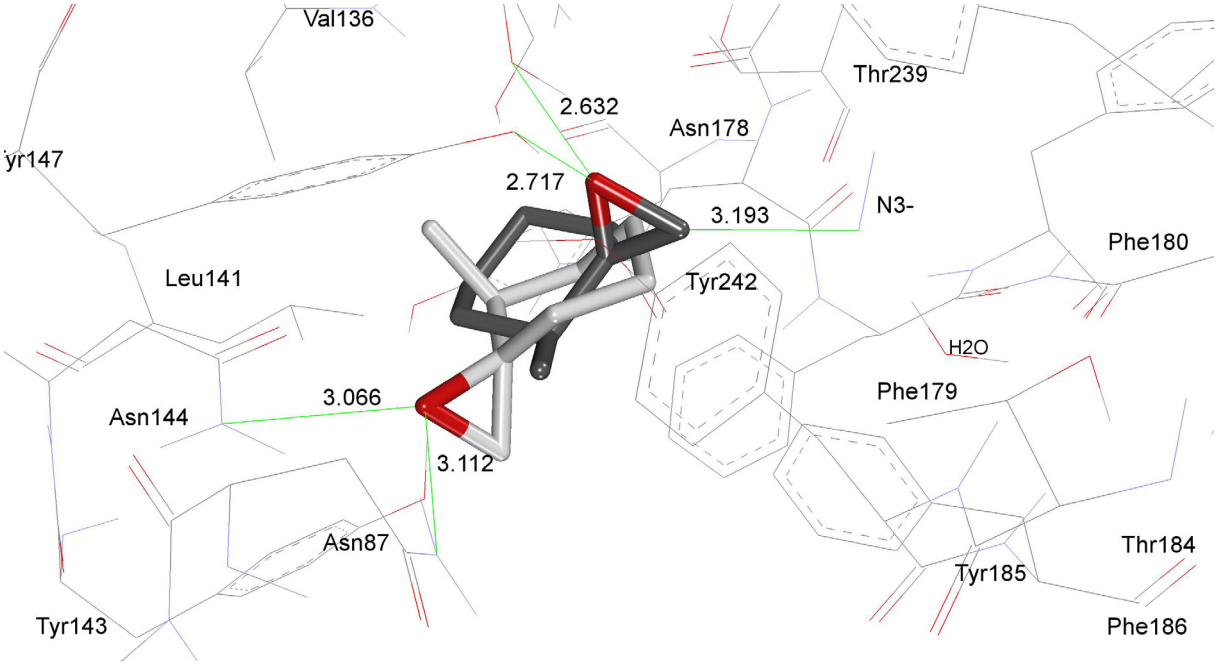


Fig. S4 (3*R*,4*S*)-**1d**-HheA complexes derived from docking studies: overlay of (3*R*,4*S*)-**1d**$_{O\text{-}ax}$ (grey) and (3*R*,4*S*)-**1d**$_{O\text{-}eq}$ (white). HheA active site is represented by some structurally important amino acids. Only polar hydrogen atoms are presented. Interatomic distances are given in Å.

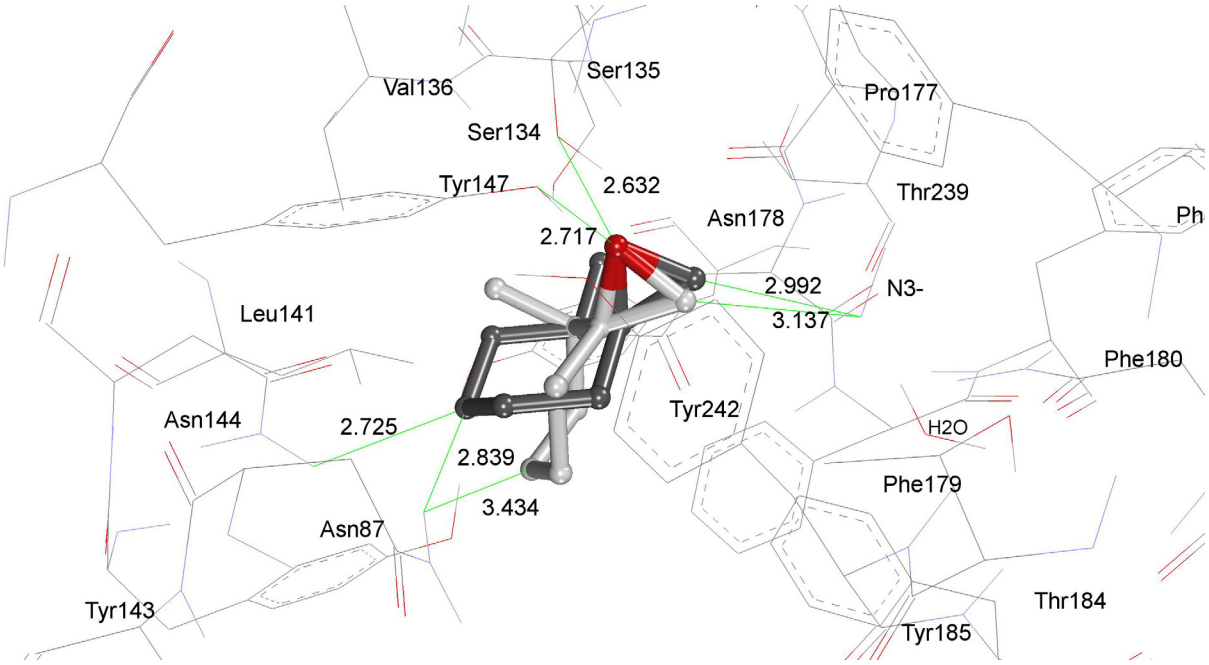


Fig. S5 (3*S*,4*R*)-**1d**-HheA complexes derived from docking studies: overlay of (3*S*,4*R*)-**1d**$_{O\text{-}ax}$ (grey) and (3*S*,4*R*)-**1d**$_{O\text{-}eq}$ (white). HheA active site is represented by some structurally important amino acids. Only polar hydrogen atoms are presented. Interatomic distances are given in Å.

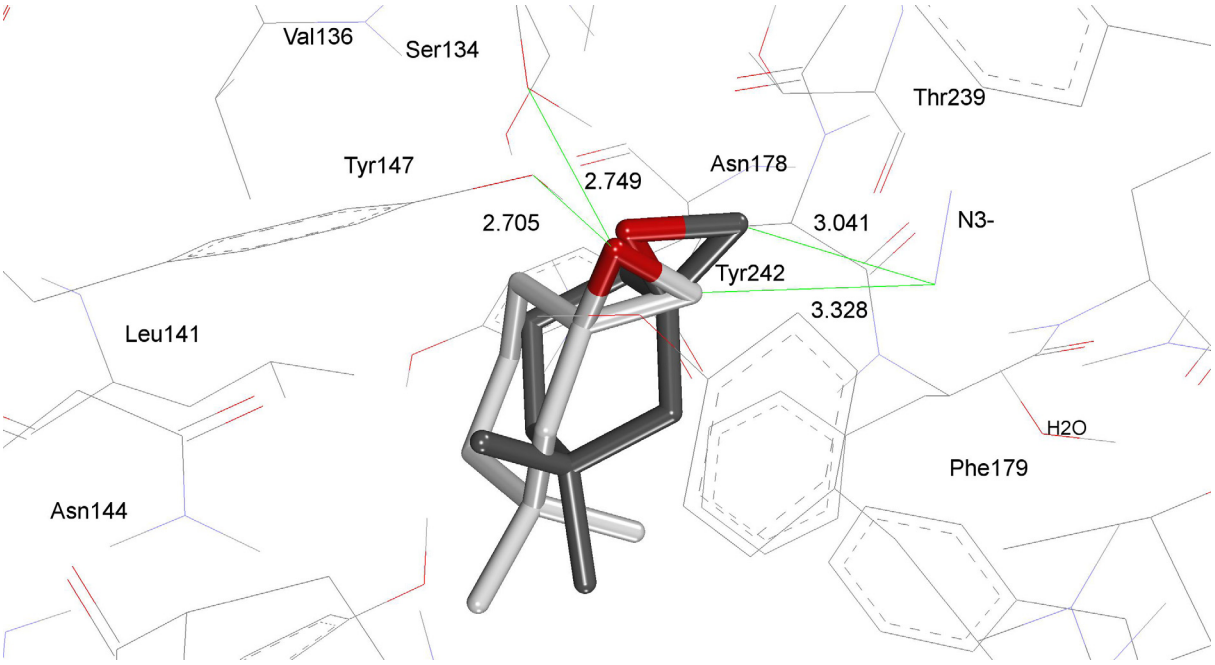


Fig. S6 (*R*)-**1f**-HheA complexes derived from docking studies: overlay of (*R*)-**1f**$_{O\text{-}ax}$ (grey) and (*R*)-**1f**$_{O\text{-}eq}$ (white). HheA active site is represented by some structurally important amino acids. Only polar hydrogen atoms are presented. Interatomic distances are given in Å.

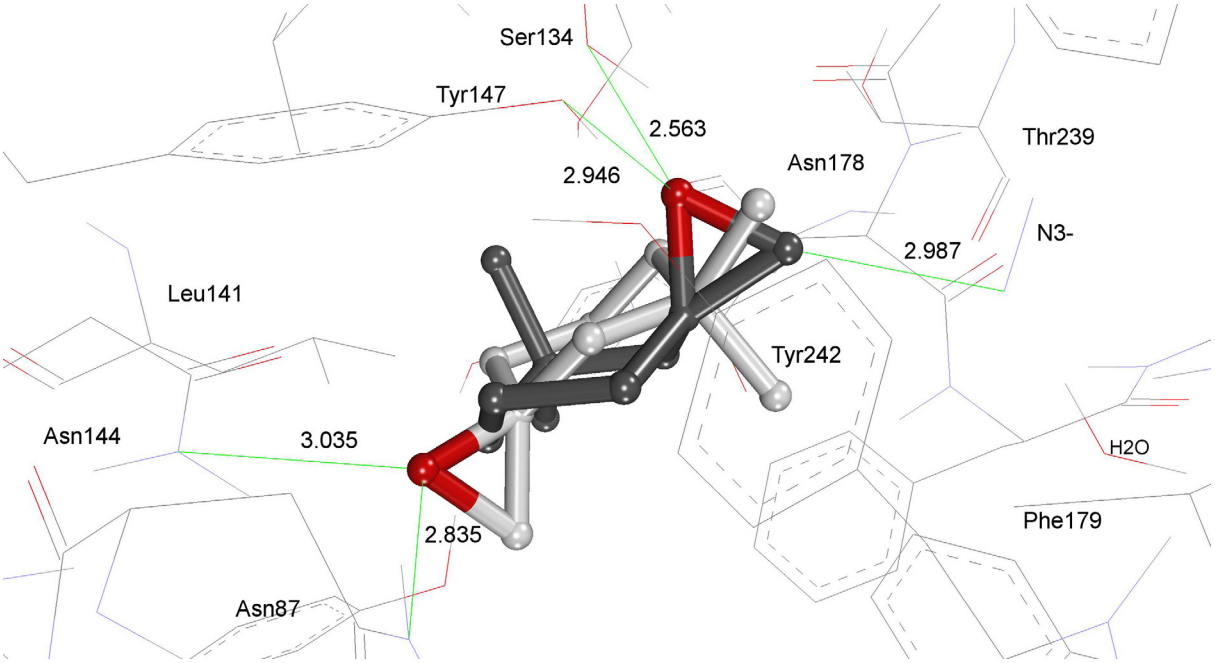


Fig. S7 (*S*)-**1f**-HheA complexes derived from docking studies: overlay of (*S*)-**1f**$_{O\text{-}ax}$ (grey) and (*S*)-**1f**$_{O\text{-}eq}$ (white). HheA active site is represented by some structurally important amino acids. Only polar hydrogen atoms are presented. Interatomic distances are given in Å.

3.3. Overlay of equatorial and axial lowest energy conformers in the active site of HheC for 1d and 1f enantiomers

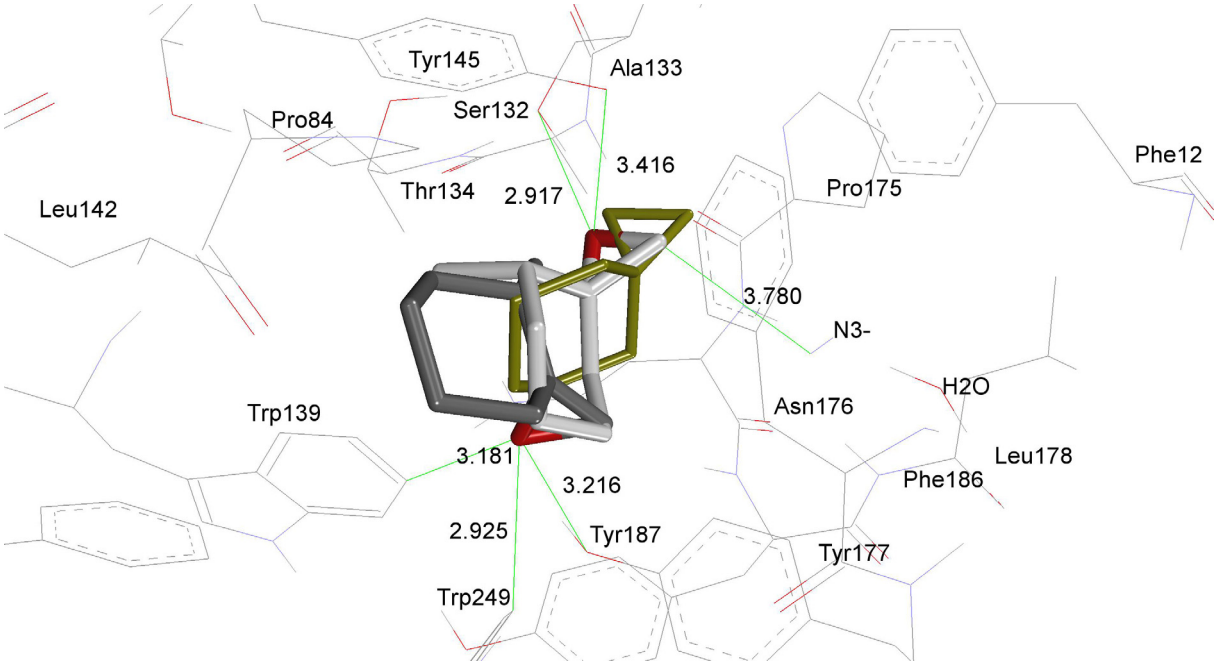


Fig. S8 (3*R*,4*S*)-**1d**-HheC complexes derived from docking studies: overlay of (3*R*,4*S*)-**1d**$_{O\text{-}ax}$ (grey) and (3*R*,4*S*)-**1d**$_{O\text{-}eq}$ (white). HheC active site is represented by some structurally important amino acids. Only polar hydrogen atoms are presented. Interatomic distances are given in Å.

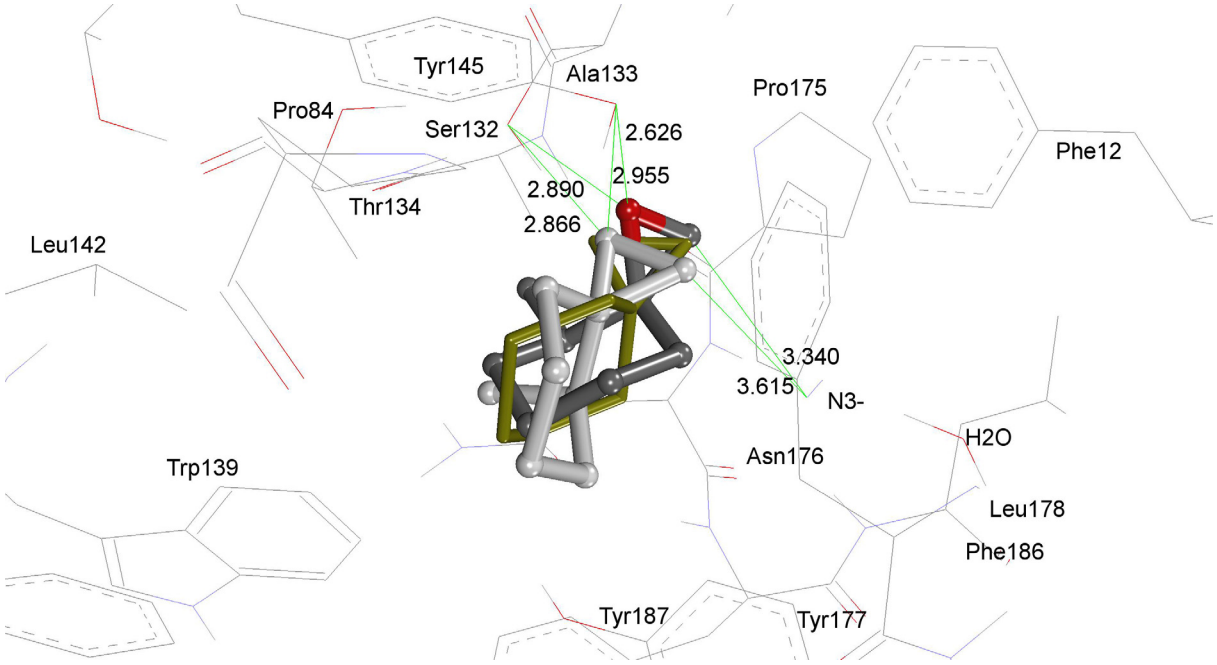


Fig. S9 (3*S*,4*R*)-**1d**-HheC complexes derived from docking studies: overlay of (3*S*,4*R*)-**1d**$_{O\text{-}ax}$ (grey) and (3*S*,4*R*)-**1d**$_{O\text{-}eq}$ (white). HheC active site is represented by some structurally important amino acids. Only polar hydrogen atoms are presented. Interatomic distances are given in Å.

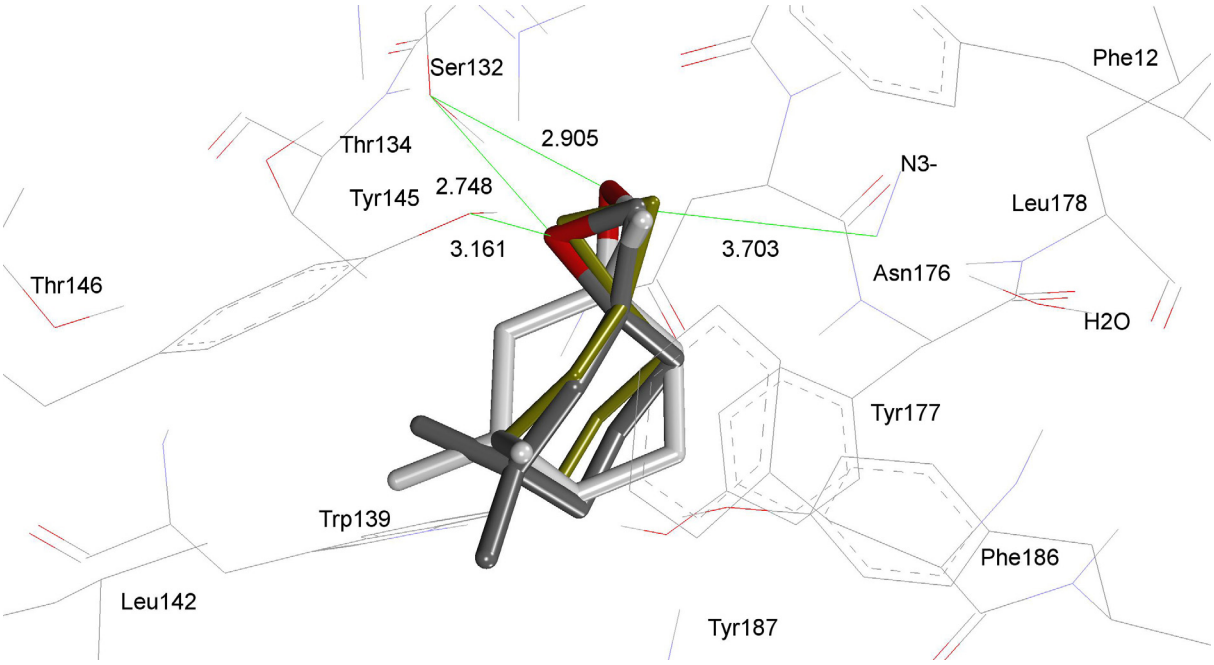


Fig. S10 (*R*)-**1f**-HheC complexes derived from docking studies: overlay of (*R*)-**1f**$_{O\text{-}ax}$ (grey) and (*R*)-**1f**$_{O\text{-}eq}$ (white). HheC active site is represented by some structurally important amino acids. Only polar hydrogen atoms are presented. Interatomic distances are given in Å.

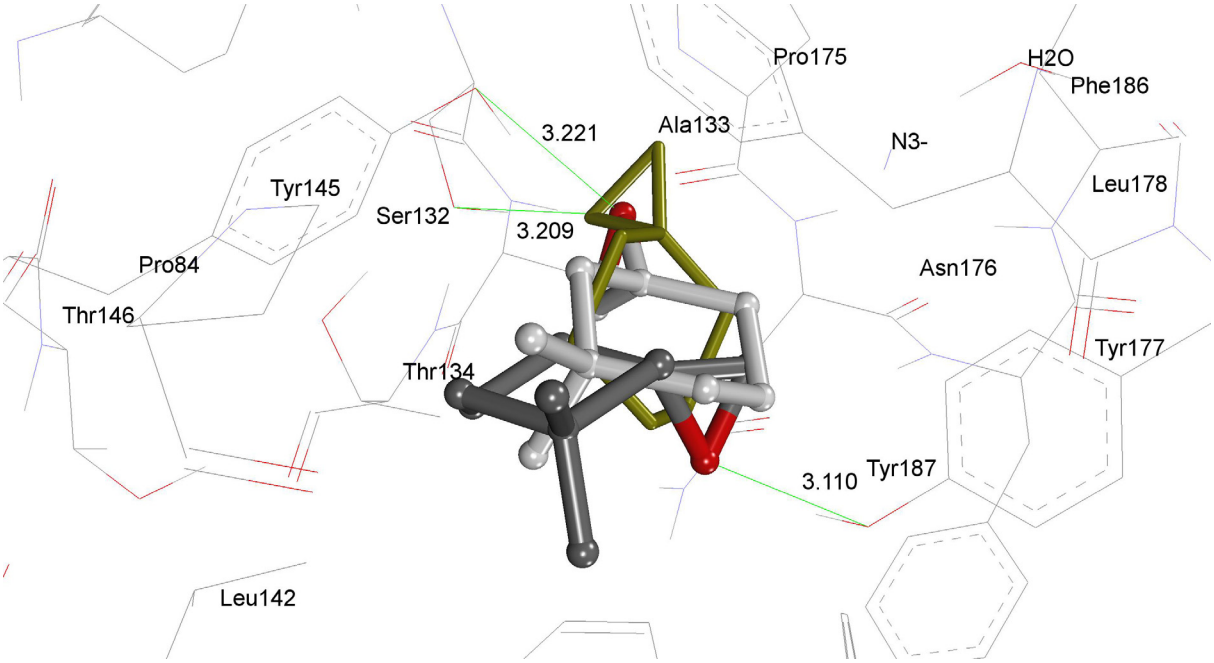
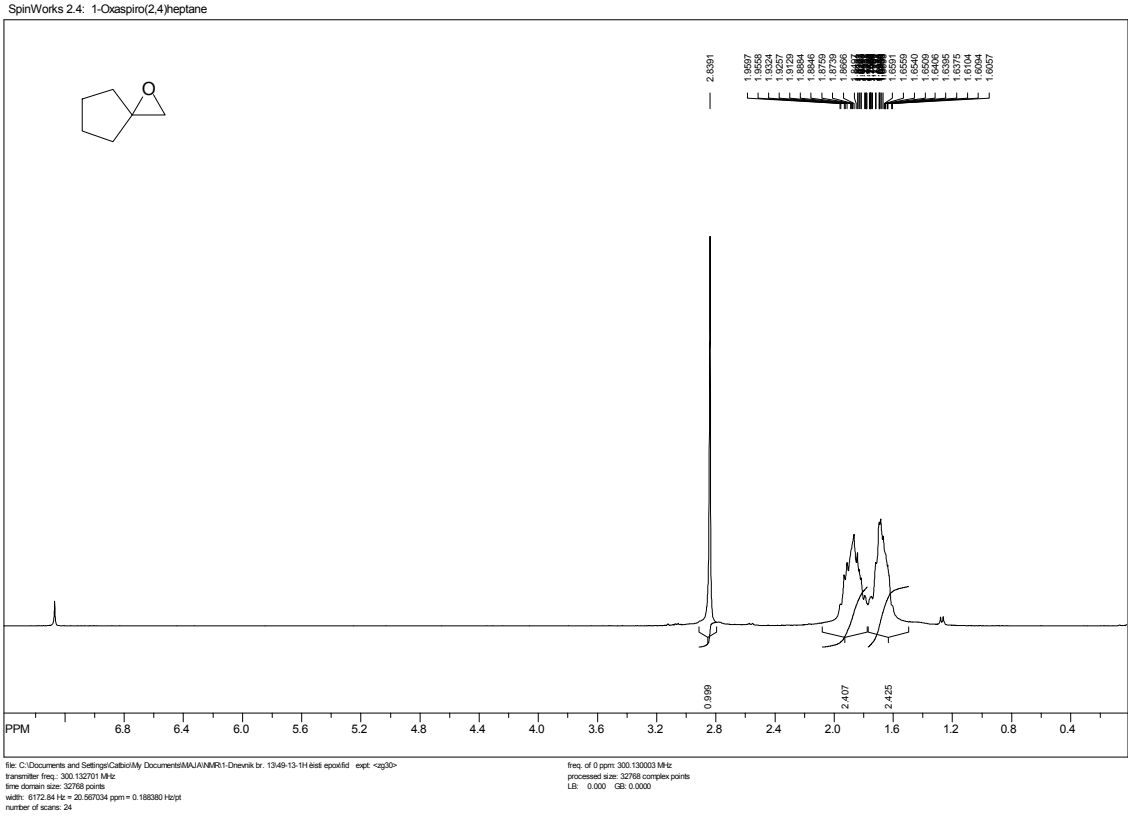
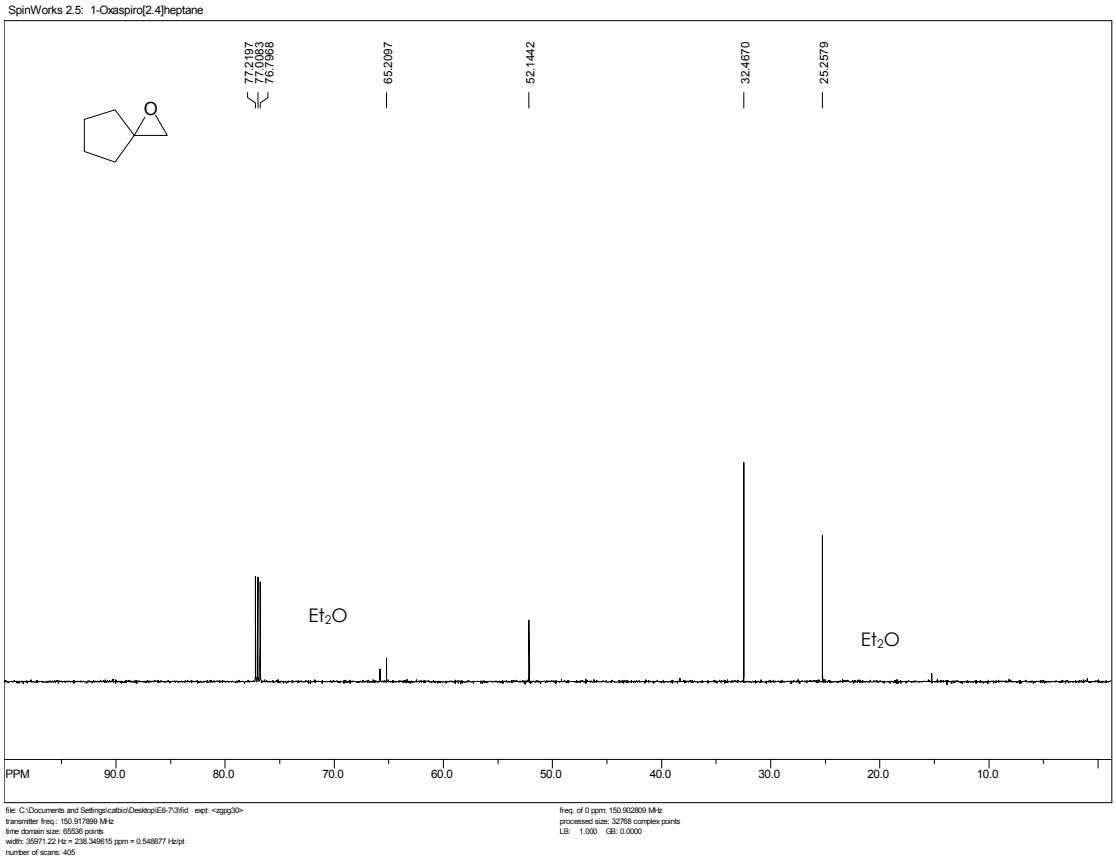


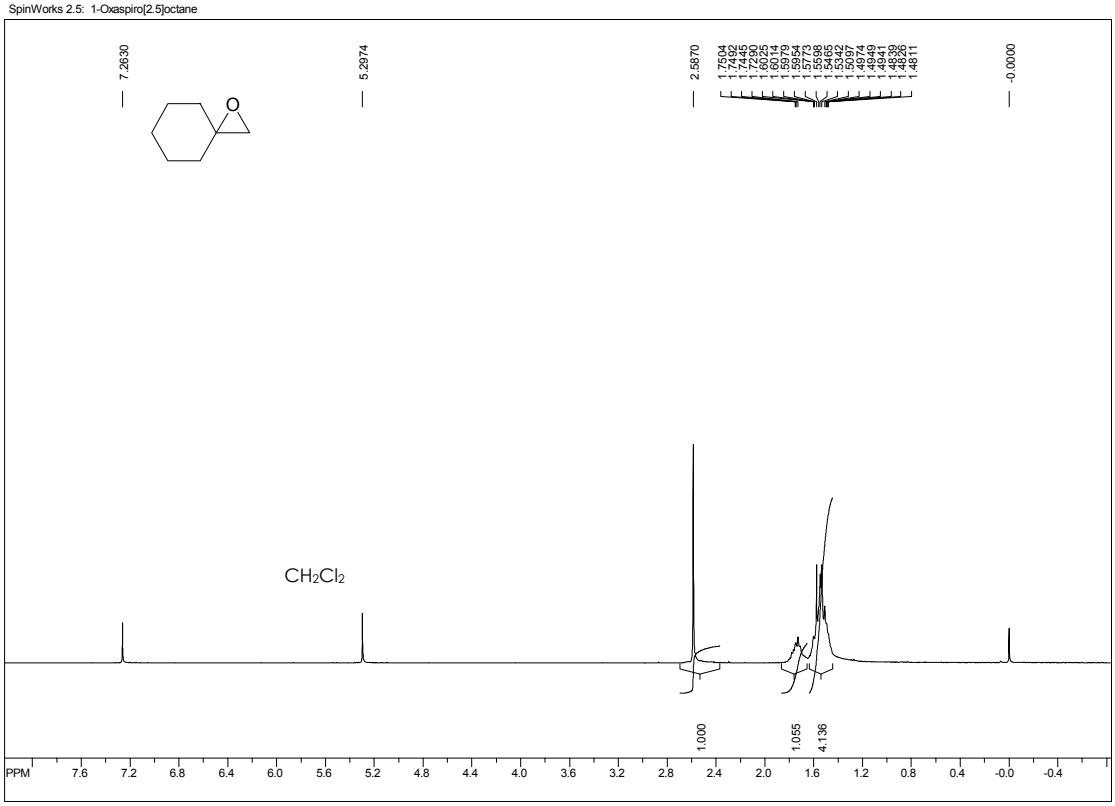
Fig. S11 (*S*)-**1f**-HheC complexes derived from docking studies: overlay of (*S*)-**1f**$_{O\text{-}ax}$ (grey) and (*S*)-**1f**$_{O\text{-}eq}$ (white). HheC active site is represented by some structurally important amino acids. Only polar hydrogen atoms are presented. Interatomic distances are given in Å.

4. NMR spectra





SpinWorks 2.5: 1-Oxaspiro[2.5]octane



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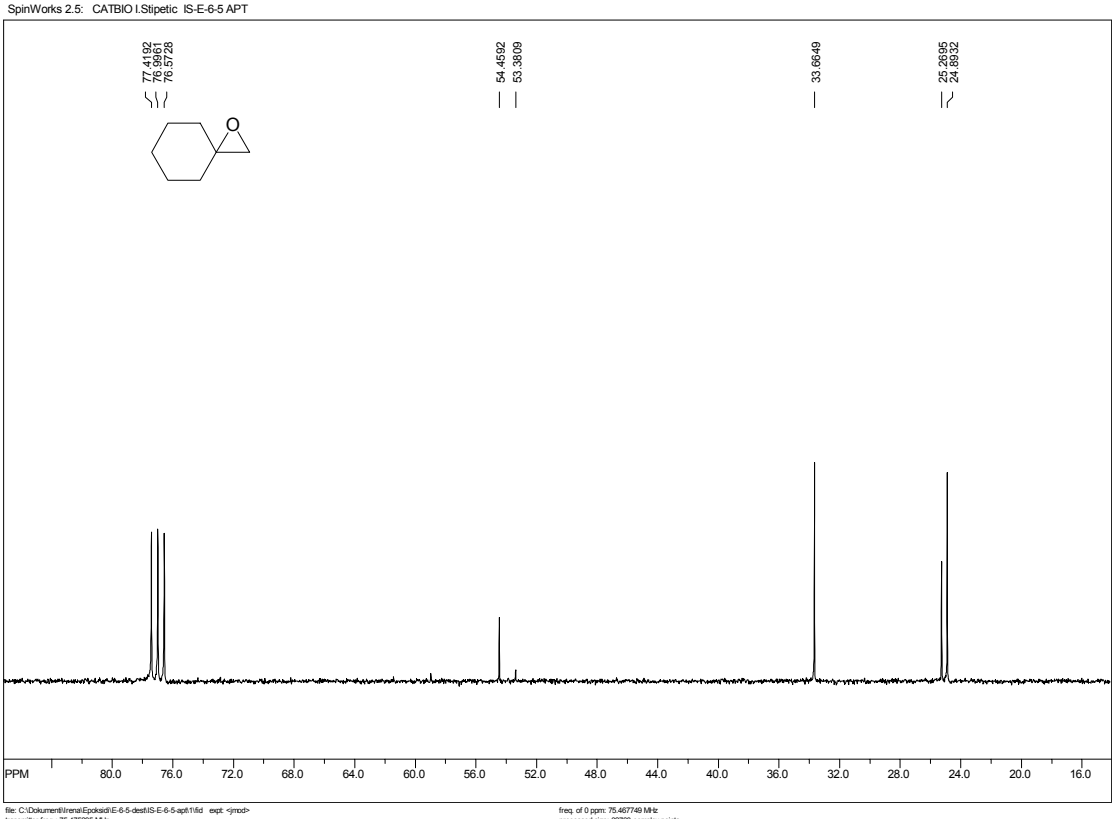

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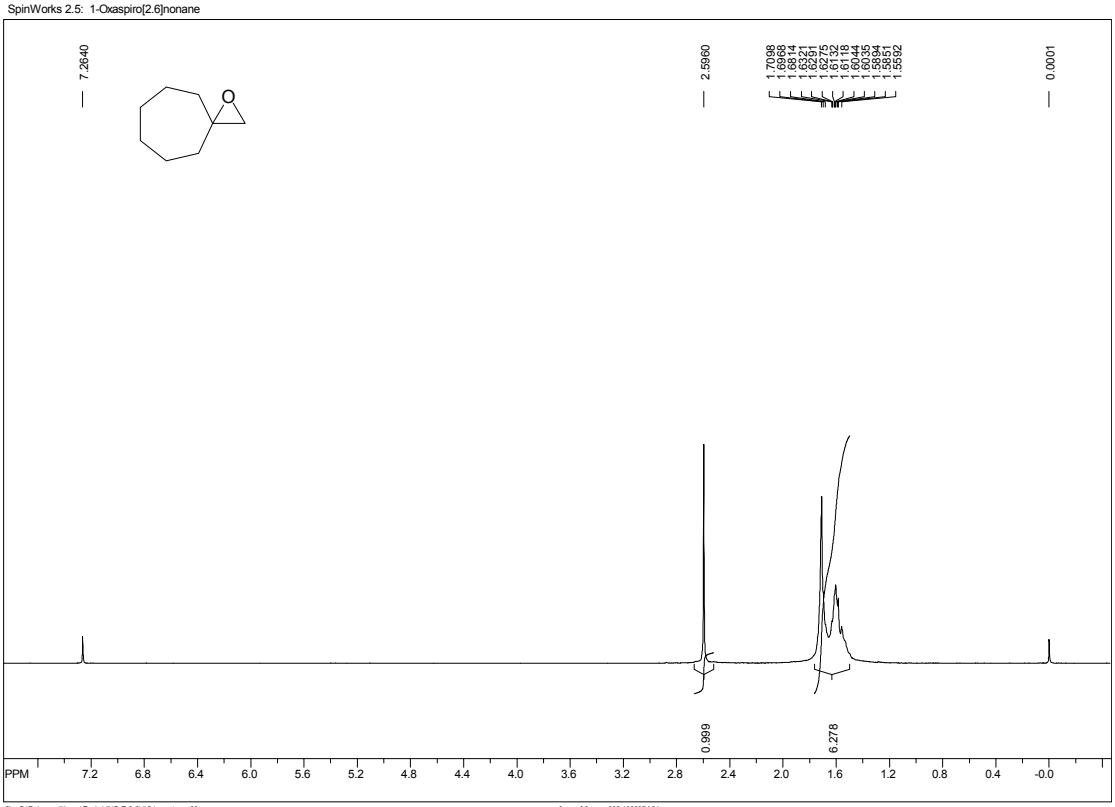
SpinWorks 2.5: 1-Oxaspiro[2.6]nonane



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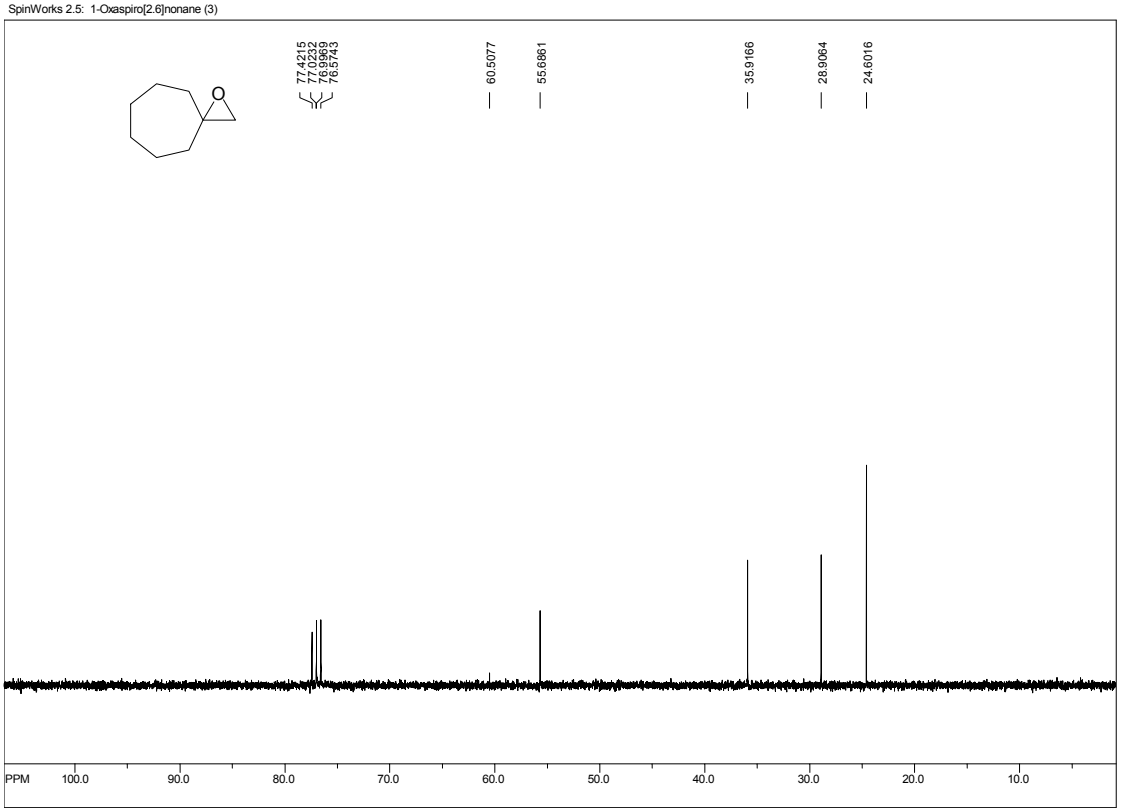

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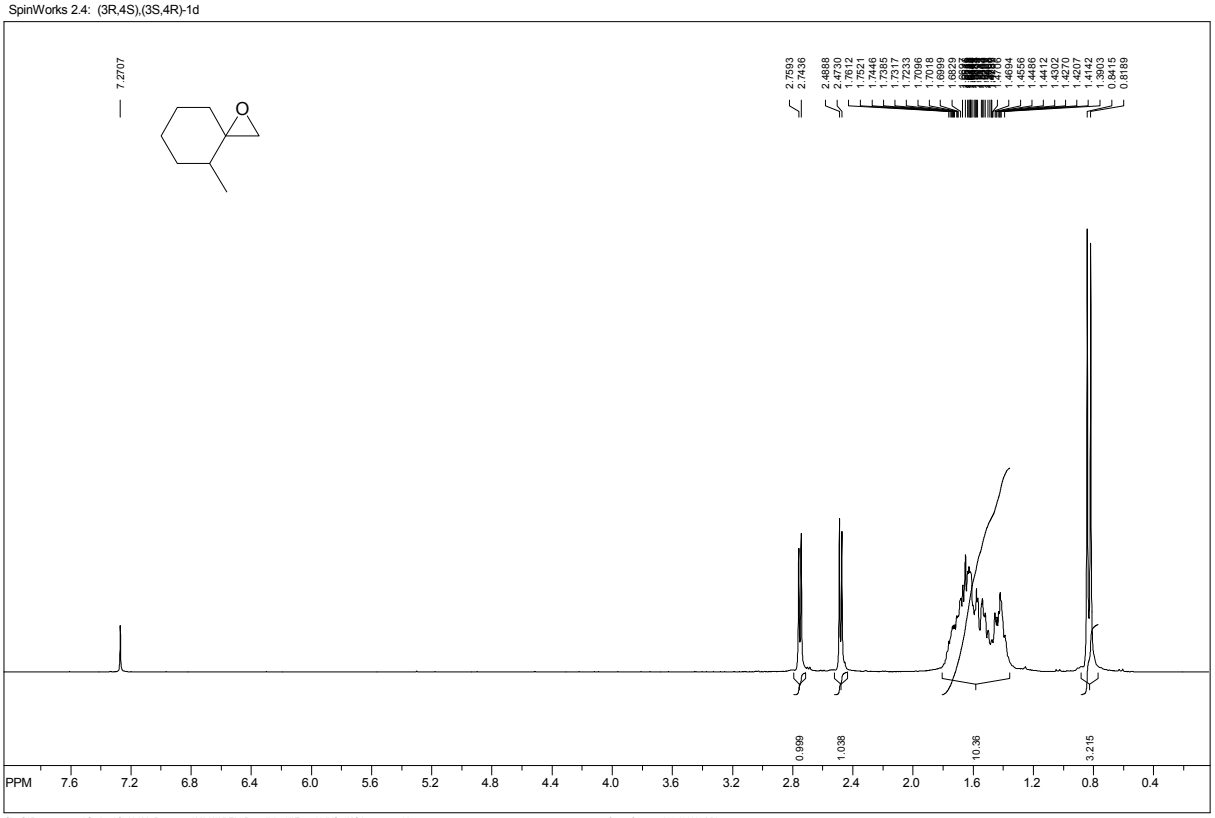

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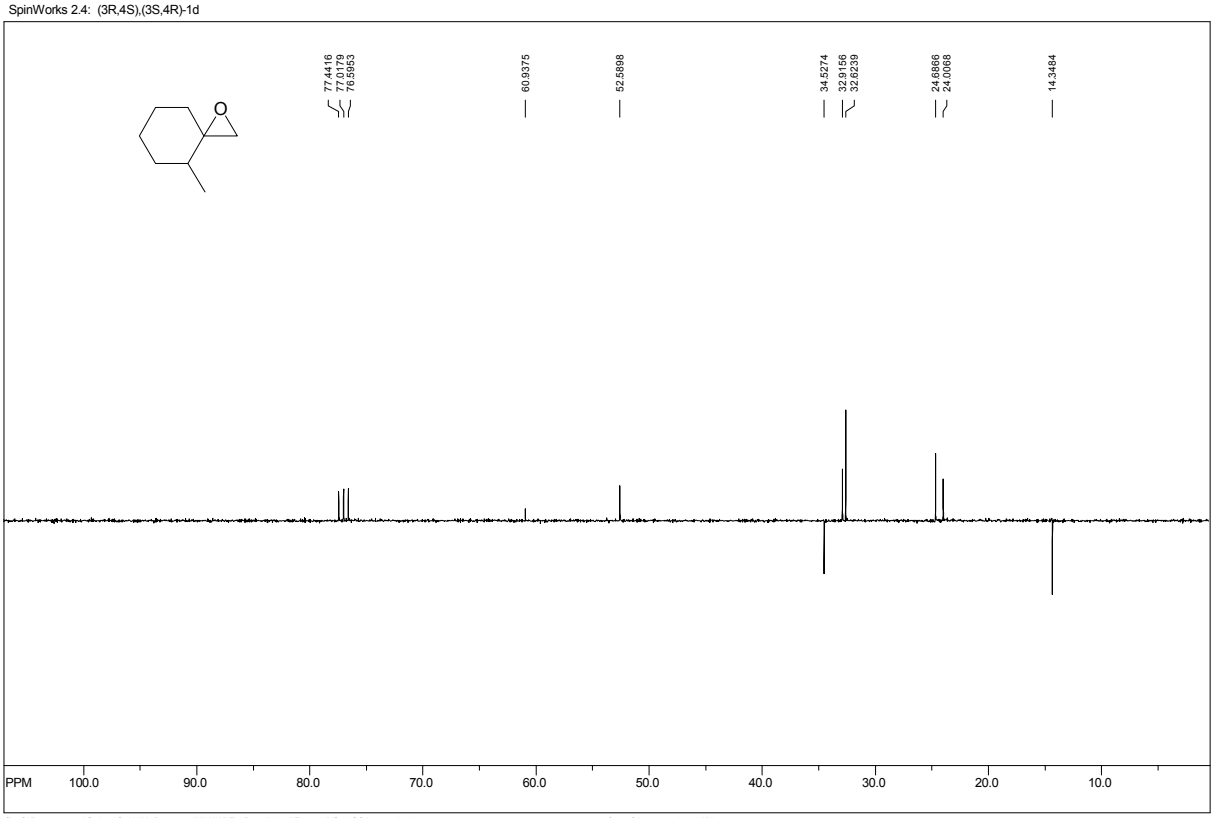

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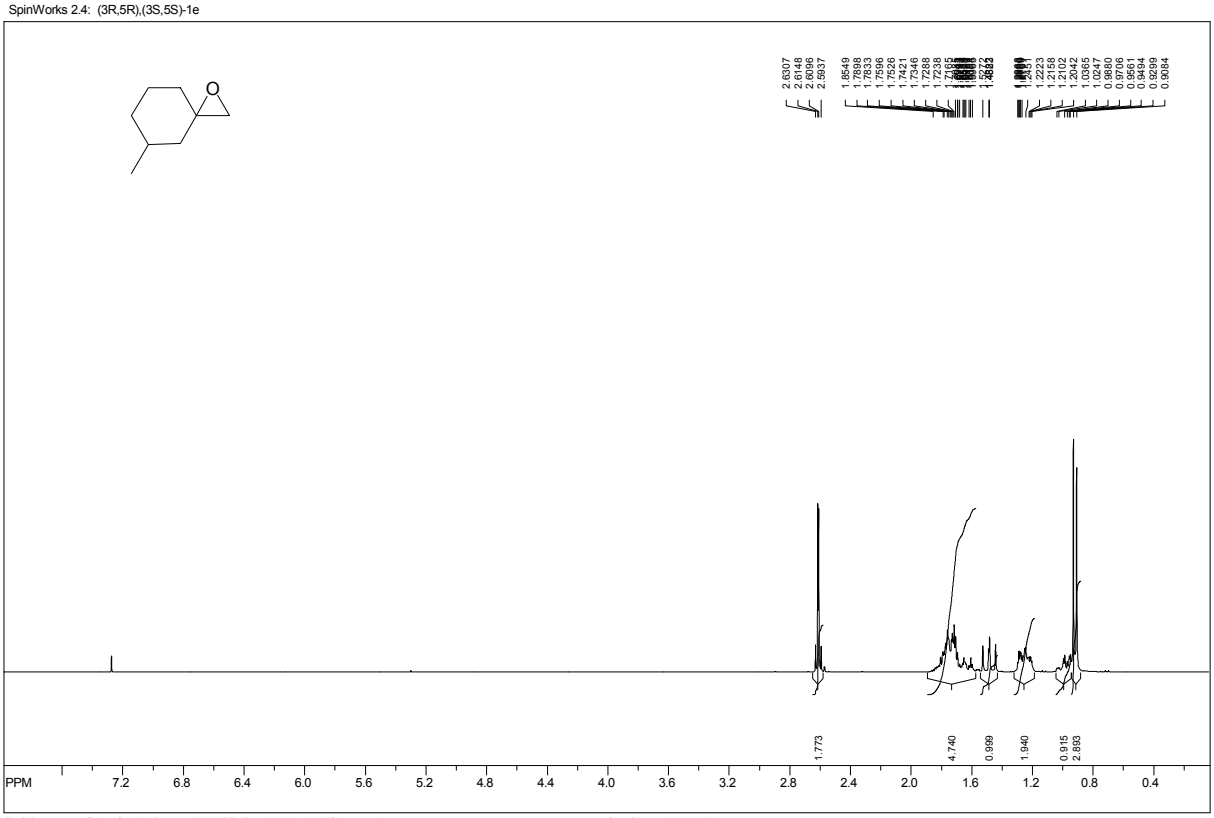

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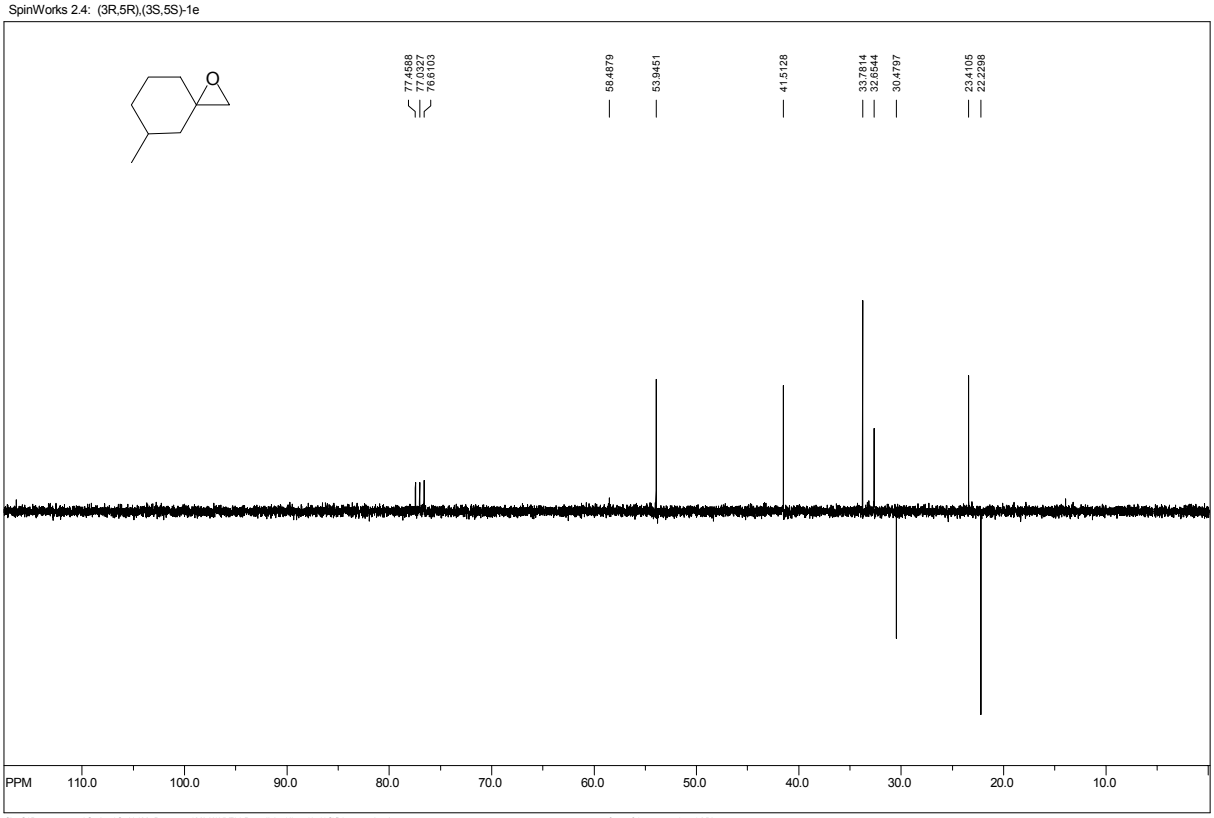

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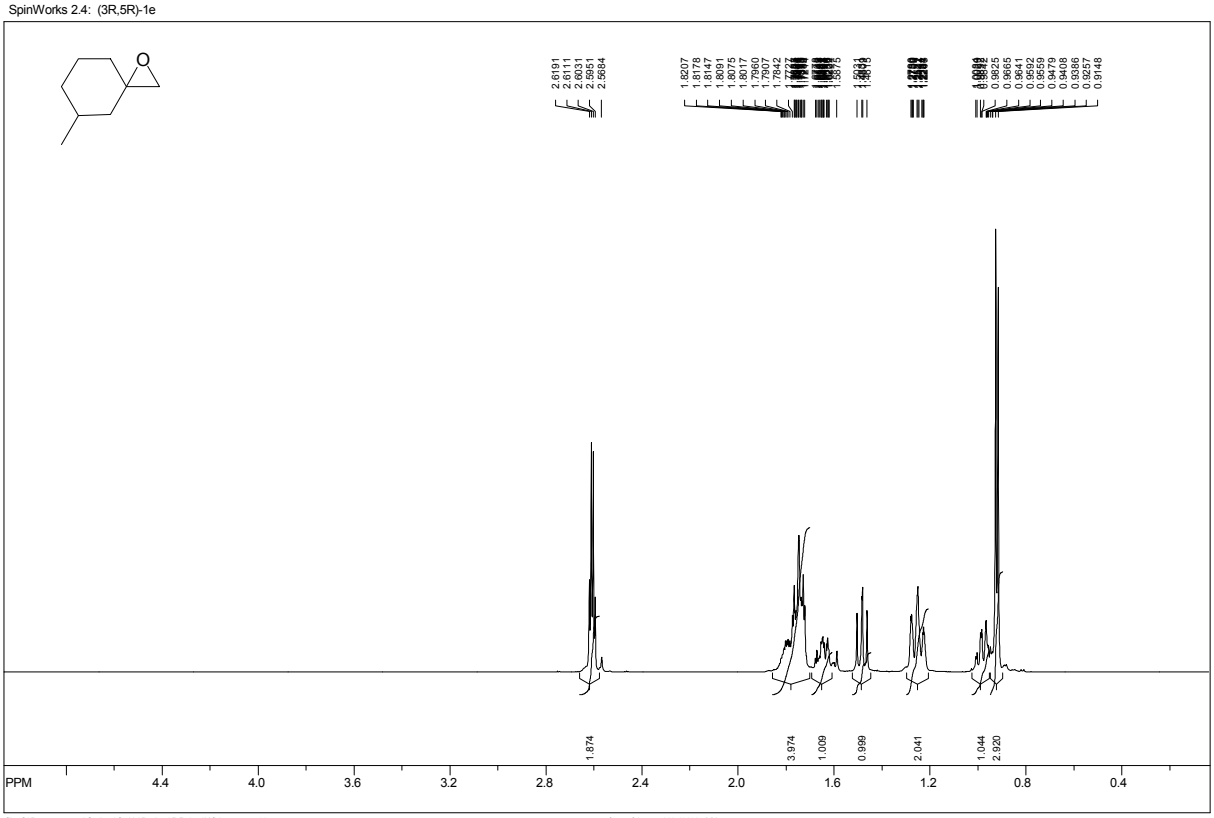

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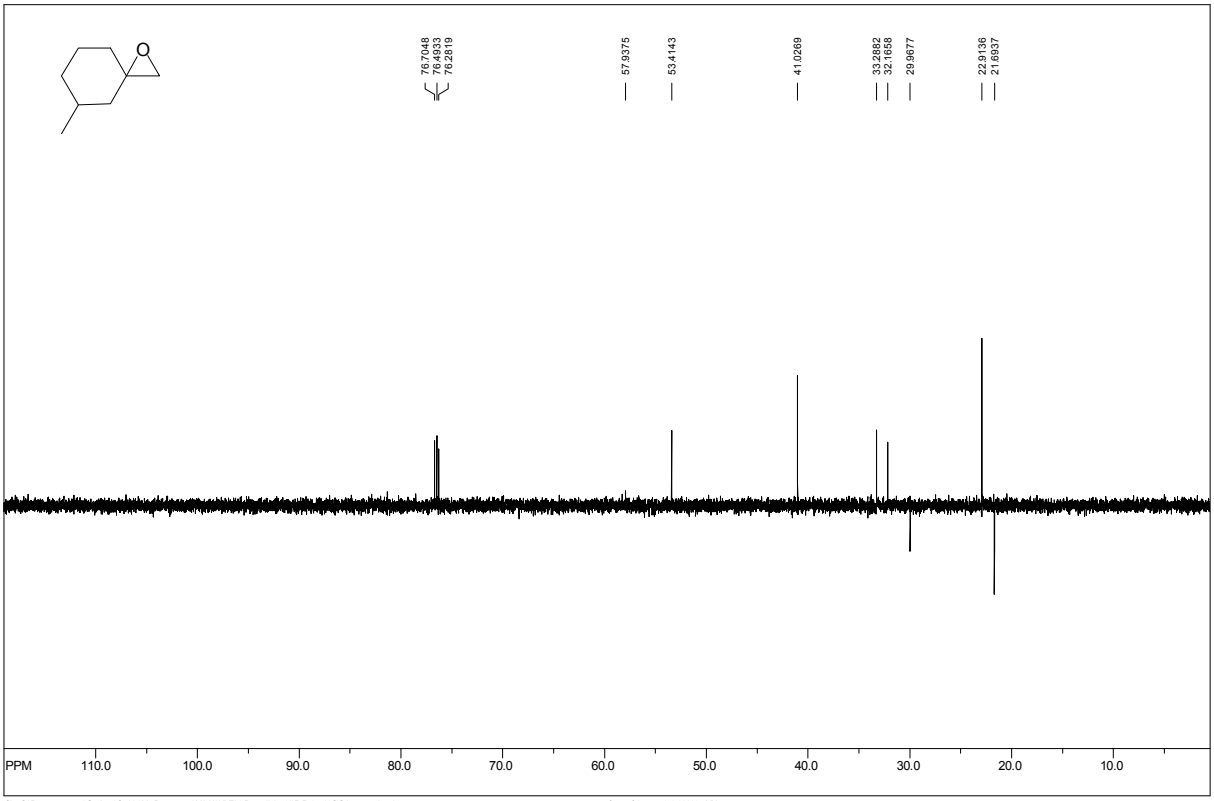

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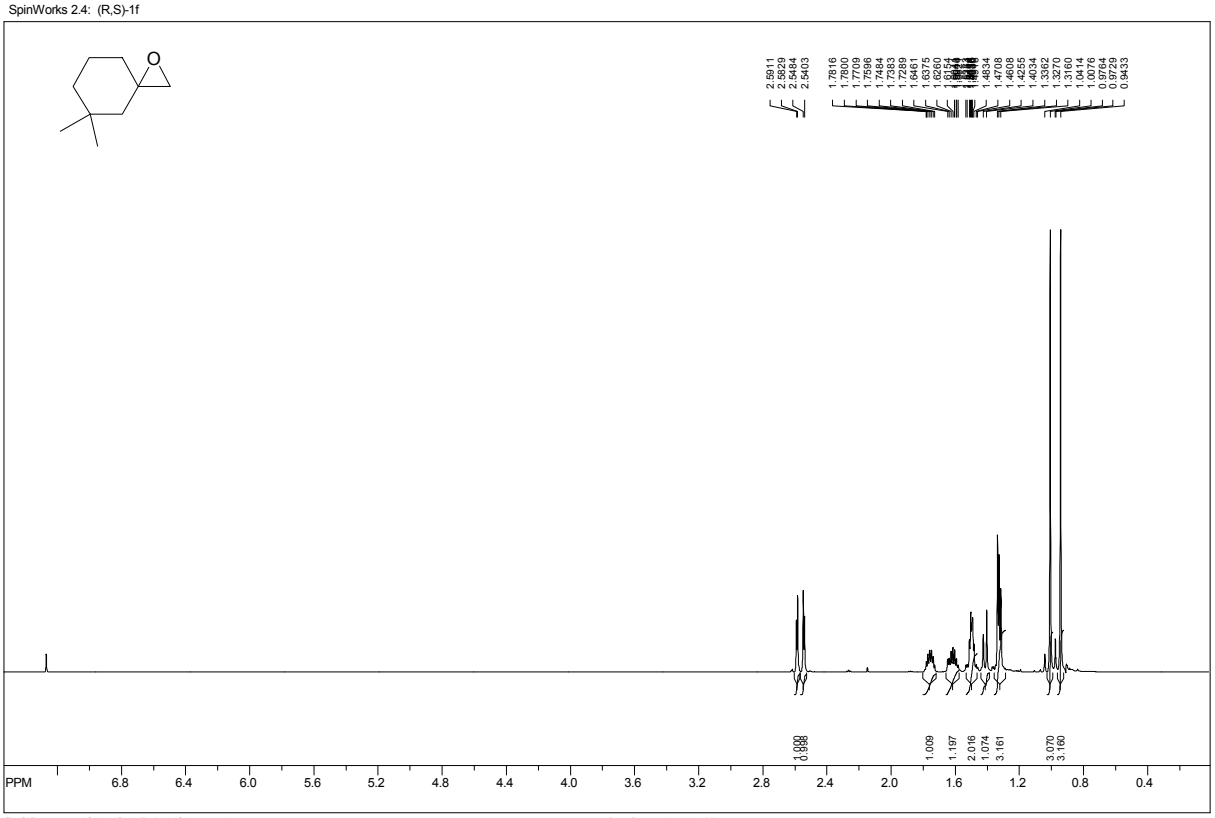

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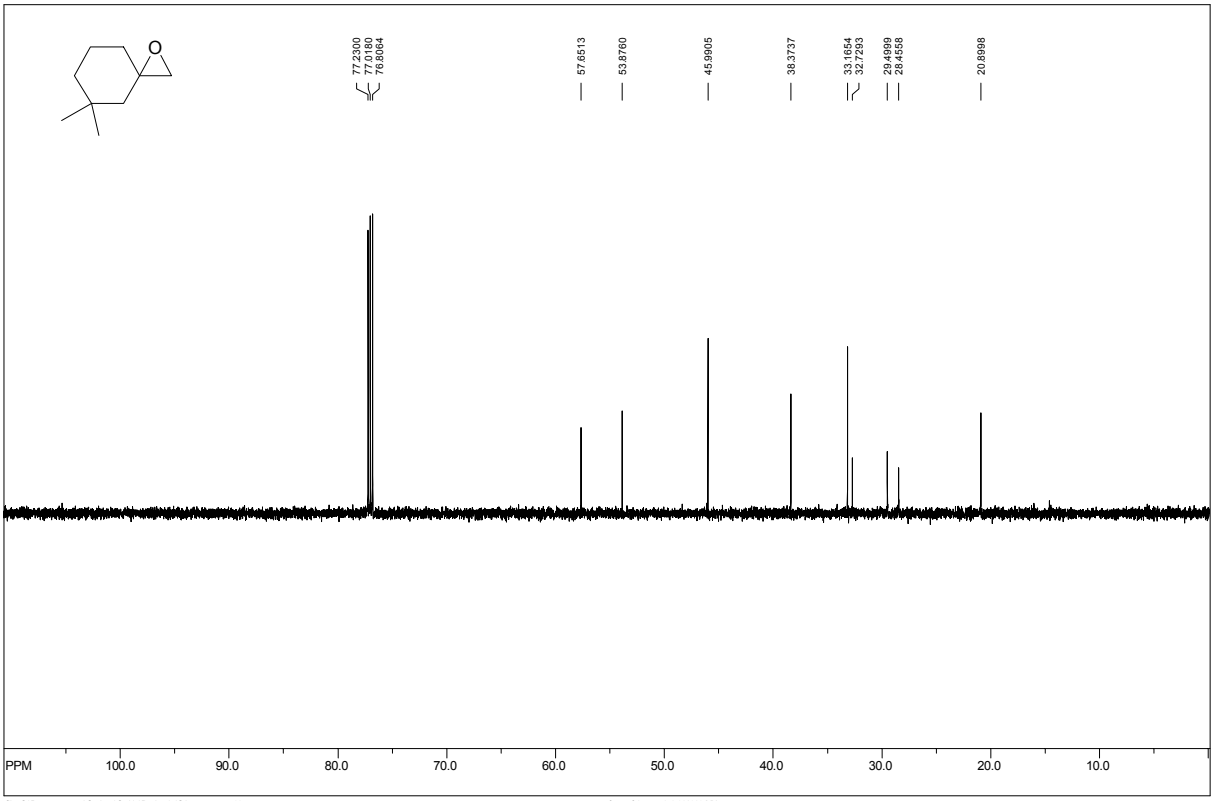
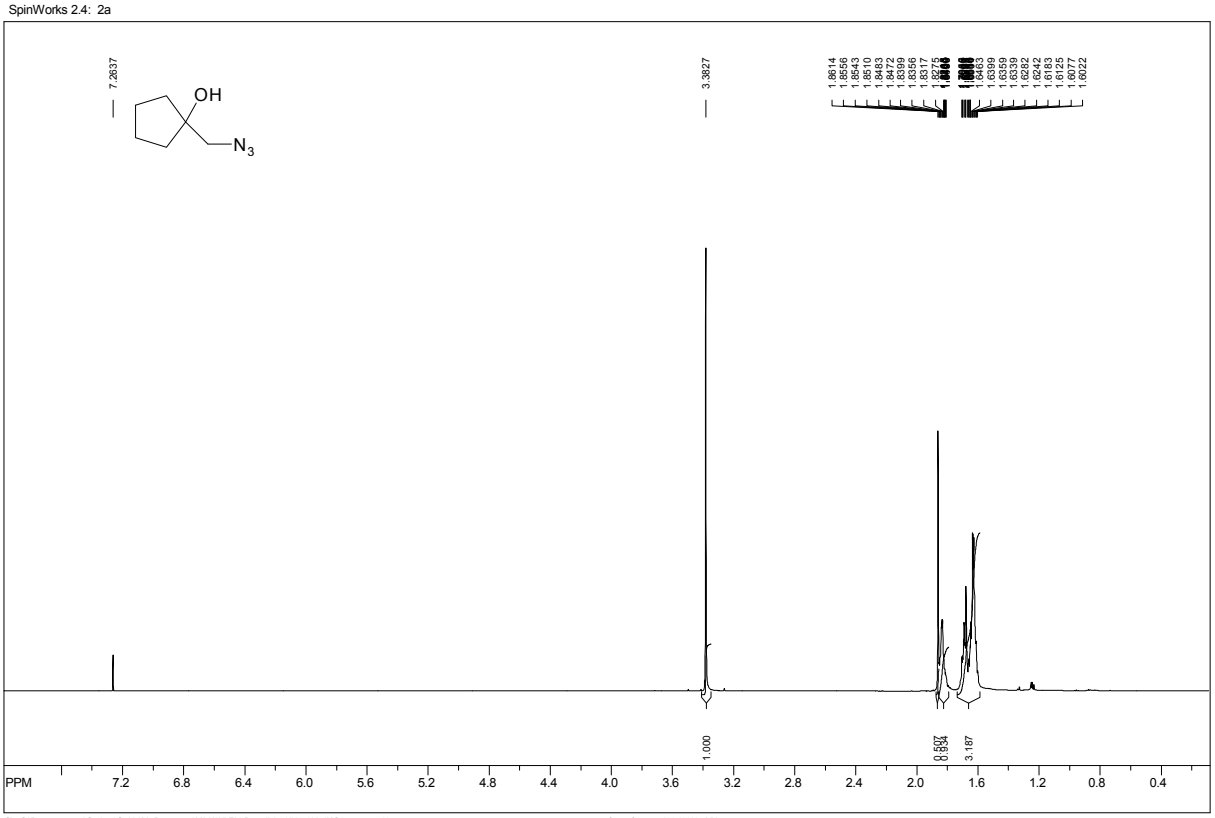
SpinWorks 2.4: (R,S)-1f



file: C:\Documents and Settings\Catbio\Desktop\4\fid expt: <zgpg30>
transmitter freq.: 150.917899 MHz
time domain size: 65536 points
width: 35971.22 Hz = 238.349615 ppm = 0.548877 Hz/pt
number of scans: 168

freq. of 0 ppm: 150.902809 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

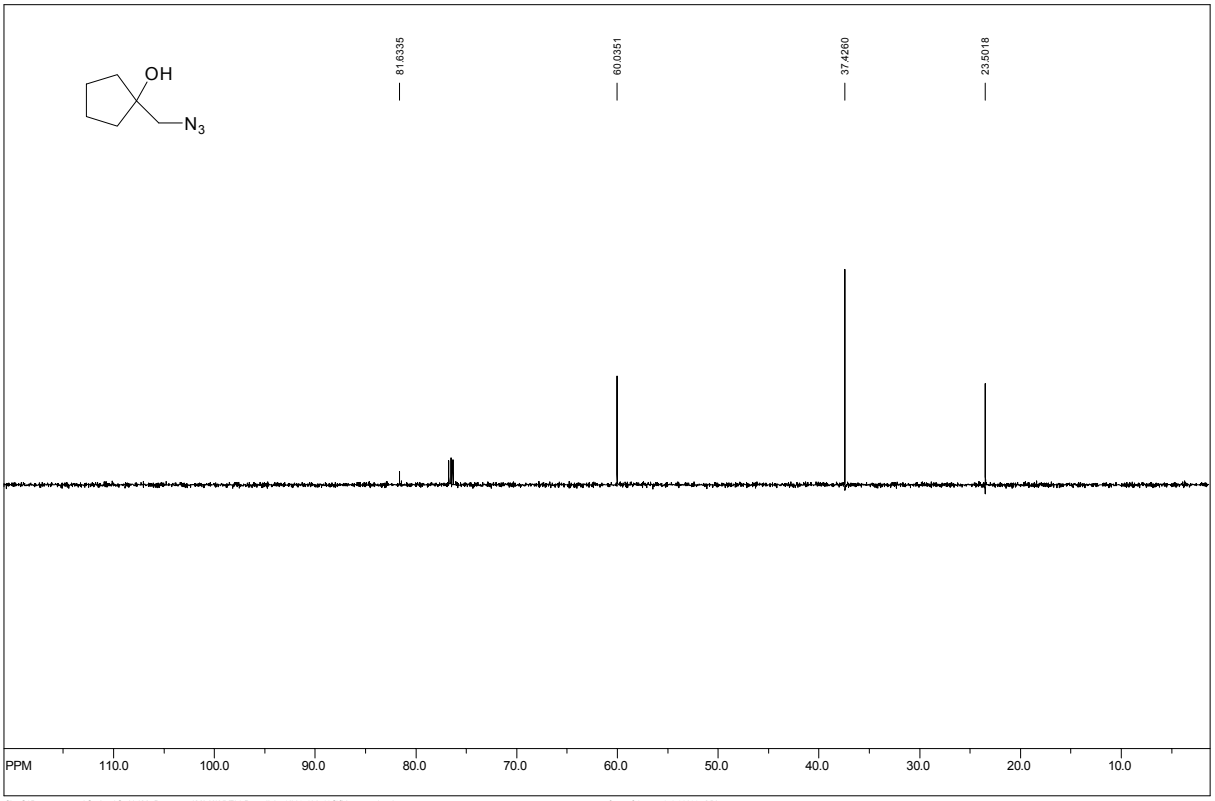
SpinWorks 2.4: 2a



file: C:\Documents and Settings\Catbio\My Documents\MAJA\NMR\1-Dnevnik br 12\28-12A-1H\fid expt: <zg30>
transmitter freq.: 600.133901 MHz
time domain size: 32768 points
width: 9541.98 Hz = 15.899760 ppm = 0.291198 Hz/pt
number of scans: 12

freq. of 0 ppm: 600.130007 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

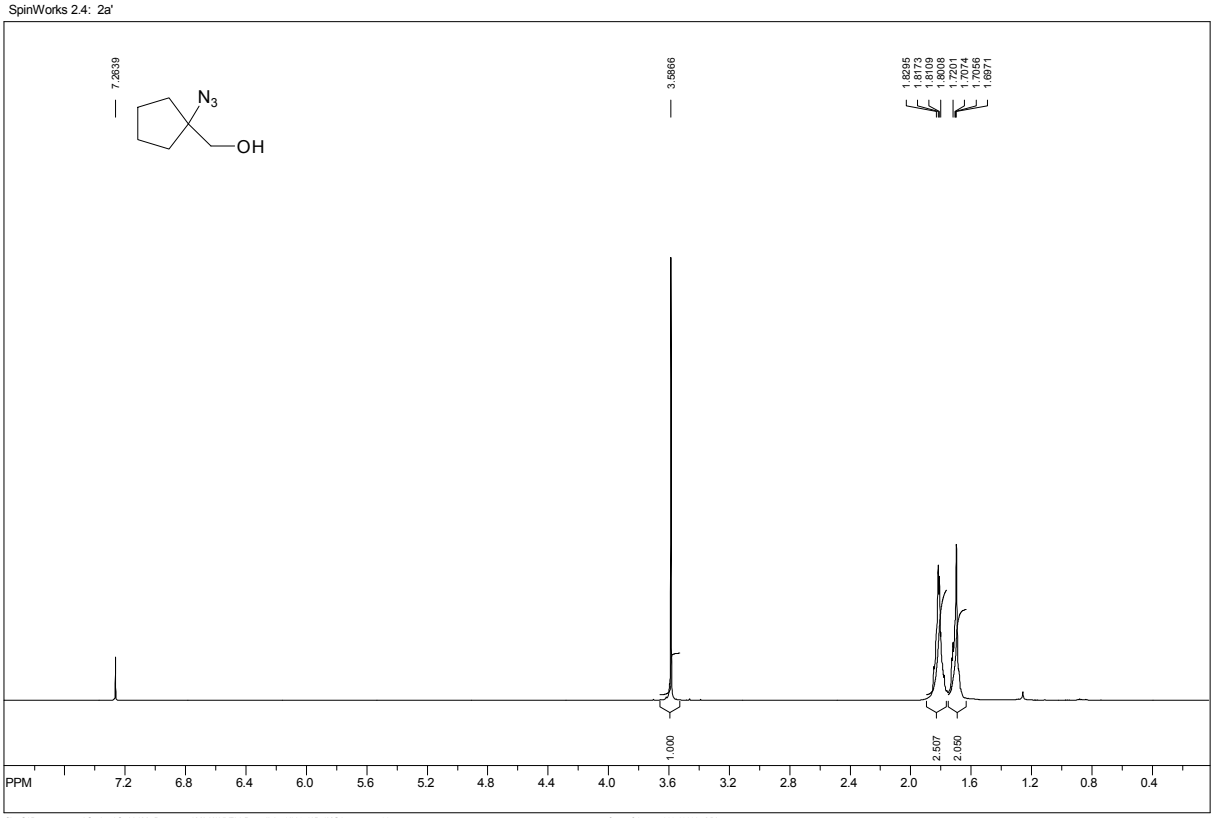
SpinWorks 2.4: 2a



file: C:\Documents and Settings\Catbio\My Documents\MAJA\NMR\1-Dnevnik br 12\28-12A-13C\fid expt: <jmod>
transmitter freq.: 150.917899 MHz
time domain size: 65536 points
width: 35971.22 Hz = 238.349615 ppm = 0.548877 Hz/pt
number of scans: 1233

freq. of 0 ppm: 150.902884 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

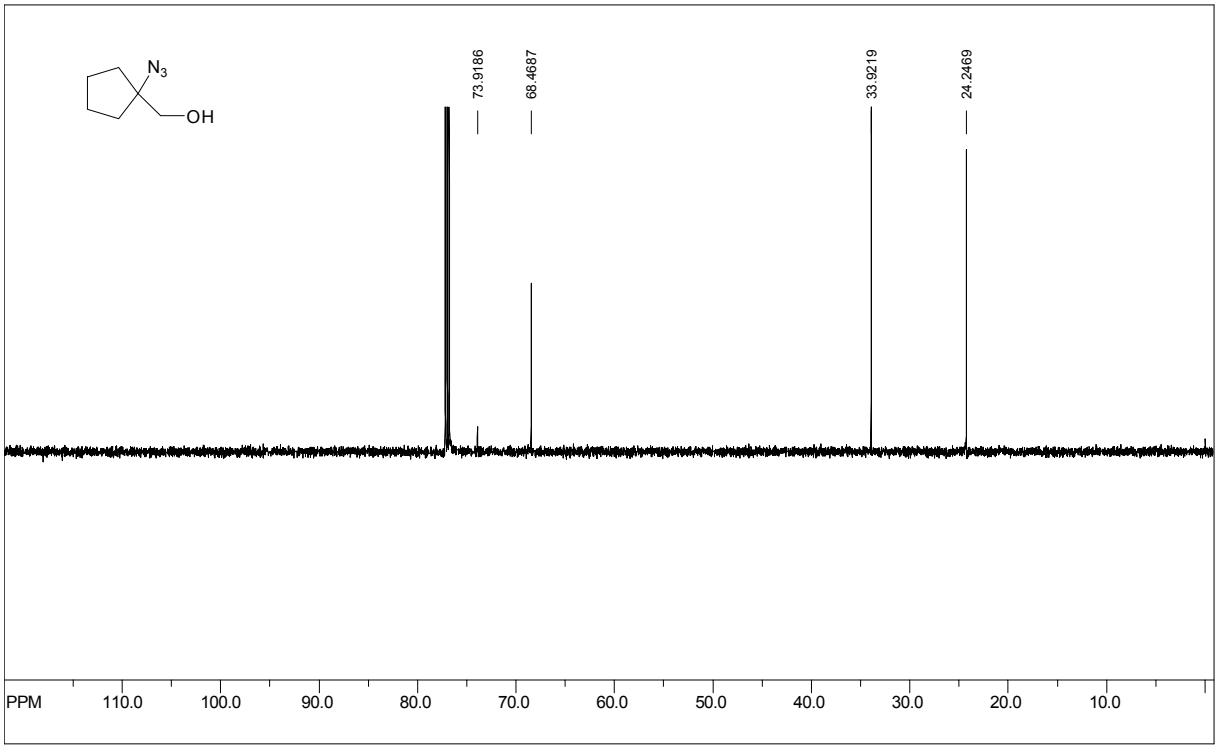
SpinWorks 2.4: 2a'



file: C:\Documents and Settings\Catbio\My Documents\MAJA\NMR\1-Dnevnik br 12\28-12B-1H\fid expt: <zg30>
transmitter freq.: 600.133901 MHz
time domain size: 32768 points
width: 9541.98 Hz = 15.899760 ppm = 0.291198 Hz/pt
number of scans: 12

freq. of 0 ppm: 600.130007 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

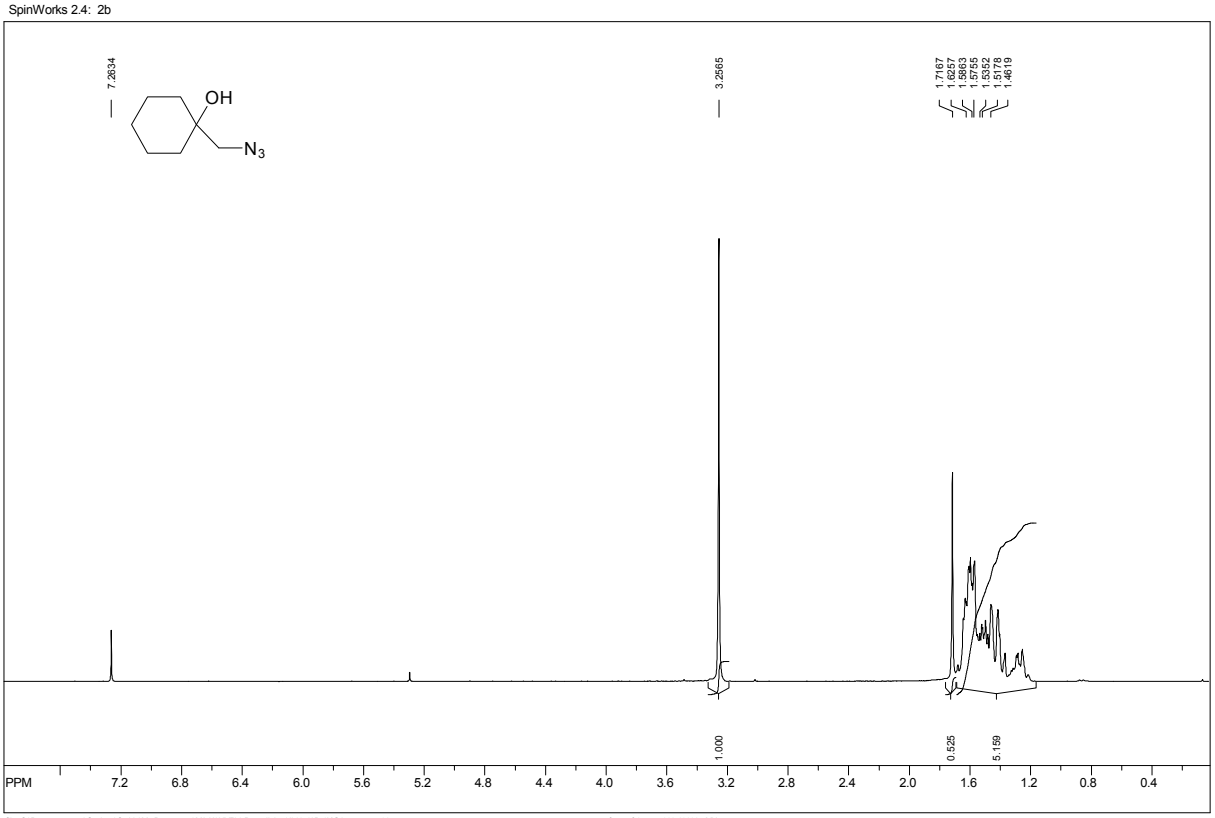
SpinWorks 2.4: Maja 2a*



file: C:\Documents and Settings\Catbio\Desktop\2\fid expt: <zgpg30>
transmitter freq.: 150.917899 MHz
time domain size: 65536 points
width: 35971.22 Hz = 238.349615 ppm = 0.548877 Hz/pt
number of scans: 574

freq. of 0 ppm: 150.902809 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

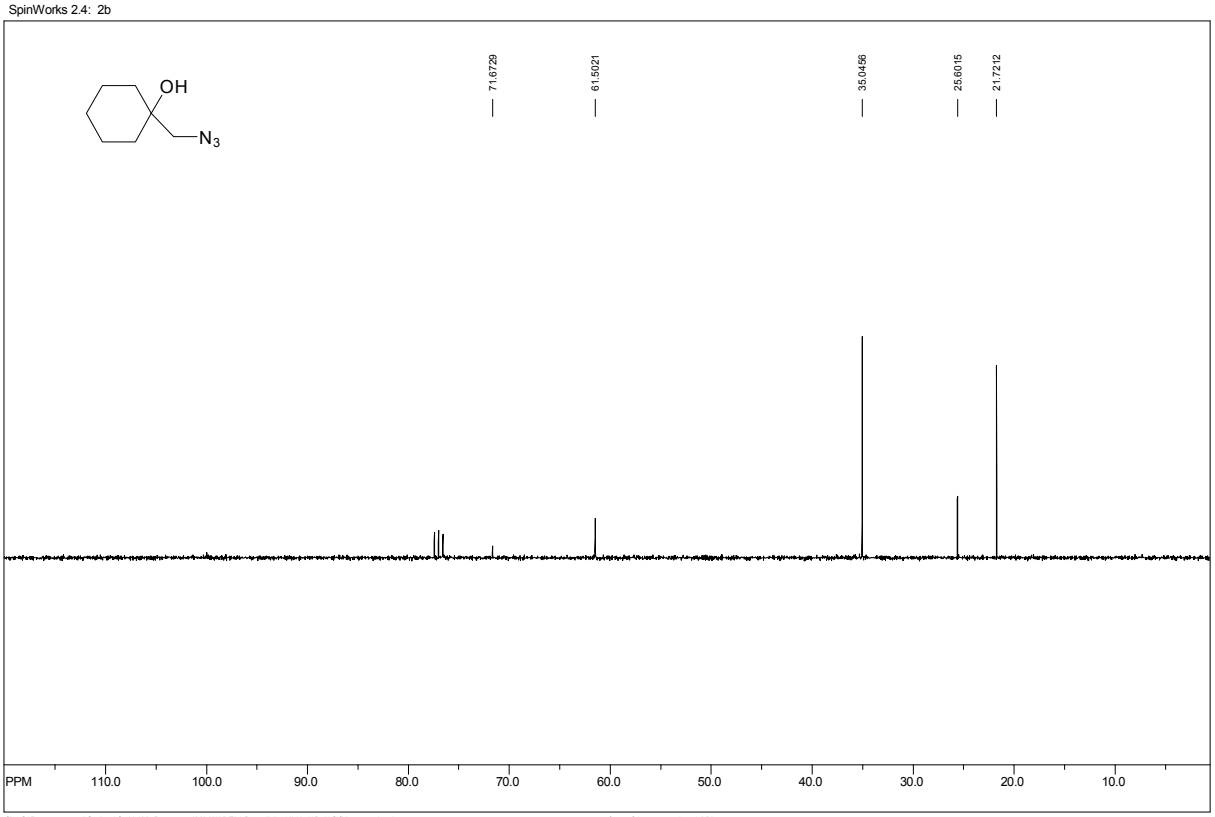
SpinWorks 2.4: 2b



file: C:\Documents and Settings\Catbio\My Documents\MAJA\NMR\1-Dnevnik br 12\10-12B-1H\fid expt: <zg30>
transmitter freq.: 300.131853 MHz
time domain size: 32768 points
width: 6172.84 Hz = 20.567092 ppm = 0.188380 Hz/pt
number of scans: 16

freq. of 0 ppm: 300.130005 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

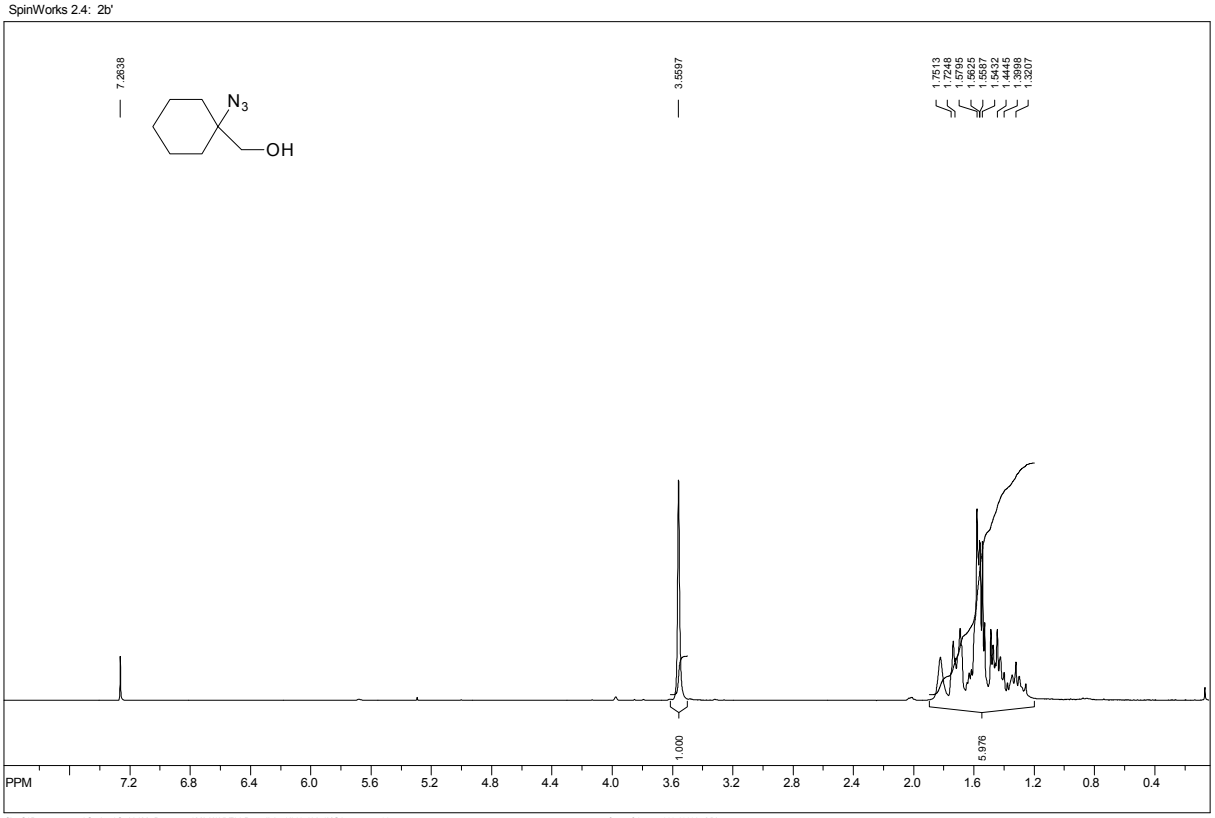
SpinWorks 2.4: 2b



file: C:\Documents and Settings\Catbio\My Documents\MAJA\NMR\1-Dnevnik br 12\10-12B-13C\fid expt: <jmod>
transmitter freq.: 75.475295 MHz
time domain size: 65536 points
width: 17985.61 Hz = 238.297995 ppm = 0.274439 Hz/pt
number of scans: 794

freq. of 0 ppm: 75.467749 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

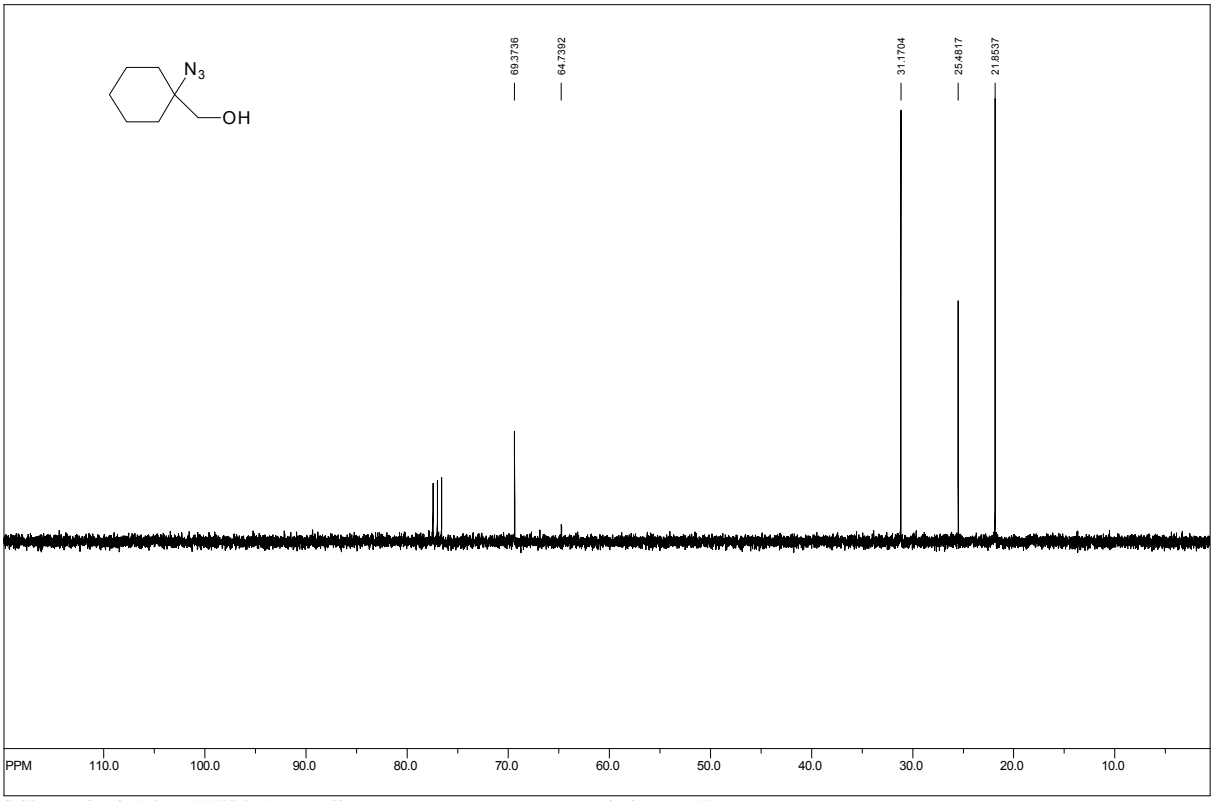
SpinWorks 2.4: 2b'



file: C:\Documents and Settings\Catbio\My Documents\MAJA\NMR\1-Dnevnik br 12\10-12A-1H\fid expt: <zg30>
transmitter freq.: 300.131853 MHz
time domain size: 32768 points
width: 6172.84 Hz = 20.567092 ppm = 0.188380 Hz/pt
number of scans: 24

freq. of 0 ppm: 300.130005 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

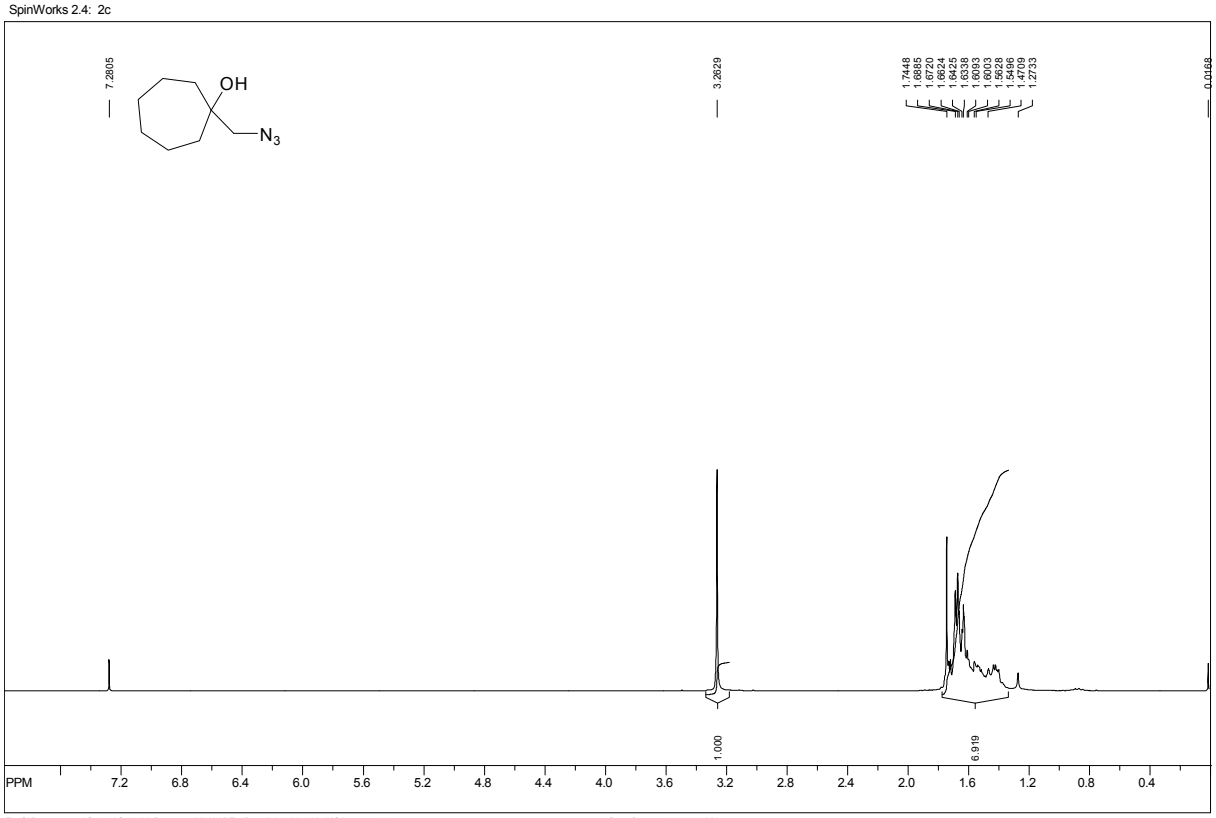
SpinWorks 2.4: 2b'



file: C:\Documents and Settings\Catbio\My Documents\MAJA\NMR\1-Dnevnik br 12\10-12A-13C\fid expt: <jmod>
transmitter freq.: 75.475295 MHz
time domain size: 65536 points
width: 17985.61 Hz = 238.297995 ppm = 0.274439 Hz/pt
number of scans: 425

freq. of 0 ppm: 75.467749 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

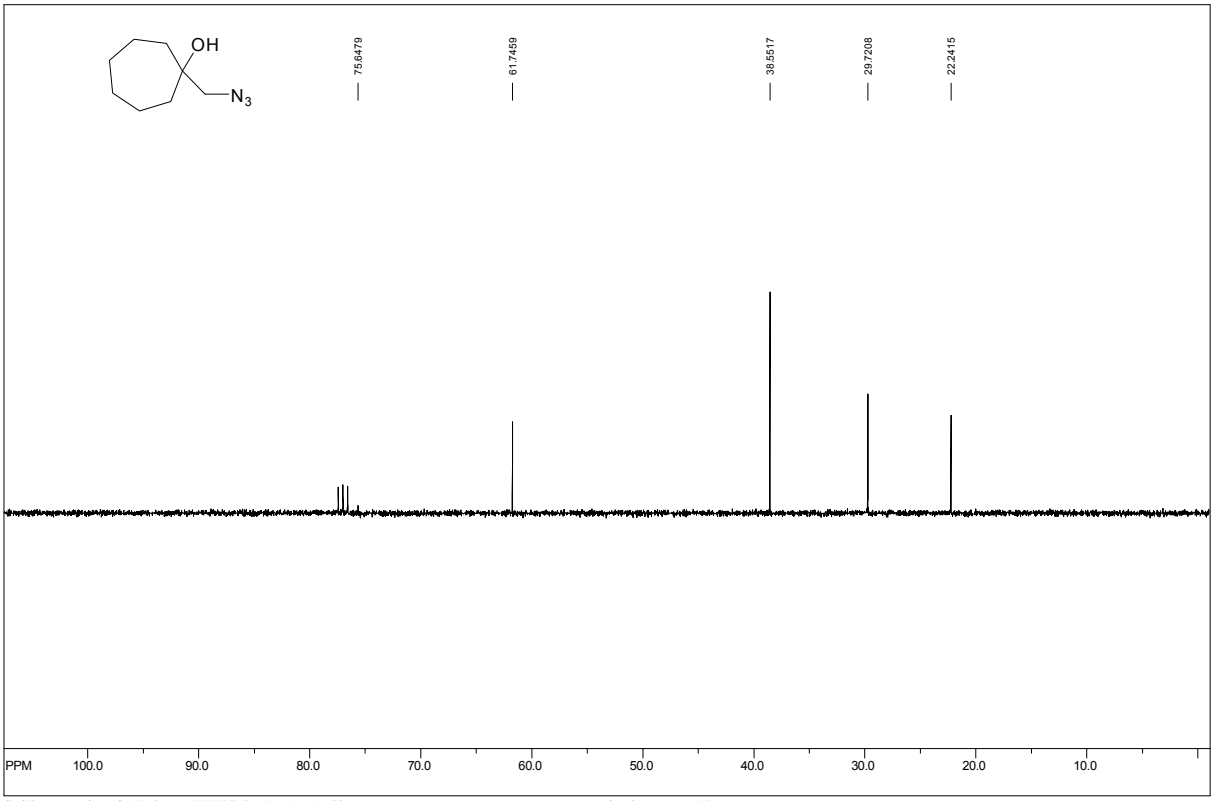
SpinWorks 2.4: 2c



file: C:\Documents and Settings\Catbio\My Documents\MAJA\NMR\1-Dnevnik br 12\27-12A-1H\fid expt: <zg30>
transmitter freq.: 300.131853 MHz
time domain size: 32768 points
width: 6172.84 Hz = 20.567092 ppm = 0.188380 Hz/pt
number of scans: 24

freq. of 0 ppm: 300.130000 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

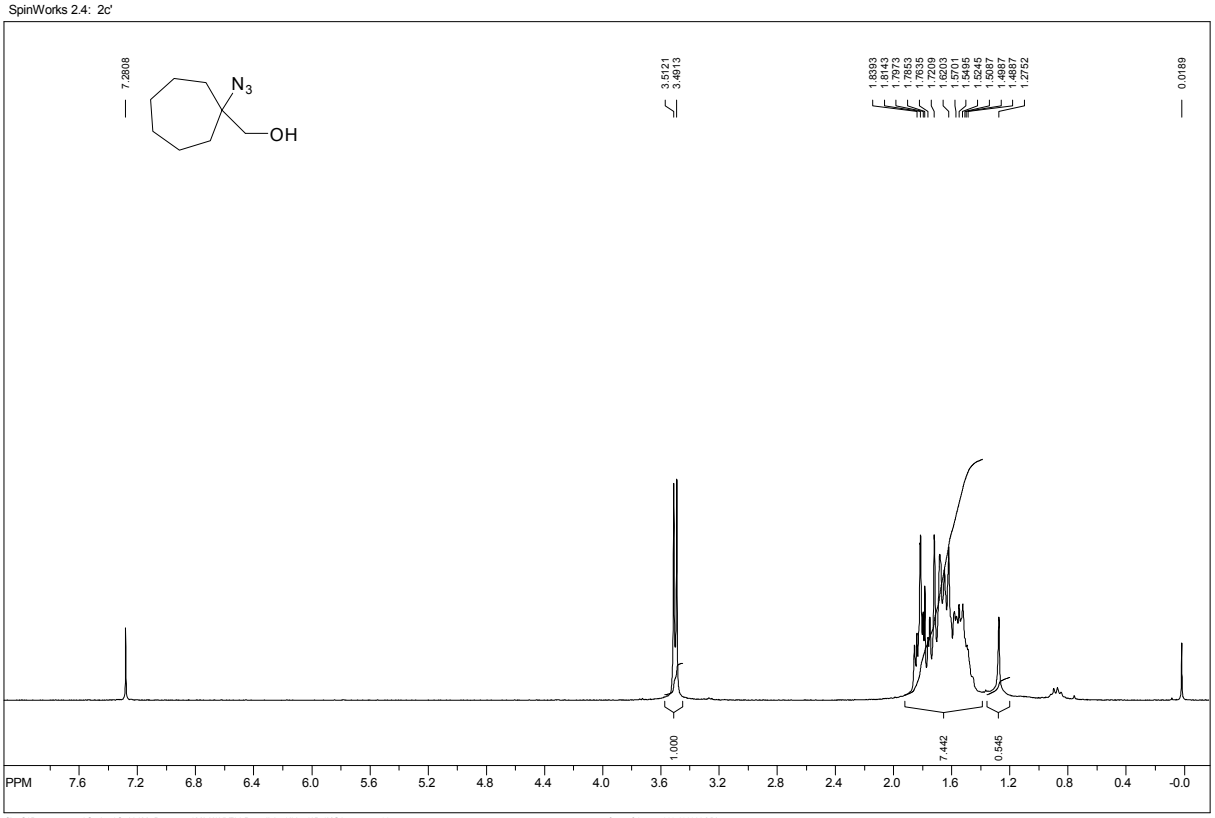
SpinWorks 2.4: 2c



file: C:\Documents and Settings\Catbio\My Documents\MAJA\NMR\1-Dnevnik br 12\27-12A-13C\fid expt: <jmod>
transmitter freq.: 75.475295 MHz
time domain size: 65536 points
width: 17985.61 Hz = 238.297995 ppm = 0.274439 Hz/pt
number of scans: 541

freq. of 0 ppm: 75.467749 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

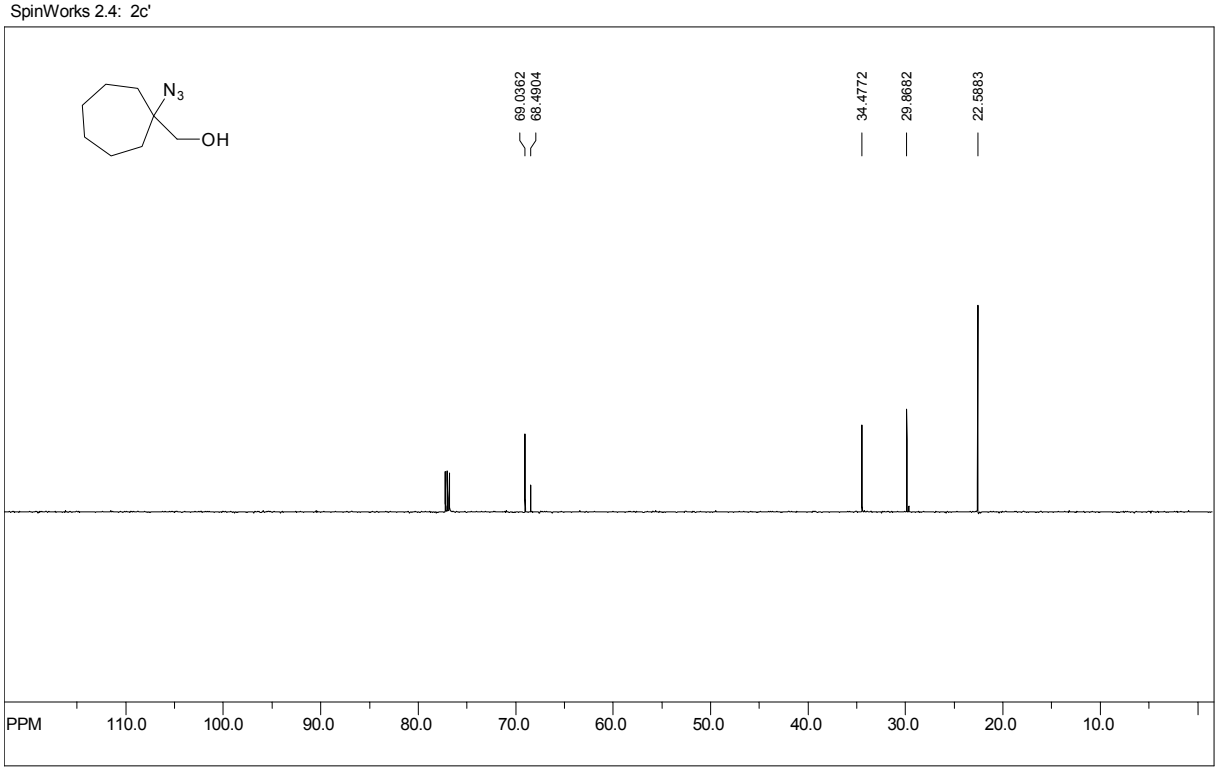
SpinWorks 2.4: 2c'



file: C:\Documents and Settings\Catbio\My Documents\MAJA\NMR\1-Dnevnik br 12\27-12B-1H\fid expt: <zg30>
transmitter freq.: 300.131853 MHz
time domain size: 32768 points
width: 6172.84 Hz = 20.567092 ppm = 0.188380 Hz/pt
number of scans: 24

freq. of 0 ppm: 300.130000 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

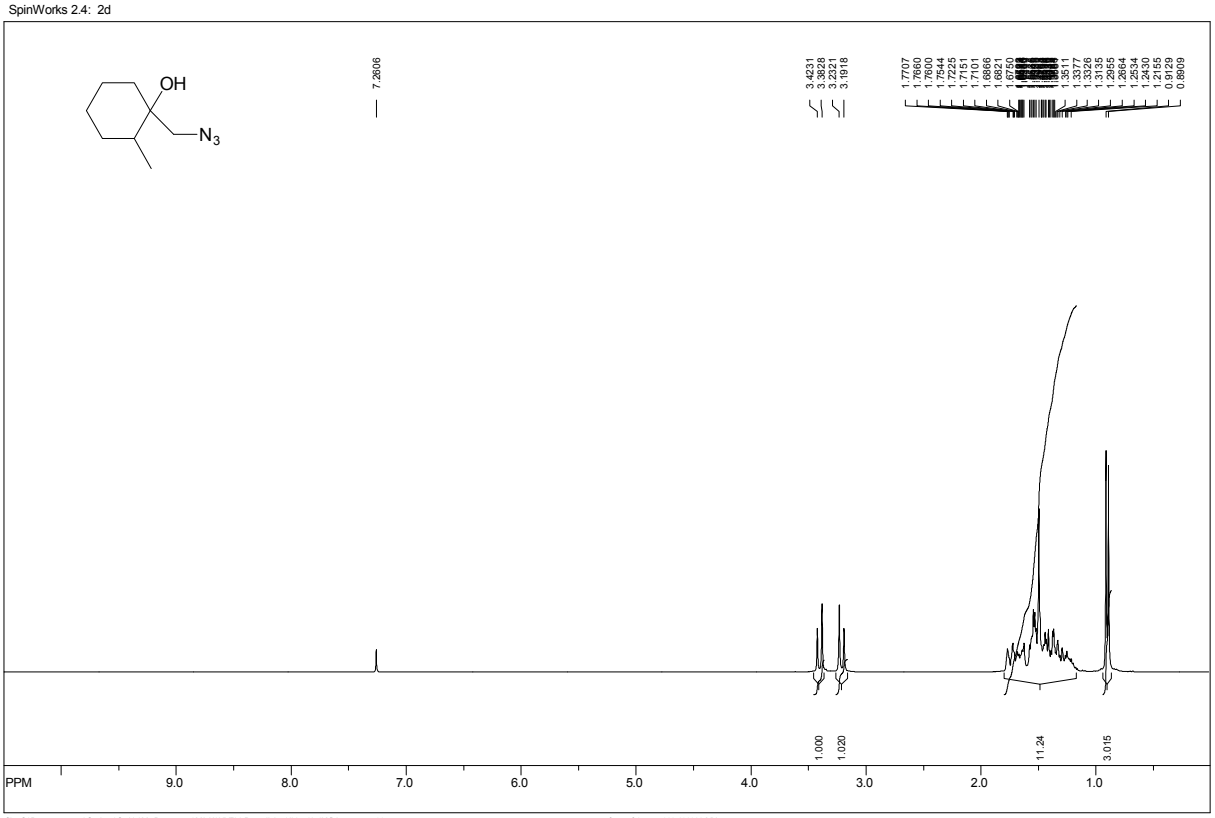
SpinWorks 2.4: 2c'



file: C:\Documents and Settings\Catbio\Desktop\4\fid expt: <zgpg30>
transmitter freq.: 150.917899 MHz
time domain size: 65536 points
width: 35971.22 Hz = 238.349615 ppm = 0.548877 Hz/pt
number of scans: 111

freq. of 0 ppm: 150.902809 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

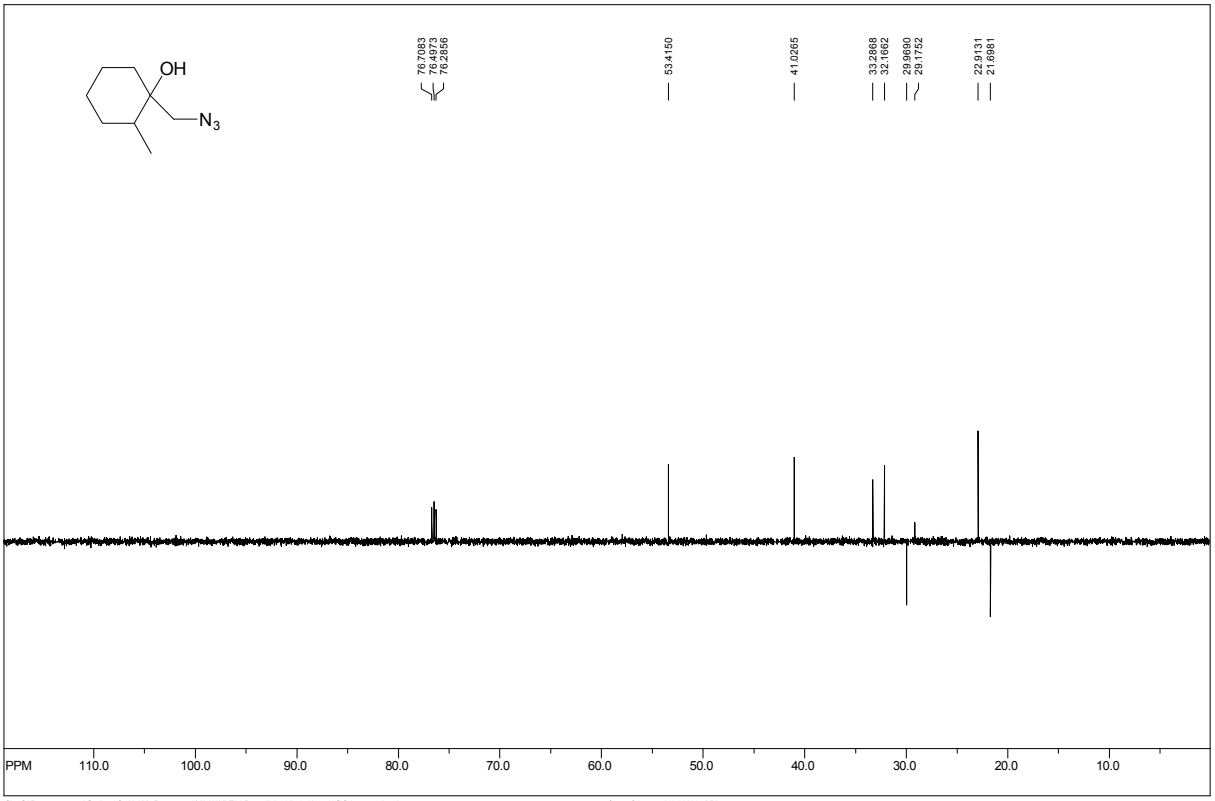
SpinWorks 2.4: 2d



file: C:\Documents and Settings\Catbio\My Documents\MAJA\NMR\1-Dnevnik br 12\64-12-1H\fid expt: <zg30>
transmitter freq.: 300.132701 MHz
time domain size: 32768 points
width: 6172.84 Hz = 20.567034 ppm = 0.188380 Hz/pt
number of scans: 9

freq. of 0 ppm: 300.130006 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

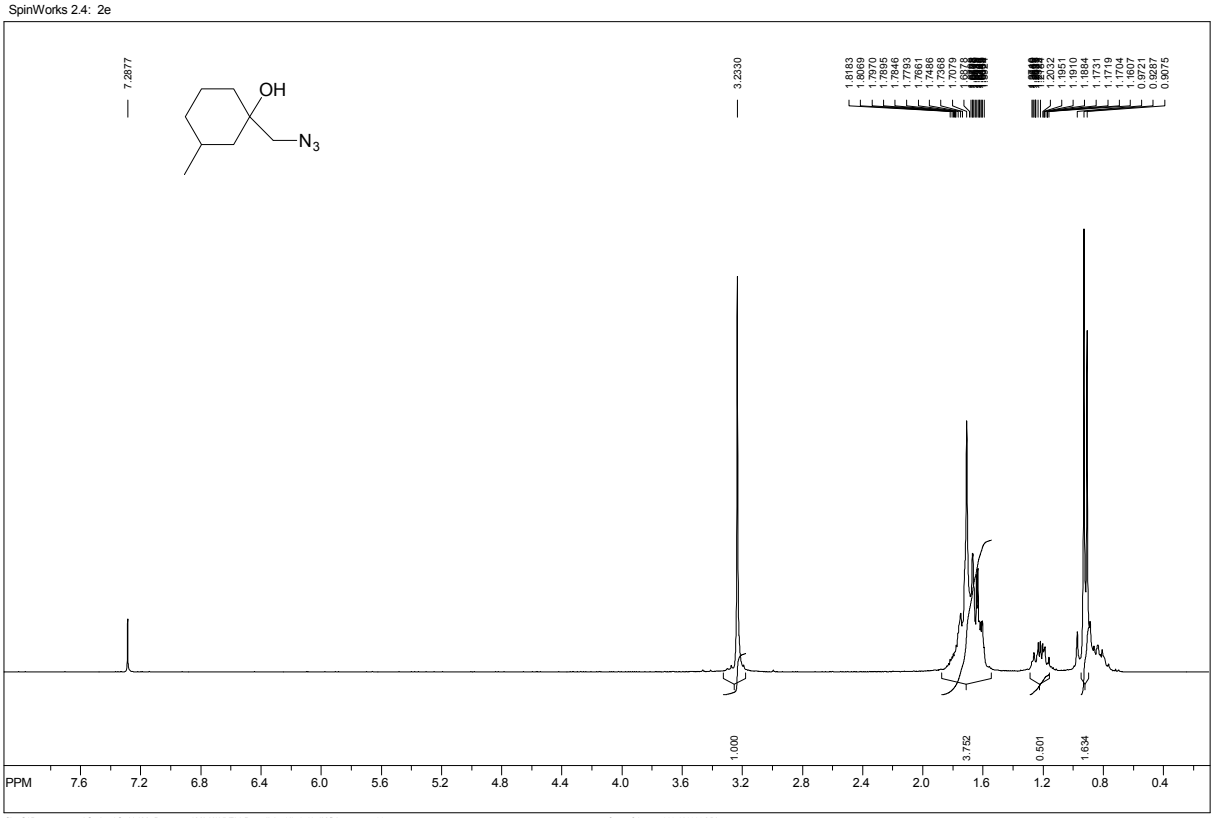
SpinWorks 2.4: 2d



file: C:\Documents and Settings\Catbio\My Documents\MAJA\NMR\1-Dnevnik br 12\46-12-rs-13C\fid expt: <jmod>
transmitter freq.: 150.917899 MHz
time domain size: 65536 points
width: 35971.22 Hz = 238.349615 ppm = 0.548877 Hz/pt
number of scans: 939

freq. of 0 ppm: 150.902884 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

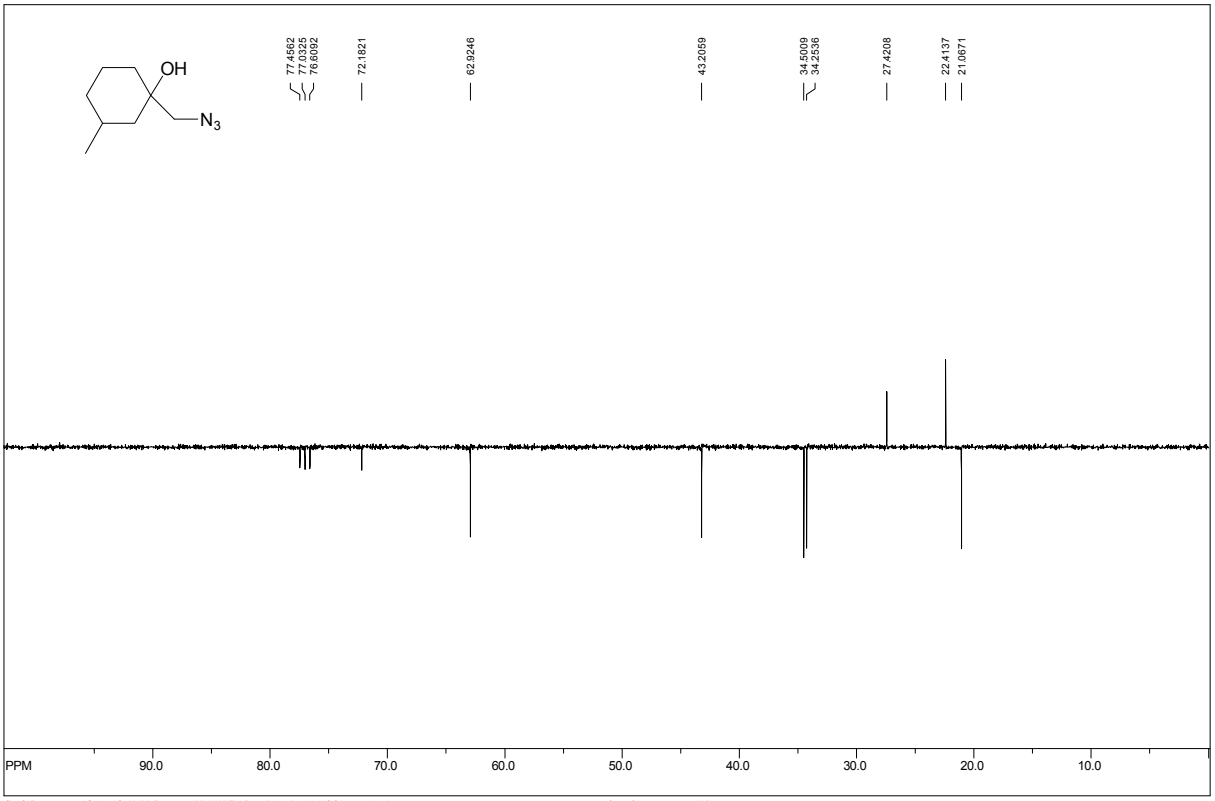
SpinWorks 2.4: 2e



file: C:\Documents and Settings\Catbio\My Documents\MAJA\NMR\1-Dnevnik br 12\56-12-1H\fid expt: <zg30>
transmitter freq.: 300.132701 MHz
time domain size: 32768 points
width: 6172.84 Hz = 20.567034 ppm = 0.188380 Hz/pt
number of scans: 8

freq. of 0 ppm: 300.129998 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

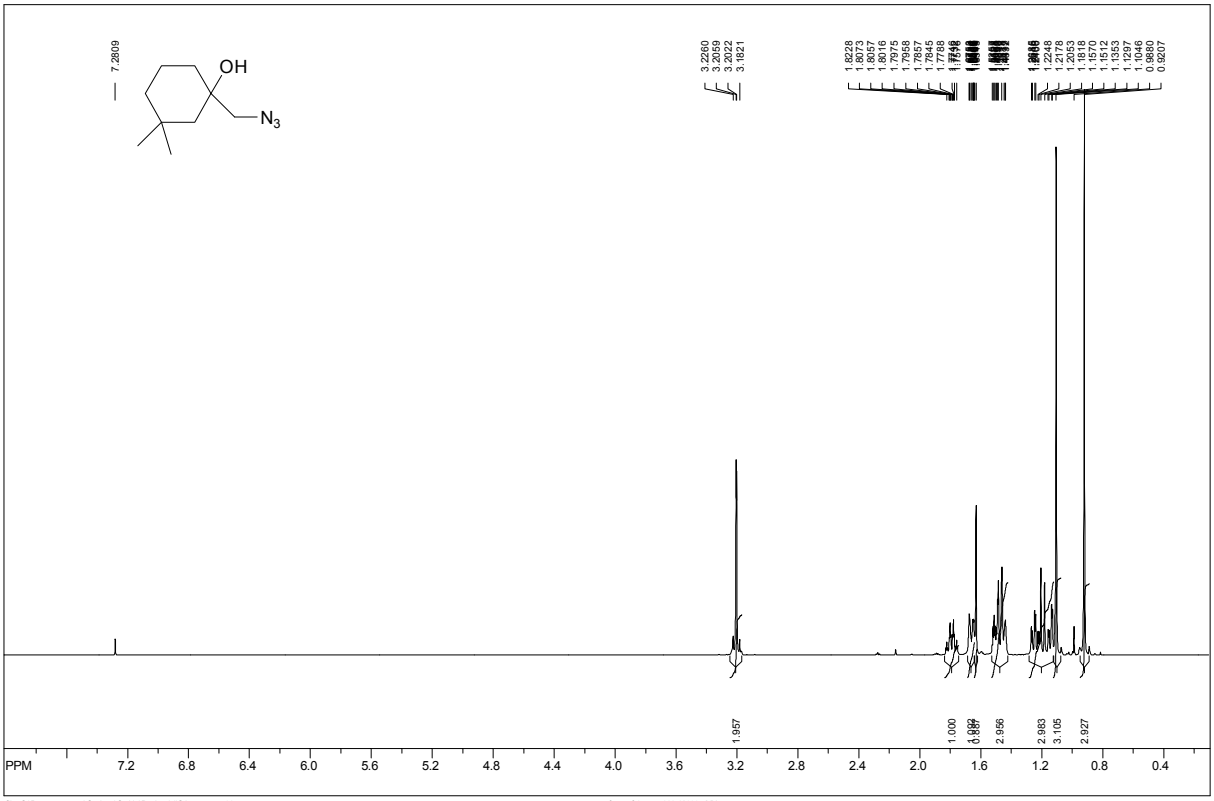
SpinWorks 2.4: 2e



file: C:\Documents and Settings\Catbio\My Documents\MAJA\NMR\1-Dnevnik br 12\56-12-13C\fid expt: <jmod>
transmitter freq.: 75.475295 MHz
time domain size: 65536 points
width: 17985.61 Hz = 238.297995 ppm = 0.274439 Hz/pt
number of scans: 469

freq. of 0 ppm: 75.467749 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

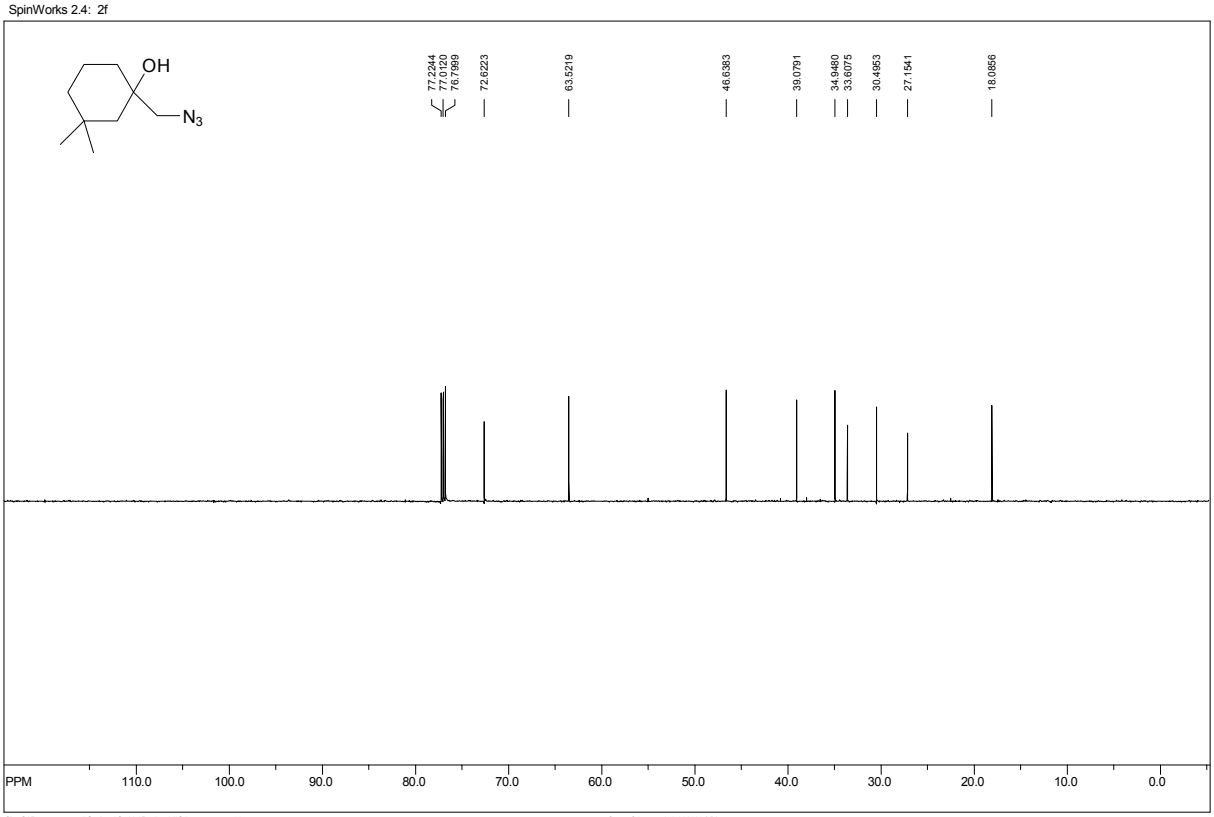
SpinWorks 2.4: 2f



file: C:\Documents and Settings\Catbio\Desktop\1\fid expt: <zg30>
transmitter freq.: 600.133901 MHz
time domain size: 32768 points
width: 9541.98 Hz = 15.899760 ppm = 0.291198 Hz/pt
number of scans: 16

freq. of 0 ppm: 600.129997 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000

SpinWorks 2.4: 2f



file: C:\Documents and Settings\Catbio\Desktop\2\fid expt: <zgpg30>
transmitter freq.: 150.917899 MHz
time domain size: 65536 points
width: 35971.22 Hz = 238.349615 ppm = 0.548877 Hz/pt
number of scans: 899

freq. of 0 ppm: 150.902809 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000