Supporting Information

for

"Cyclobutane amino acid analogues of furanomycin obtained by a formal [2+2] cycloaddition strategy promoted by methylaluminoxane"

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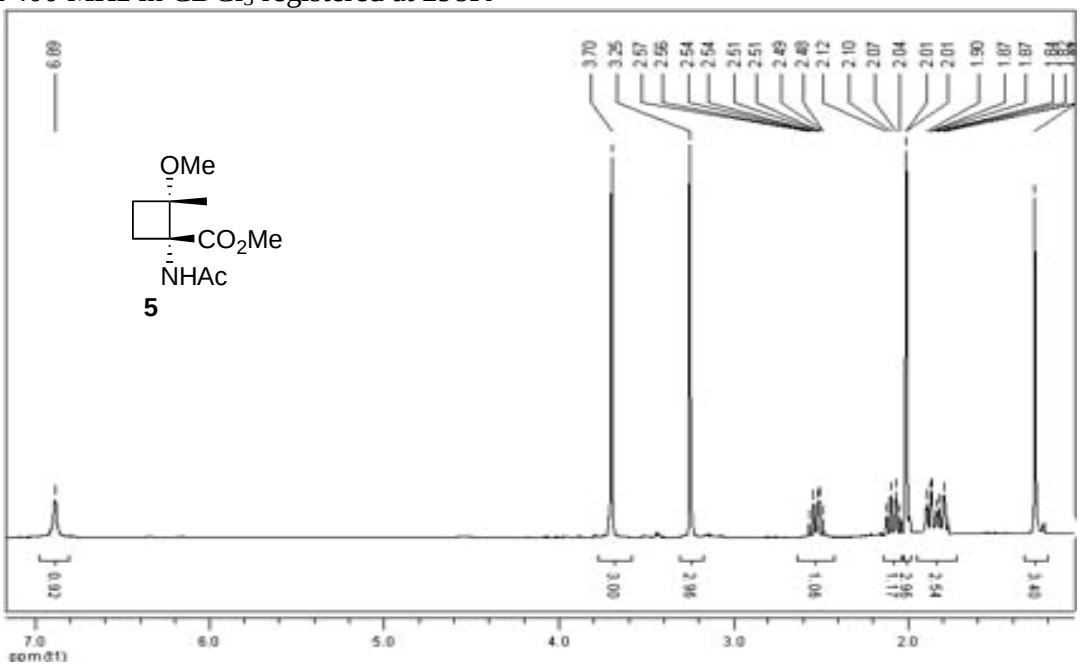
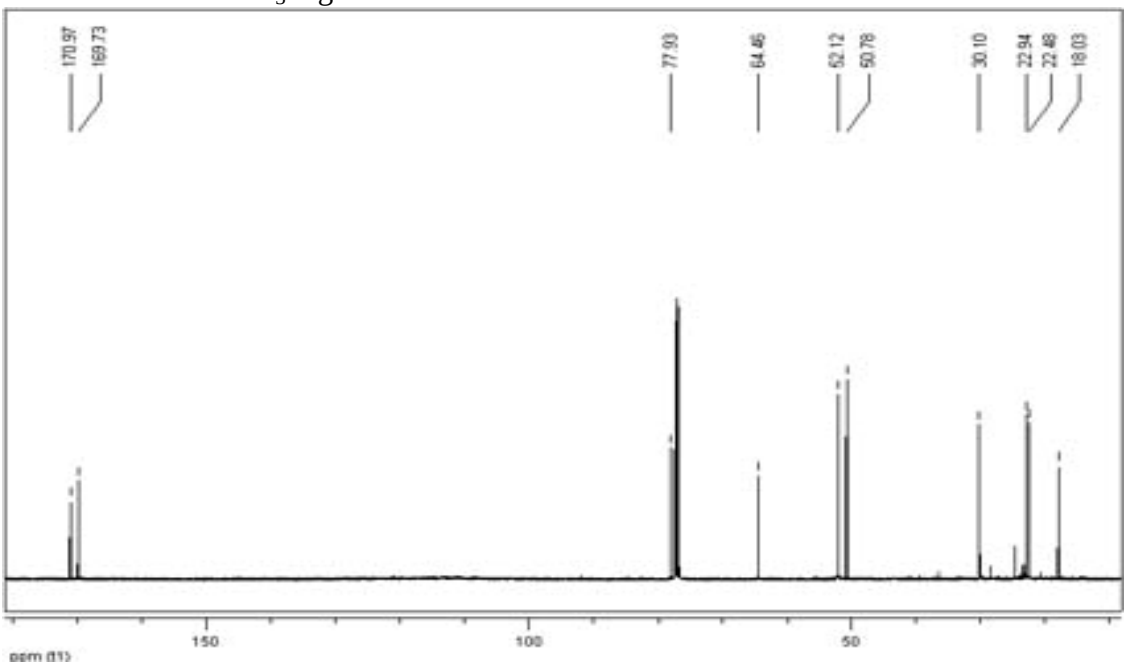
(1*R*,2*S*)- and (1*S*,2*R*)-1-Acetamido-2-methoxy-2-methylcyclobutan-1-carboxylic acid methyl ester (5)

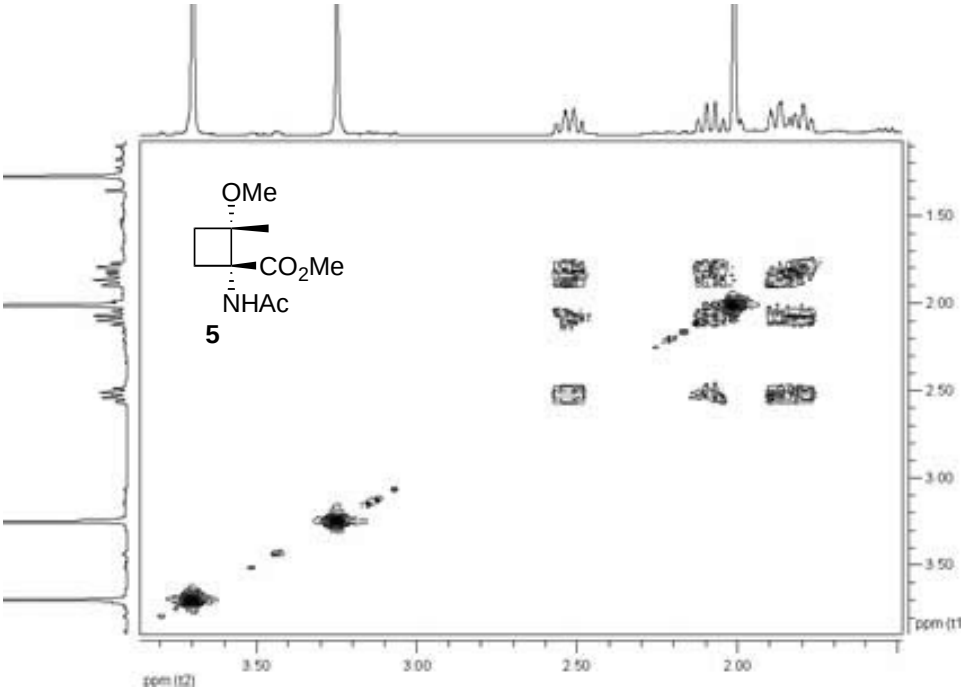
^{1}H NMR 400 MHz in $CDCl_3$ registered at 298K



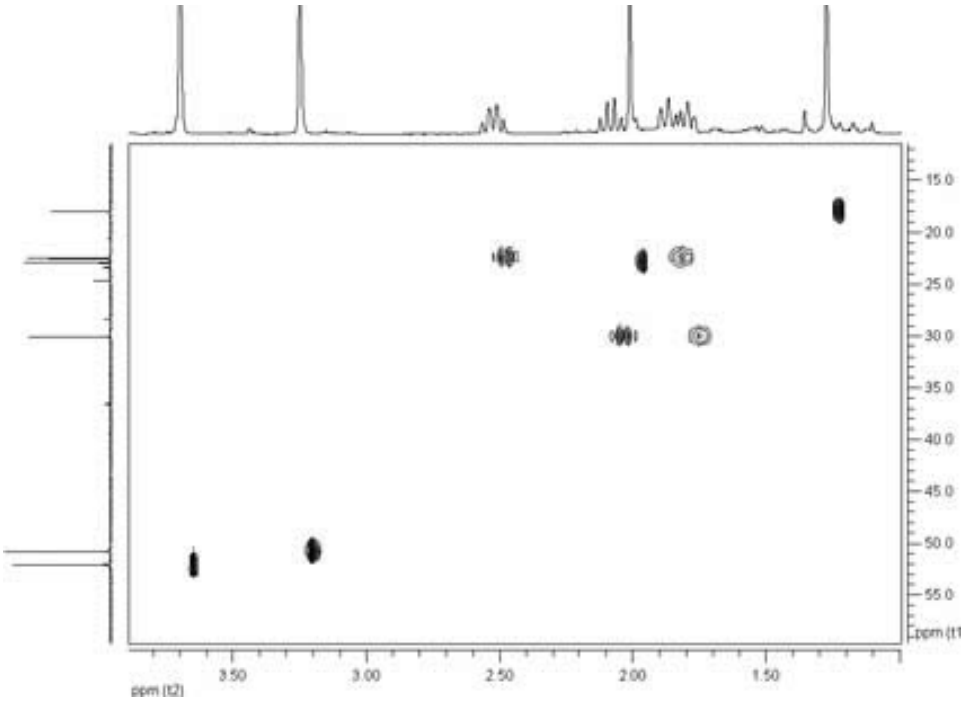
^{13}C NMR 100 MHz in $CDCl_3$ registered at 298K



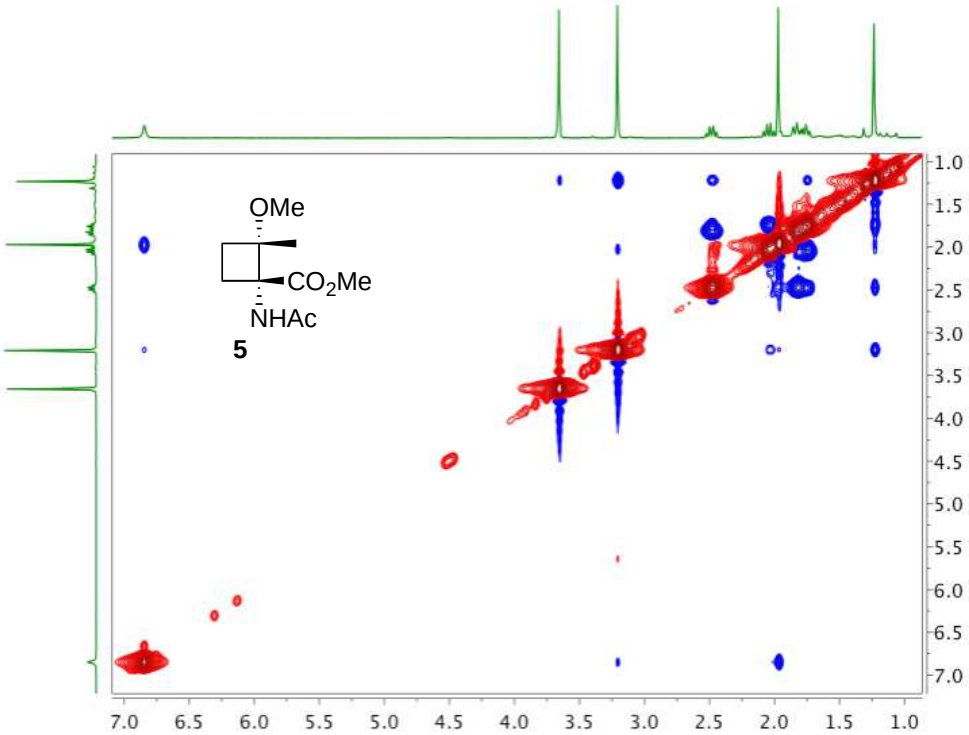
COSY in $CDCl_3$ registered at 298K



HSQC in $CDCl_3$ registered at 298K

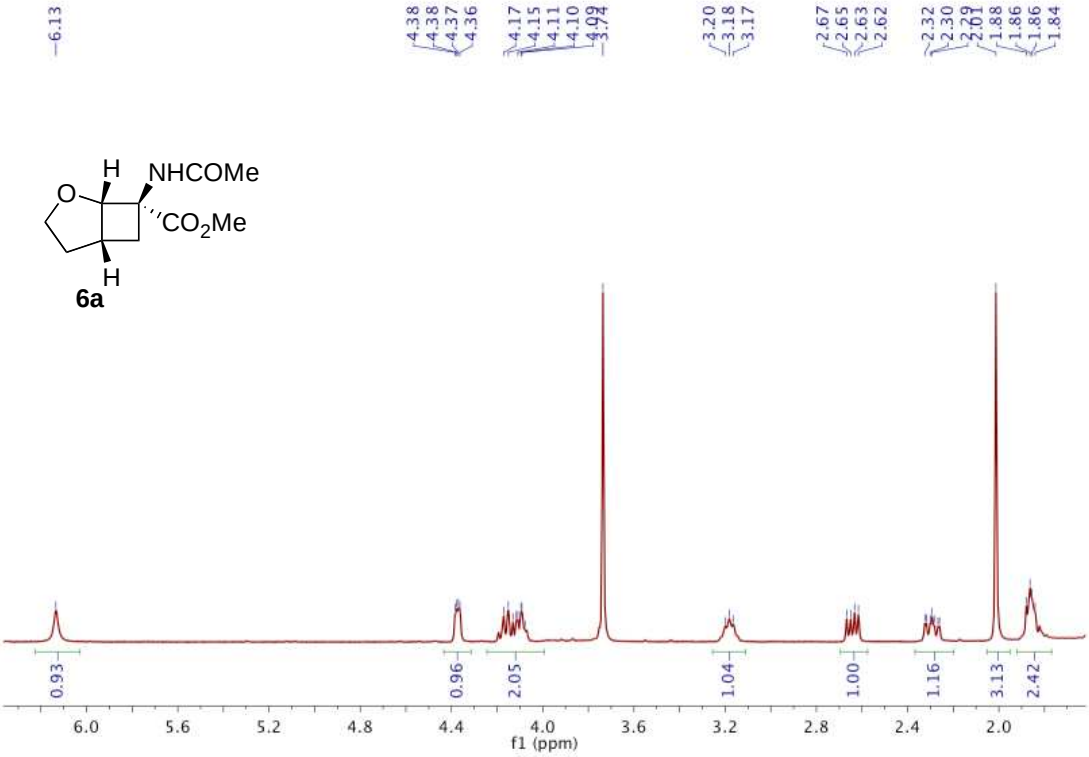


2D-NOESY (800 ms) in $CDCl_3$ registered at 298K

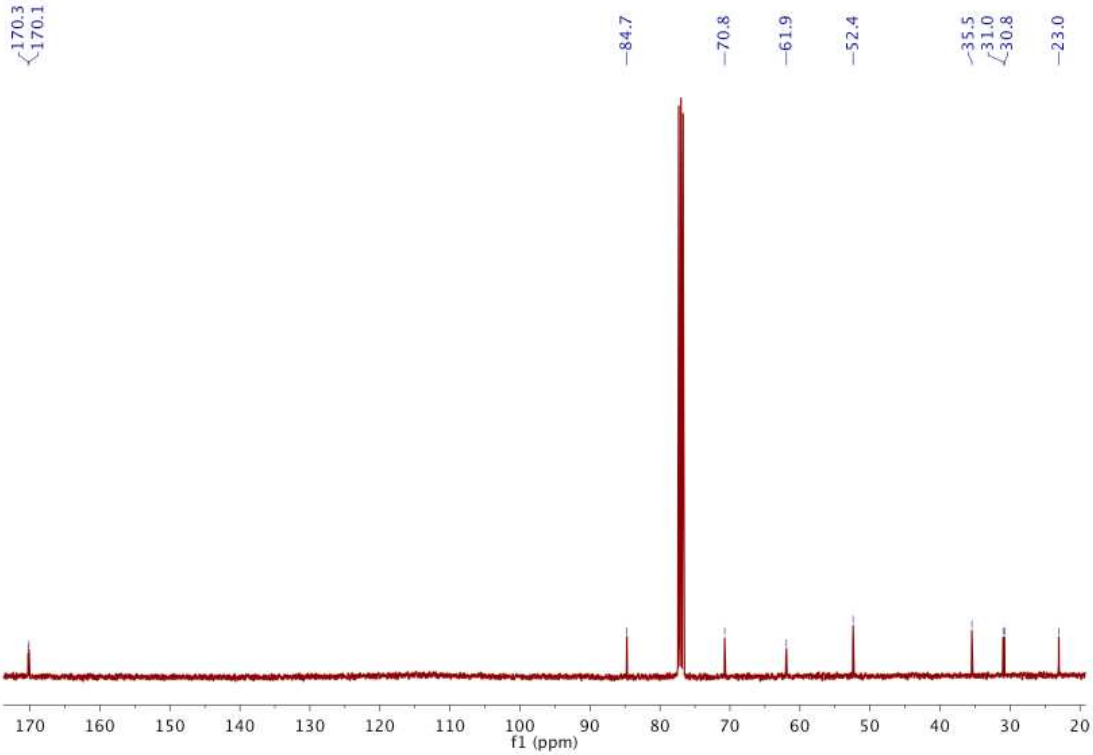


(1*S*,5*R*,7*S*)- and (1*R*,5*S*,7*R*)-7-Acetamido-2-oxabicyclo[3.2.0]heptan-7-carboxylic acid methyl ester (6a)

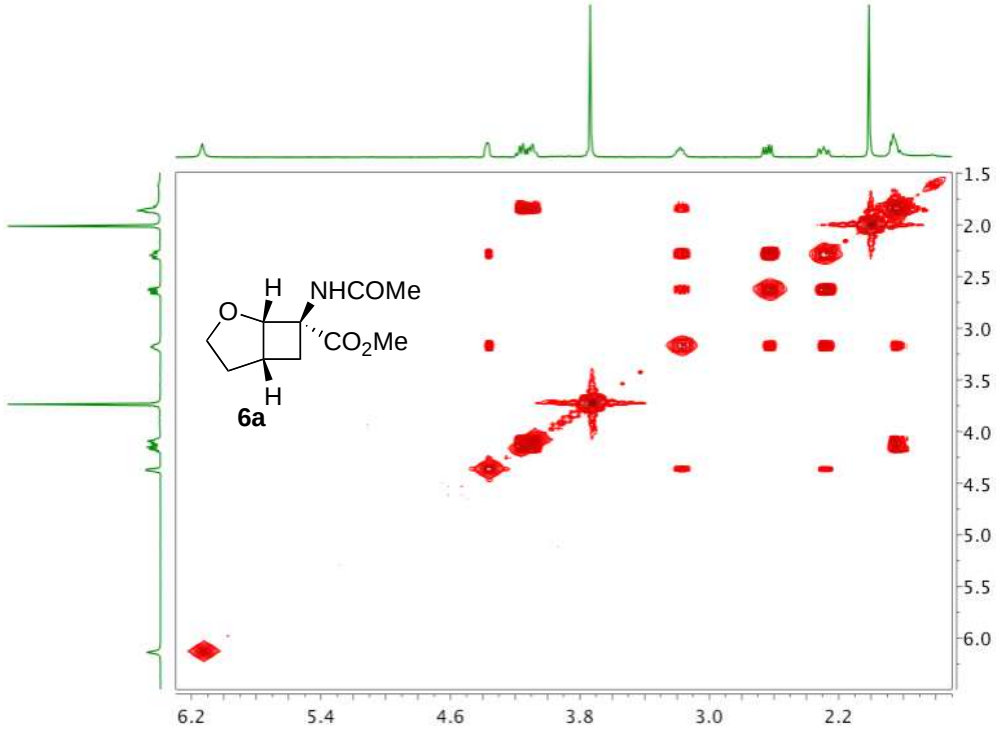
^{1}H NMR 400 MHz in $CDCl_3$ registered at 298K



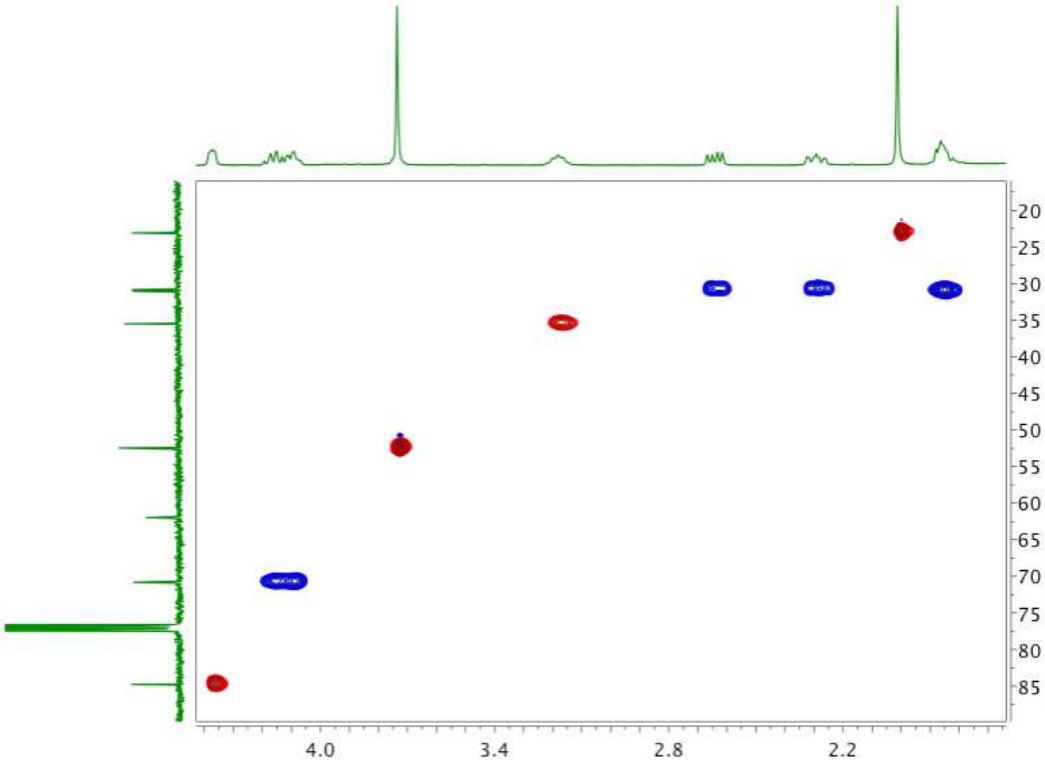
^{13}C NMR 100 MHz in $CDCl_3$ registered at 298K



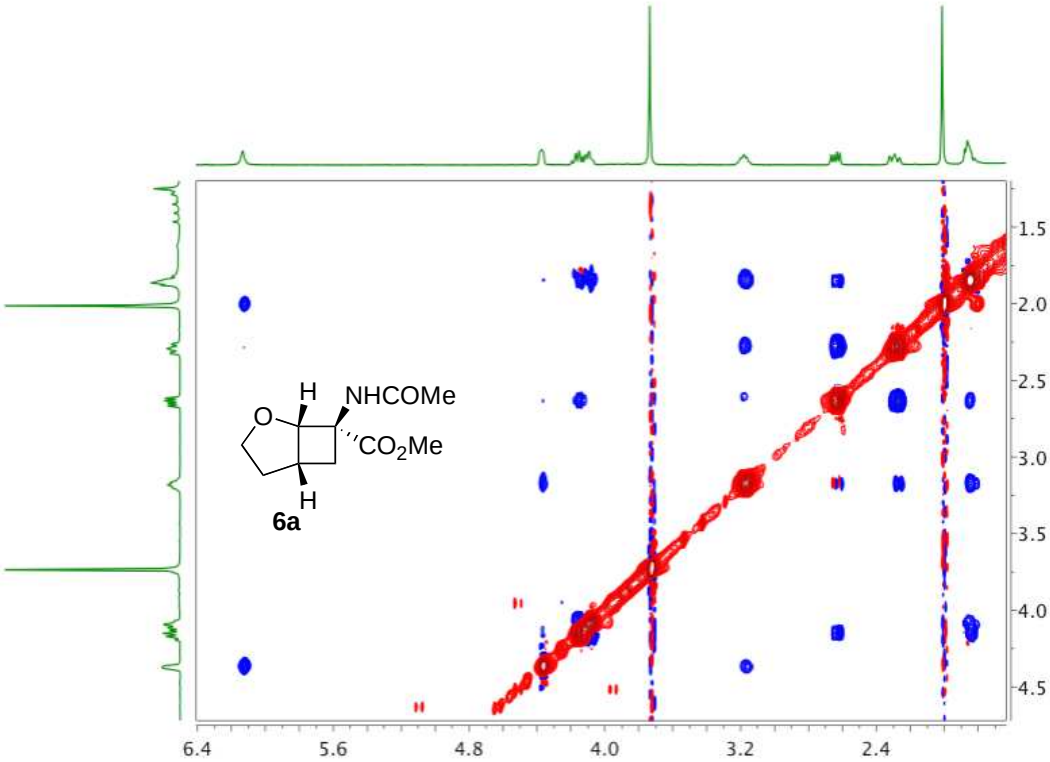
COSY in $CDCl_3$ registered at 298K



HSQC in $CDCl_3$ registered at 298K

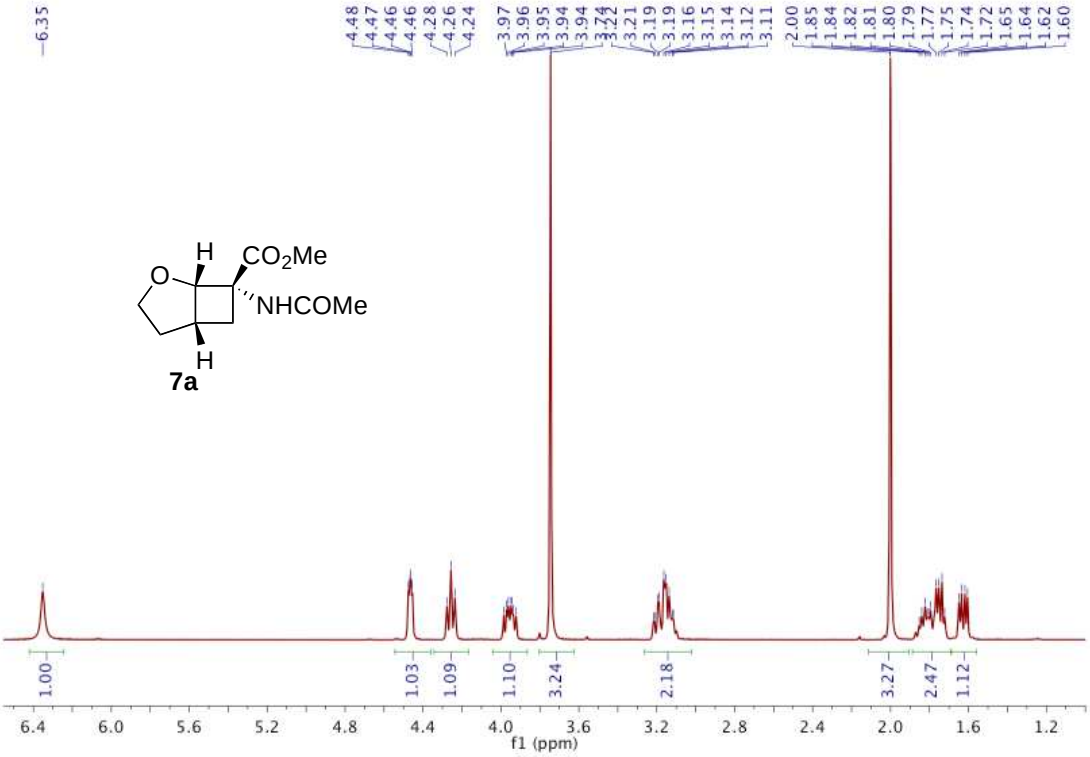


2D-NOESY (800 ms) in $CDCl_3$ registered at 298K

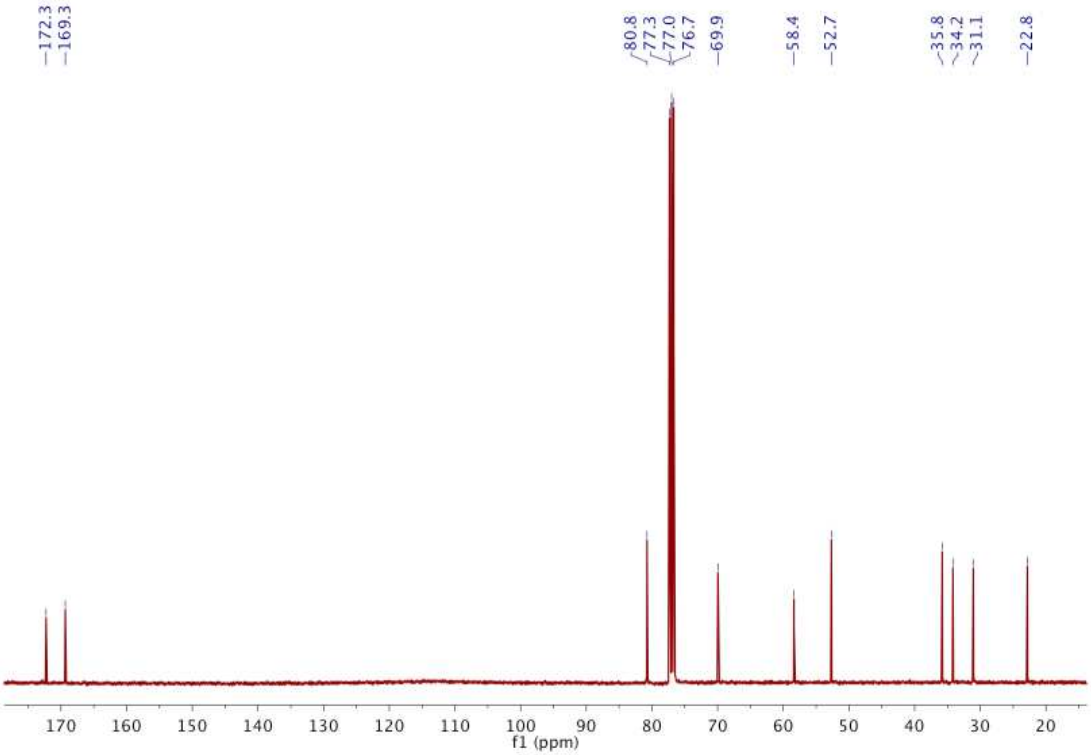


(1*S*,5*R*,7*R*)- and (1*R*,5*S*,7*S*)-7-acetamido-2-oxabicyclo[3.2.0]heptan-7-carboxylic acid methyl ester (7a)

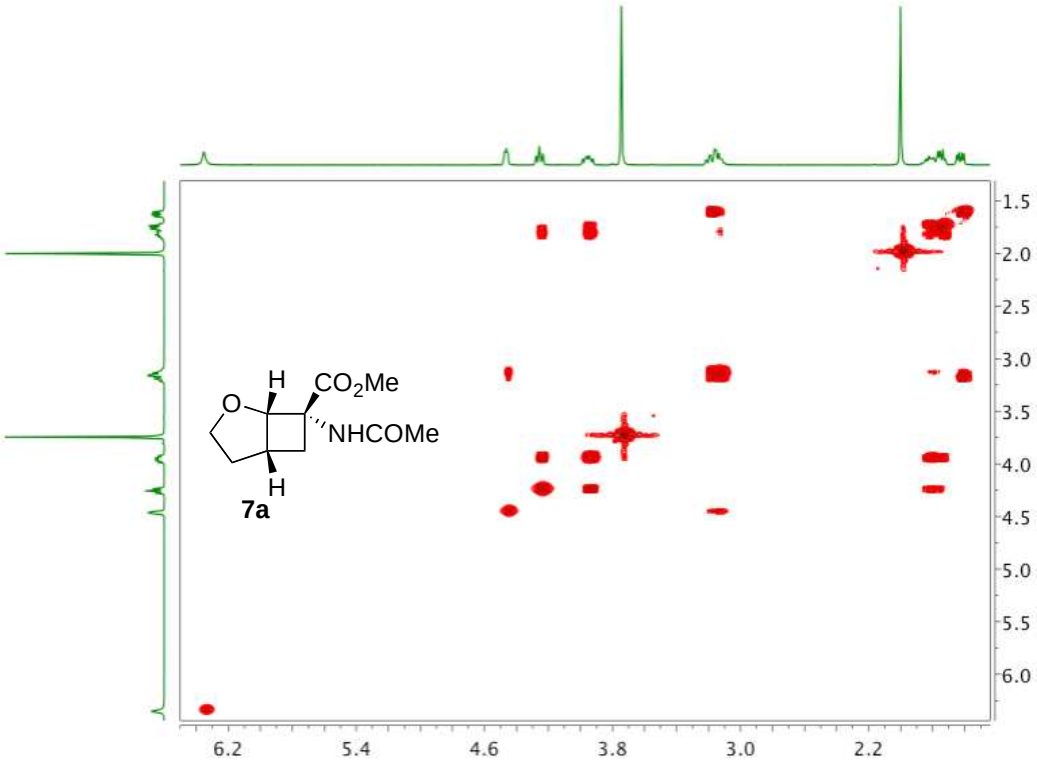
^{1}H NMR 400 MHz in $CDCl_3$ registered at 298K



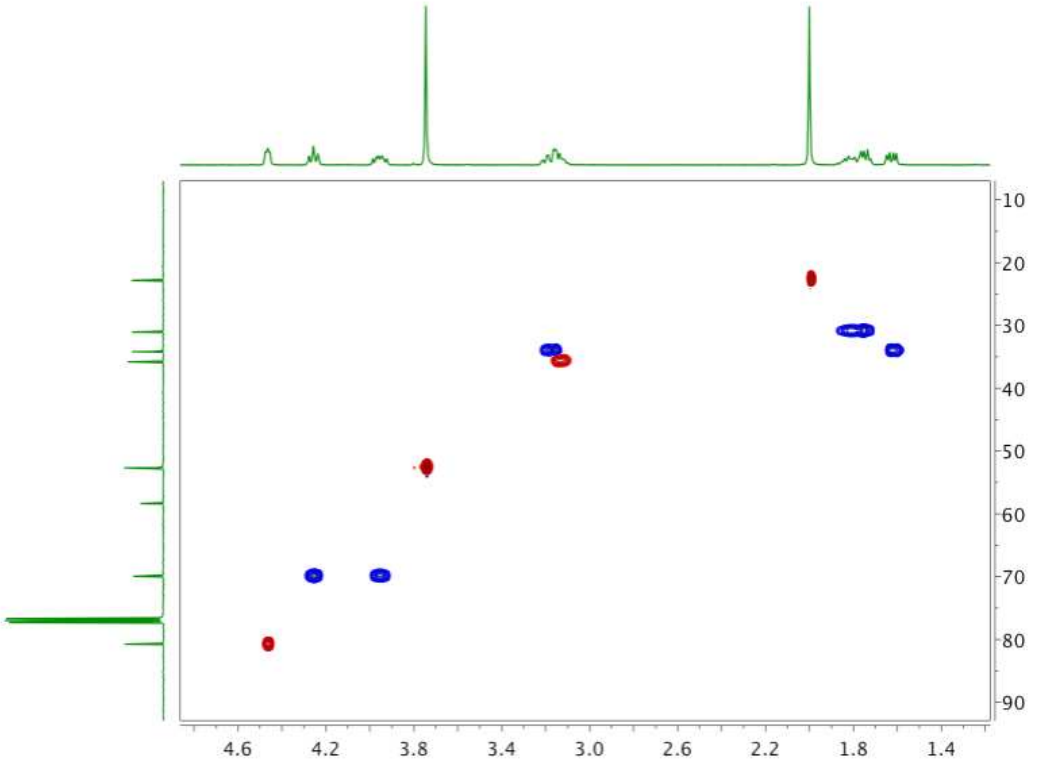
^{13}C NMR 100 MHz in $CDCl_3$ registered at 298K



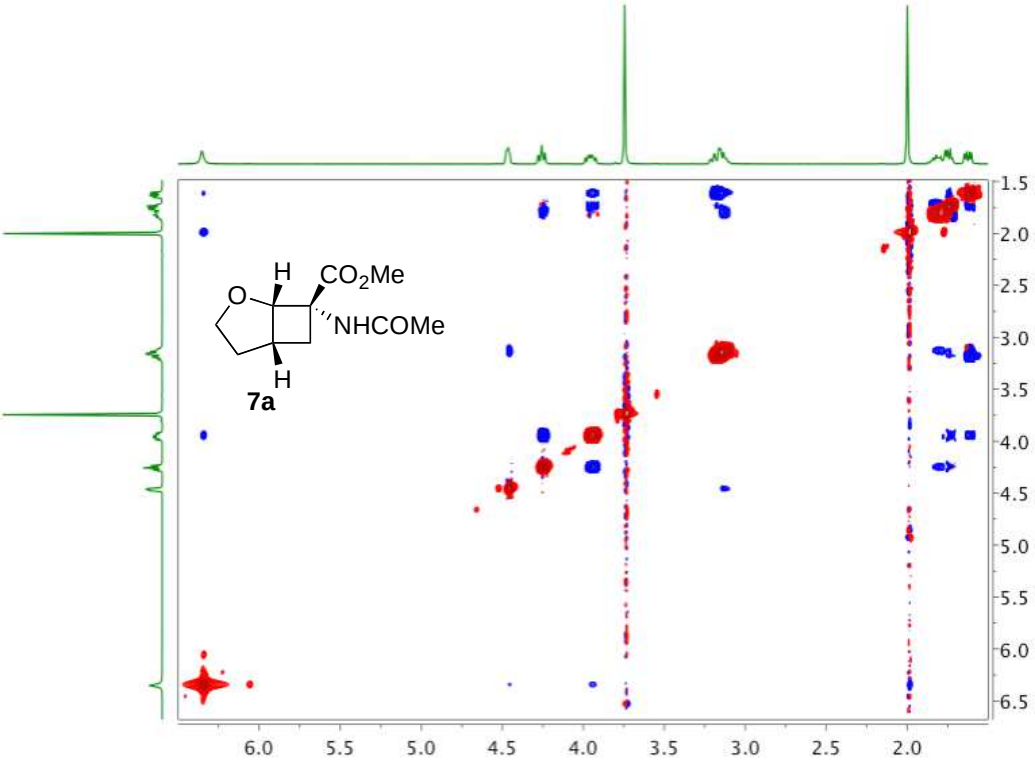
COSY in $CDCl_3$ registered at 298K



HSQC in $CDCl_3$ registered at 298K

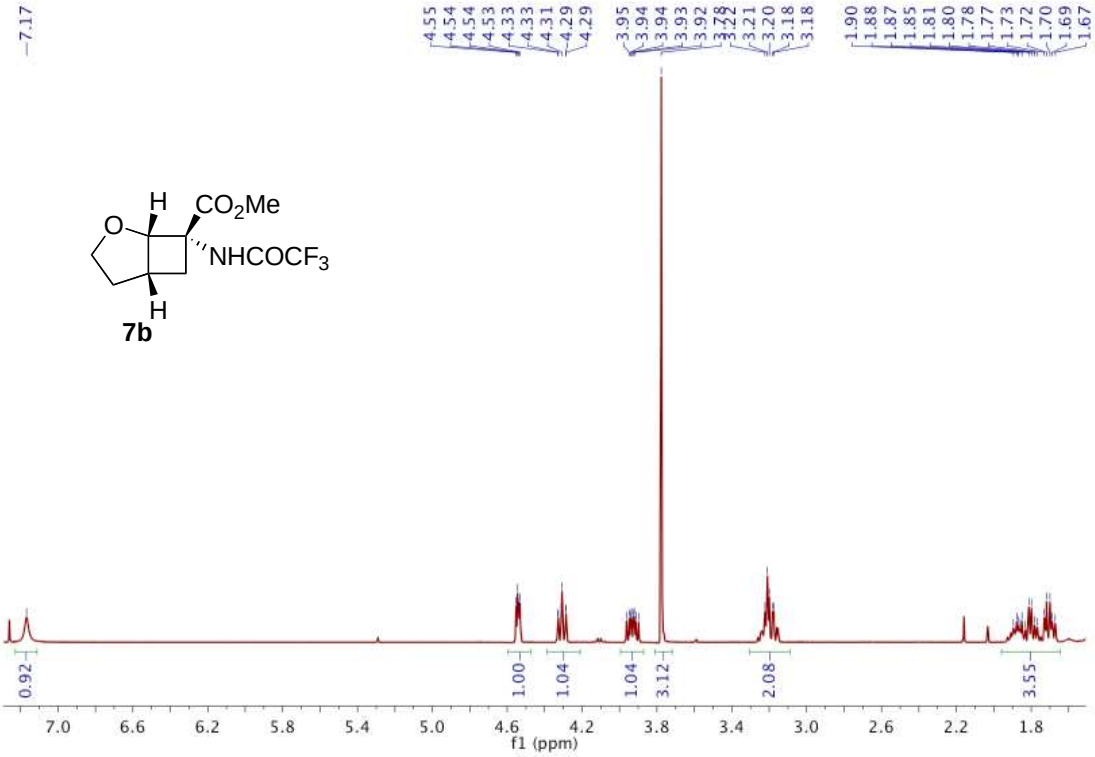


2D-NOESY (800 ms) in $CDCl_3$ registered at 298K

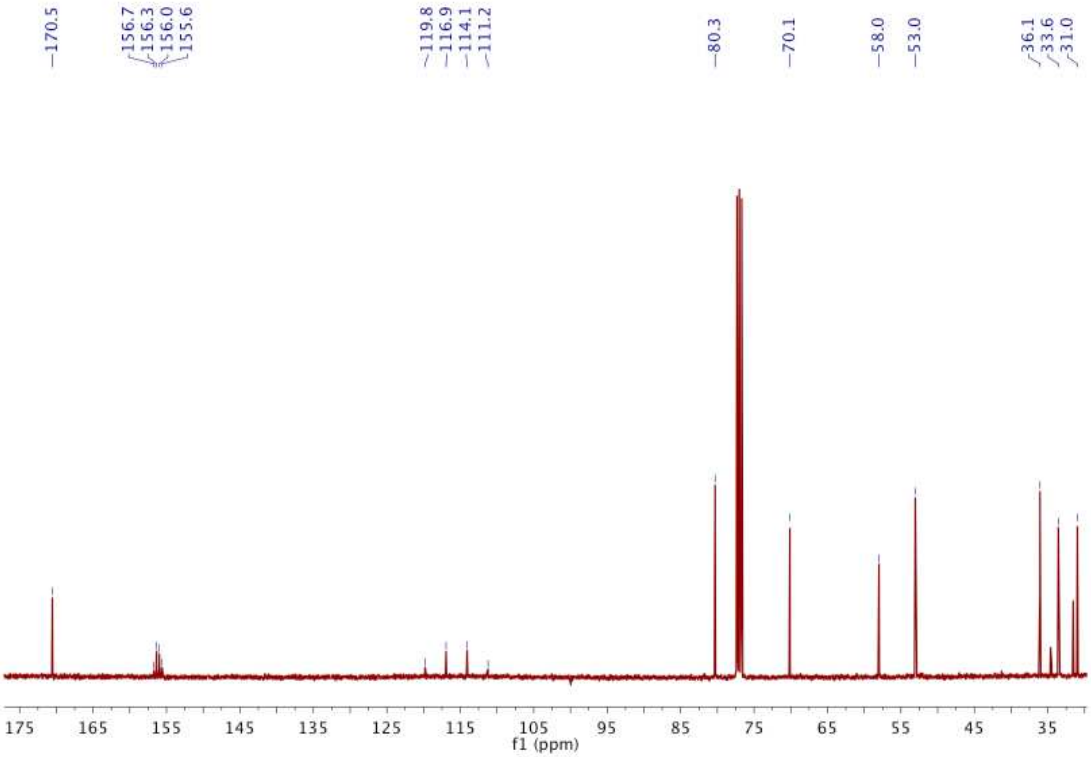


(1*S*,5*R*,7*R*)- and (1*R*,5*S*,7*S*)-7-(2',2',2'-trifluoroacetamido)-2-oxabicyclo[3.2.0]heptan-7-carboxylic acid methyl ester (7b)

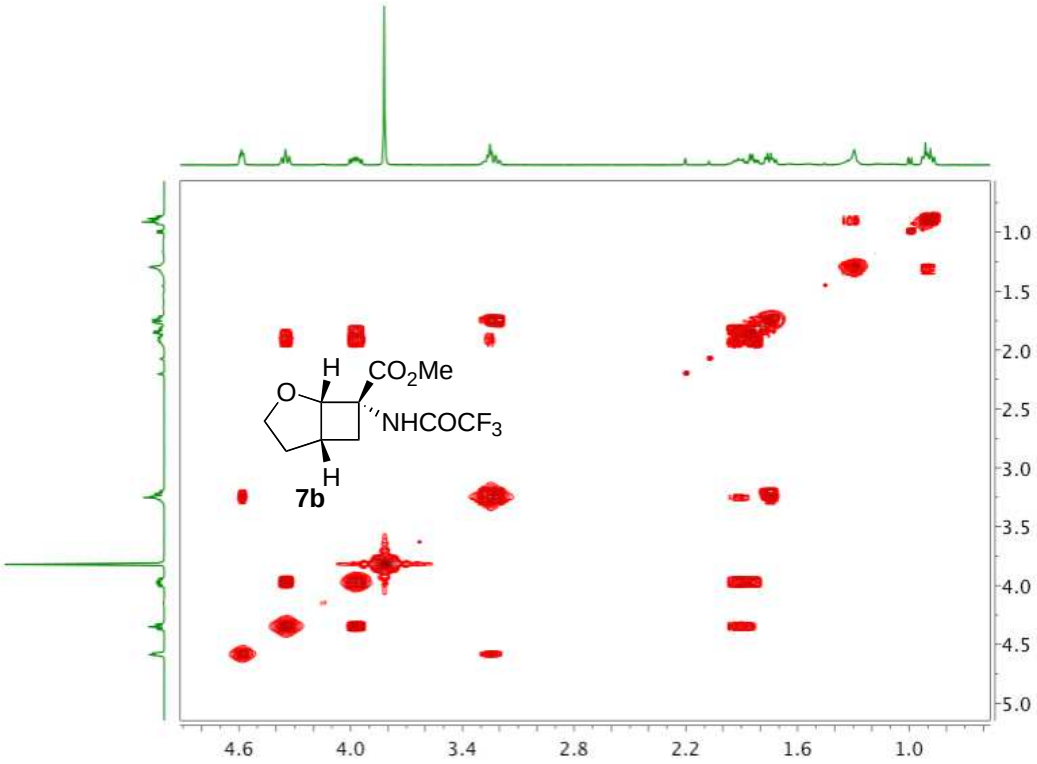
^{1}H NMR 400 MHz in $CDCl_3$ registered at 298K



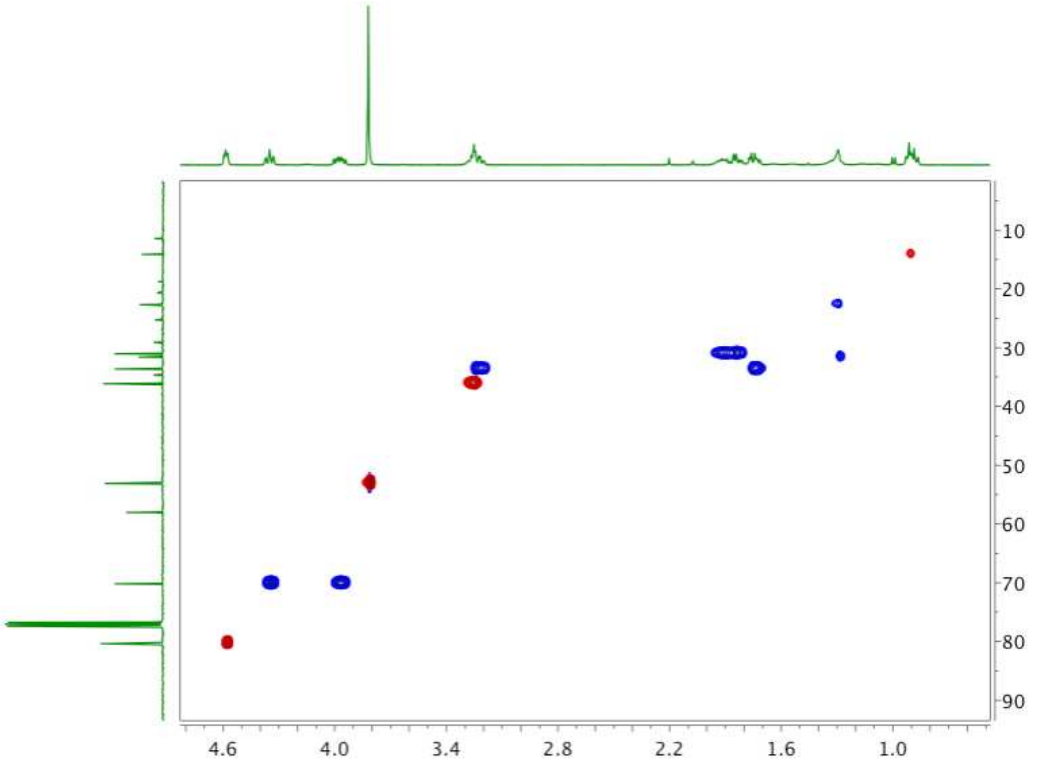
^{13}C NMR 100 MHz in $CDCl_3$ registered at 298K



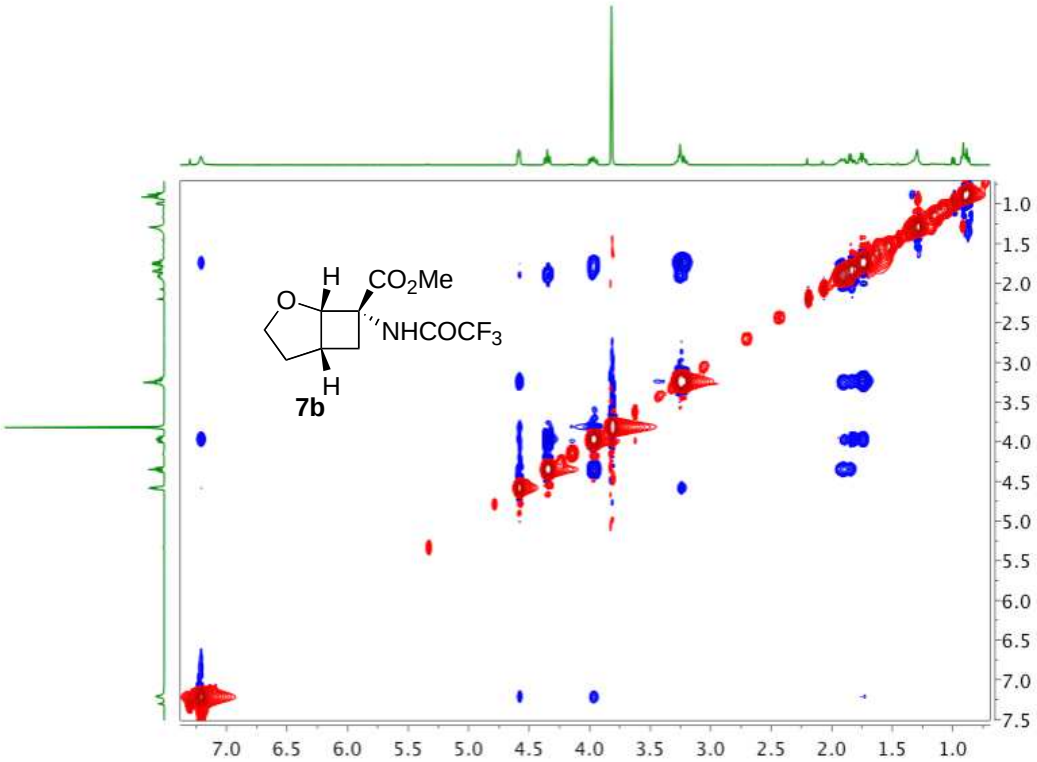
COSY in $CDCl_3$ registered at 298K



HSQC in $CDCl_3$ registered at 298K

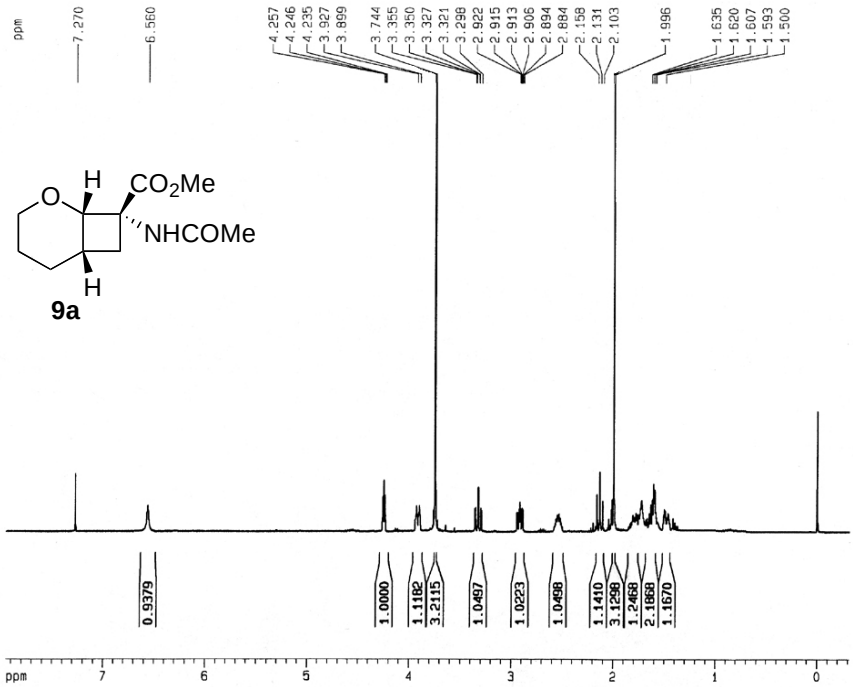


2D-NOESY (800 ms) in $CDCl_3$ registered at 298K

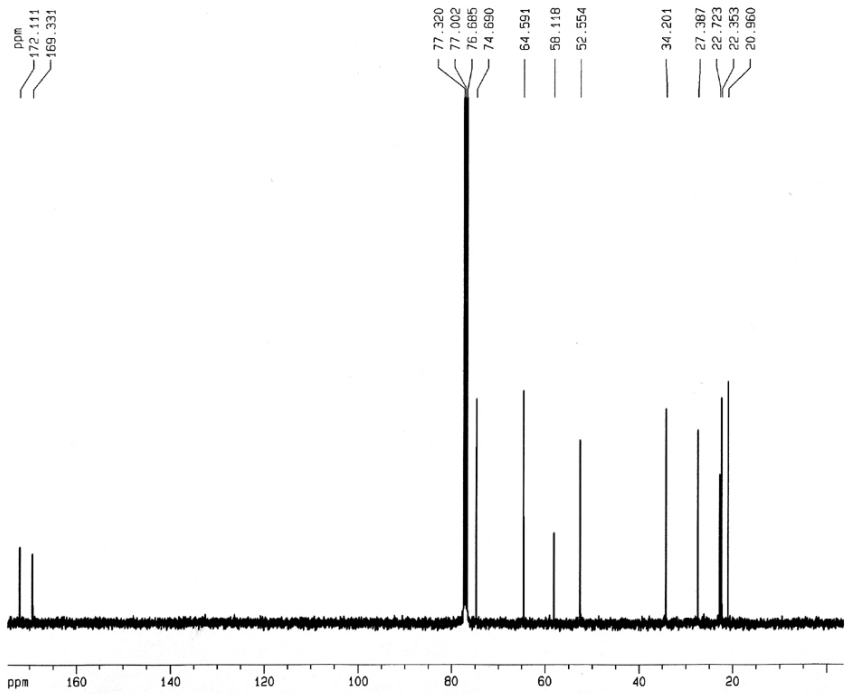


(1*S*,6*S*,8*R*)- and (1*R*,6*R*,8*S*)-8-Acetamido-2-oxabycyclo[4.2.0]octan-8-carboxylic acid methyl ester (9a)

^{1}H NMR 300 MHz in $CDCl_3$ registered at 298K

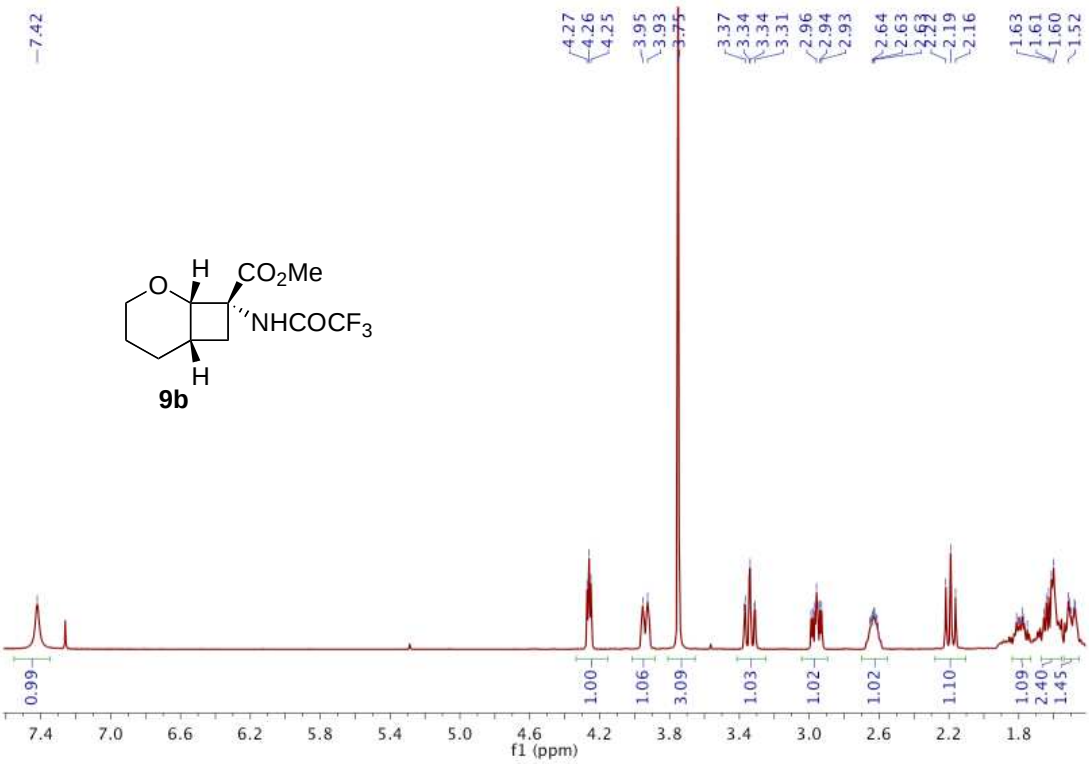


^{13}C NMR 75 MHz in $CDCl_3$ registered at 298K

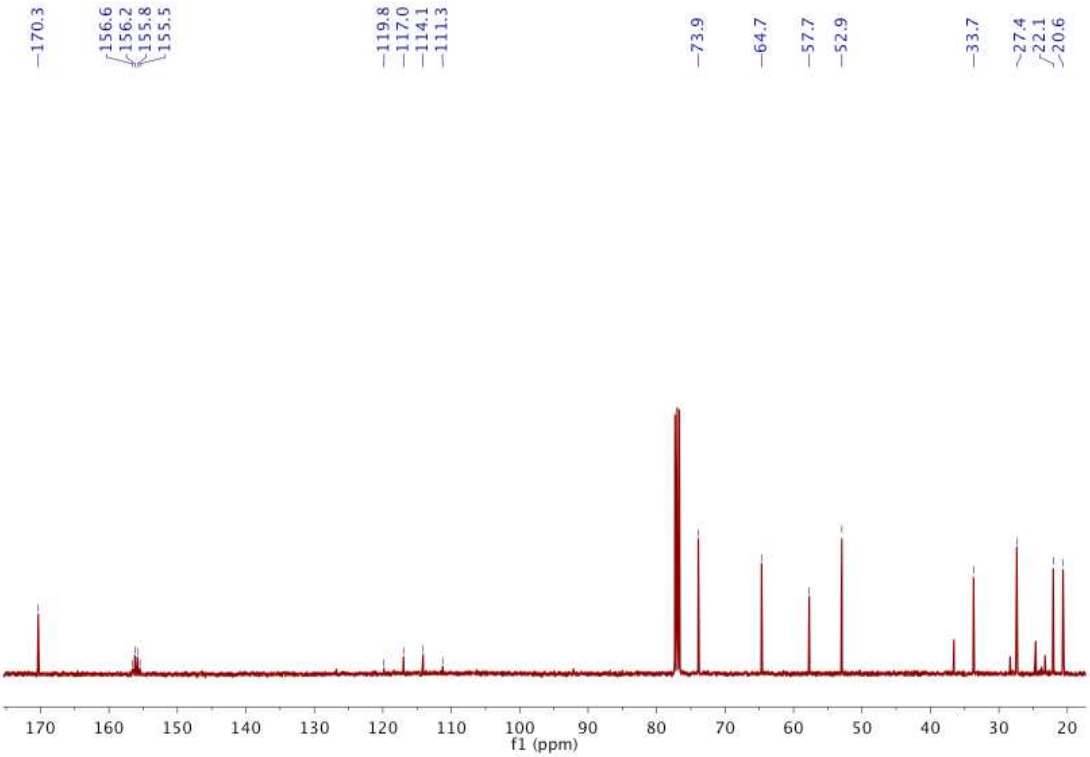


(1*S*,6*S*,8*R*)- and (1*R*,6*R*,8*S*)-8-(2',2',2'-Trifluoroacetamido)-2-oxabicyclo[4.2.0]octan-8-carboxylic acid methyl ester (9b)

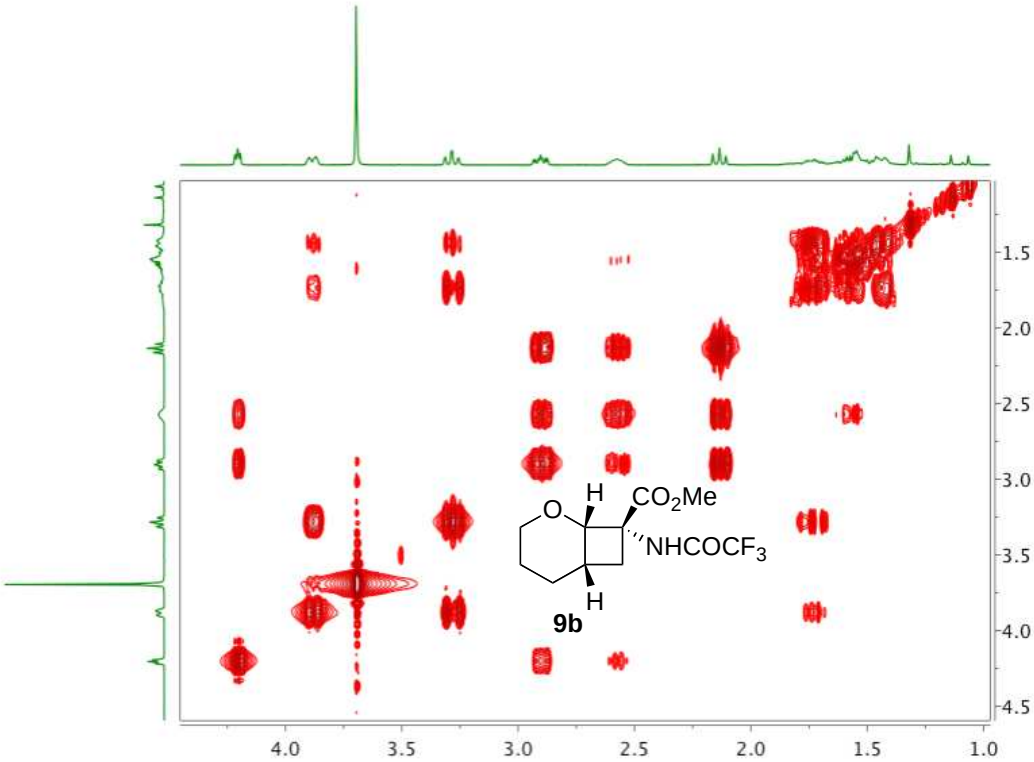
^{1}H NMR 400 MHz in $CDCl_3$ registered at 298K



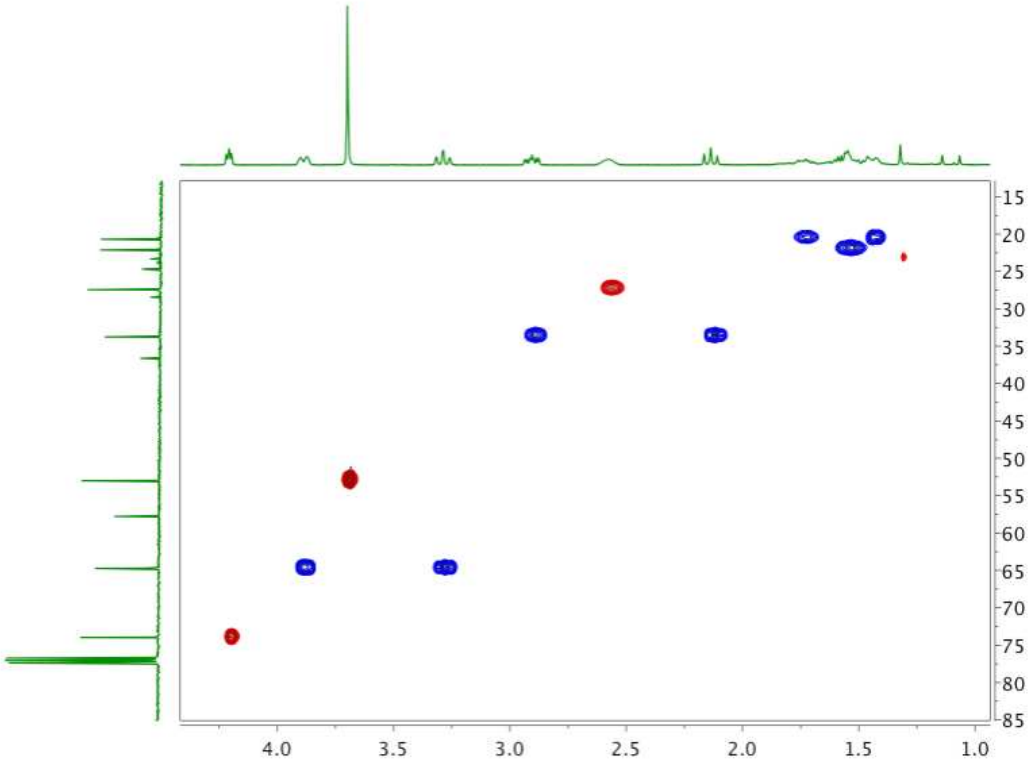
^{13}C NMR 100 MHz in $CDCl_3$ registered at 298K



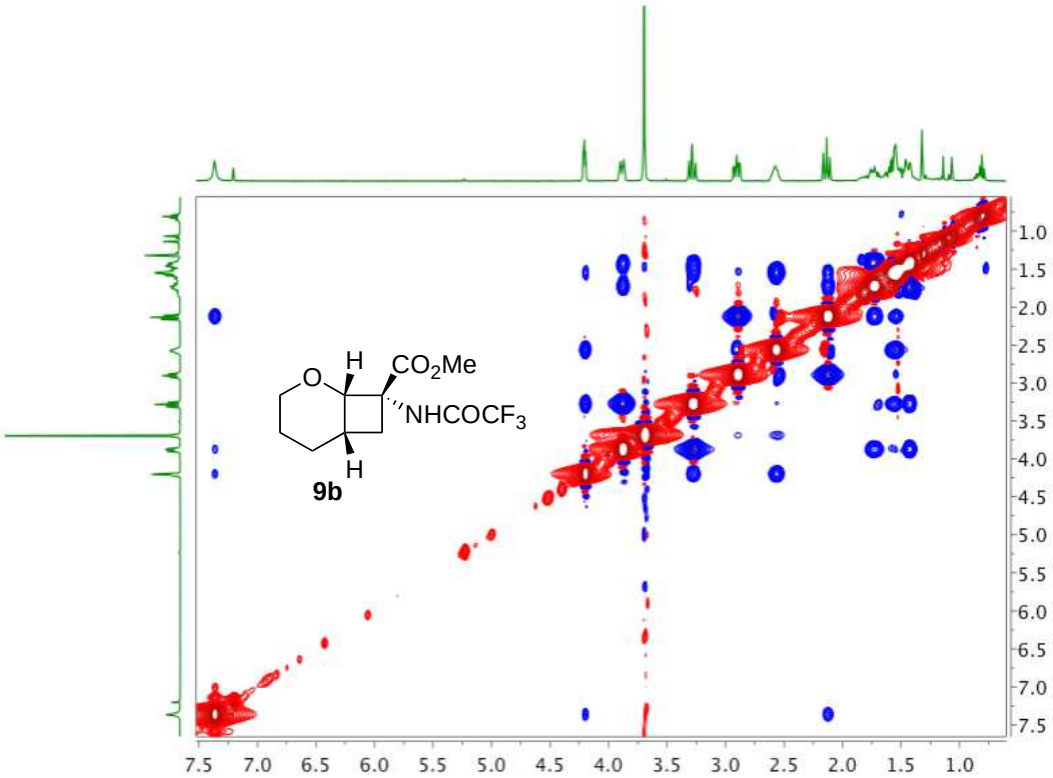
COSY in $CDCl_3$ registered at 298K



HSQC in $CDCl_3$ registered at 298K

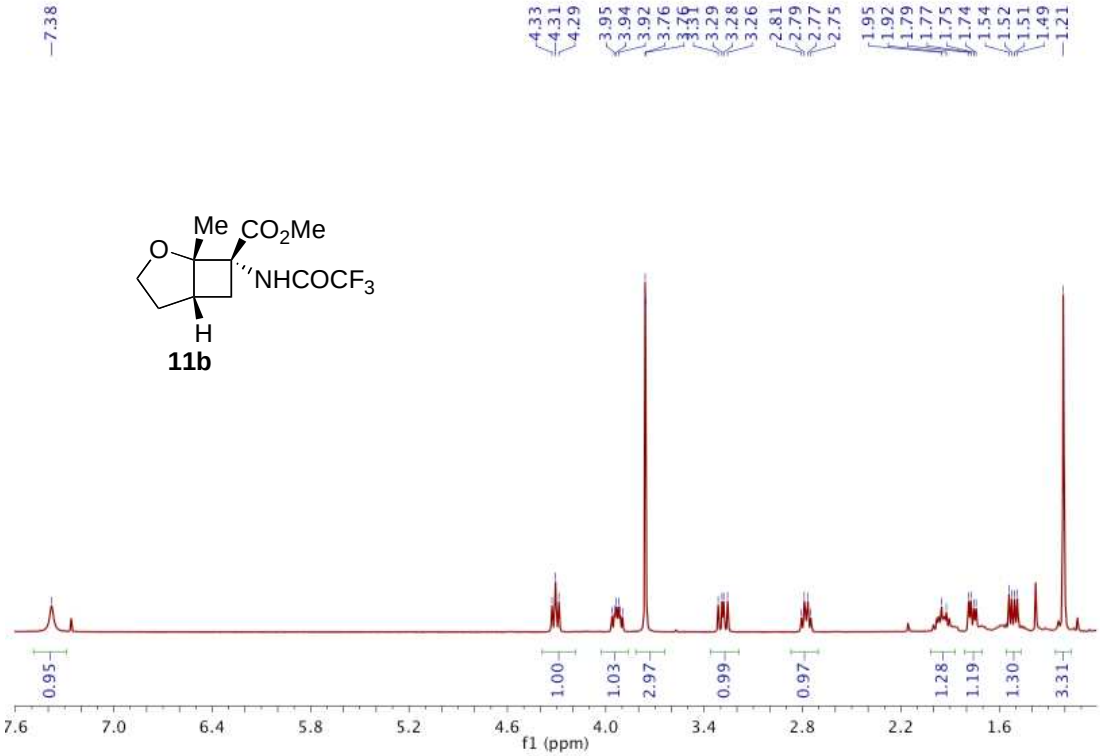


2D-NOESY (800 ms) in $CDCl_3$ registered at 298K

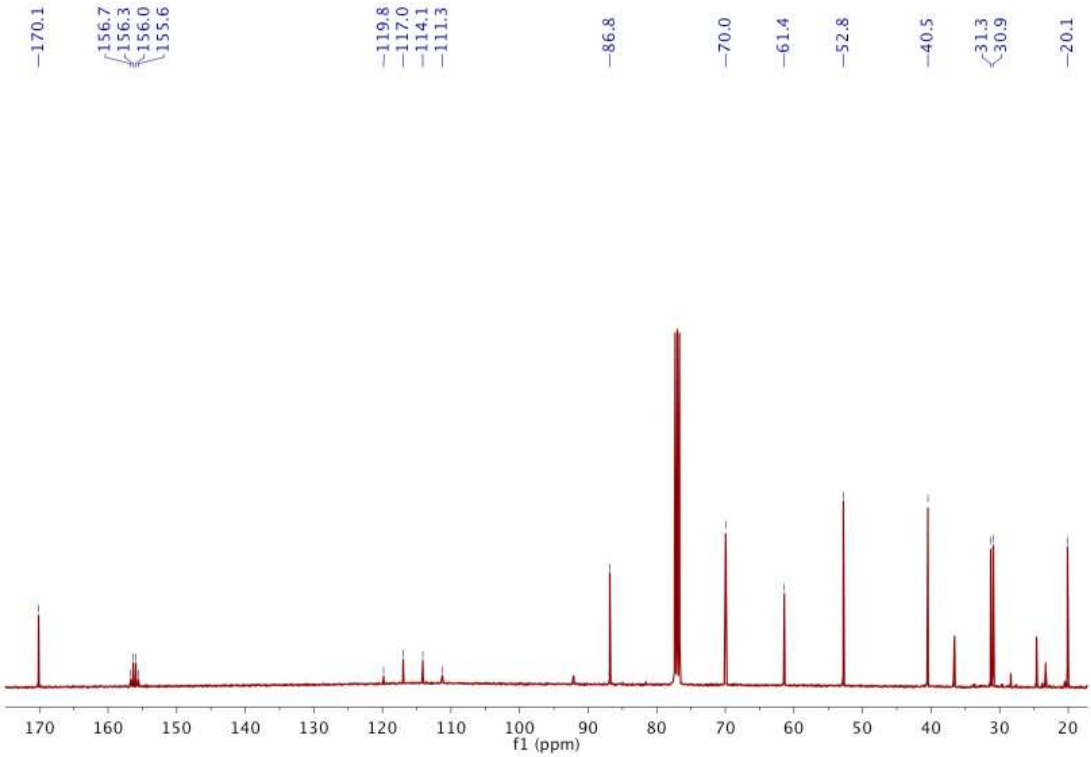


(1*S*,5*S*,7*R*)- and (1*R*,5*R*,7*S*)-1-Methyl-7-(2',2',2'-trifluoroacetamido)-2-oxabicyclo[3.2.0]heptan-7-carboxylic acid methyl ester (11b)

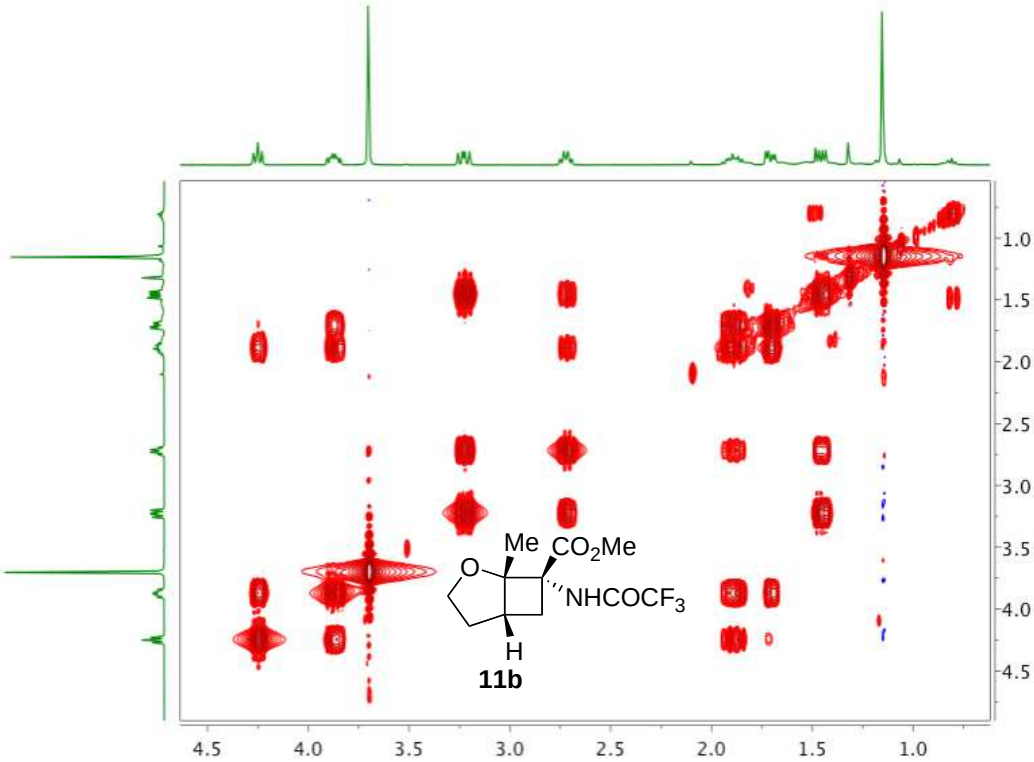
^{1}H NMR 400 MHz in $CDCl_3$ registered at 298K



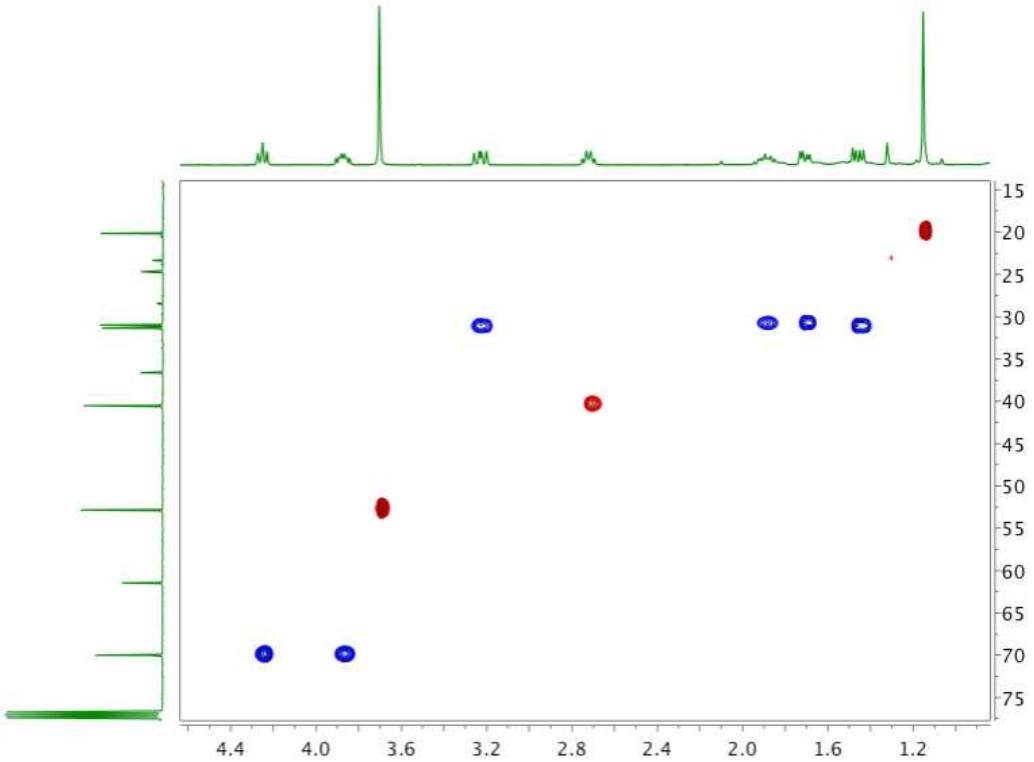
^{13}C NMR 100 MHz in $CDCl_3$ registered at 298K



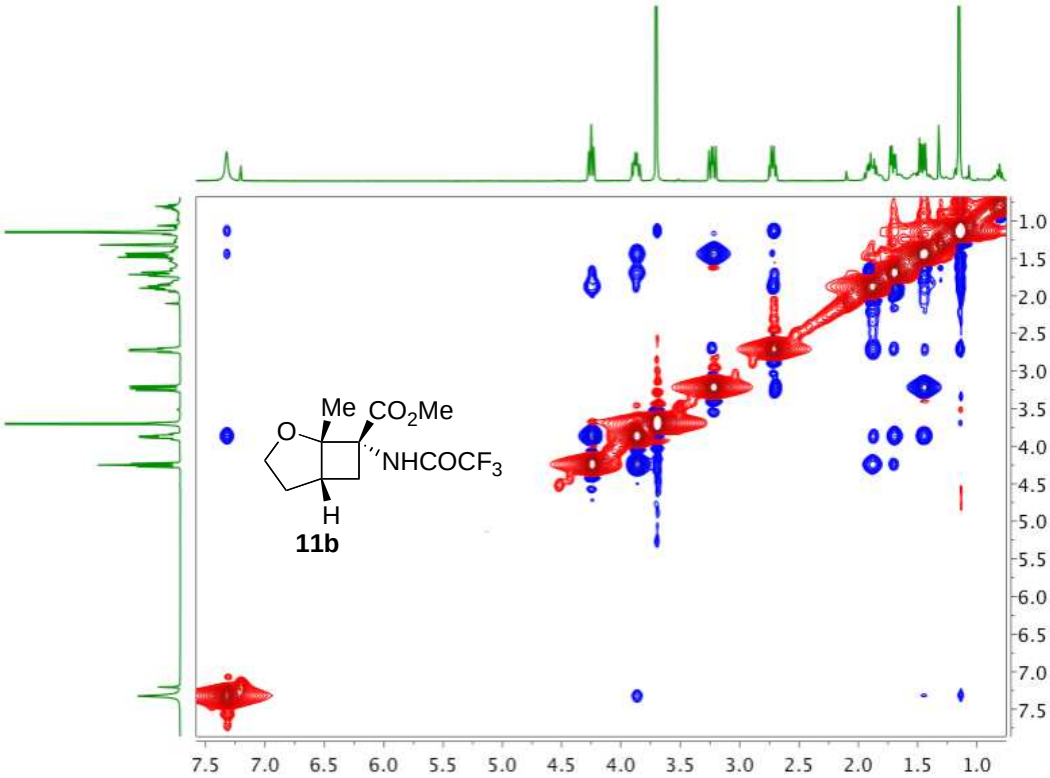
COSY in $CDCl_3$ registered at 298K



HSQC in $CDCl_3$ registered at 298K

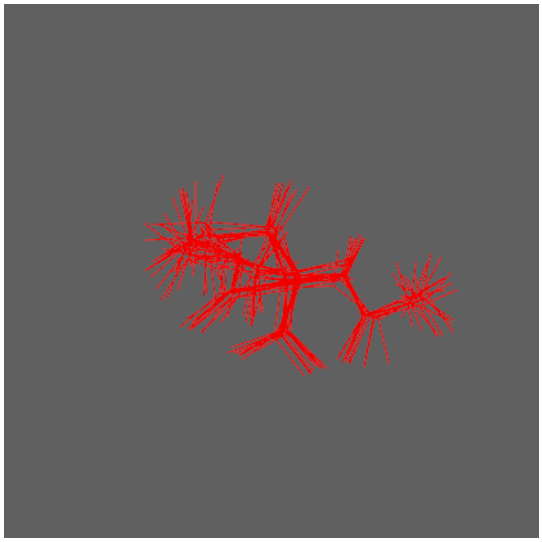


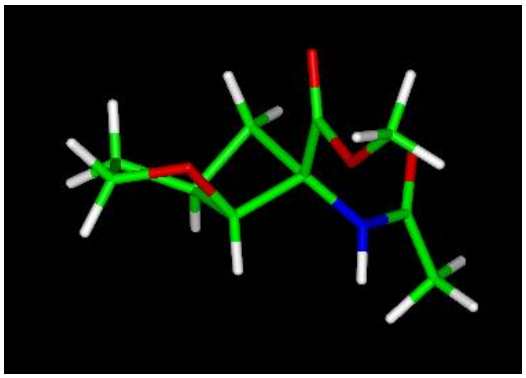
2D-NOESY (800 ms) in $CDCl_3$ registered at 298K



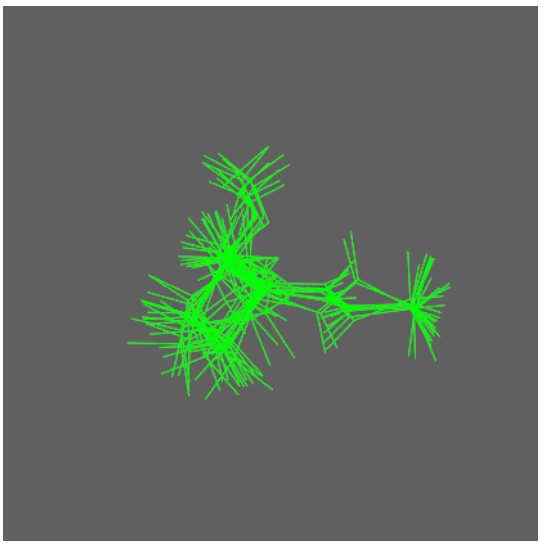
PDB files obtained from the 80 ns MD-tar simulations in implicit solvent (dielectric constant = 4 to simulate the $CHCl_3$ environment) are showed as 3D objects in the following figures (Adobe Reader 8.0 or higher is required).

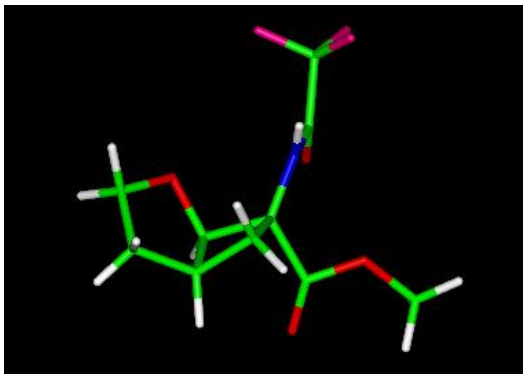
Compound 6a



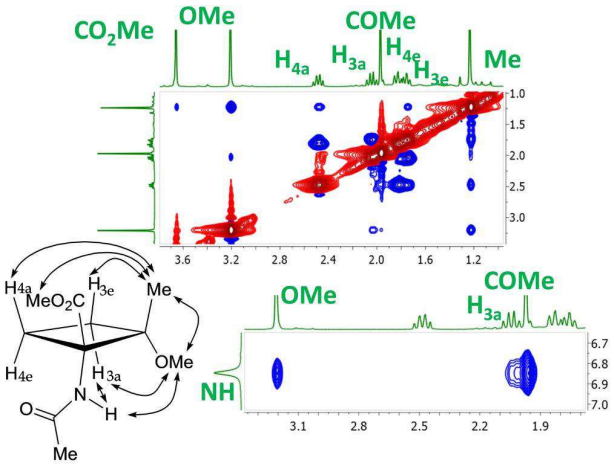


Compound 7b

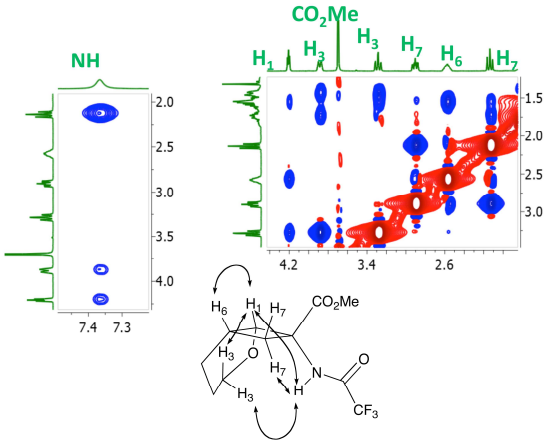




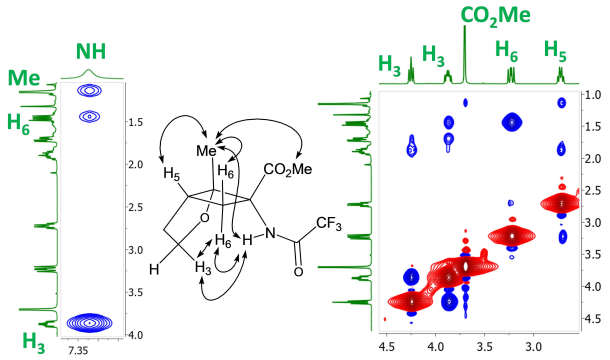
Figures corresponding to NOEs of compounds 5, 9b and 11b



NOE cross-peaks of compound **5**.

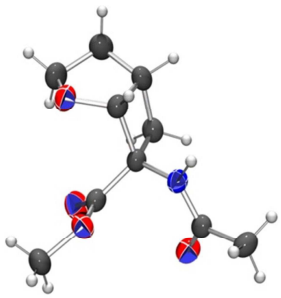


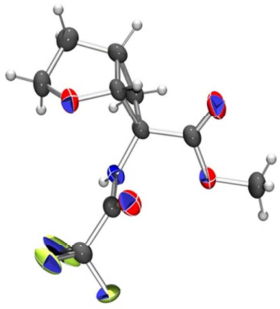
NOE cross-peaks of compound **9b**.

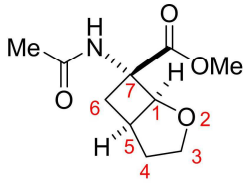


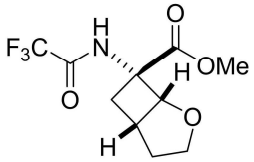
NOE cross-peaks of compound **11b**.

X-ray (ORTEP) of compounds 6a and 7b







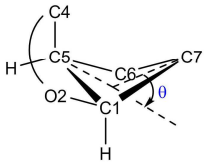


Compound **6a**

ϕ = CO-N-C7-CO = -60
ψ = N-C7-CO-O = -60
χ^1 = N-C7-C1-O2 = 142
χ^2 = C7-C1-O2-C3 = 88

Compound **7b**

ϕ = CO-N-C7-CO = 60
ψ = N-C7-CO-O = 30
χ^1 = N-C7-C1-O2 = -14
χ^2 = C7-C1-O2-C3 = -83



Atom coordinates for compounds 6a and 7b

PDB files of one representative frame obtained from the 80 ns MD-tar simulations in implicit solvent (dielectric constant = 4 to simulatethe $CHCl_3$ environment)for compounds **6a** and **7b**.

Compound **6a**

```
ATOM      1  O3  M6A     1       2.334  -1.237   1.741  0.00  0.00
ATOM      2  C5  M6A     1       2.636  -0.109   1.516  0.00  0.00
ATOM      3  C13 M6A     1       3.619   0.567   2.380  0.00  0.00
ATOM      4 AH13 M6A     1       3.977  -0.149   3.097  0.00  0.00
ATOM      5 BH13 M6A     1       3.194   1.438   2.885  0.00  0.00
ATOM      6 CH13 M6A     1       4.444   0.918   1.797  0.00  0.00
ATOM      7  N1  M6A     1       1.959   0.678   0.696  0.00  0.00
ATOM      8  H1  M6A     1       2.322   1.627   0.681  0.00  0.00
ATOM      9  C8  M6A     1       0.583   0.433   0.074  0.00  0.00
ATOM     10  C4  M6A     1       0.346  -0.225  -1.327  0.00  0.00
ATOM     11  O2  M6A     1       1.190   0.471  -2.059  0.00  0.00
ATOM     12  C14 M6A     1       1.562   0.059  -3.392  0.00  0.00
ATOM     13 AH14 M6A     1       2.600   0.252  -3.523  0.00  0.00
ATOM     14 BH14 M6A     1       0.993   0.582  -4.094  0.00  0.00
ATOM     15 CH14 M6A     1       1.482  -1.079  -3.492  0.00  0.00
ATOM     16  O6  M6A     1      -0.238  -1.207  -1.745  0.00  0.00
ATOM     17  C9  M6A     1      -0.311   1.700   0.008  0.00  0.00
ATOM     18  H9  M6A     1       0.139   2.633  -0.088  0.00  0.00
ATOM     19  O7  M6A     1      -1.471   1.478  -0.912  0.00  0.00
ATOM     20  C12 M6A     1      -2.627   2.075  -0.264  0.00  0.00
ATOM     21 AH12 M6A     1      -2.700   3.138  -0.048  0.00  0.00
ATOM     22 BH12 M6A     1      -3.595   1.924  -0.835  0.00  0.00
ATOM     23  C15 M6A     1      -2.617   1.364   1.049  0.00  0.00
ATOM     24 AH15 M6A     1      -3.093   0.433   0.904  0.00  0.00
ATOM     25 BH15 M6A     1      -3.182   1.832   1.870  0.00  0.00
ATOM     26  C11 M6A     1      -1.096   1.180   1.284  0.00  0.00
ATOM     27  H11 M6A     1      -0.763   1.528   2.250  0.00  0.00
ATOM     28  C10 M6A     1      -0.613  -0.256   0.953  0.00  0.00
ATOM     29 AH10 M6A     1      -1.381  -0.782   0.345  0.00  0.00
ATOM     30 BH10 M6A     1      -0.235  -0.944   1.709  0.00  0.00
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Compound **7b**

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ATOM      1  C5  M7B     1       0.456   1.313  -1.083  0.00  0.00
ATOM      2  H5  M7B     1       0.585   2.380  -0.995  0.00  0.00
ATOM      3  O1  M7B     1      -0.802   0.872  -1.794  0.00  0.00
ATOM      4  C7  M7B     1      -0.471   0.541  -3.113  0.00  0.00
ATOM      5  H7A M7B     1      -1.264  -0.177  -3.441  0.00  0.00
ATOM      6  H7B M7B     1      -0.628   1.450  -3.718  0.00  0.00
ATOM      7  C14 M7B     1       0.976   0.025  -3.166  0.00  0.00
ATOM      8  H46 M7B     1       1.086  -1.056  -3.445  0.00  0.00
ATOM      9  H48 M7B     1       1.542   0.559  -3.891  0.00  0.00
ATOM     10  C13 M7B     1       1.498   0.288  -1.711  0.00  0.00
ATOM     11  H13 M7B     1       2.578   0.558  -1.679  0.00  0.00
ATOM     12  C12 M7B     1       1.051  -0.805  -0.679  0.00  0.00
ATOM     13  H42 M7B     1       1.911  -1.300  -0.256  0.00  0.00
ATOM     14  H44 M7B     1       0.521  -1.605  -1.228  0.00  0.00
ATOM     15  C8  M7B     1       0.362   0.301   0.126  0.00  0.00
ATOM     16  C9  M7B     1       1.635   0.818   0.955  0.00  0.00
ATOM     17  O4  M7B     1       1.419   0.140   2.103  0.00  0.00
ATOM     18  C16 M7B     1       2.267   0.497   3.286  0.00  0.00
ATOM     19  H50 M7B     1       2.072  -0.238   4.067  0.00  0.00
ATOM     20  H52 M7B     1       2.003   1.524   3.551  0.00  0.00
ATOM     21  H54 M7B     1       3.291   0.629   2.975  0.00  0.00
ATOM     22  O6  M7B     1       2.545   1.633   0.776  0.00  0.00
ATOM     23  N3  M7B     1      -0.977  -0.080   0.743  0.00  0.00
ATOM     24  H3  M7B     1      -1.358  -1.000   0.612  0.00  0.00
ATOM     25  C10 M7B     1      -1.761   0.777   1.422  0.00  0.00
ATOM     26  O2  M7B     1      -1.359   1.905   1.660  0.00  0.00
ATOM     27  C11 M7B     1      -3.245   0.264   1.583  0.00  0.00
ATOM     28  F58 M7B     1      -3.942   0.902   2.584  0.00  0.00
ATOM     29  F60 M7B     1      -3.280  -1.026   2.011  0.00  0.00
ATOM     30  F56 M7B     1      -3.902   0.415   0.415  0.00  0.00
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