

Exploring Chemical Diversity through Cascade Wagner-Meerwein Remodelling of Caryophyllene β -Lactam Derivates

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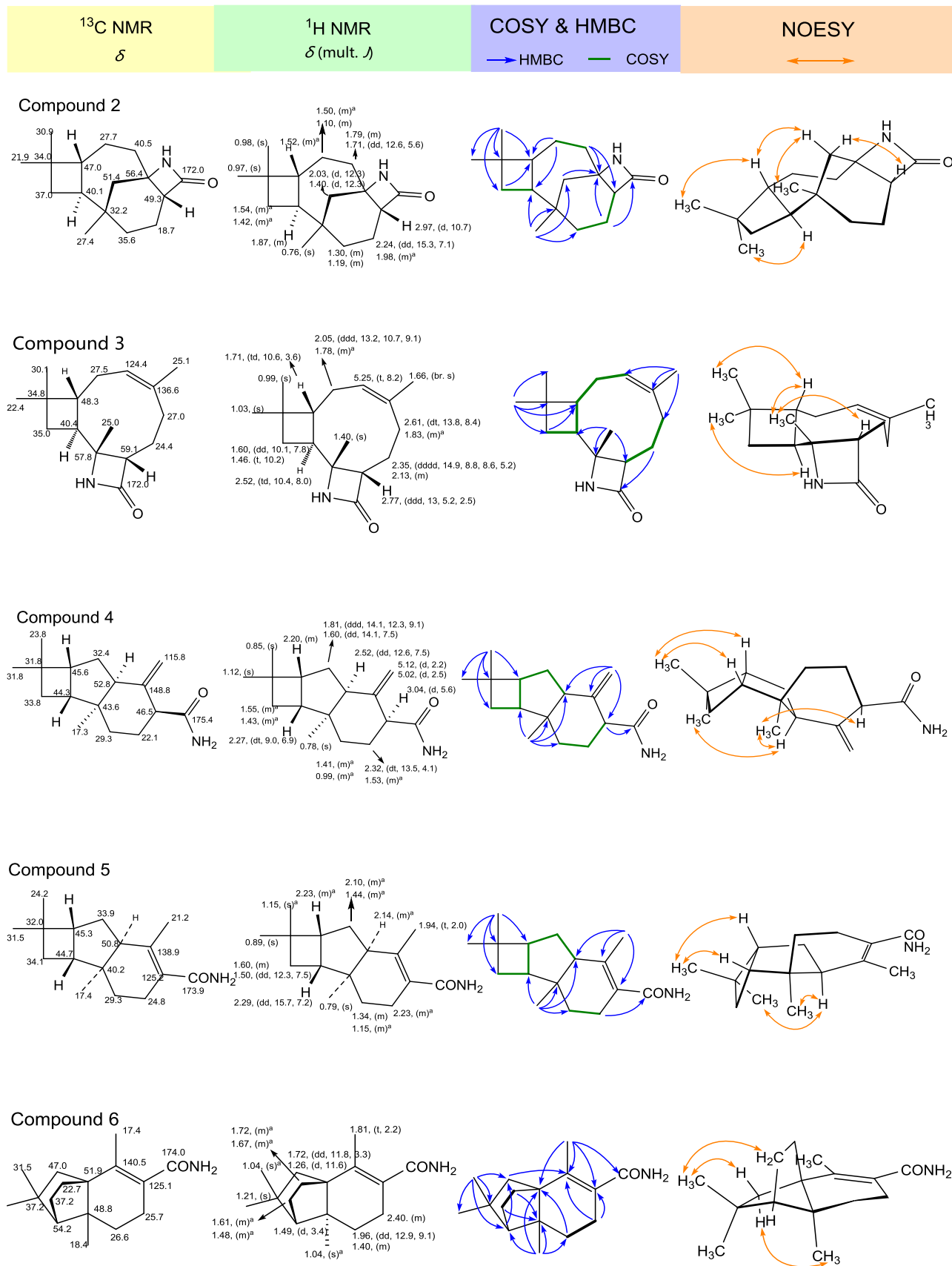
² State Key Laboratory of Medicinal Chemical Biology, Nankai University, Tianjin 300071, PR China.

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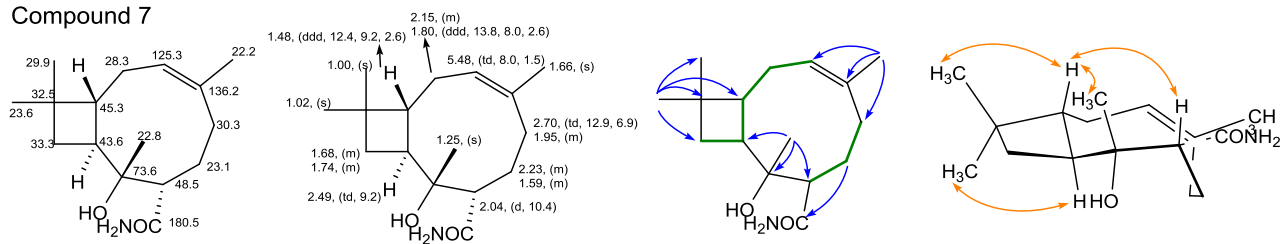
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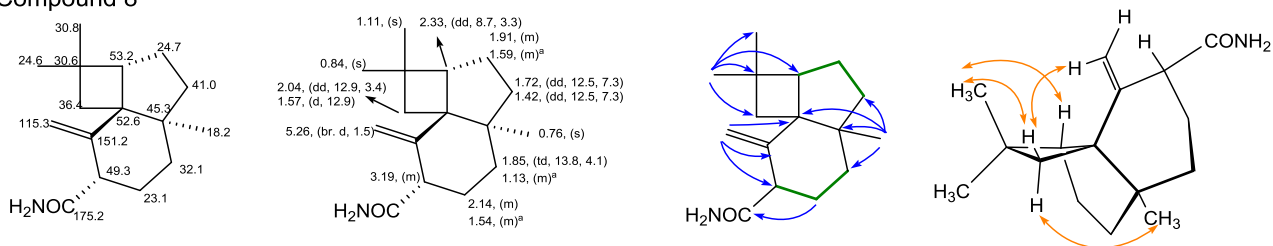
Fig S1: δ_C , δ_H and key correlations in 2D NMR of products



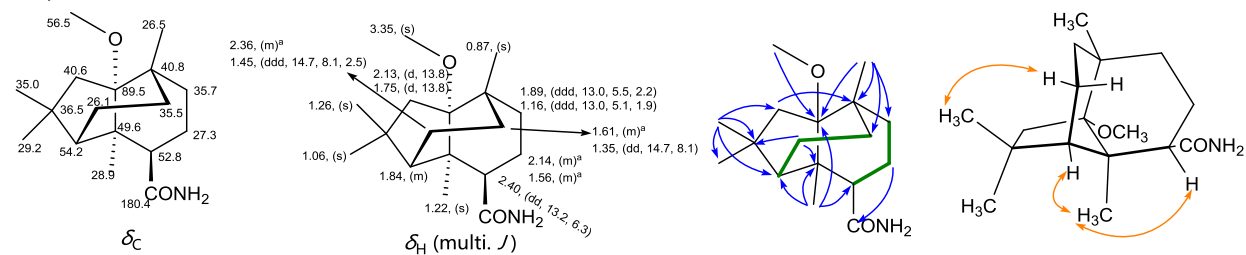
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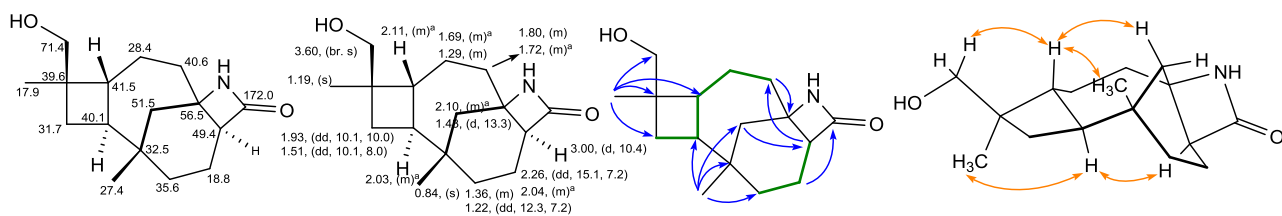
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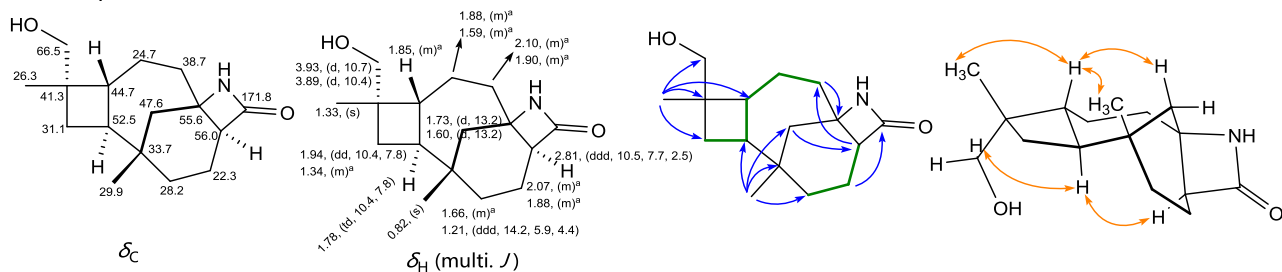
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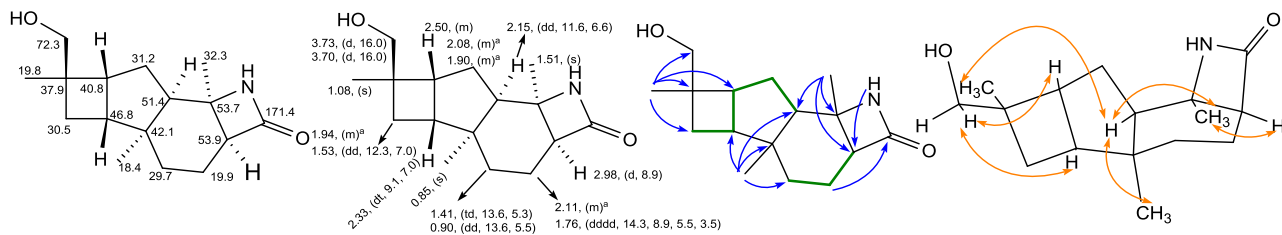
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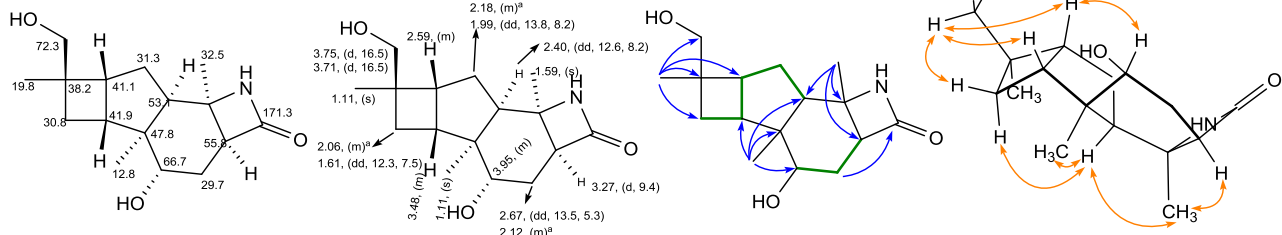
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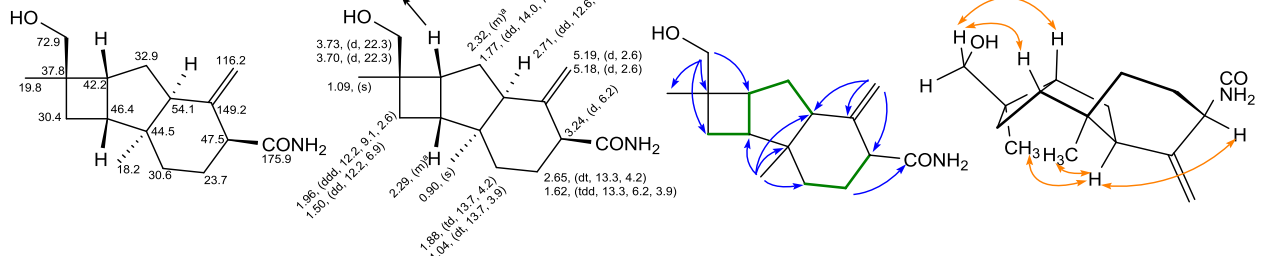
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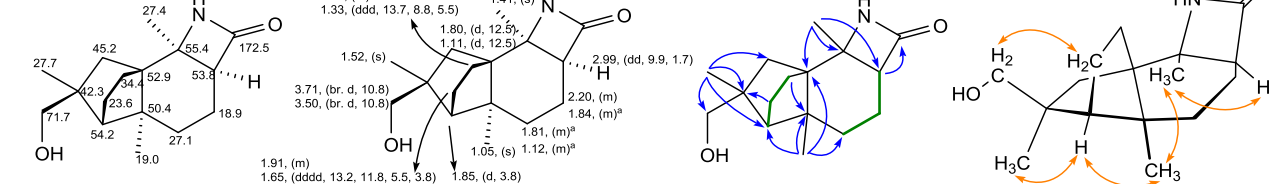
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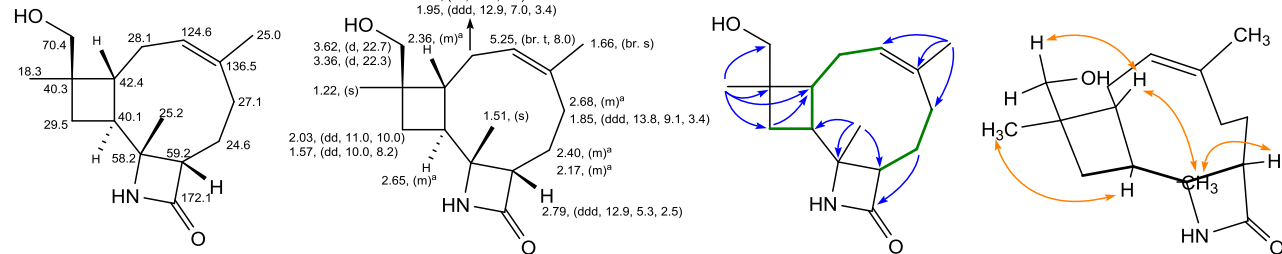
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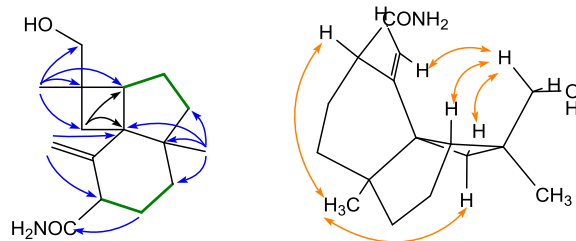
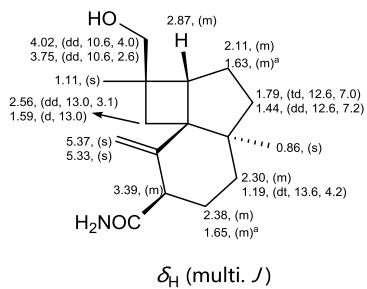
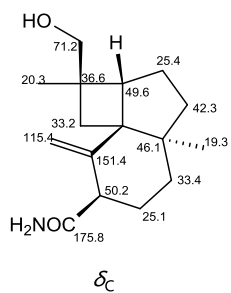
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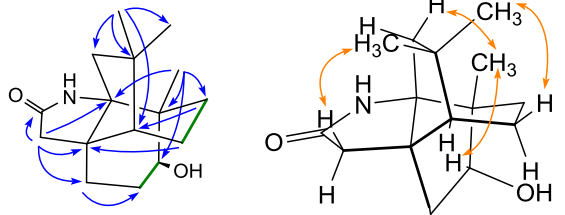
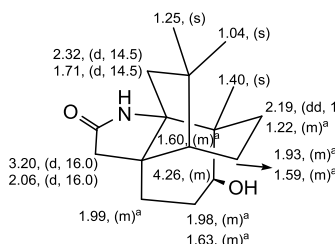
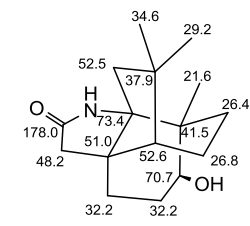
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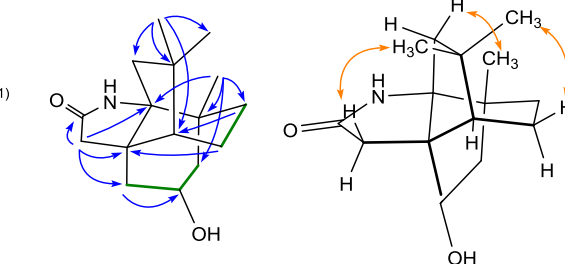
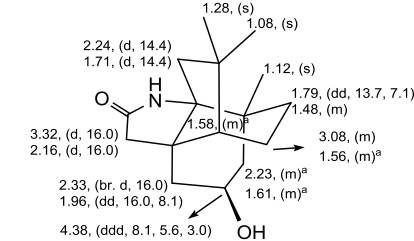
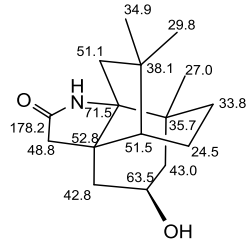
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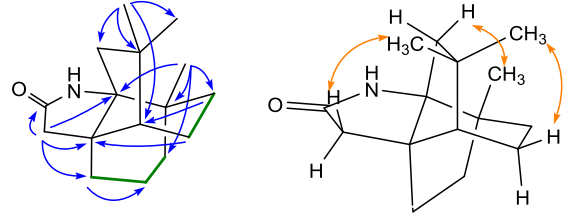
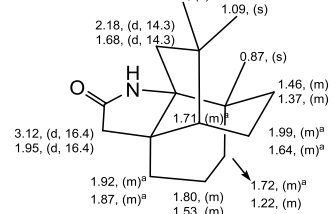
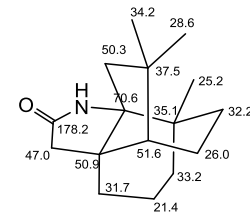
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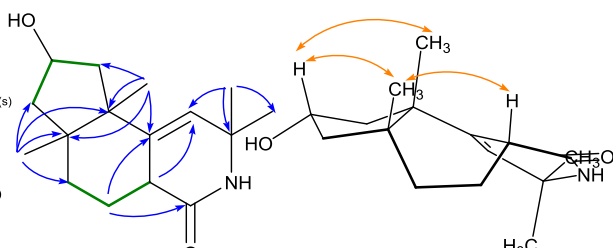
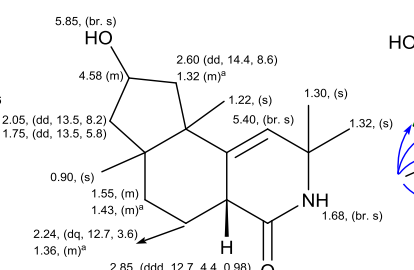
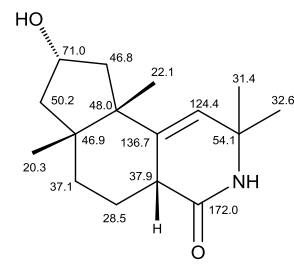
Compound 19



Compound 20

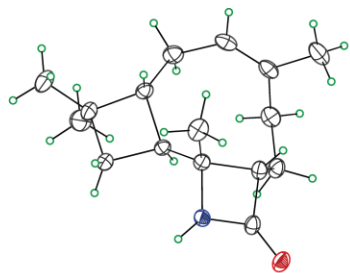


Compound 21

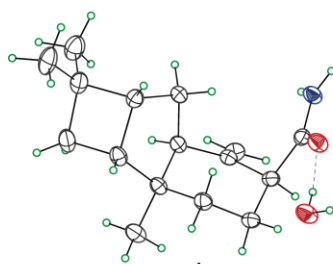


^a overlapped

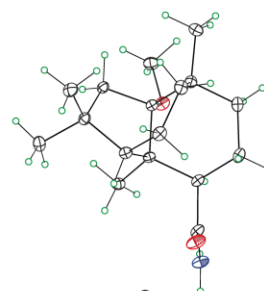
Figure S2 X-ray ORTEP views



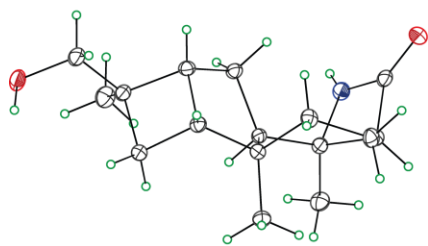
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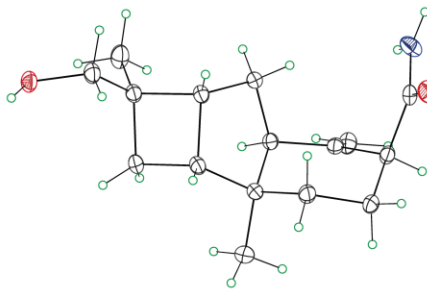
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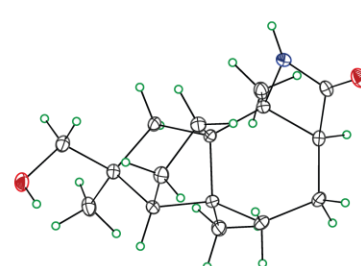
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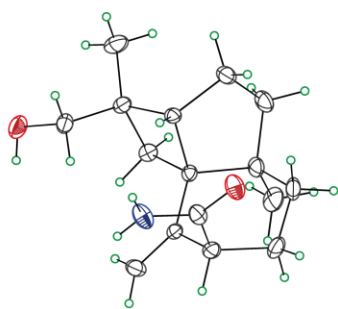
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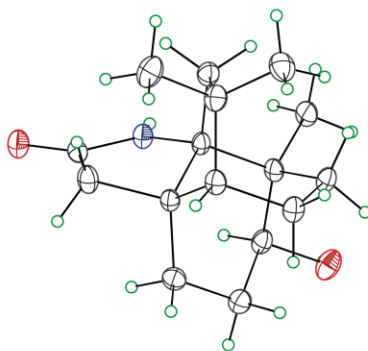
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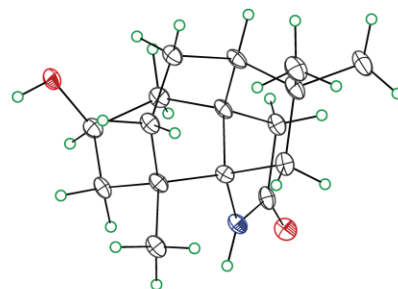
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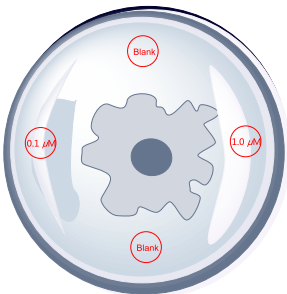


18



19

Figure S3. Anti-phytopathogenic fungus bioassay result



schematic diagram



Compound 4



Compound 8



Compound 16

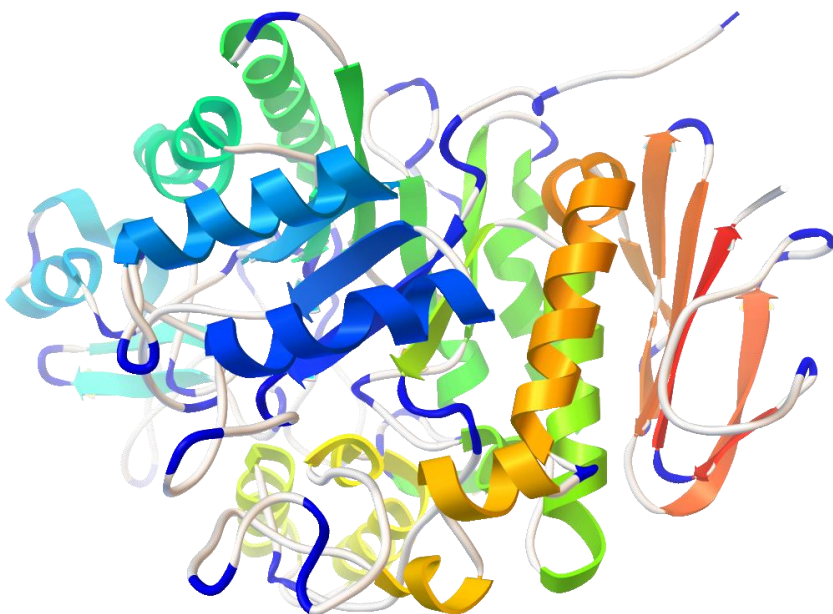


Compound 17



Positive control: hymexazol

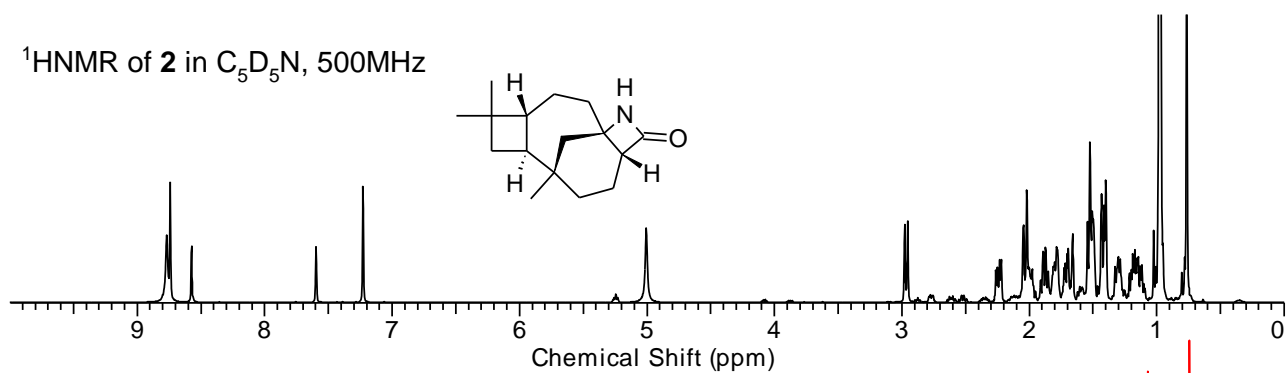
Figure S4. Homology model of α -glucosidase



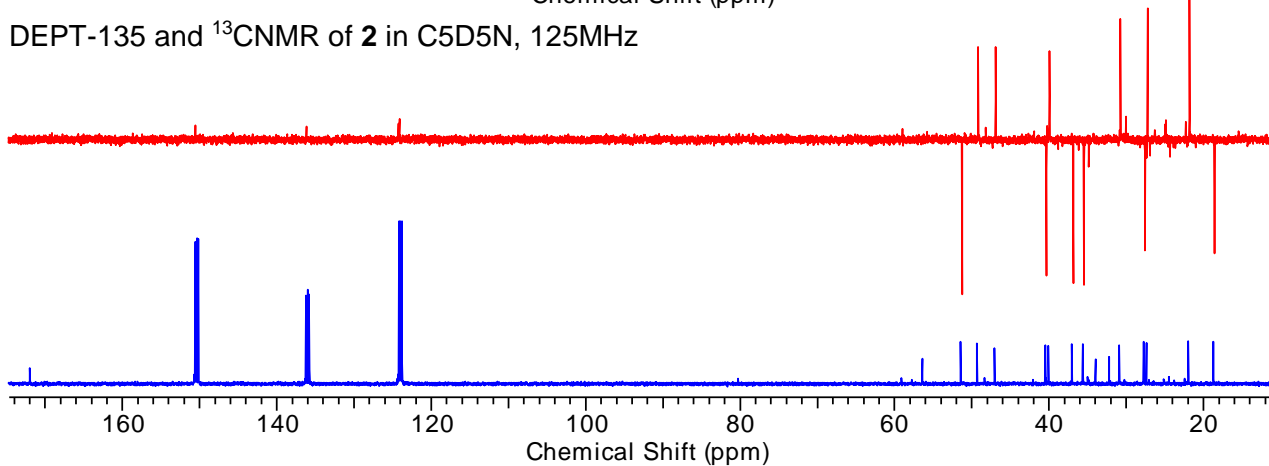
NMR spectra

Compound 2

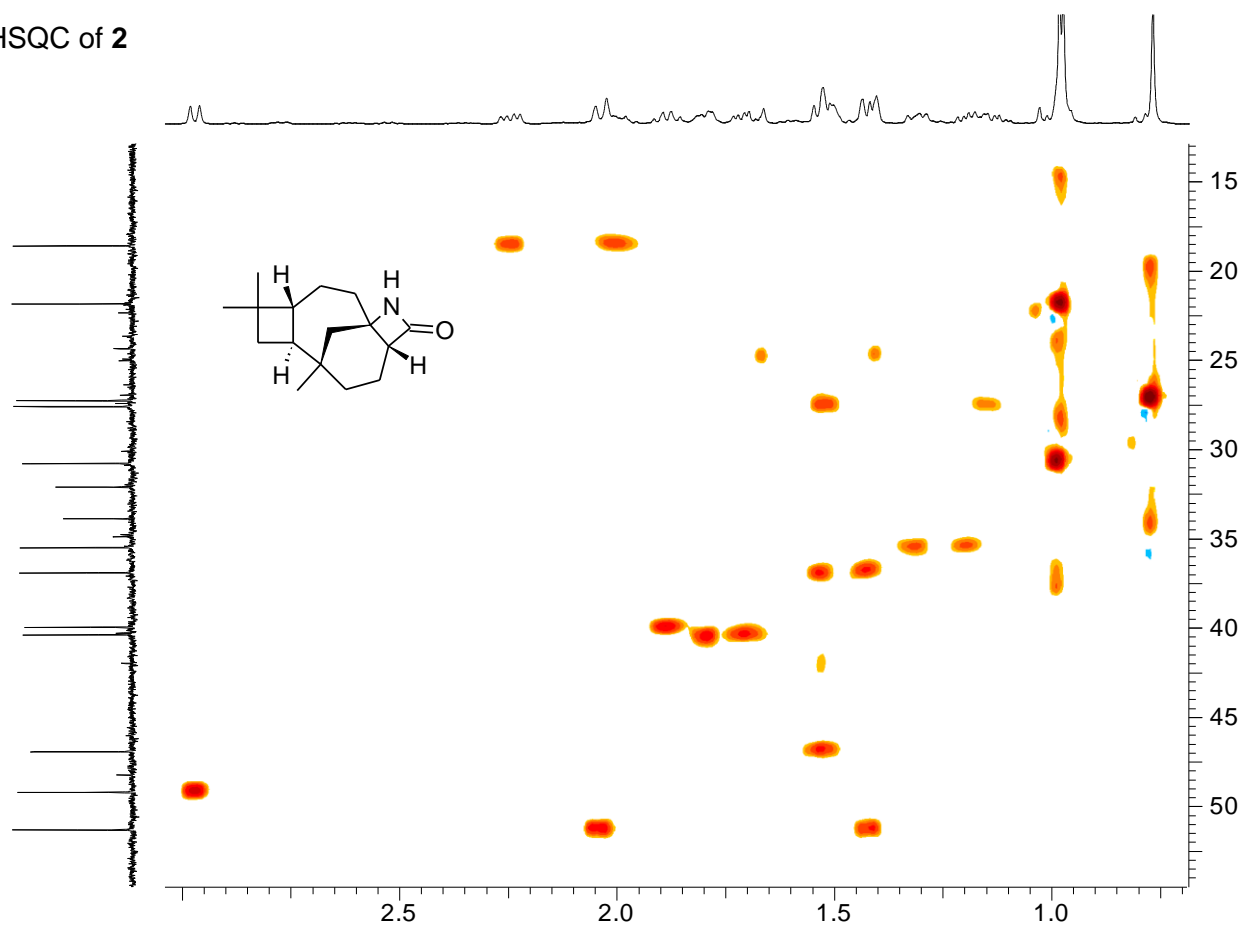
^1H NMR of **2** in $\text{C}_5\text{D}_5\text{N}$, 500MHz



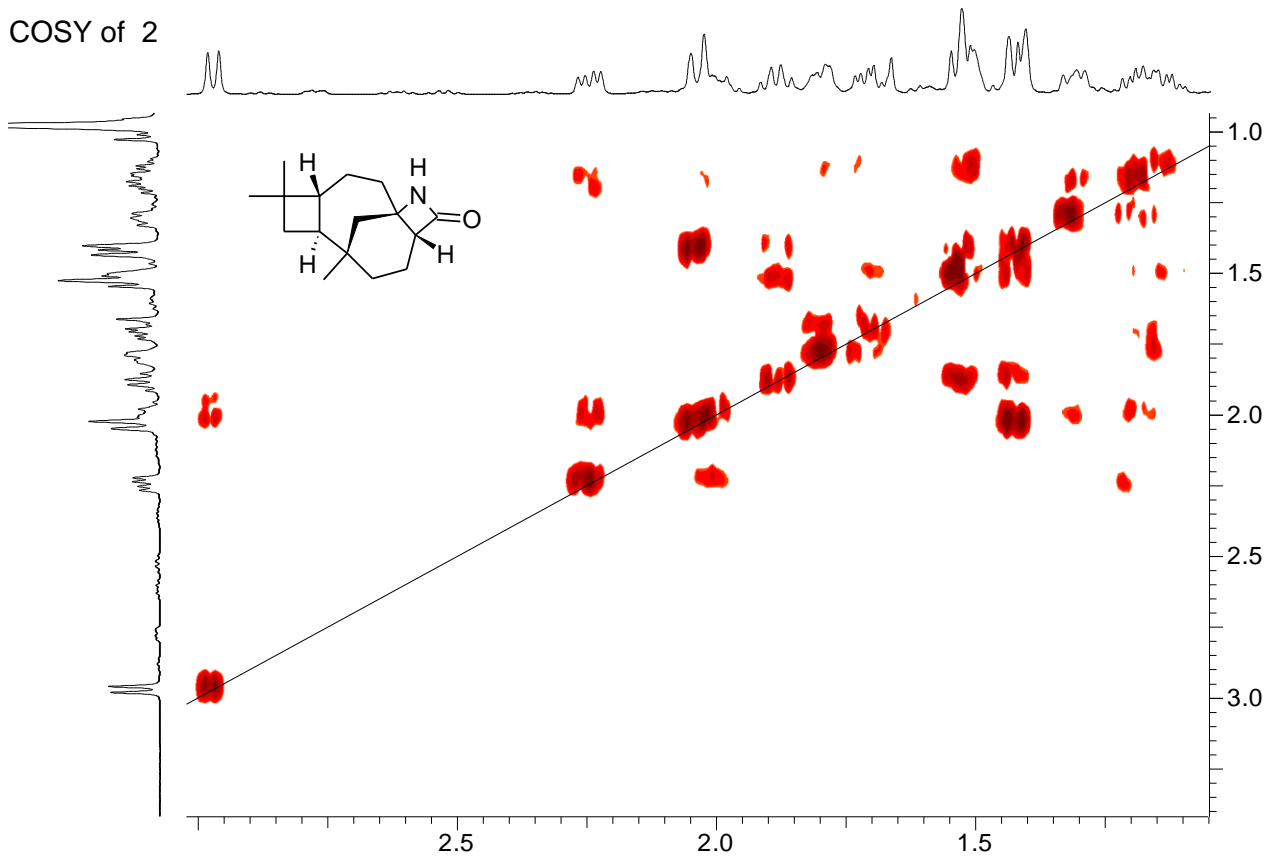
DEPT-135 and ^{13}C NMR of **2** in $\text{C}_5\text{D}_5\text{N}$, 125MHz



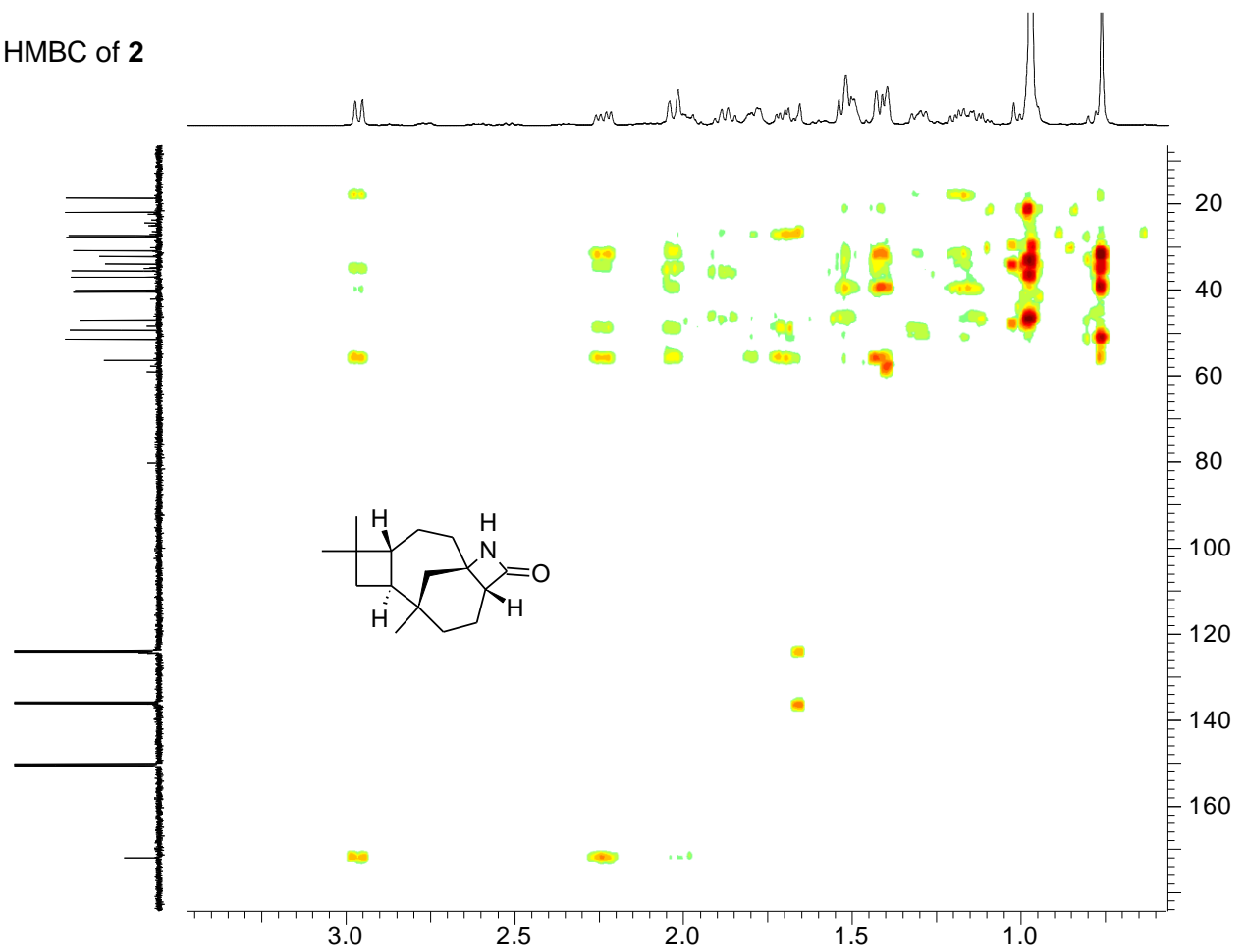
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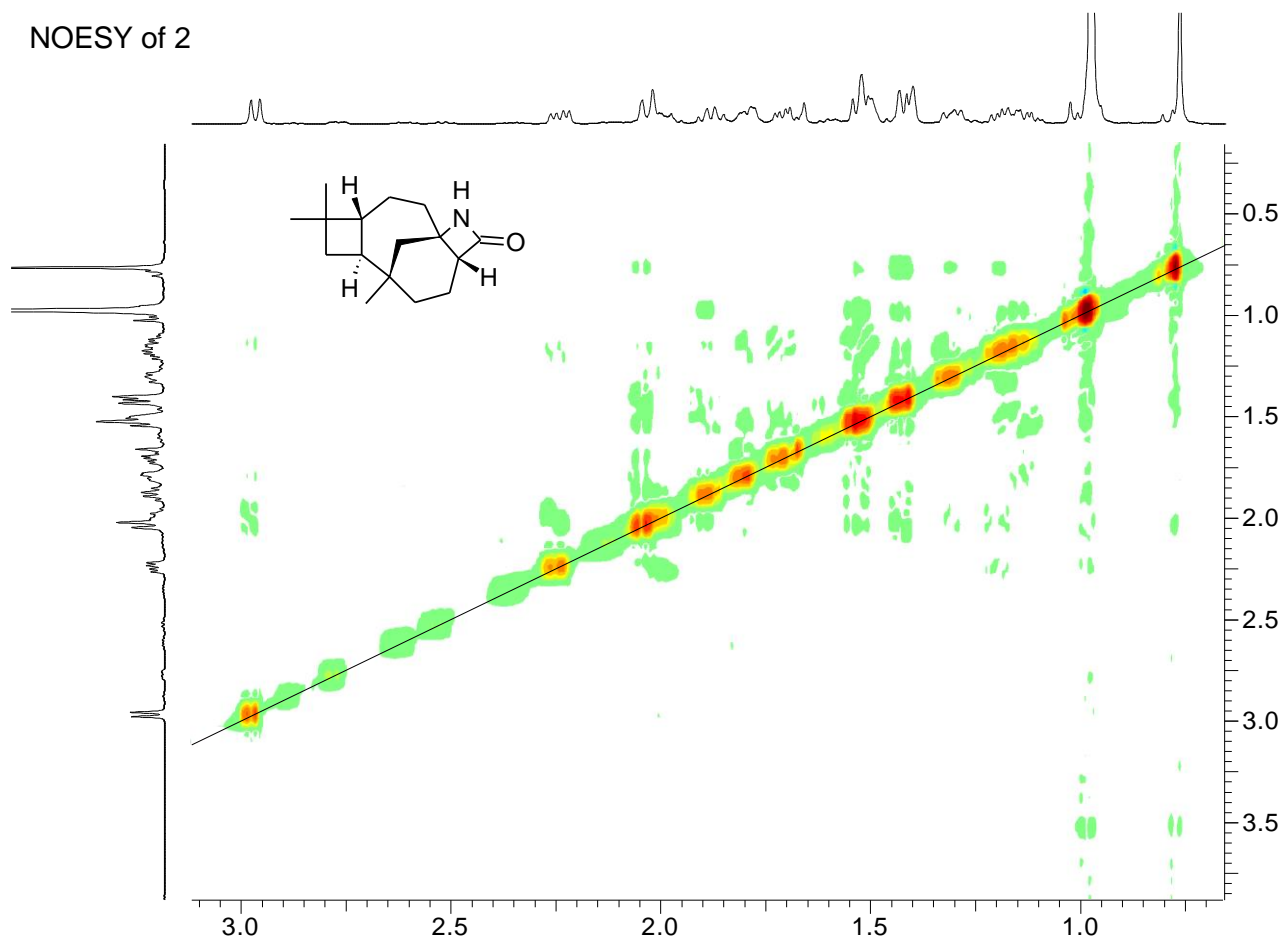
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HMBC of 2

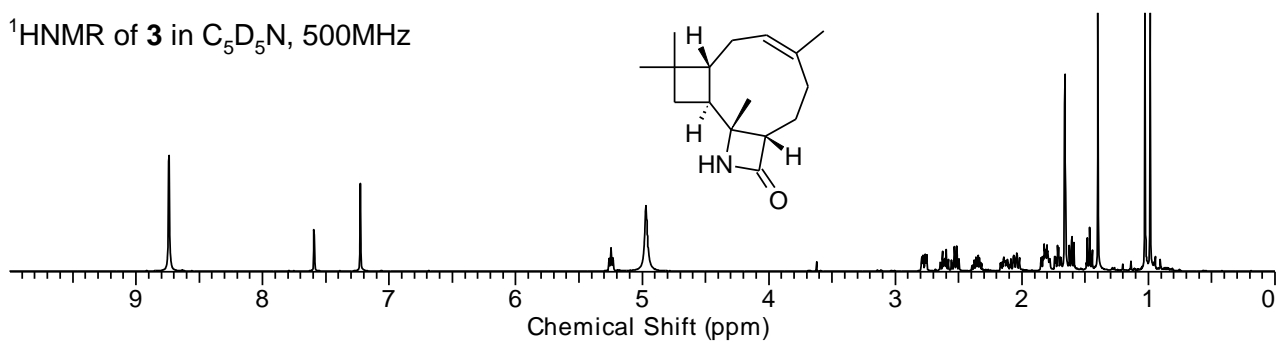


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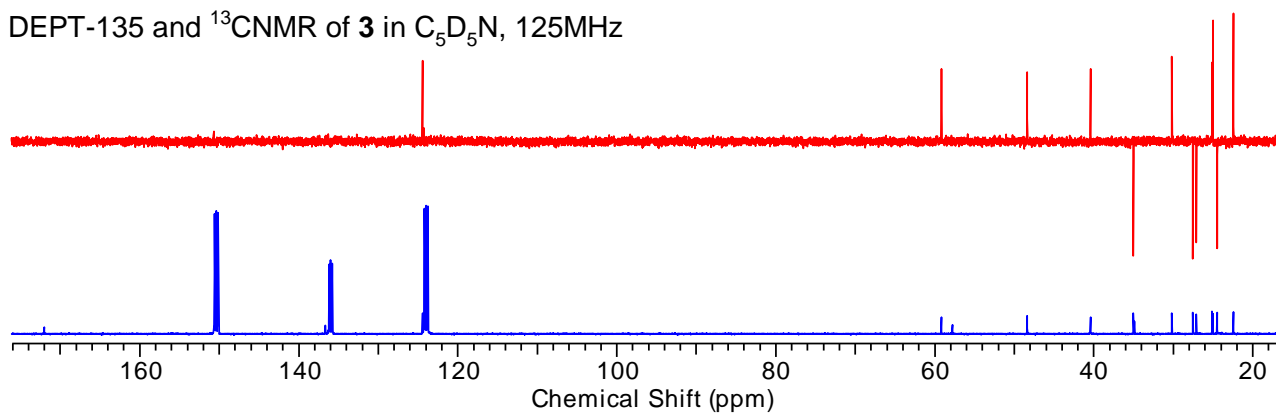


Compound 3

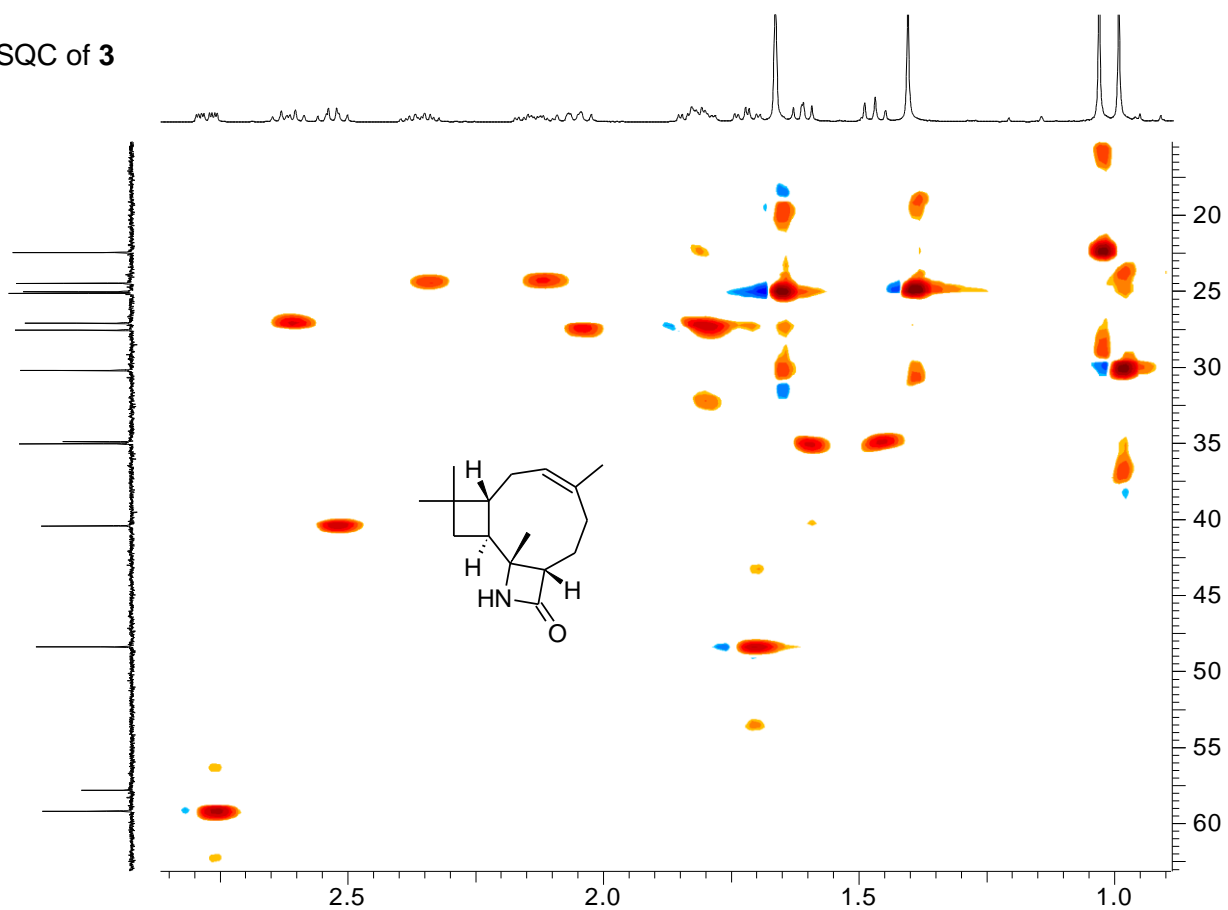
¹H NMR of 3 in C₅D₅N, 500MHz



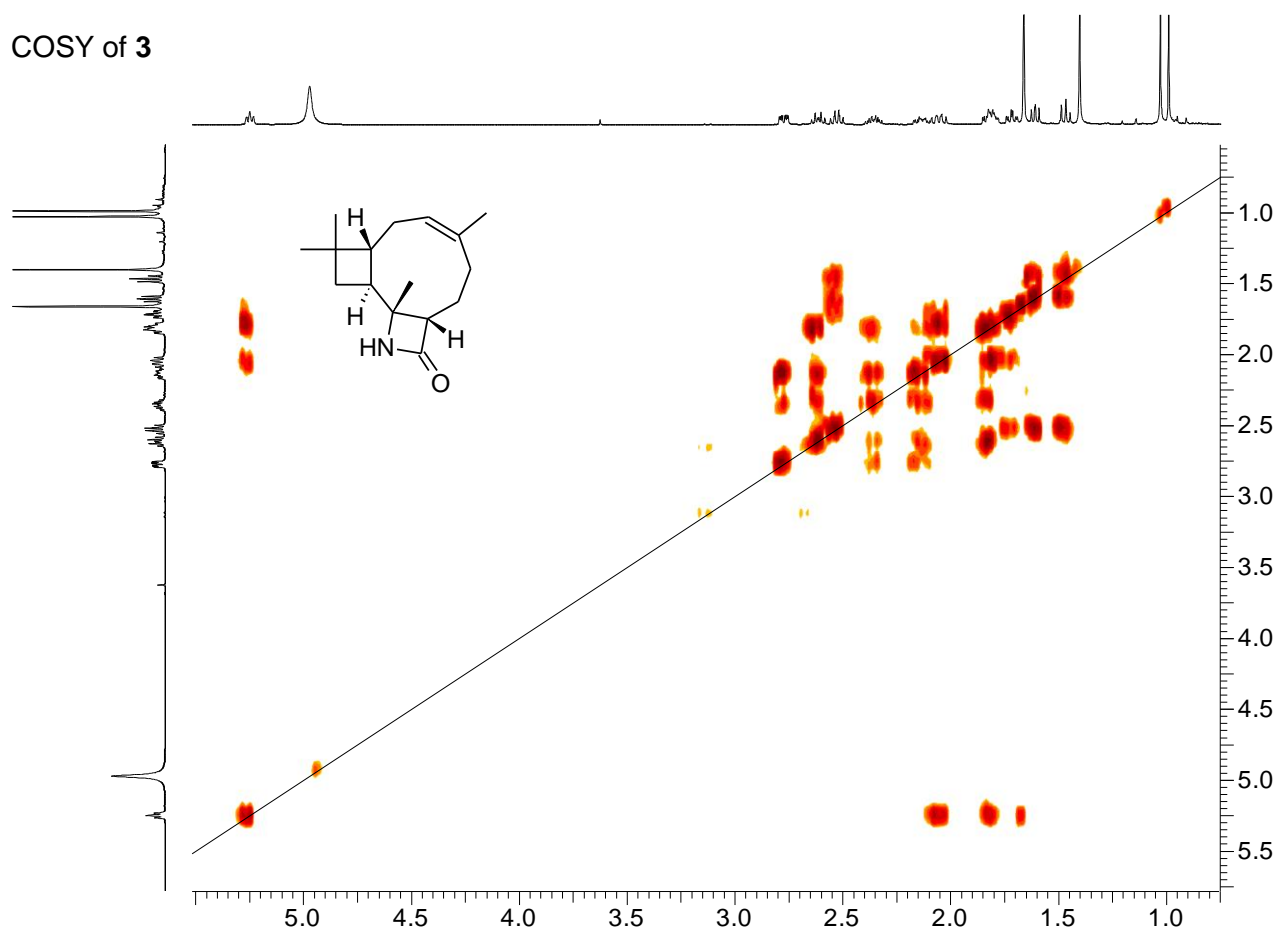
DEPT-135 and ¹³C NMR of 3 in C₅D₅N, 125MHz



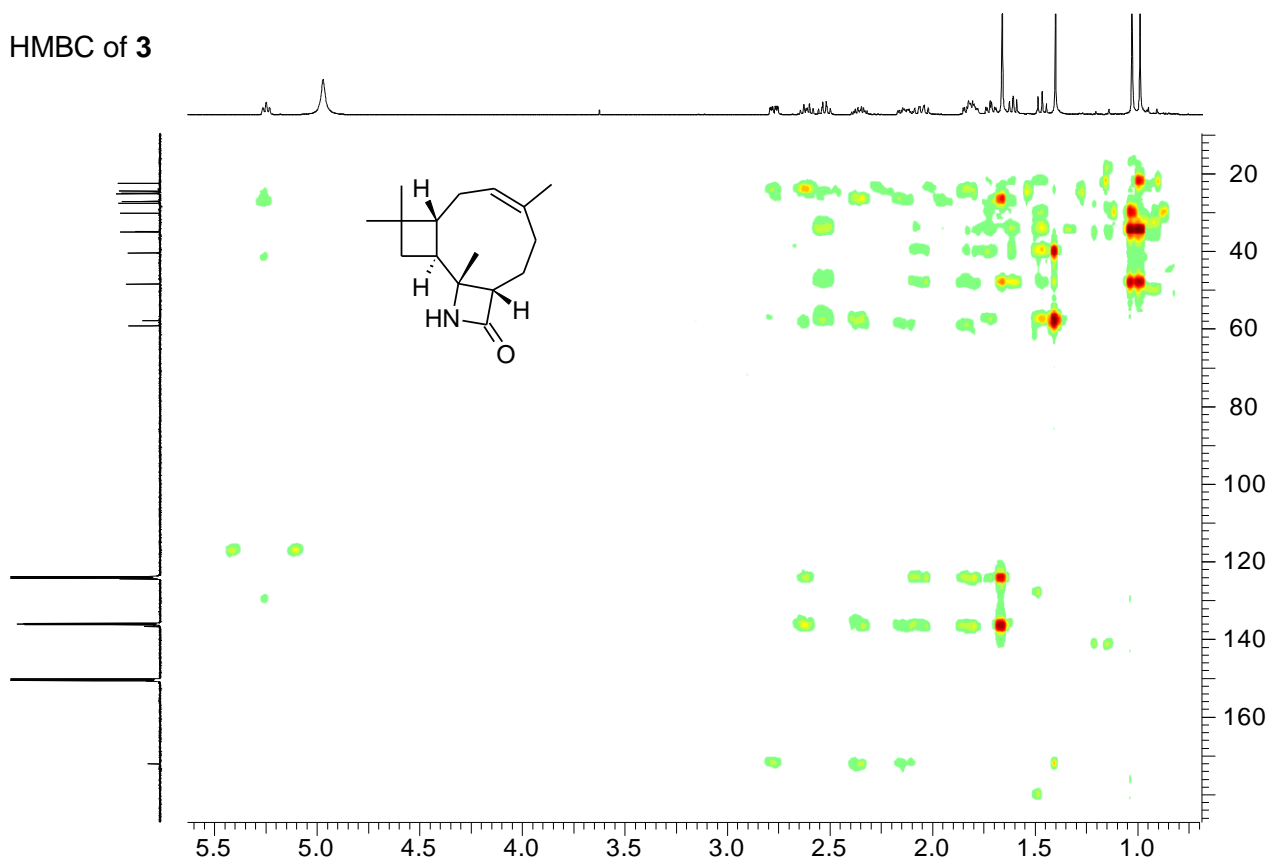
HSQC of 3



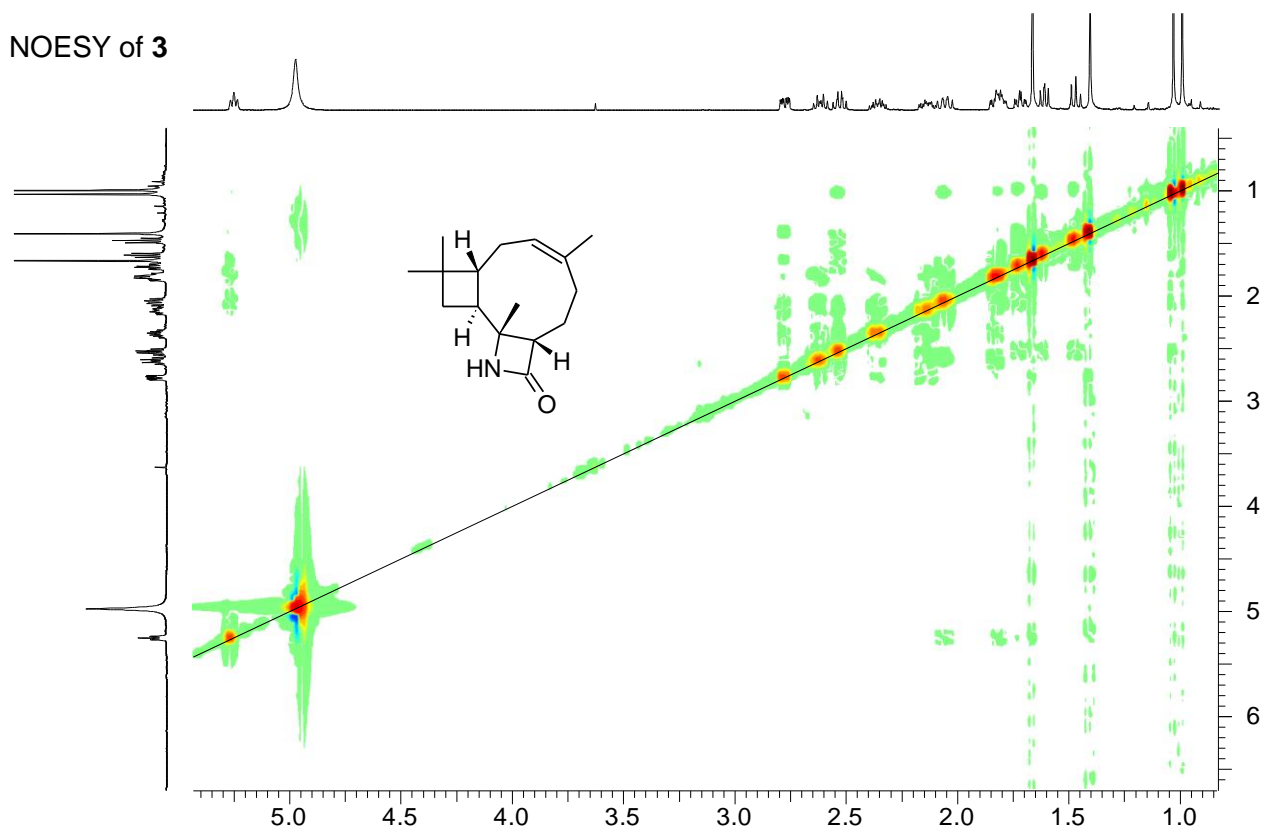
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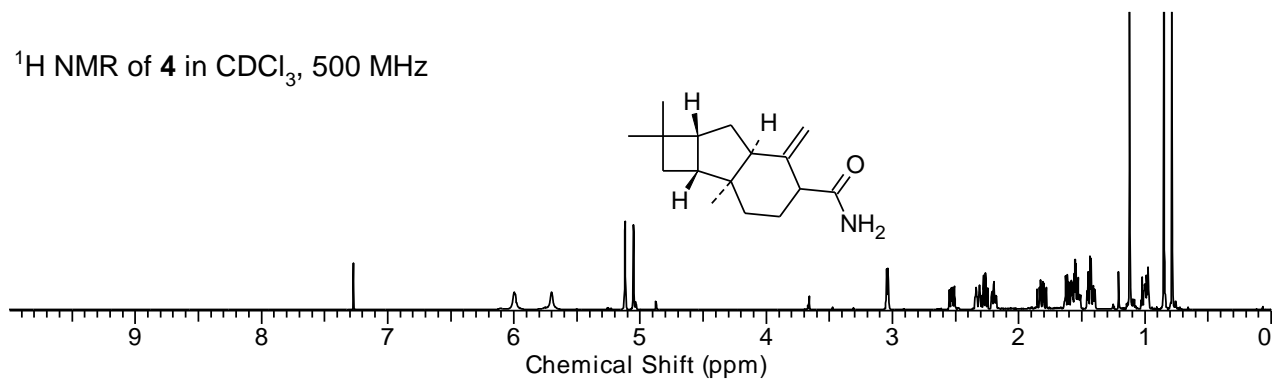


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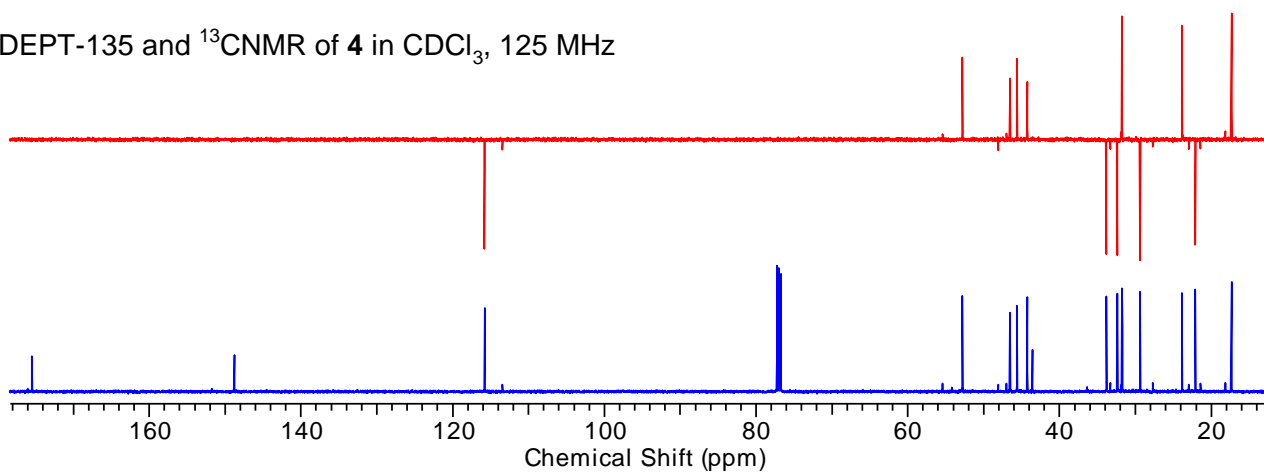


Compound 4

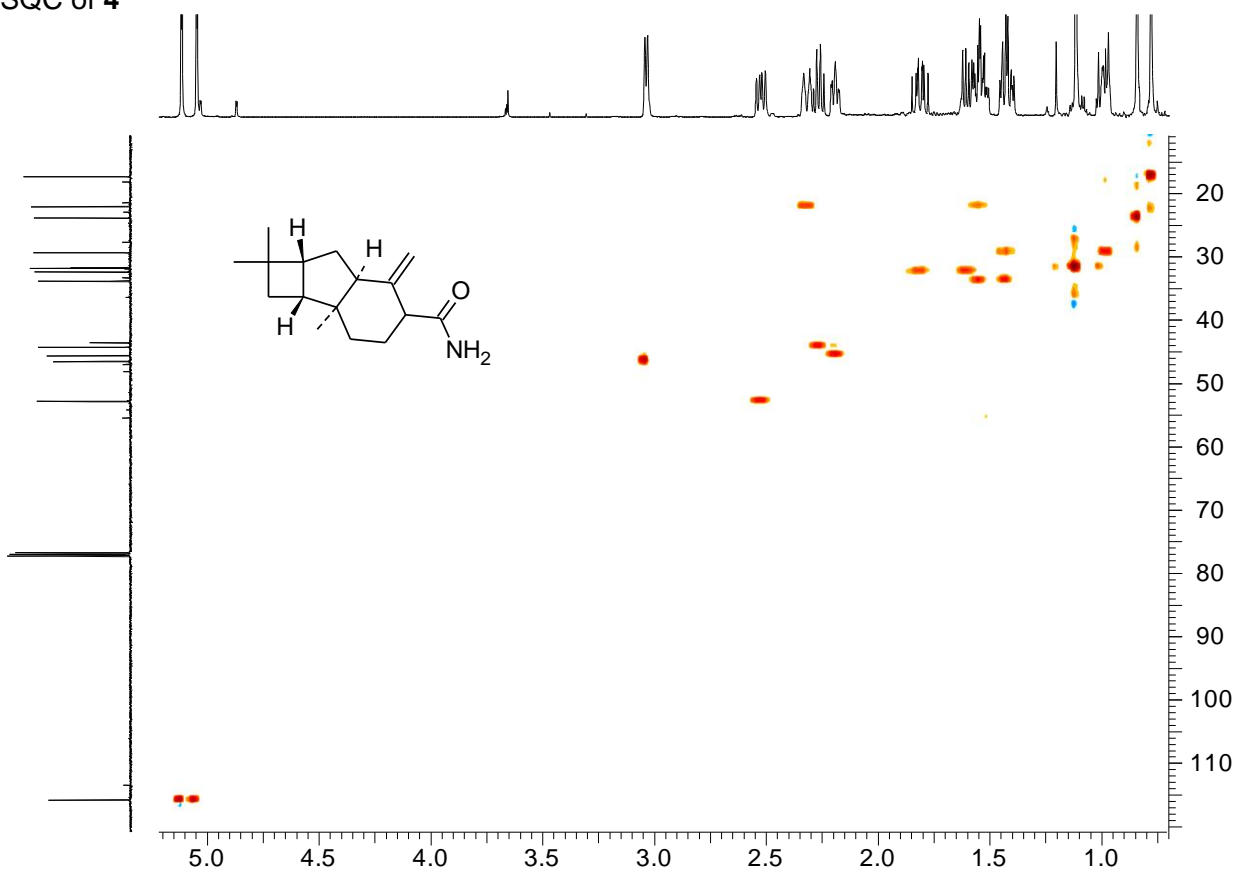
^1H NMR of **4** in CDCl_3 , 500 MHz



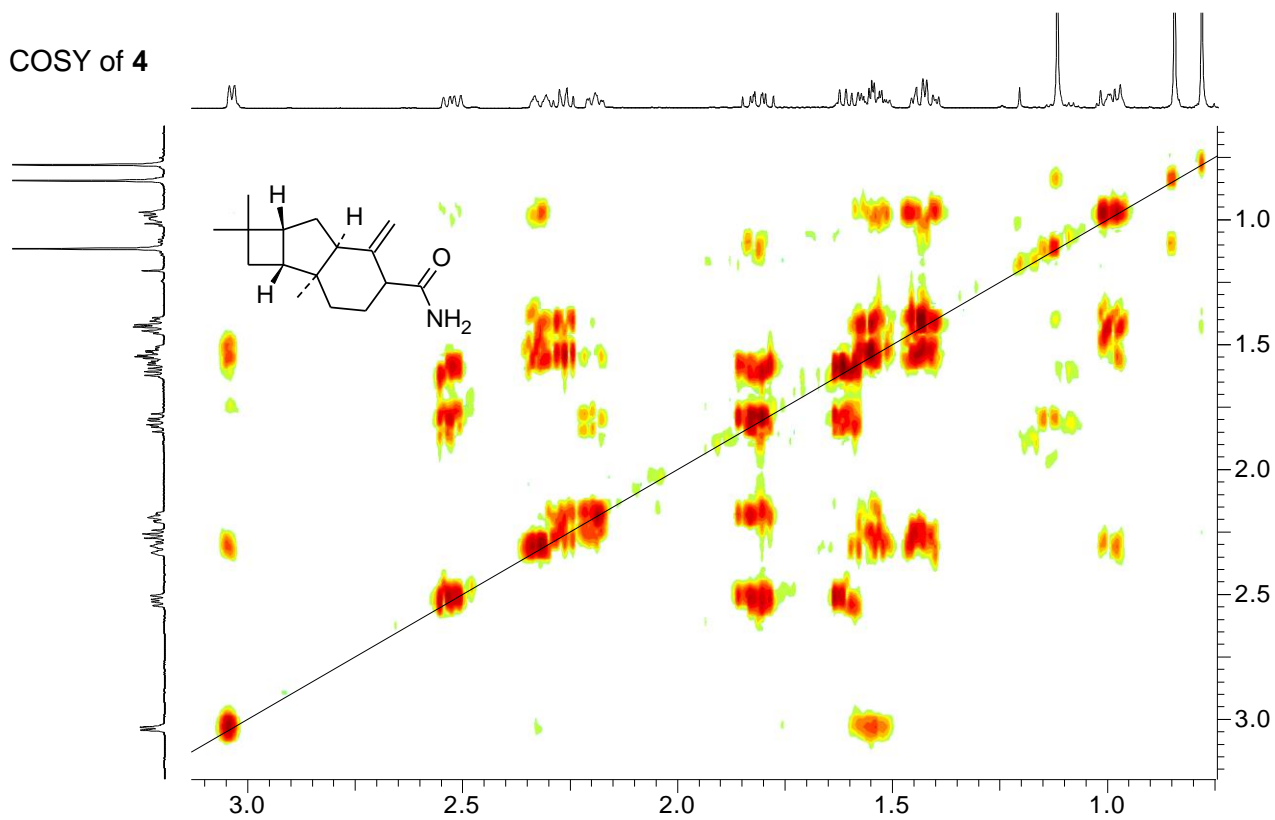
DEPT-135 and ^{13}C NMR of **4** in CDCl_3 , 125 MHz



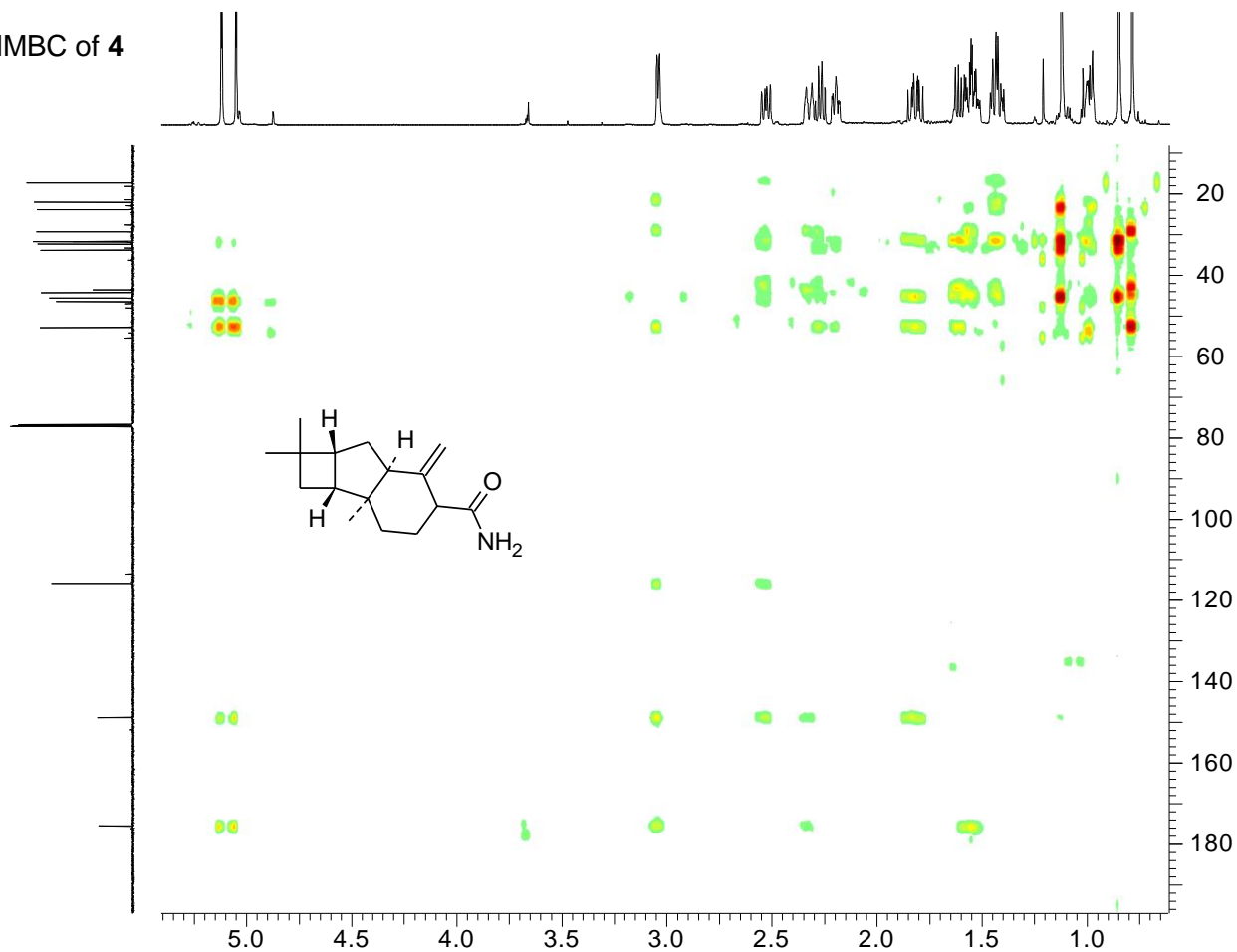
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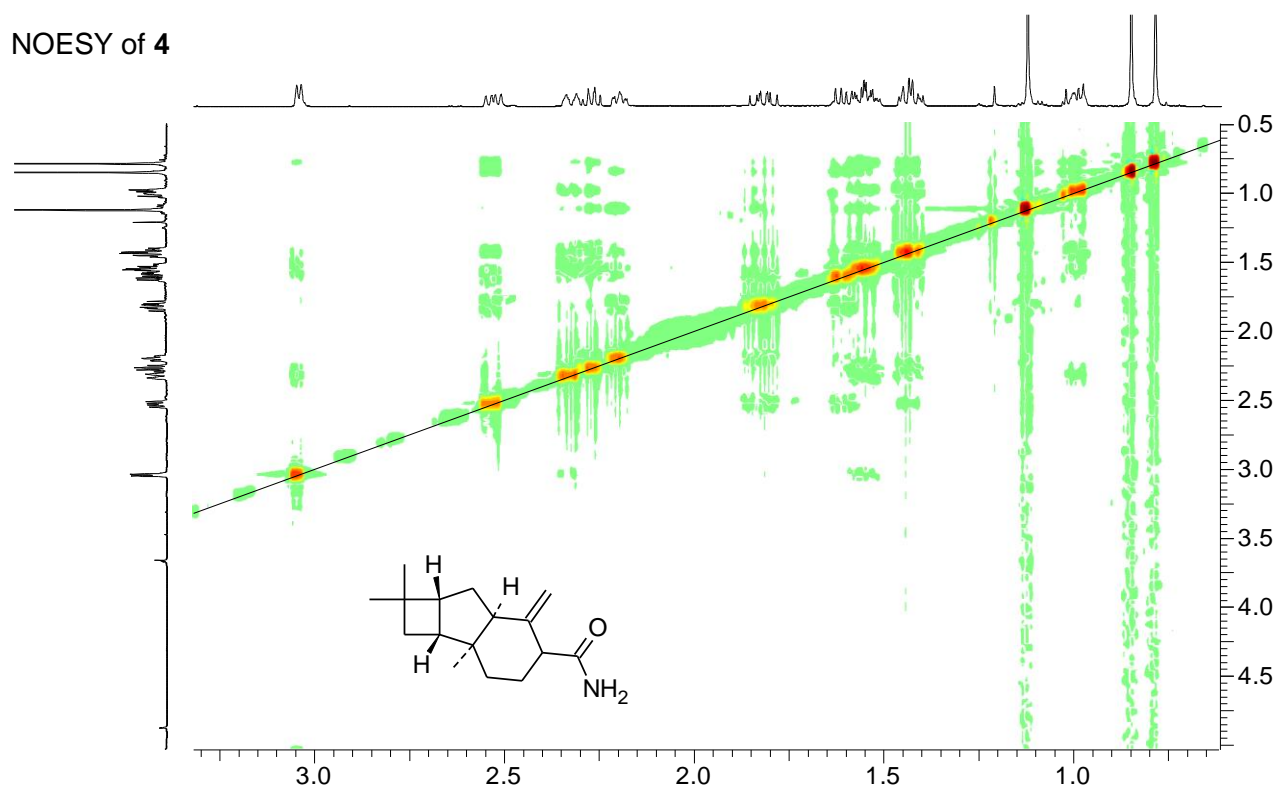
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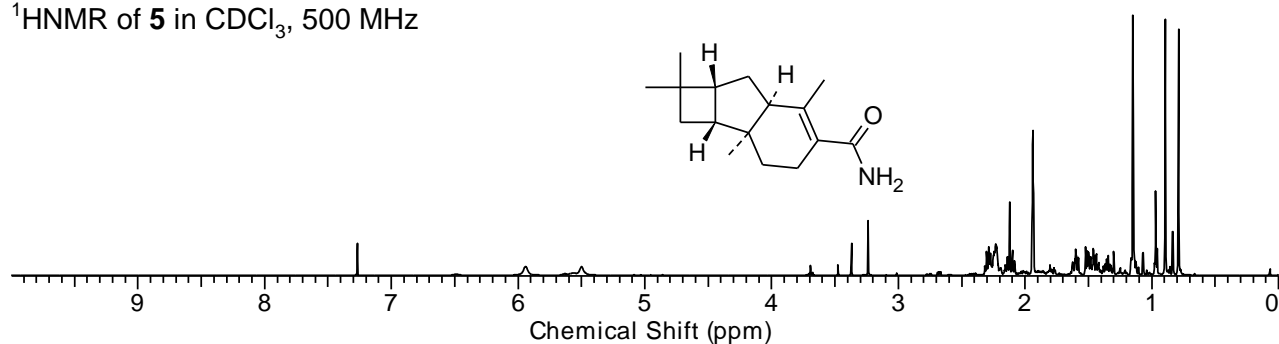


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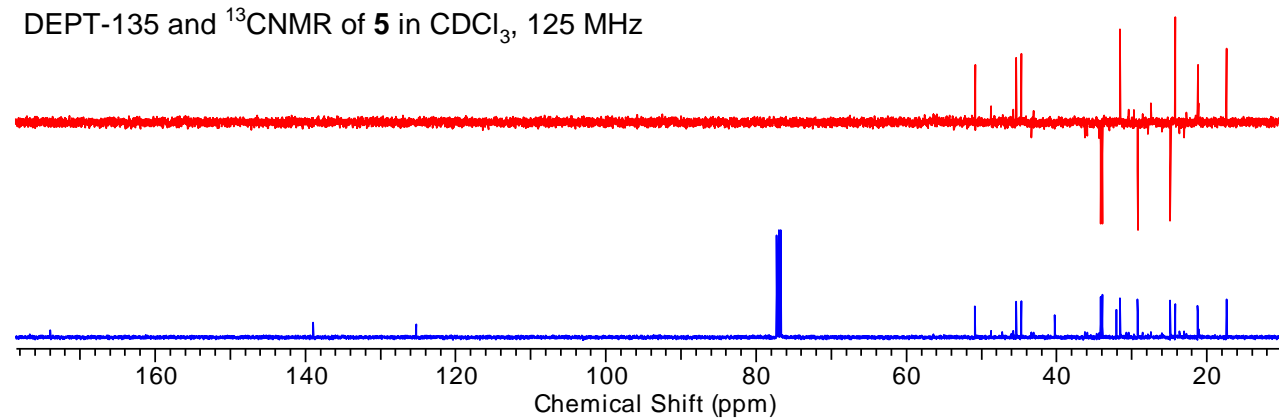


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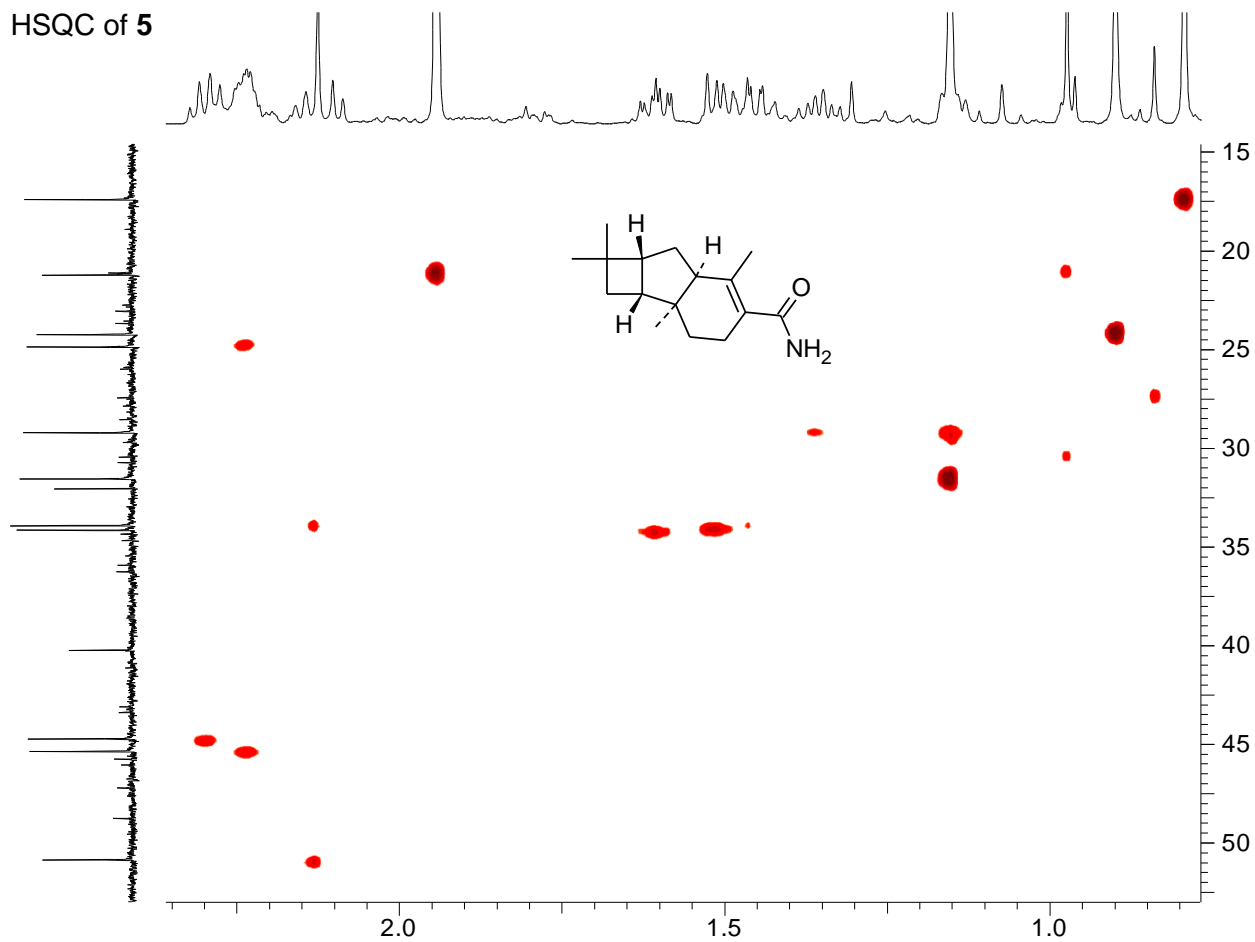
¹H NMR of 5 in CDCl₃, 500 MHz



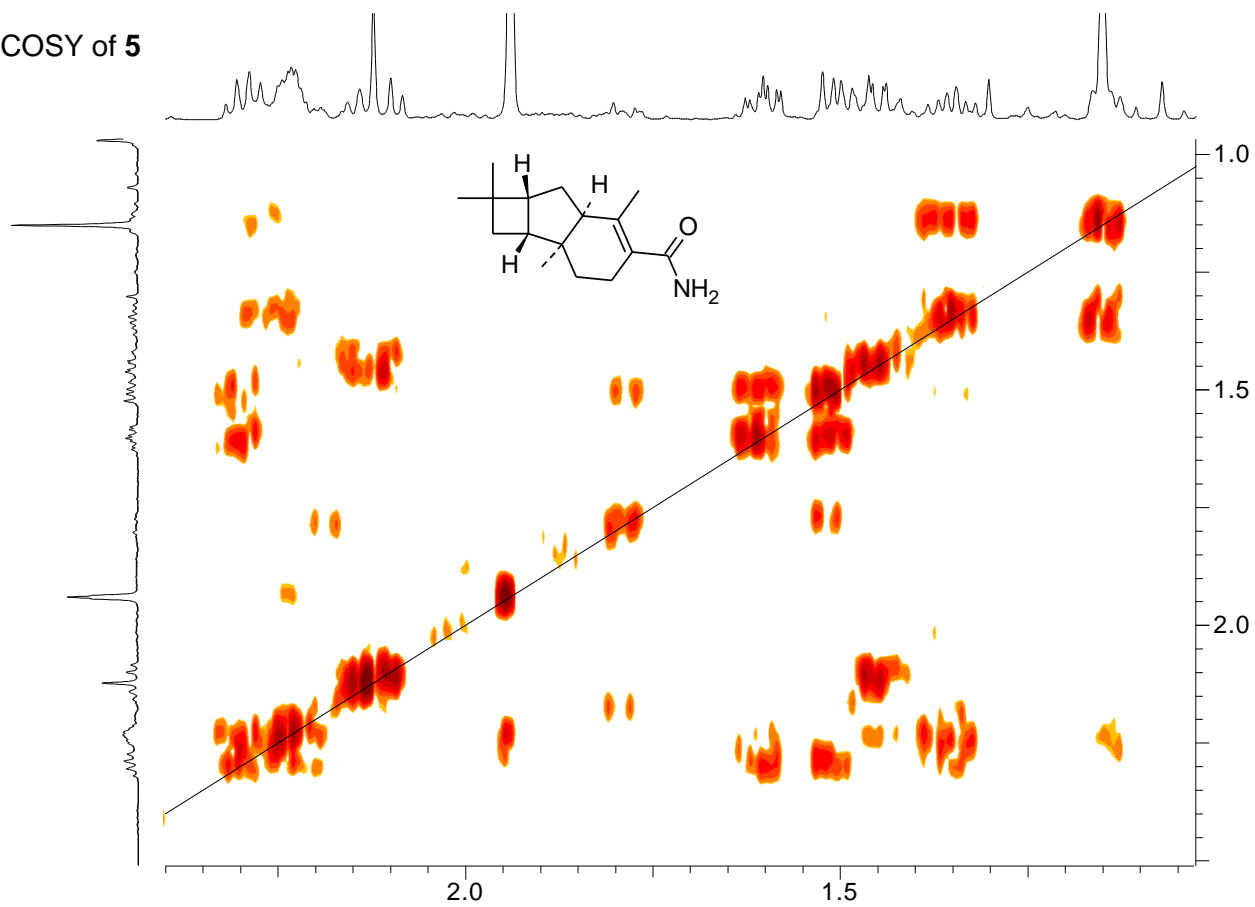
DEPT-135 and ¹³C NMR of 5 in CDCl₃, 125 MHz



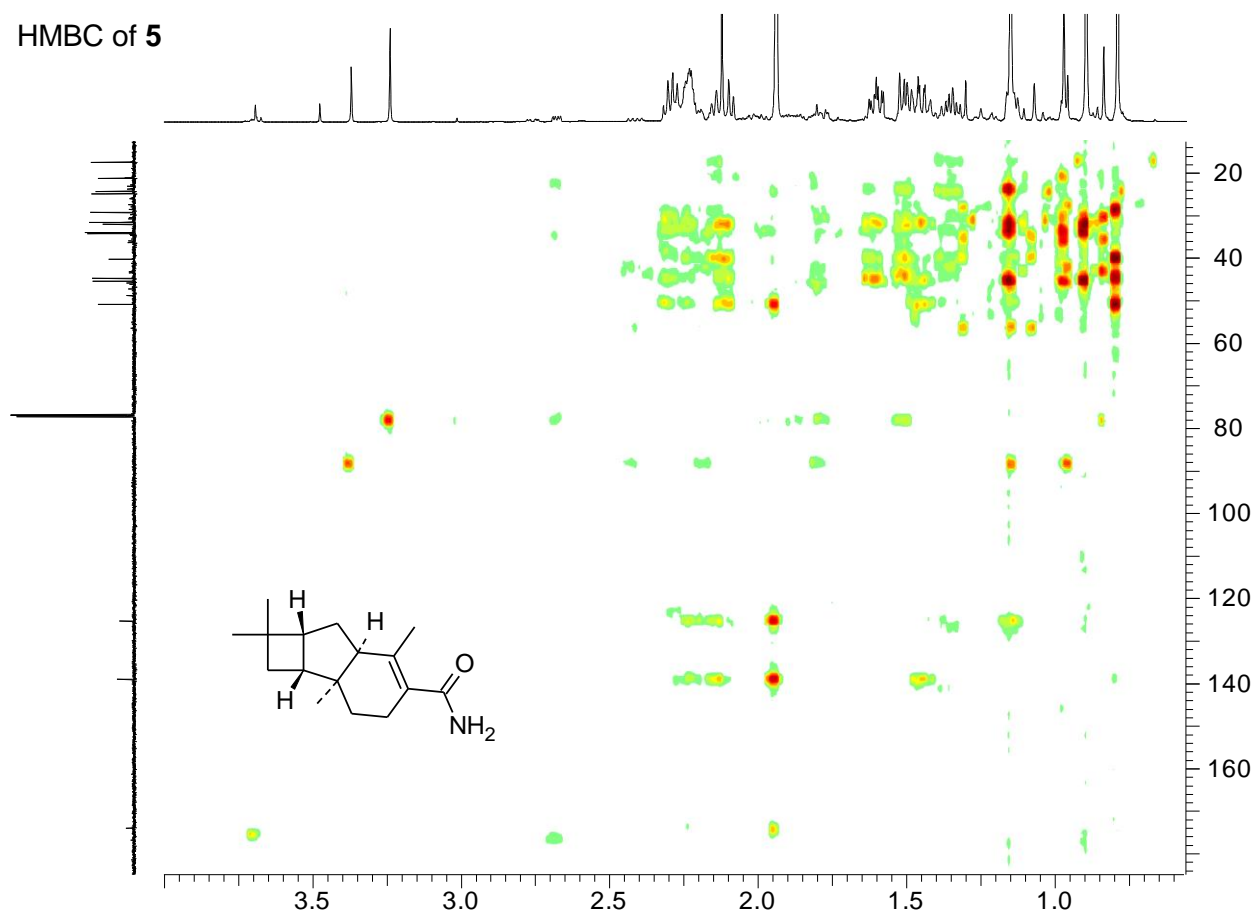
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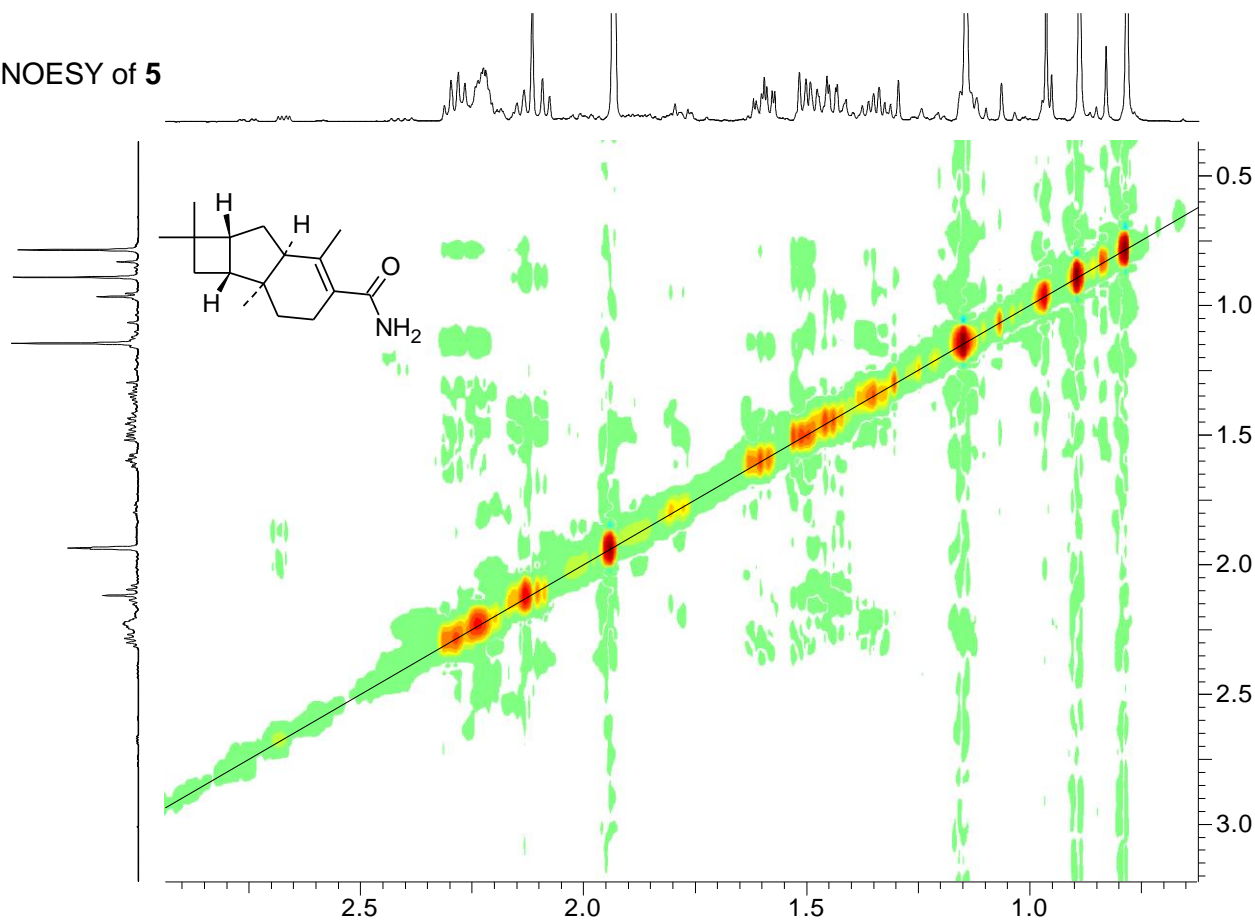
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HMBC of 5

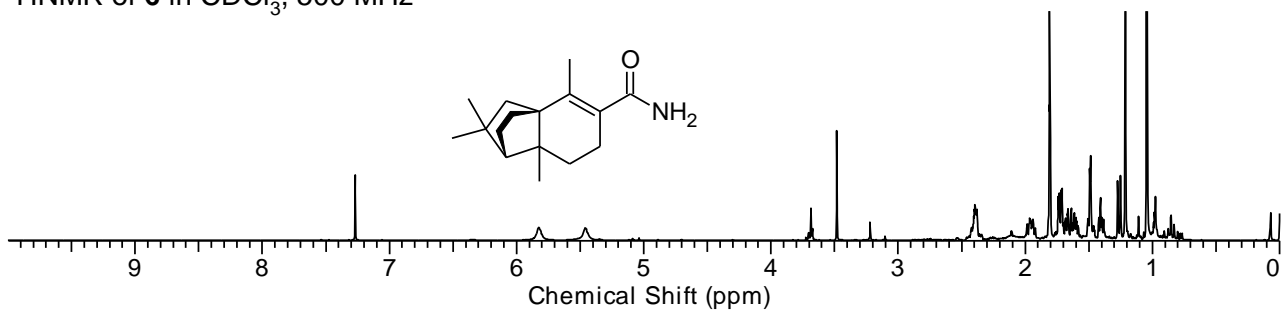


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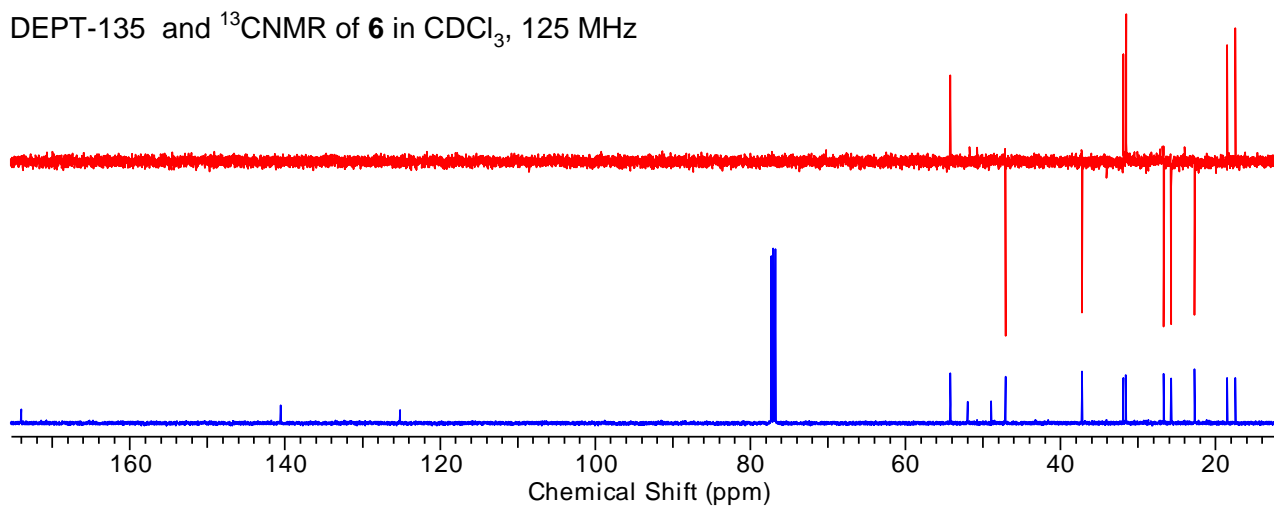


Compound 6

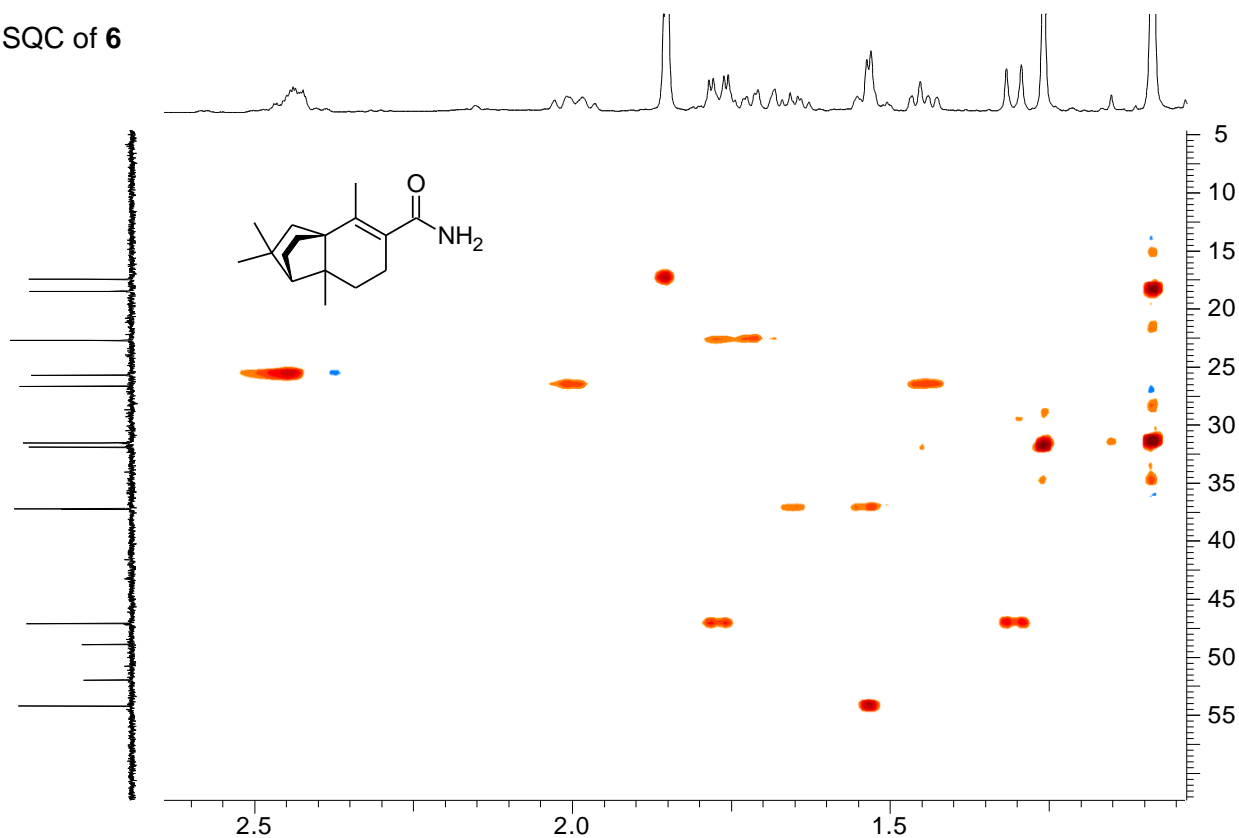
^1H NMR of **6** in CDCl_3 , 500 MHz



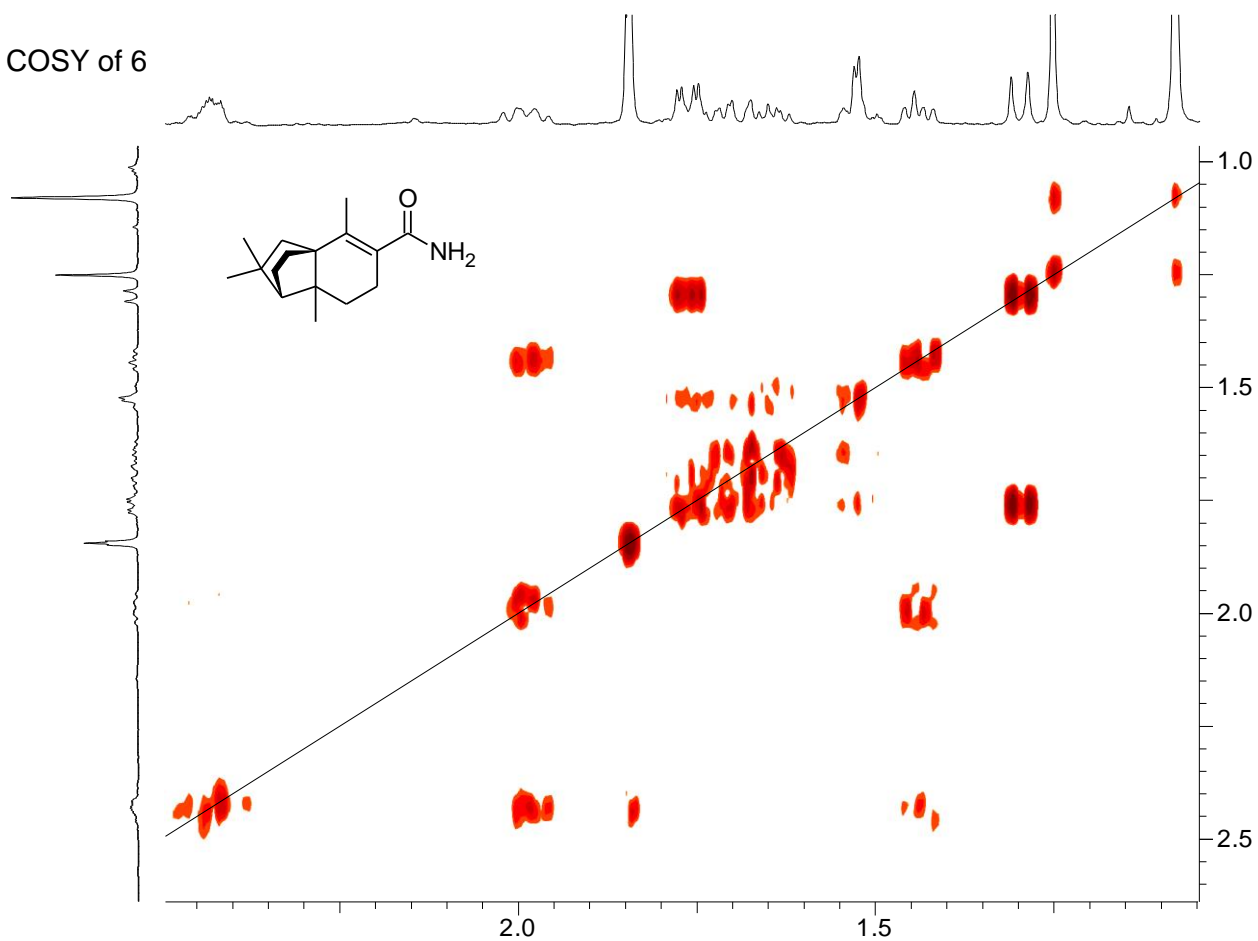
DEPT-135 and ^{13}C NMR of **6** in CDCl_3 , 125 MHz



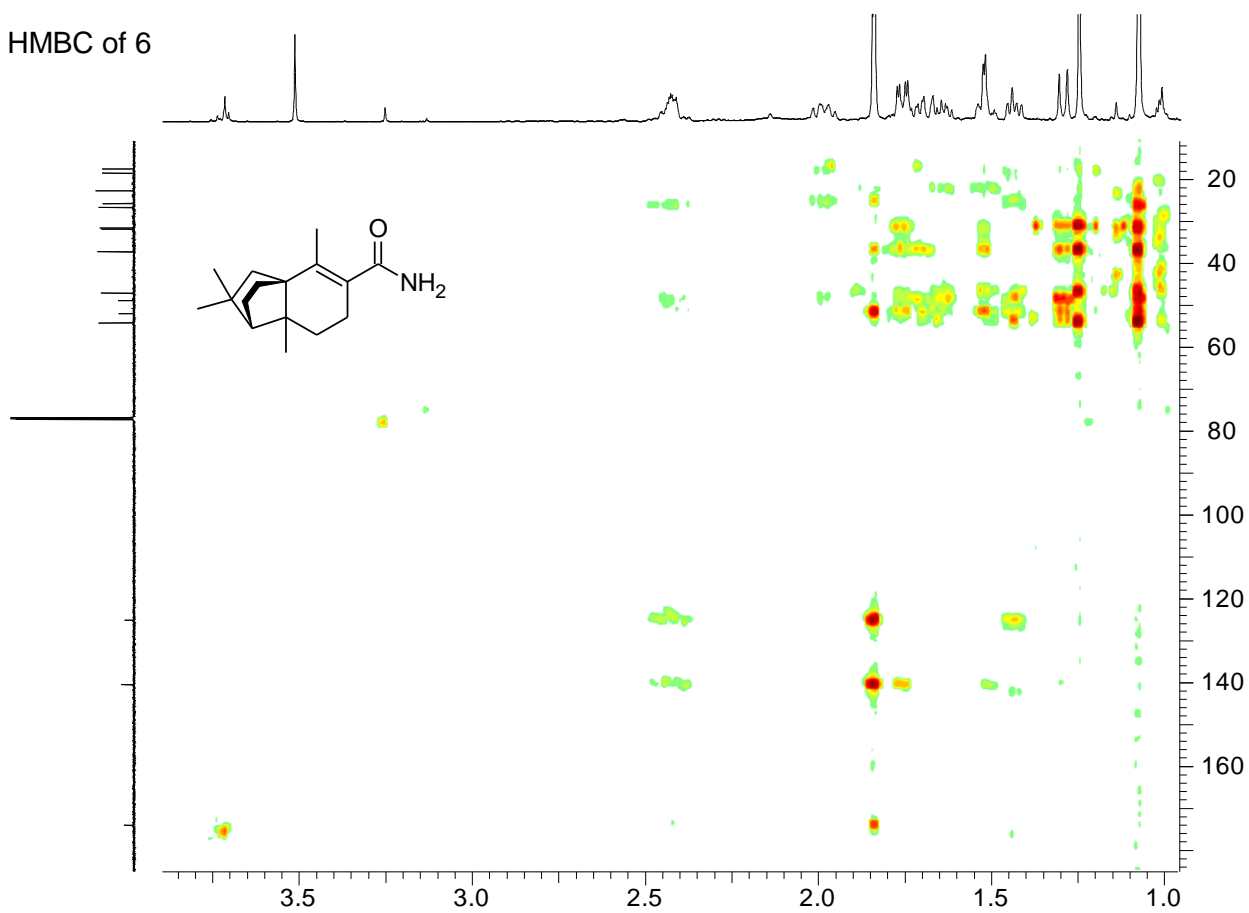
HSQC of **6**



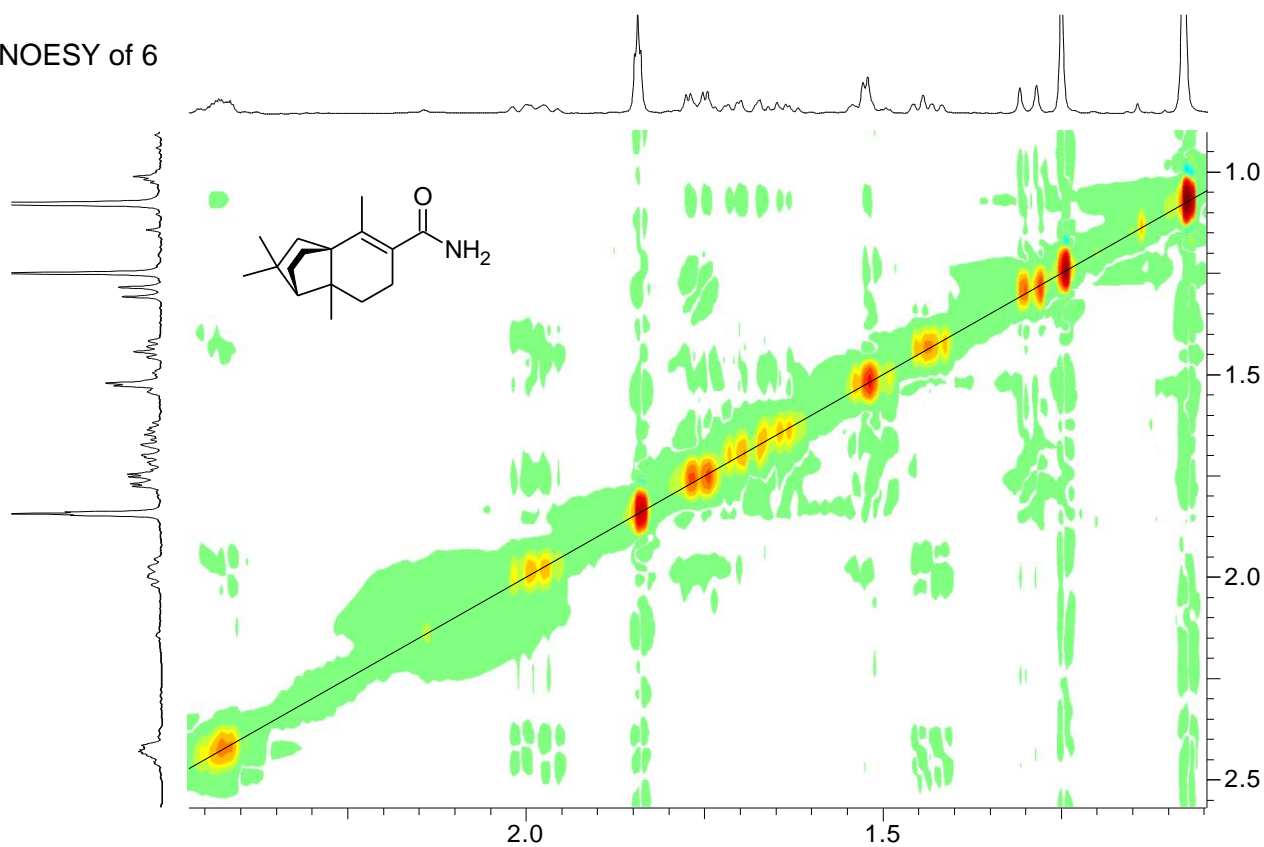
COSY of 6



HMBC of 6

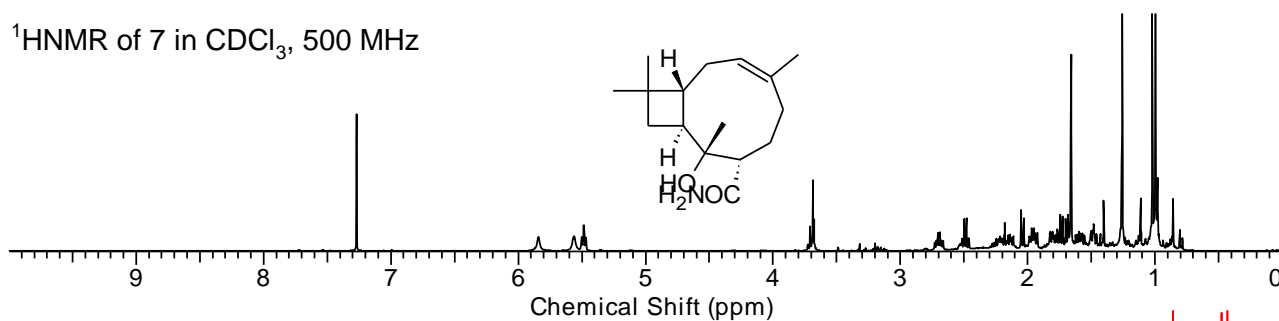


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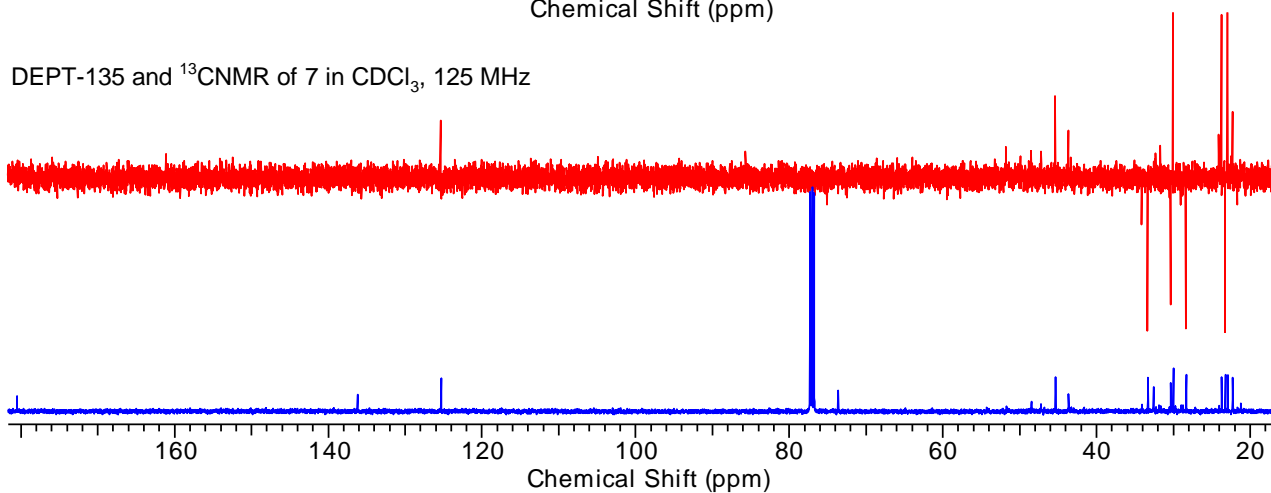


Compound 7

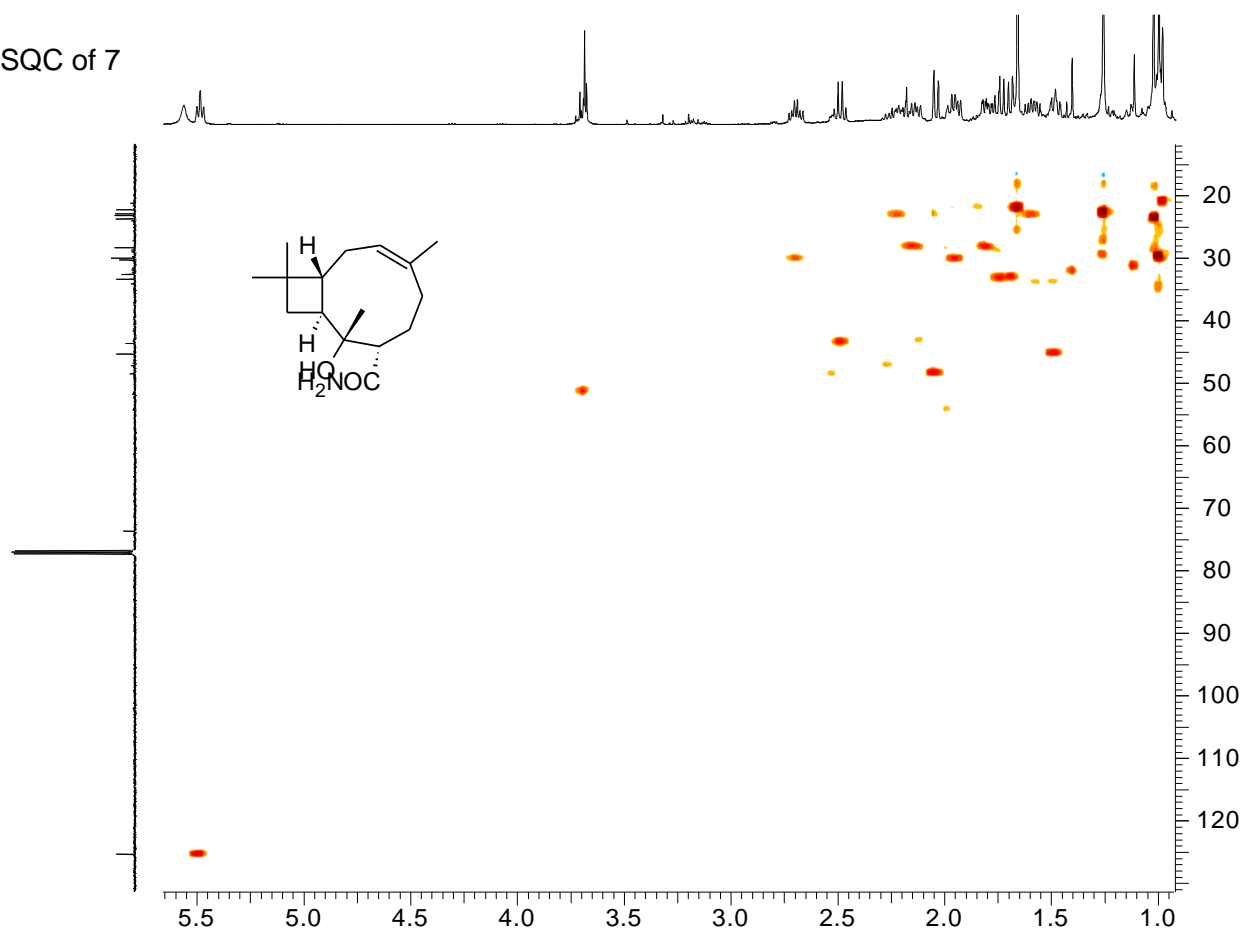
¹H NMR of 7 in CDCl₃, 500 MHz



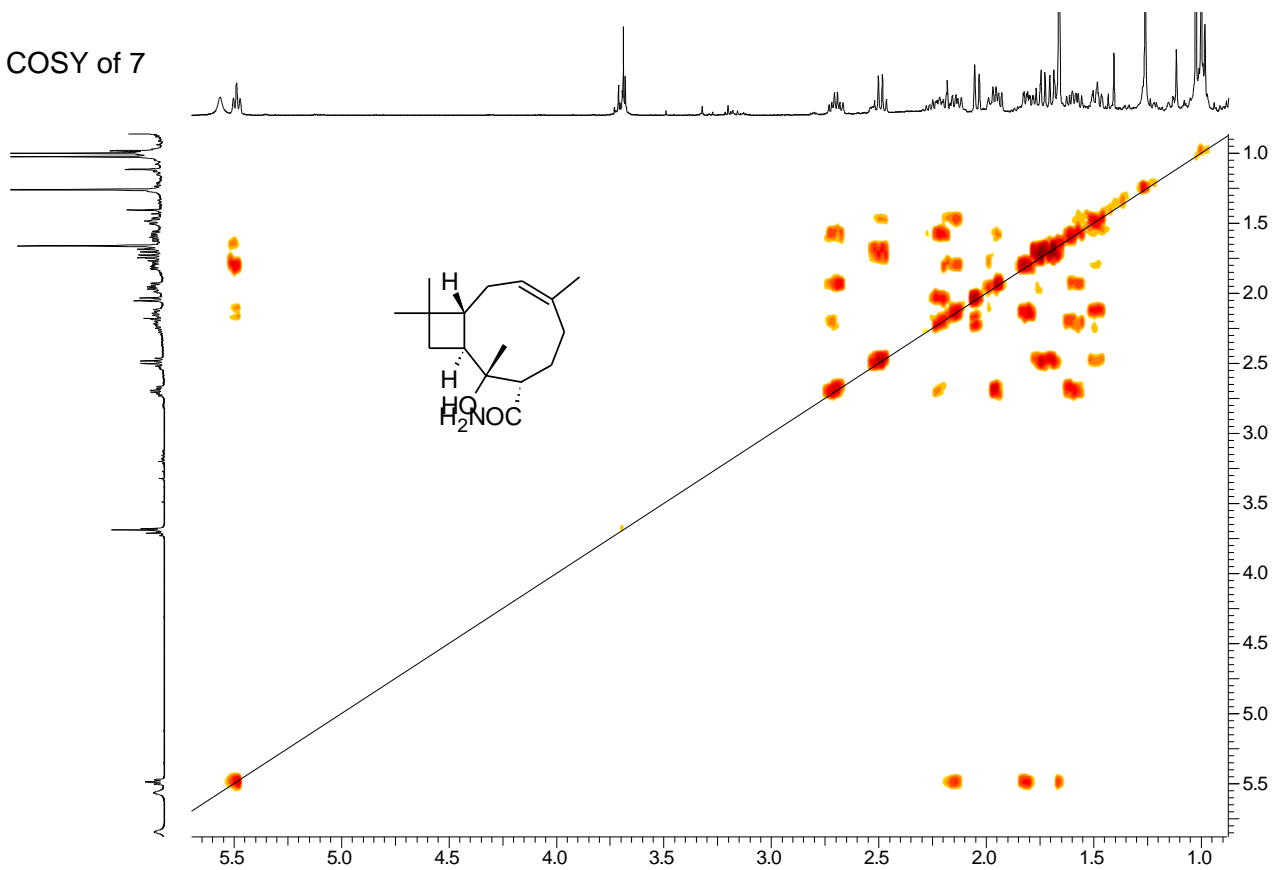
DEPT-135 and ¹³C NMR of 7 in CDCl₃, 125 MHz



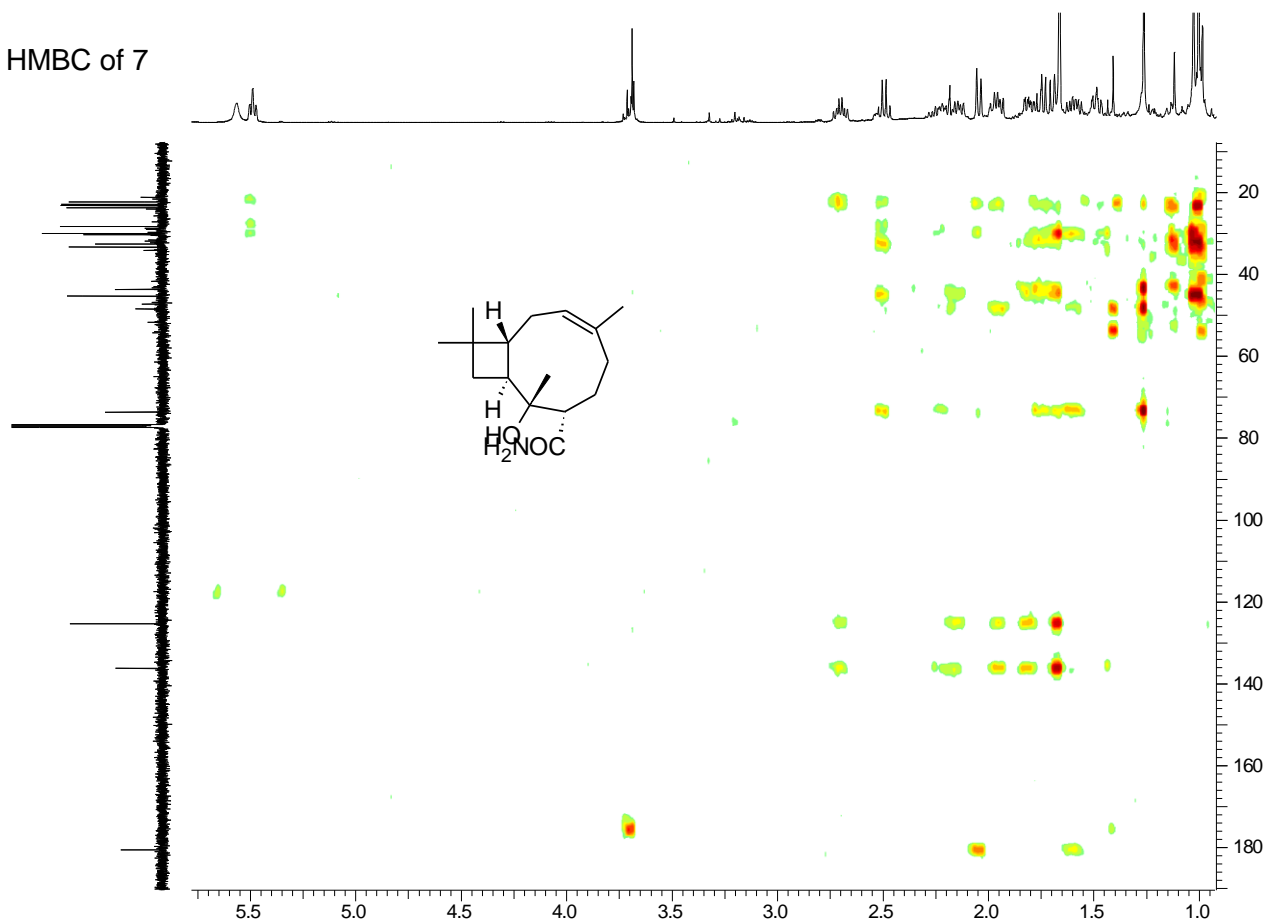
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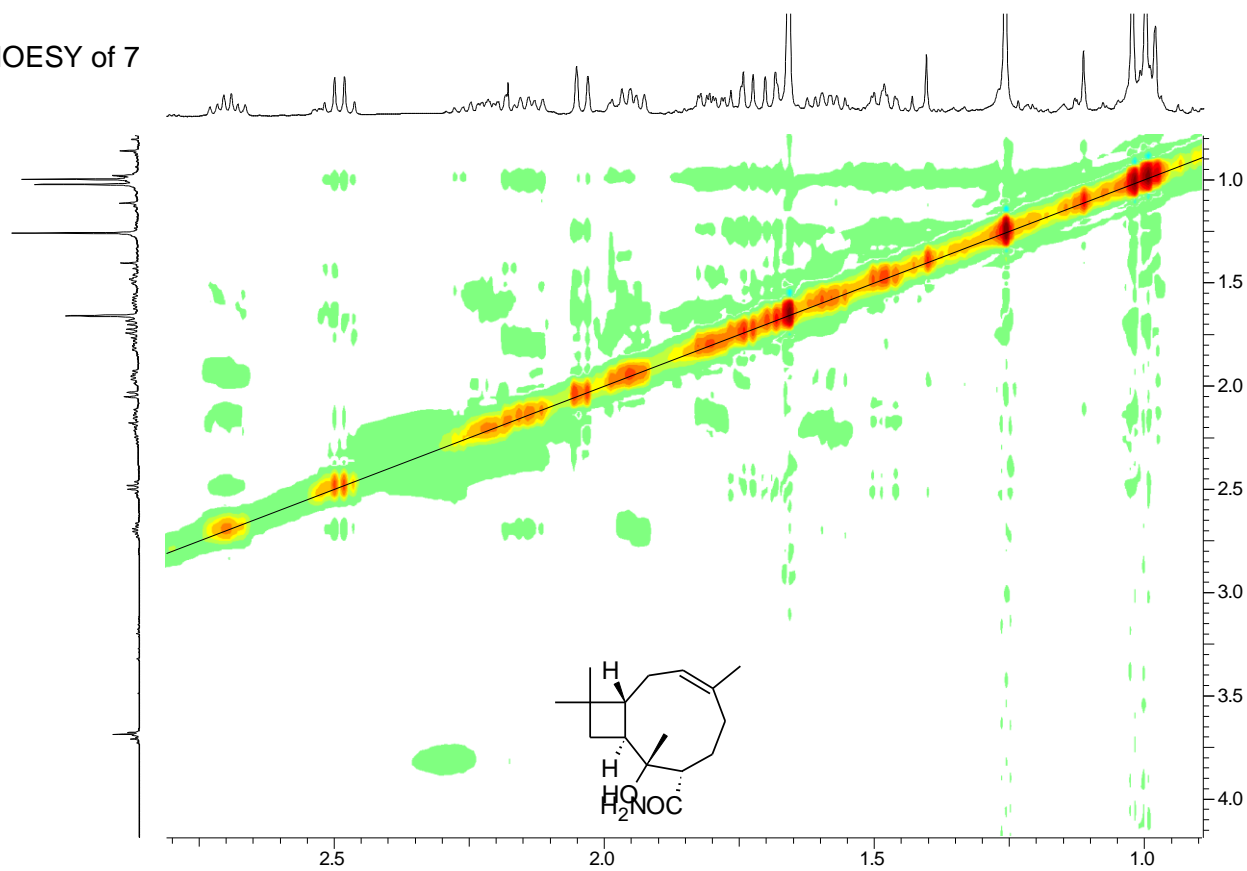
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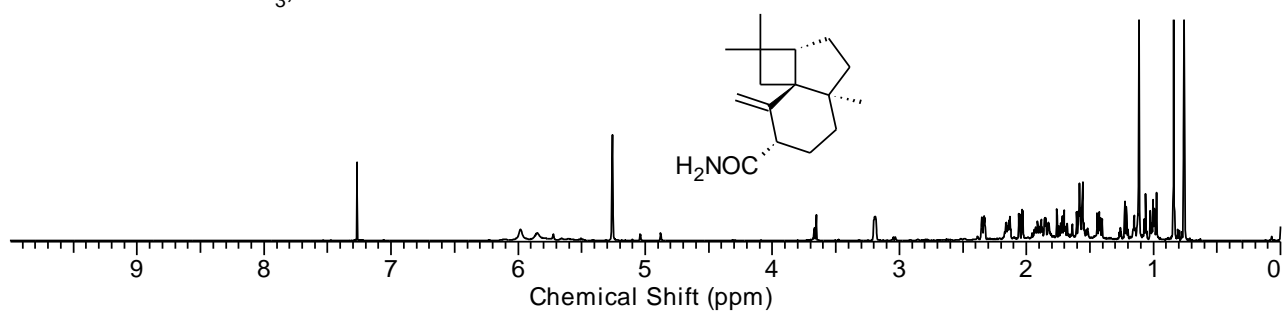


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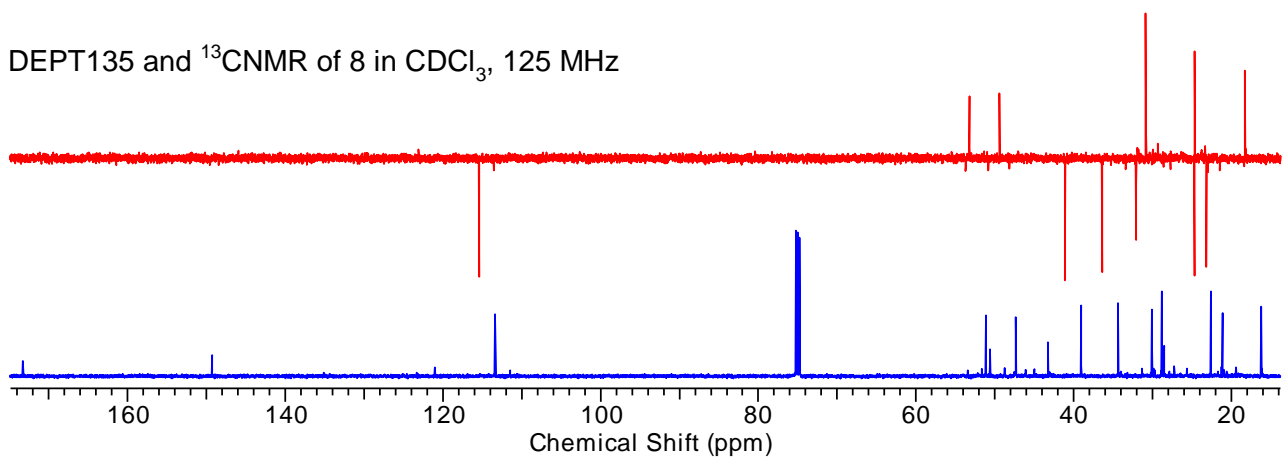


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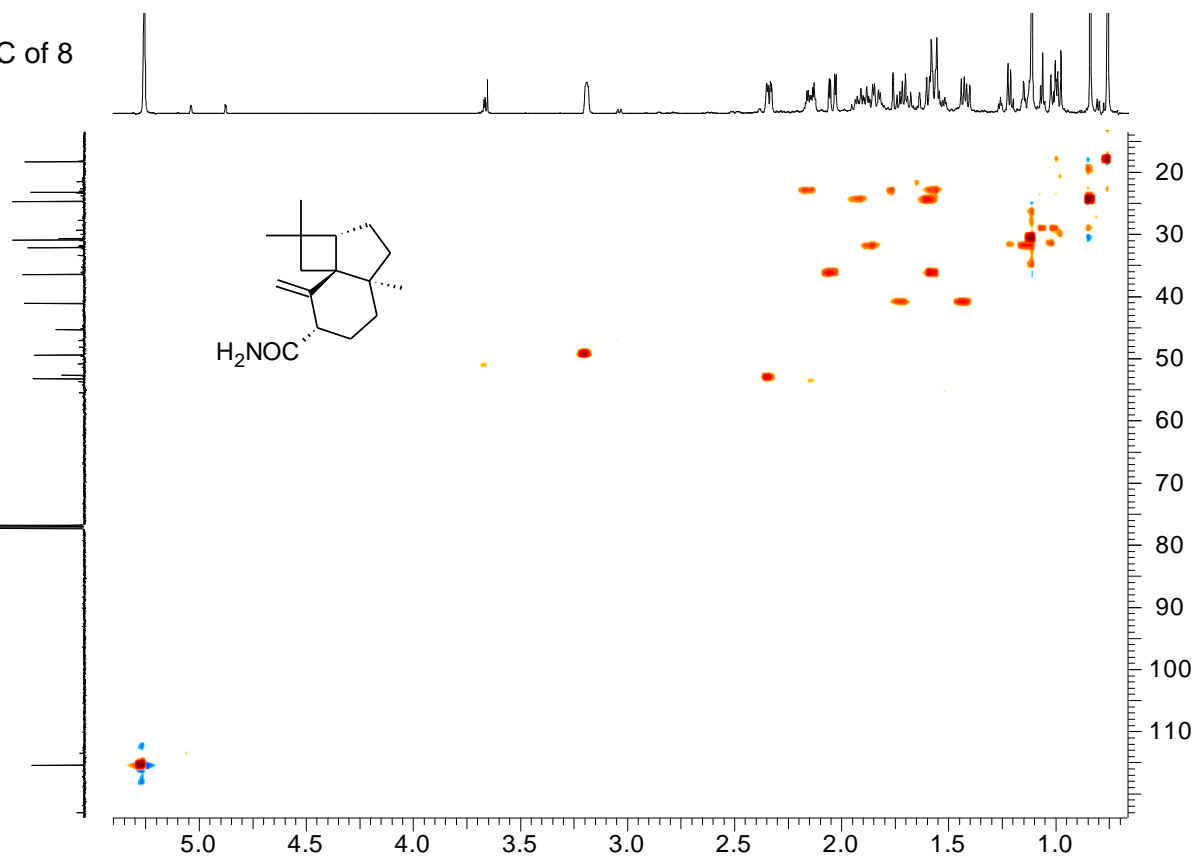
^1H NMR of 8 in CDCl_3 , 500 MHz



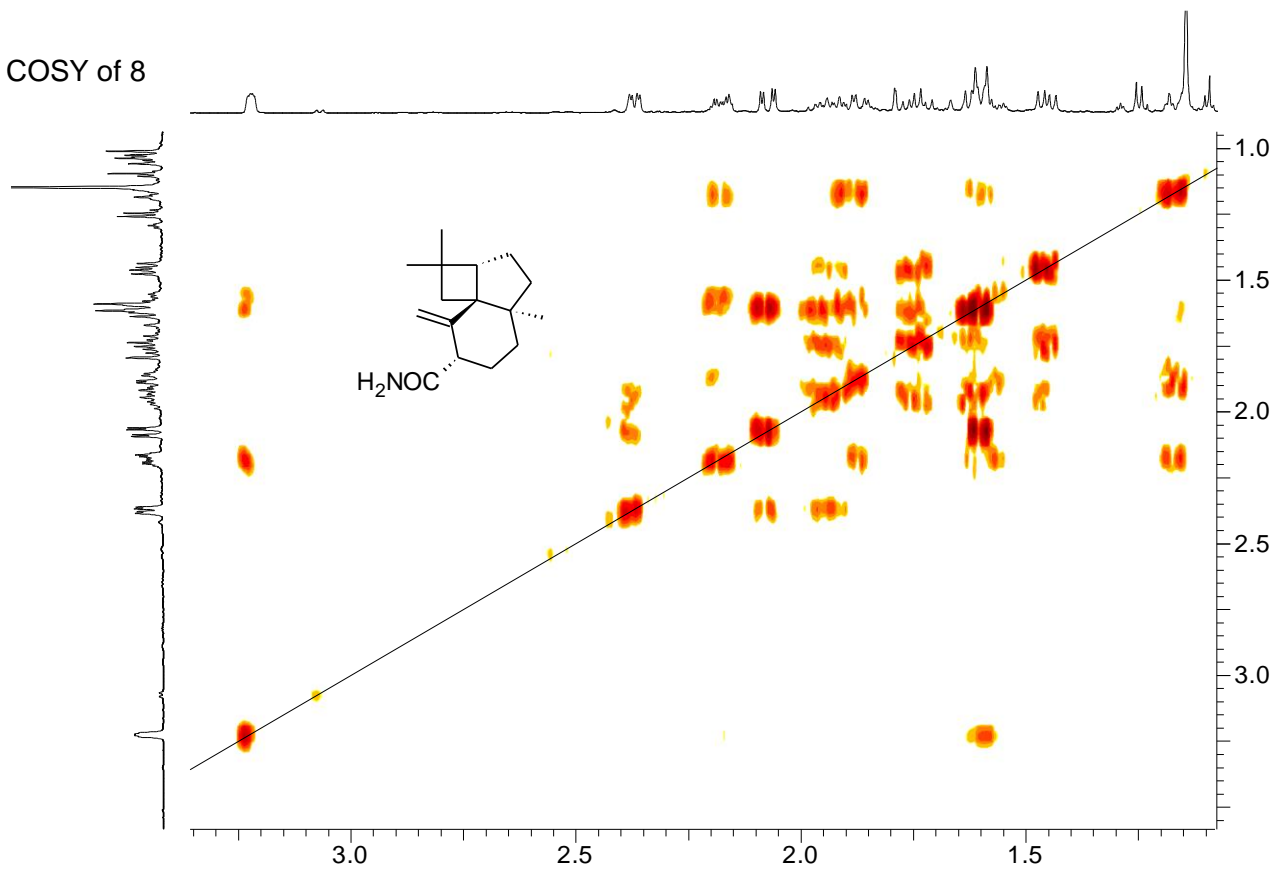
DEPT135 and ^{13}C NMR of 8 in CDCl_3 , 125 MHz



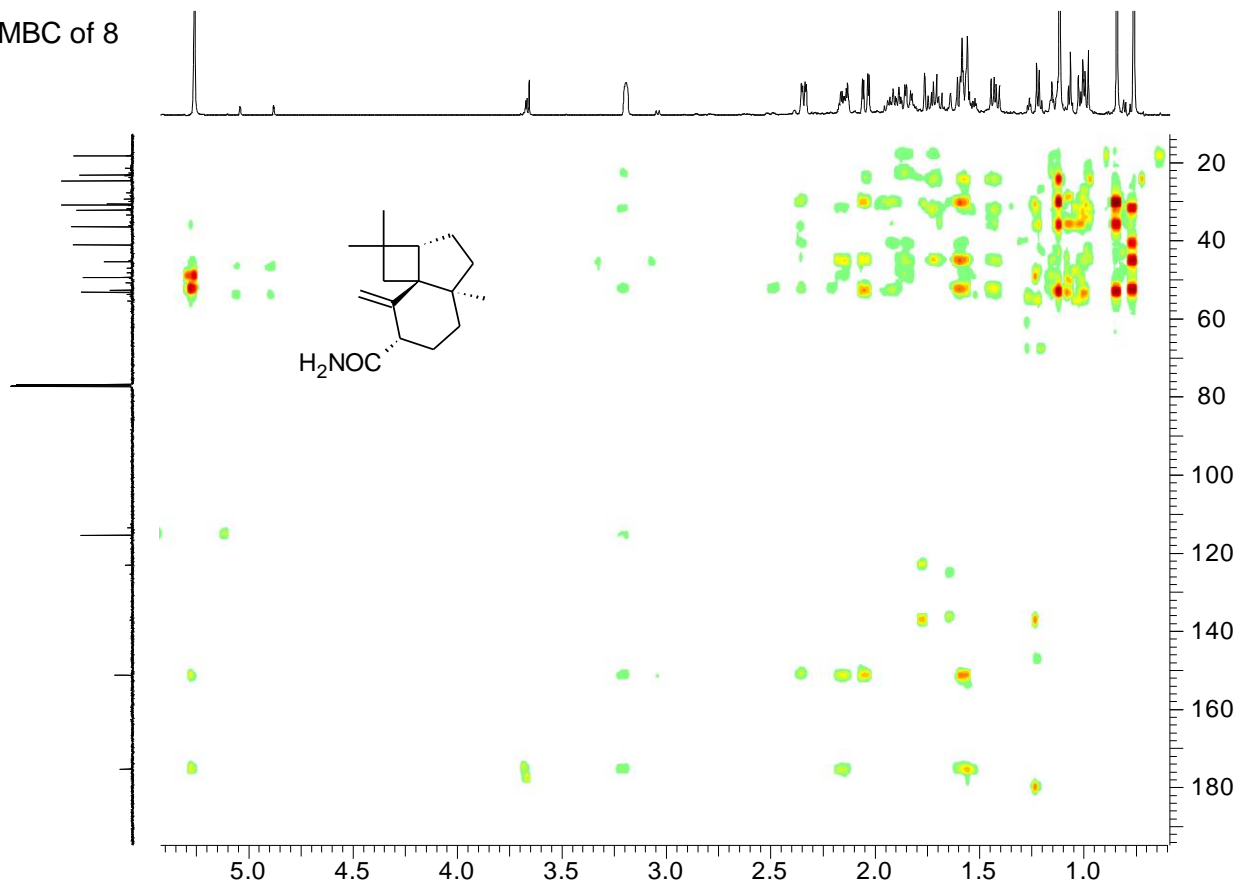
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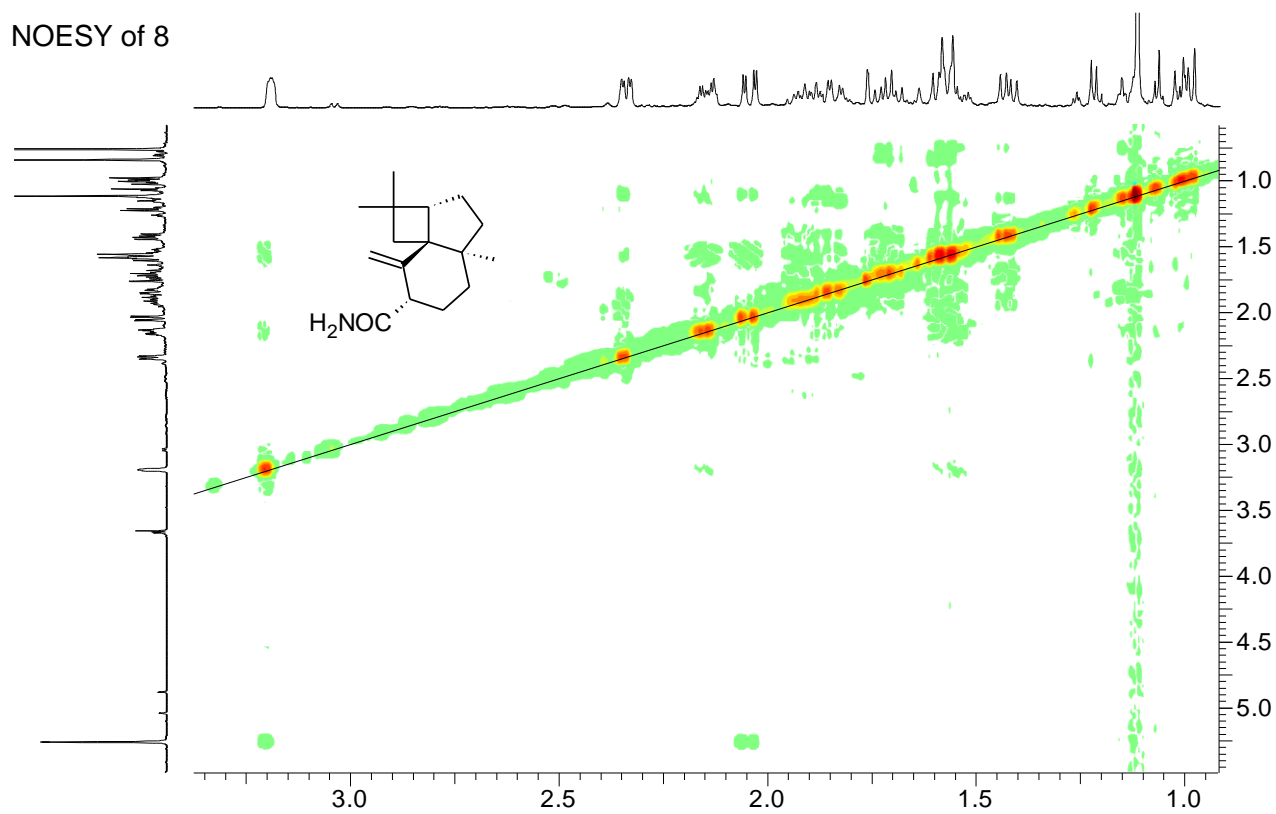
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HMBC of 8

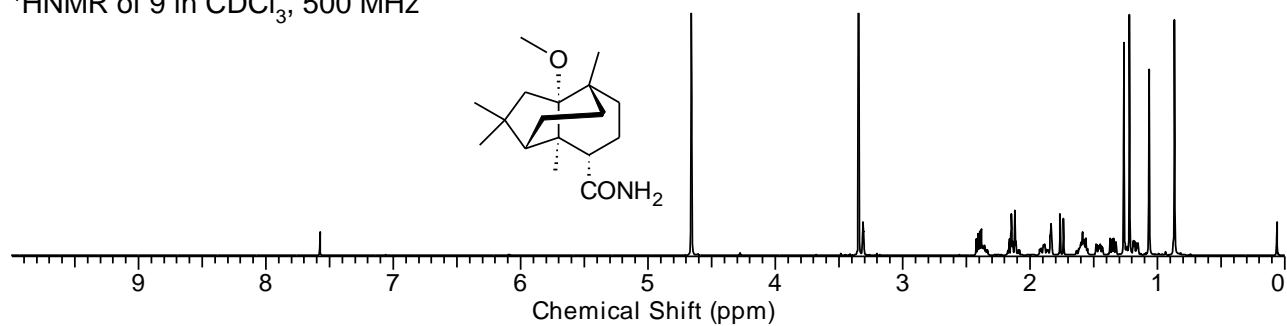


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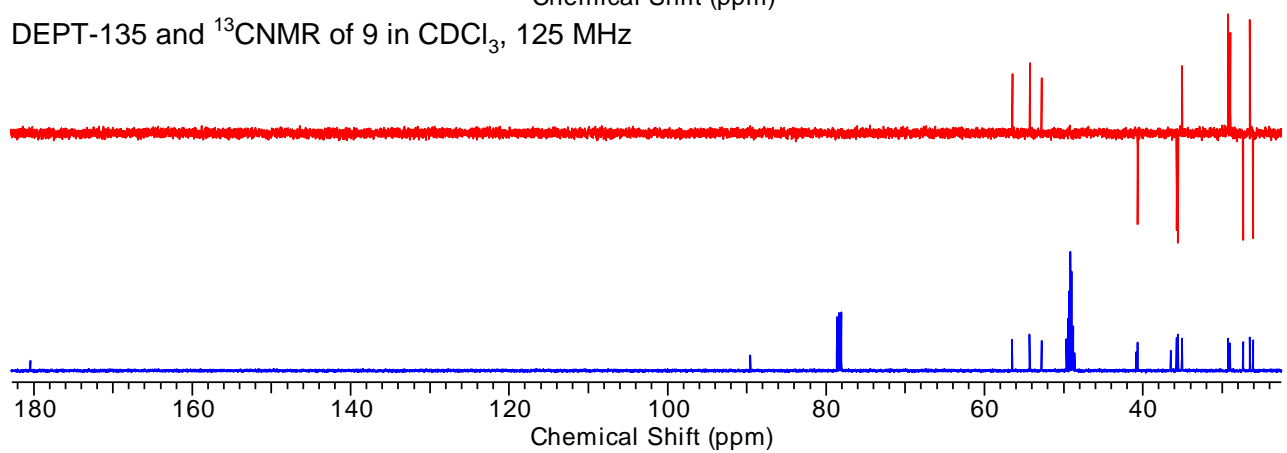


Compound 9

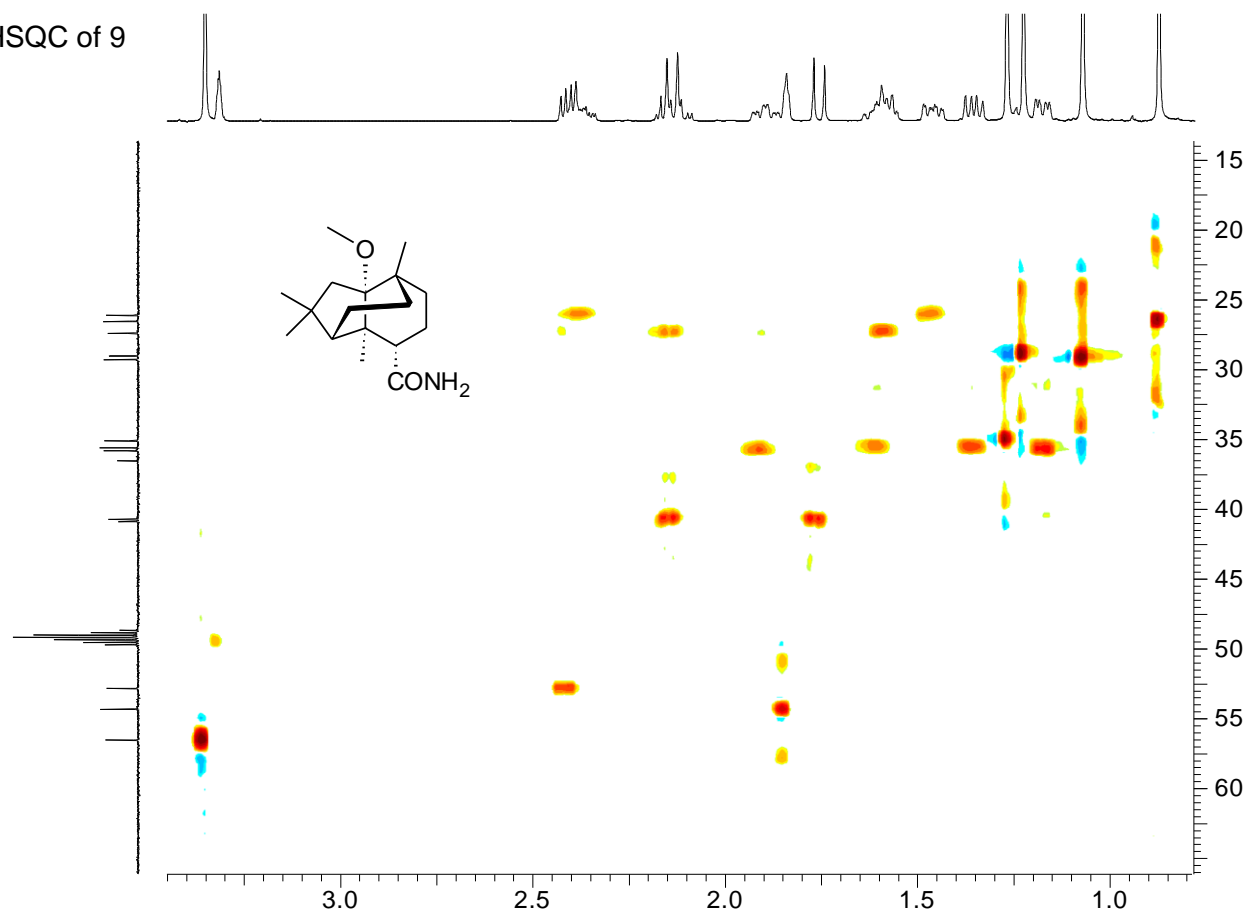
^1H NMR of 9 in CDCl_3 , 500 MHz



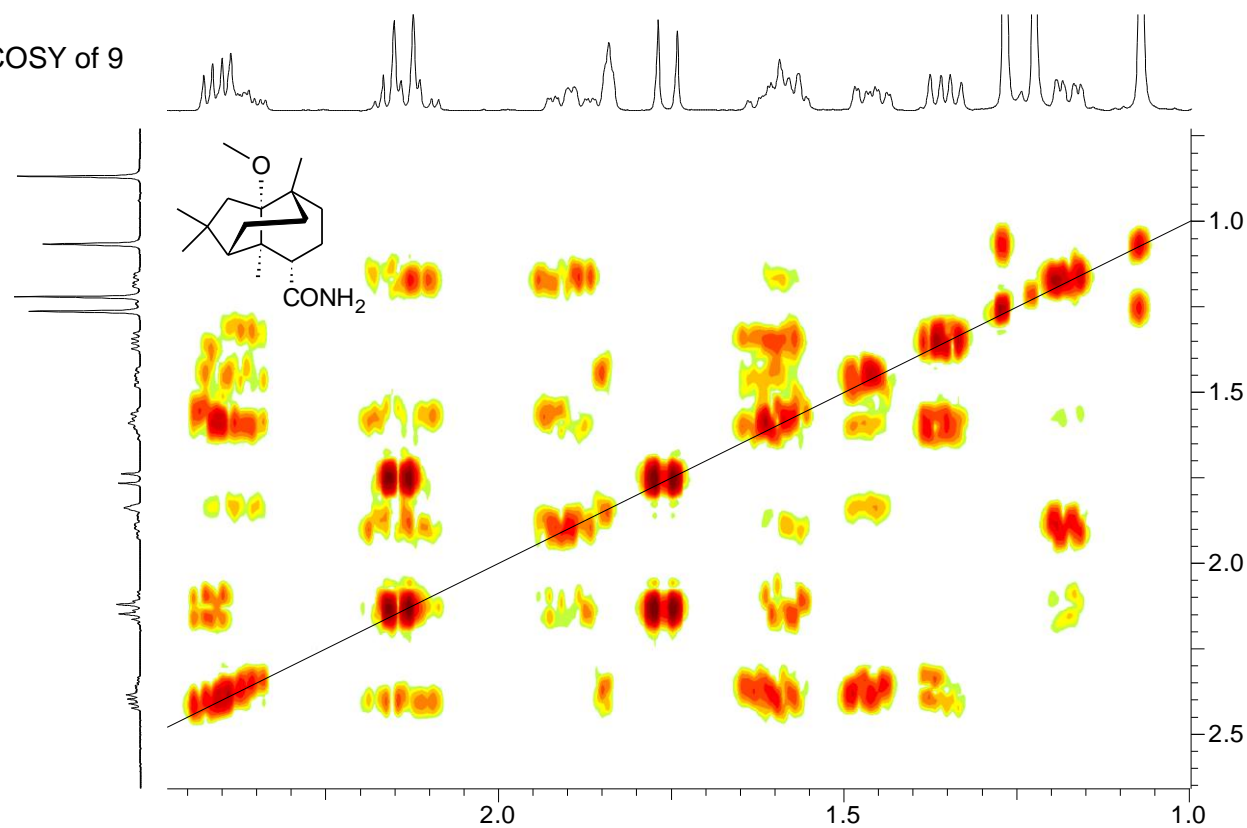
DEPT-135 and ^{13}C NMR of 9 in CDCl_3 , 125 MHz



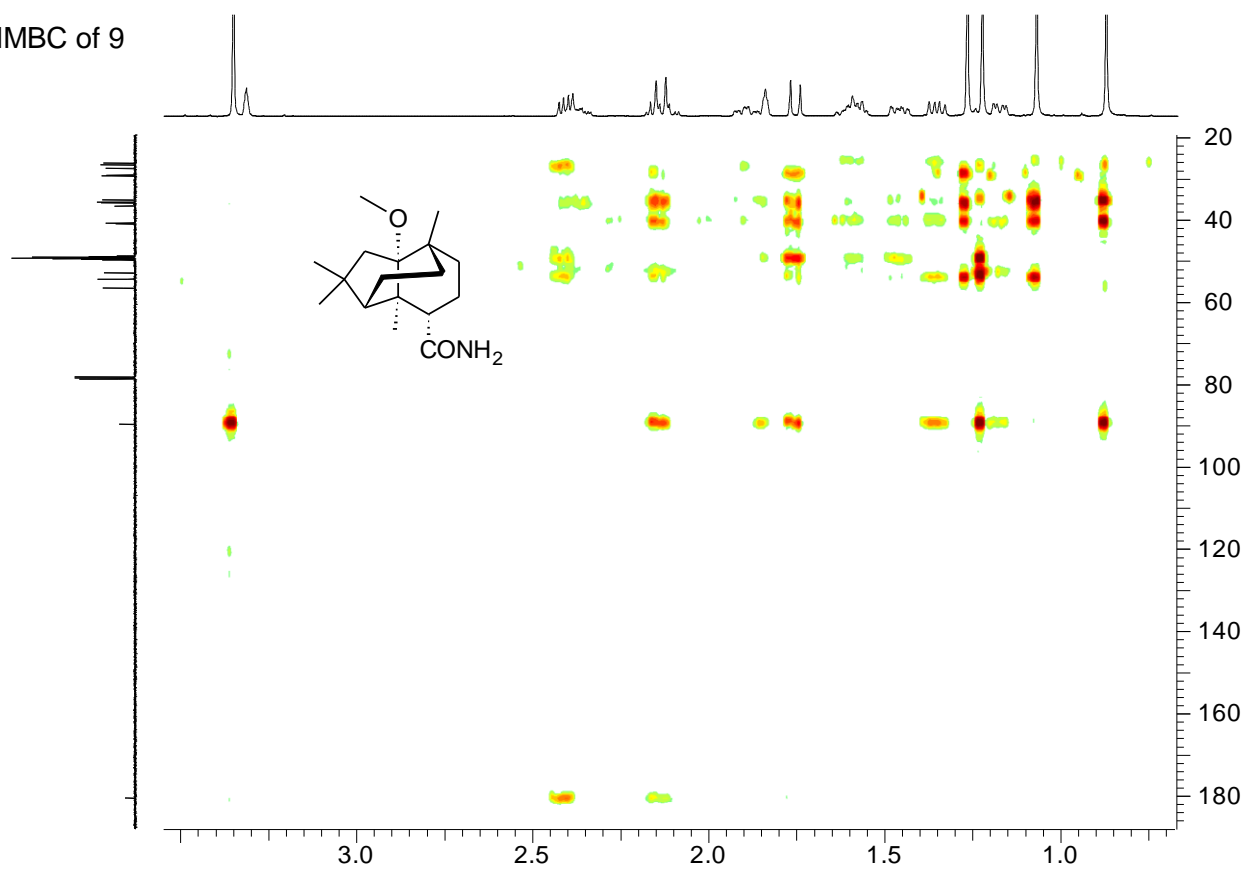
HSQC of 9



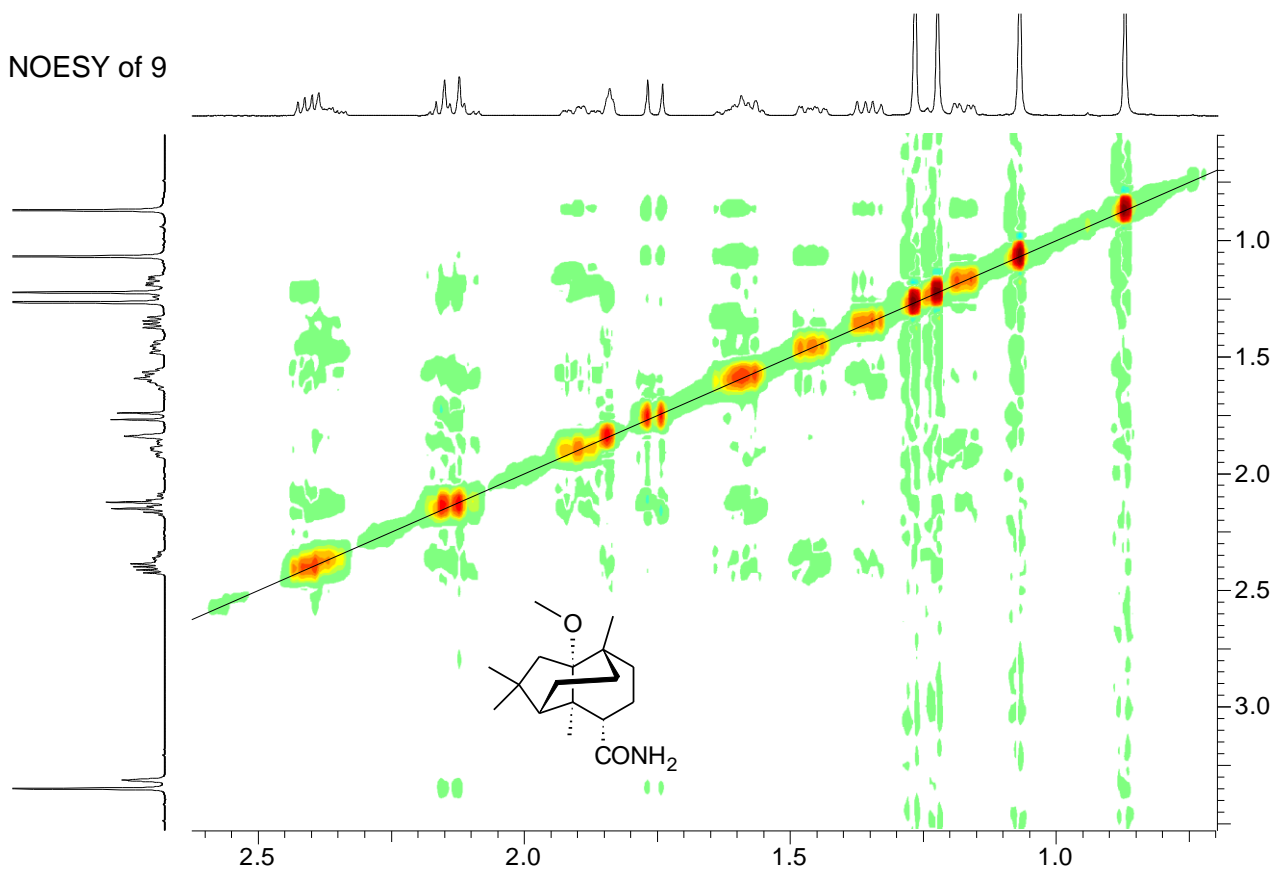
COSY of 9



HMBC of 9

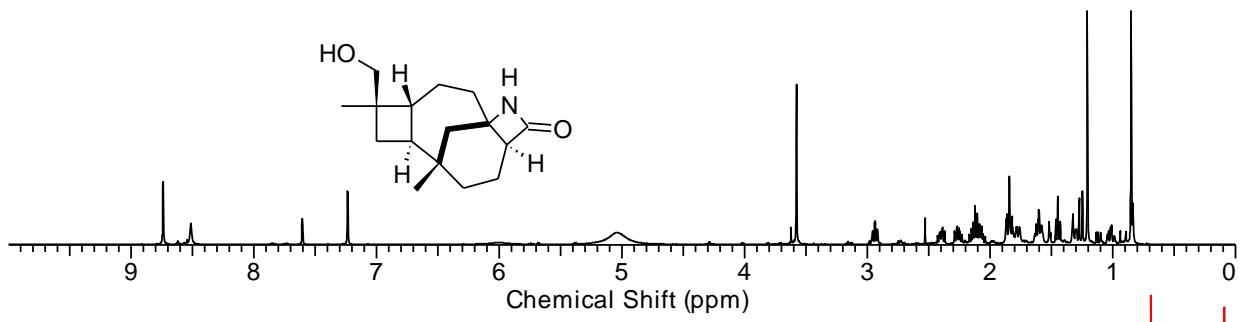


NOESY of 9

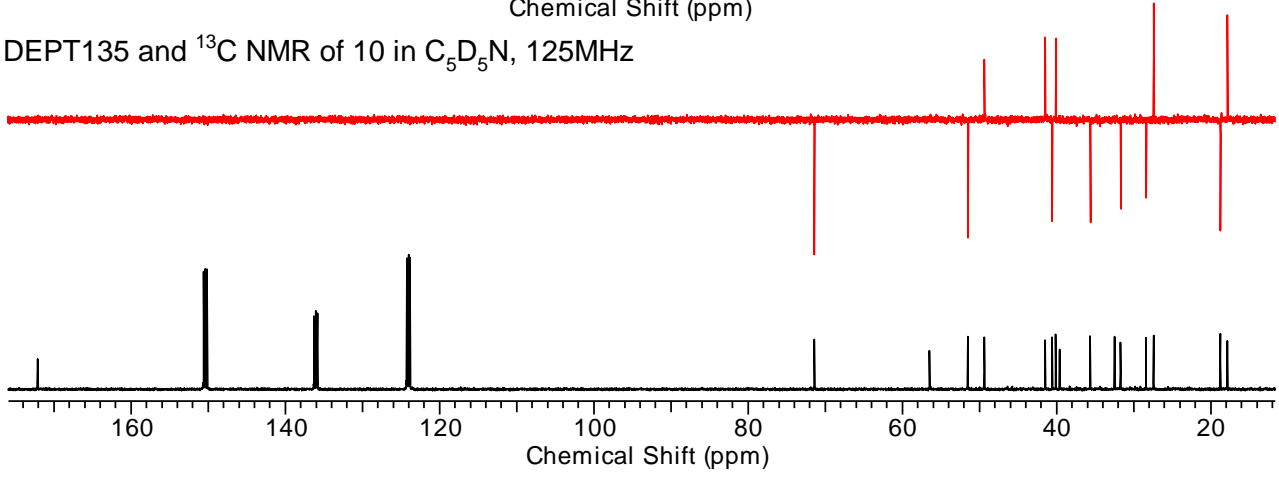


Compound 10

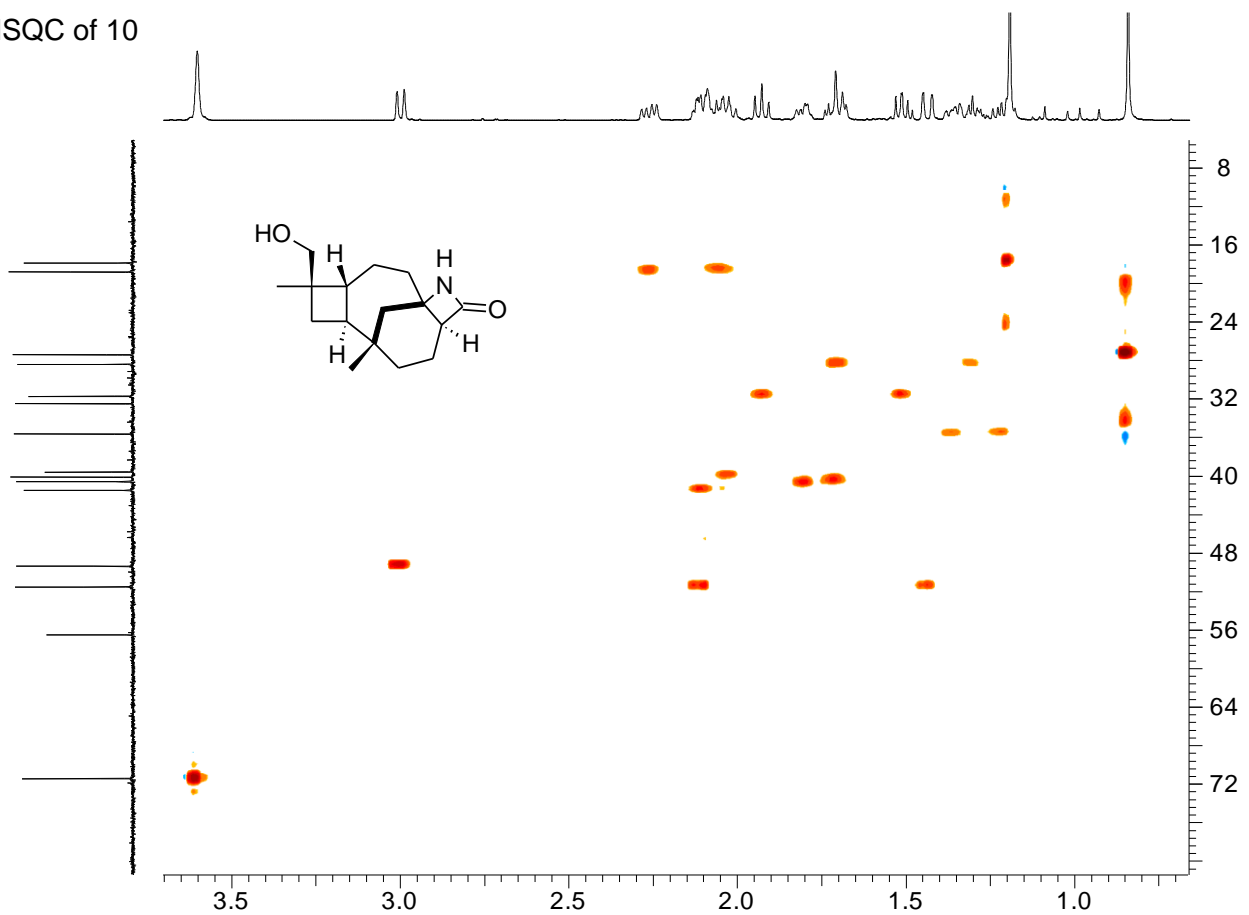
^1H NMR of 10 in $\text{C}_5\text{D}_5\text{N}$, 500MHz



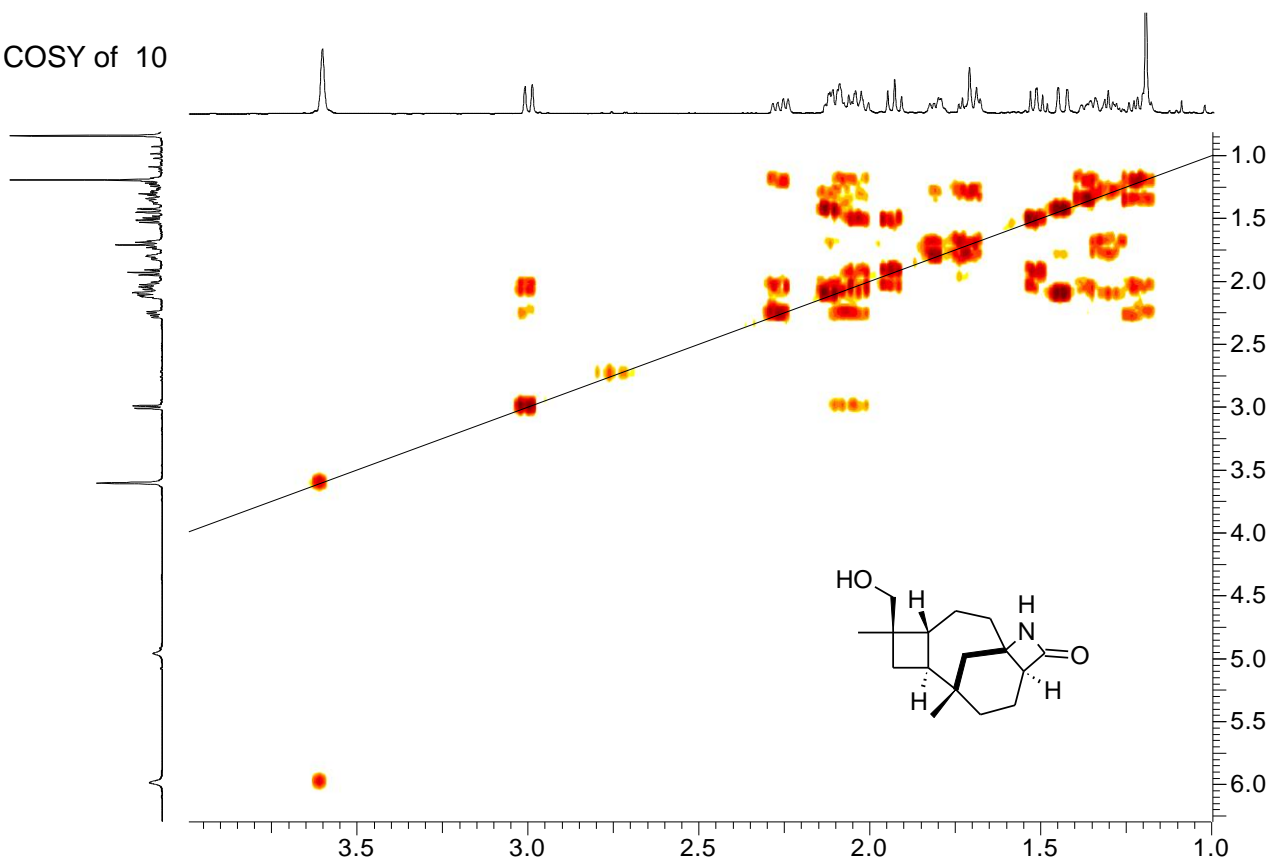
DEPT135 and ^{13}C NMR of 10 in $\text{C}_5\text{D}_5\text{N}$, 125MHz



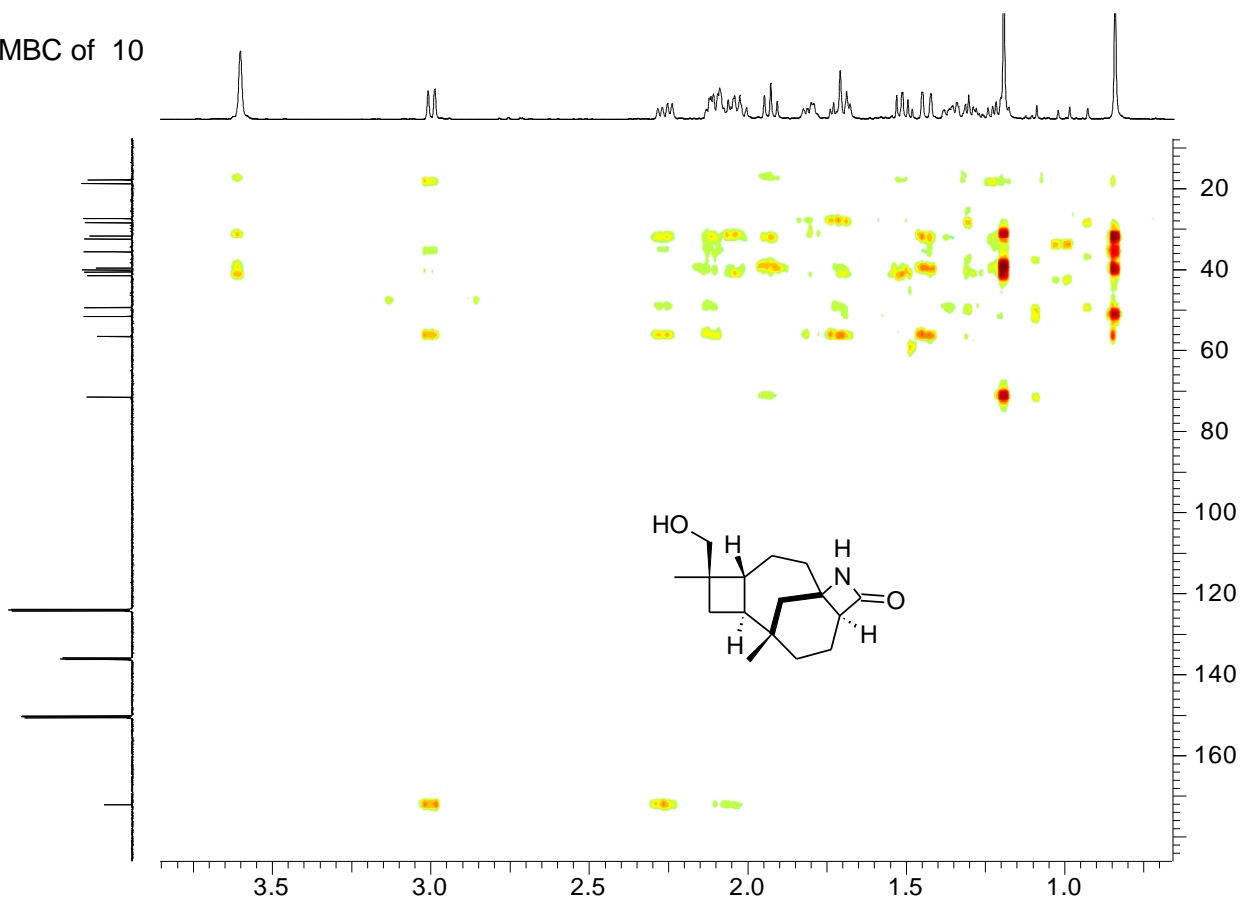
HSQC of 10

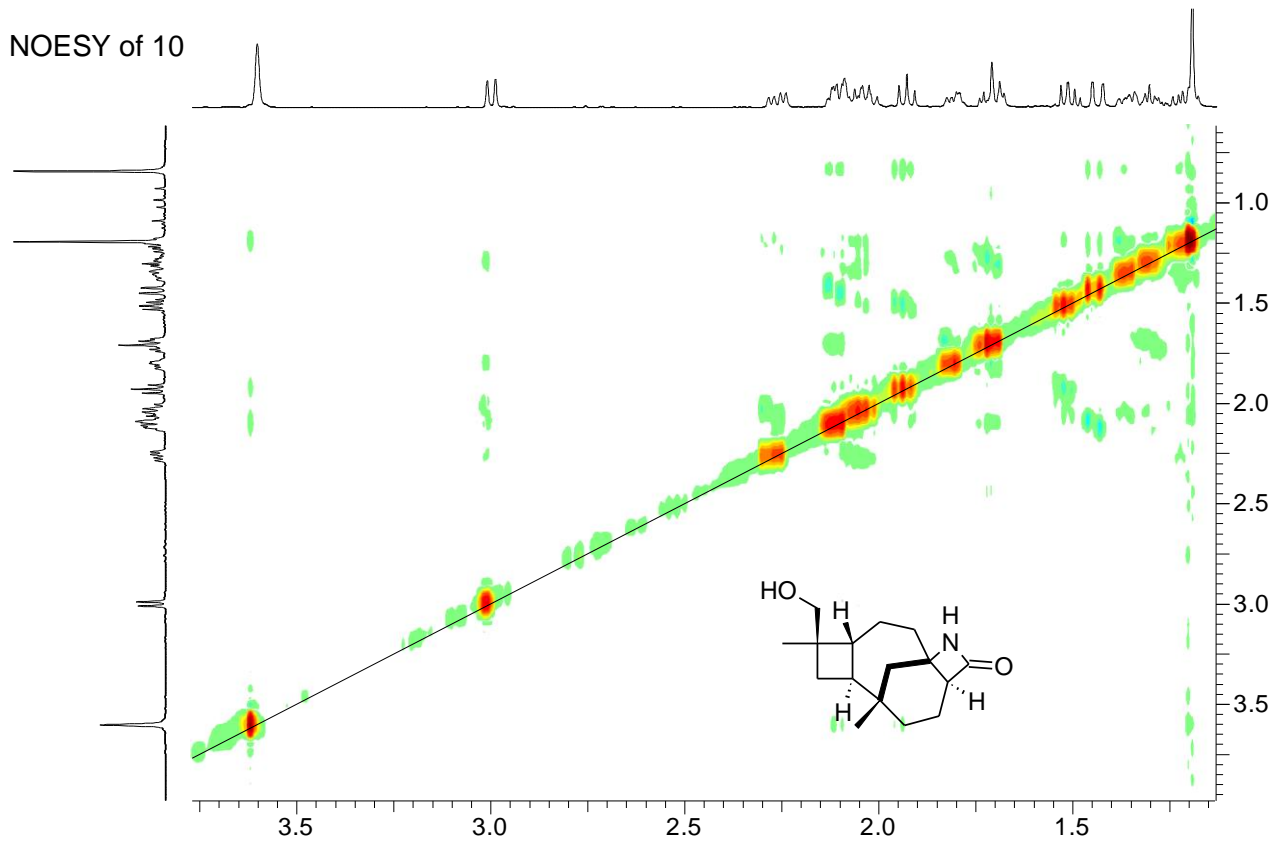


COSY of 10



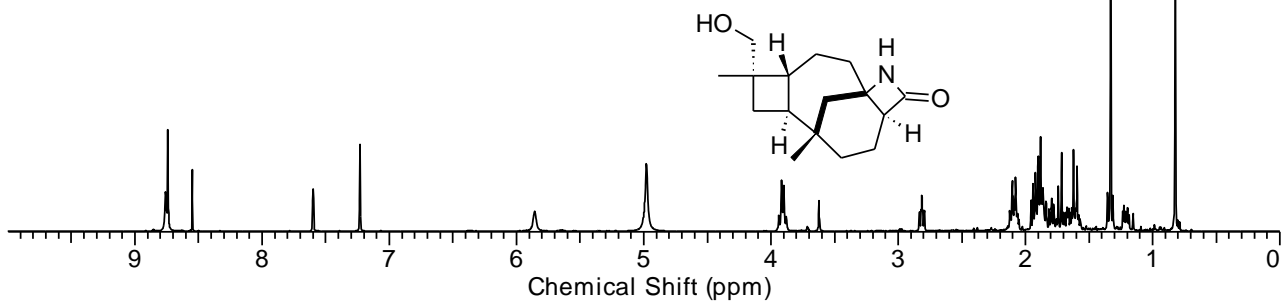
HMBC of 10



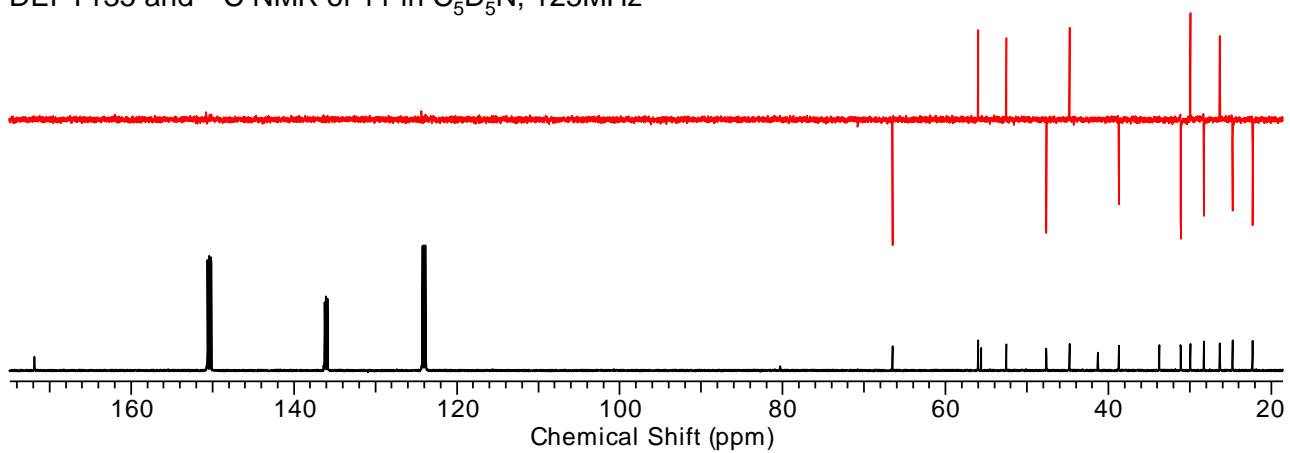


Compound 11

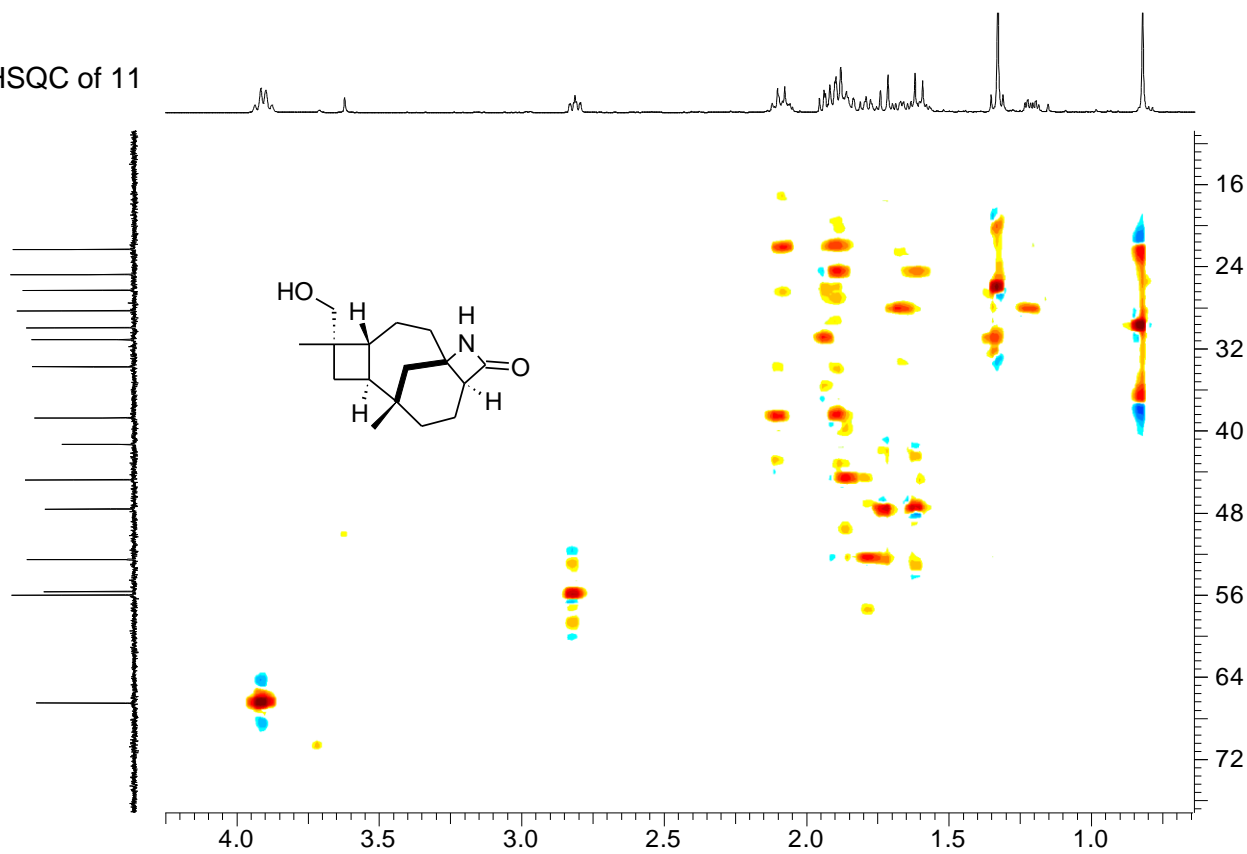
^1H NMR of 11 in $\text{C}_5\text{D}_5\text{N}$, 500MHz



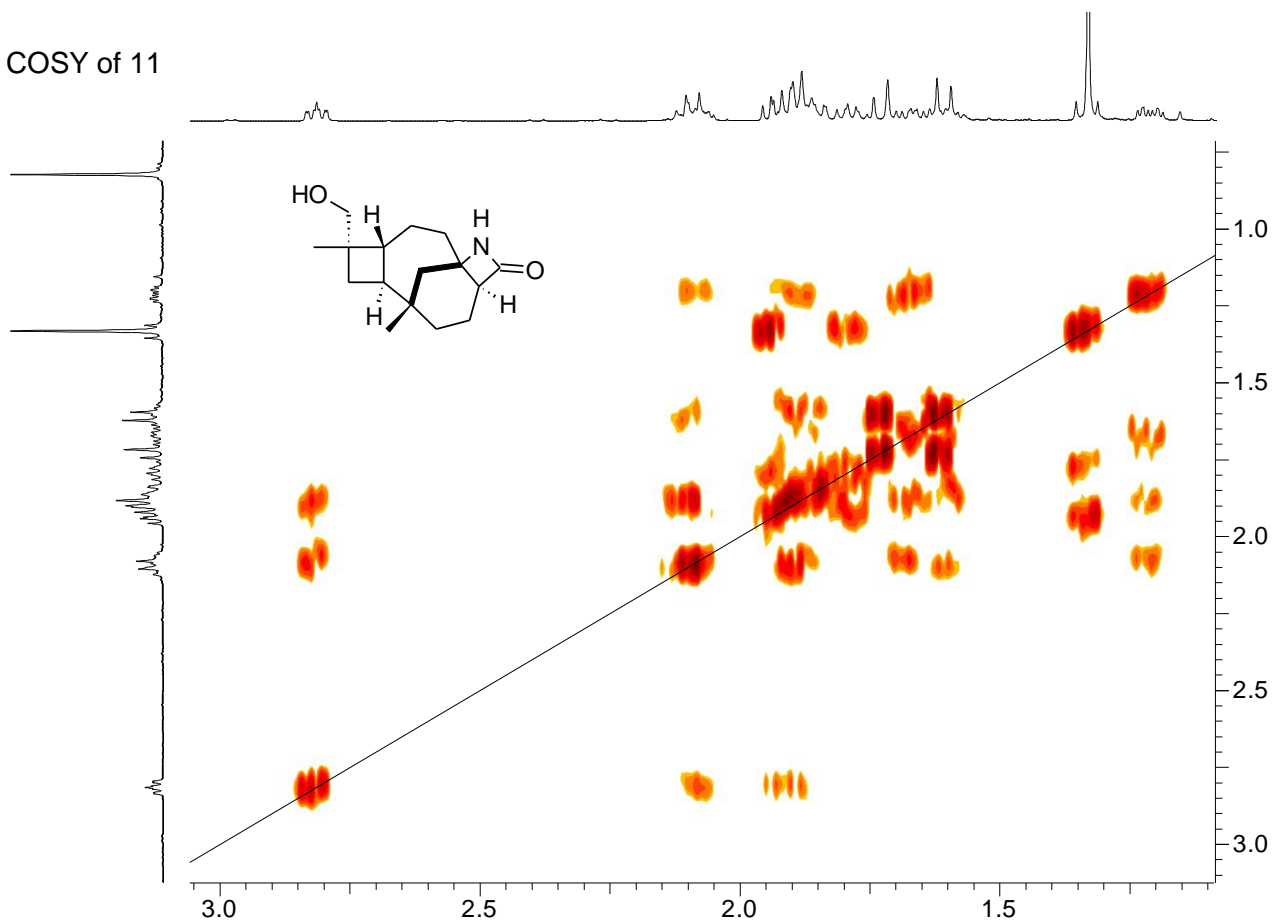
DEPT135 and ^{13}C NMR of 11 in $\text{C}_5\text{D}_5\text{N}$, 125MHz



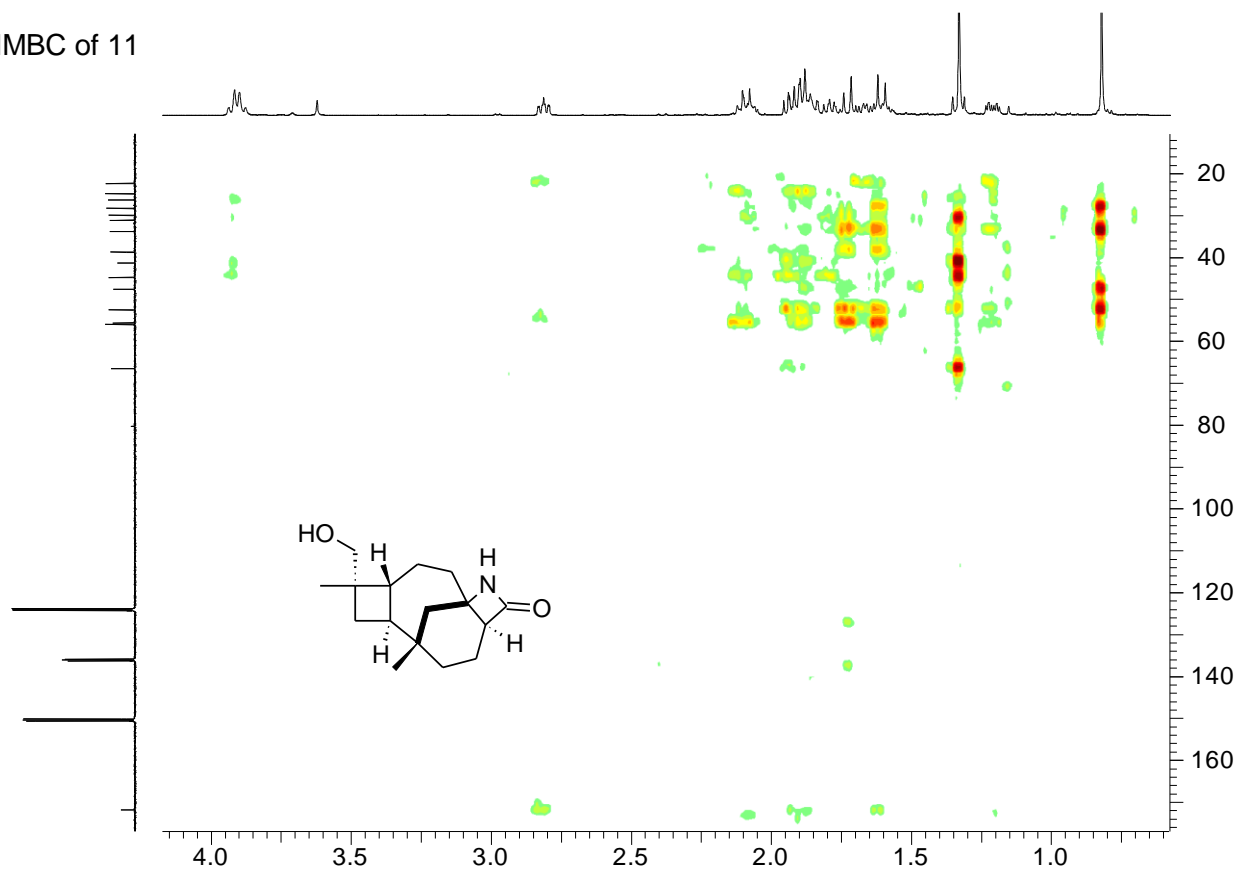
HSQC of 11



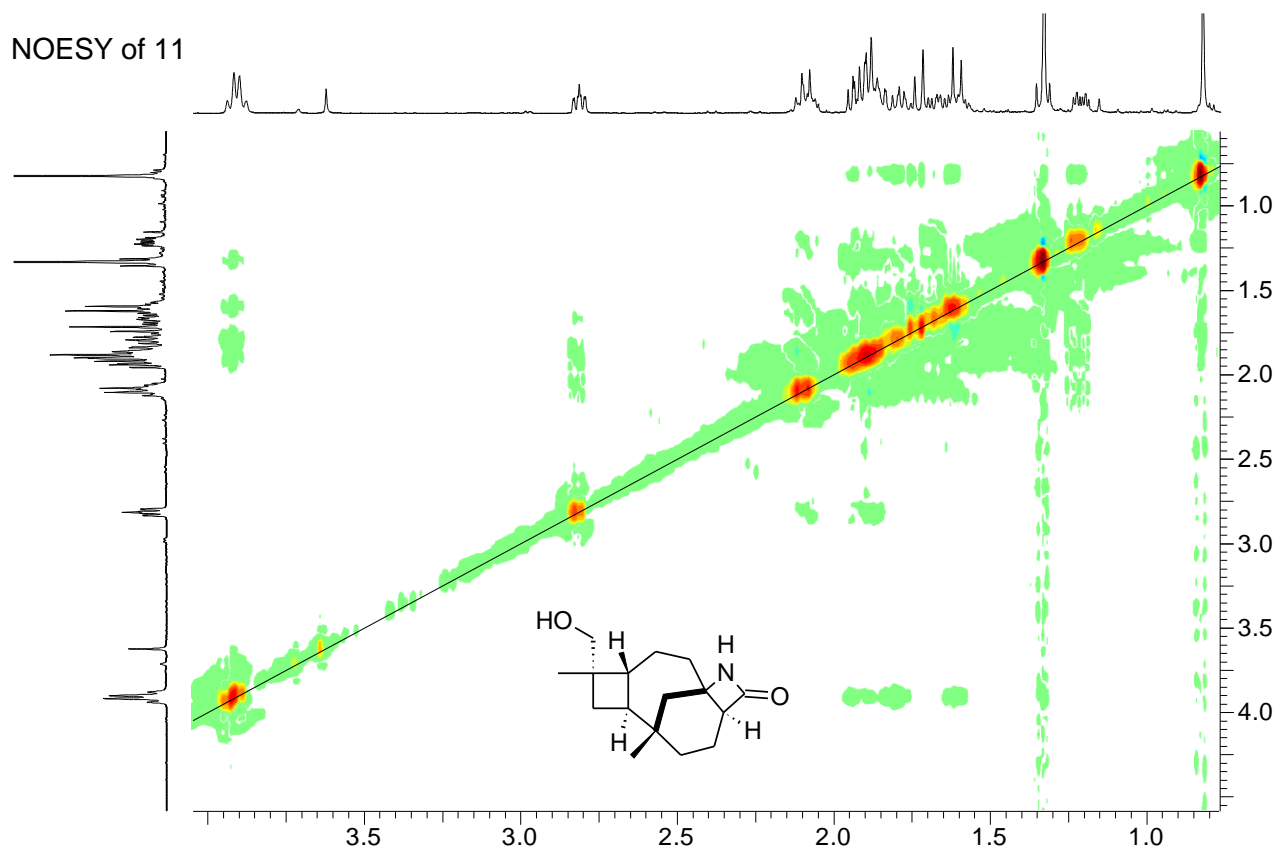
COSY of 11



HMBC of 11

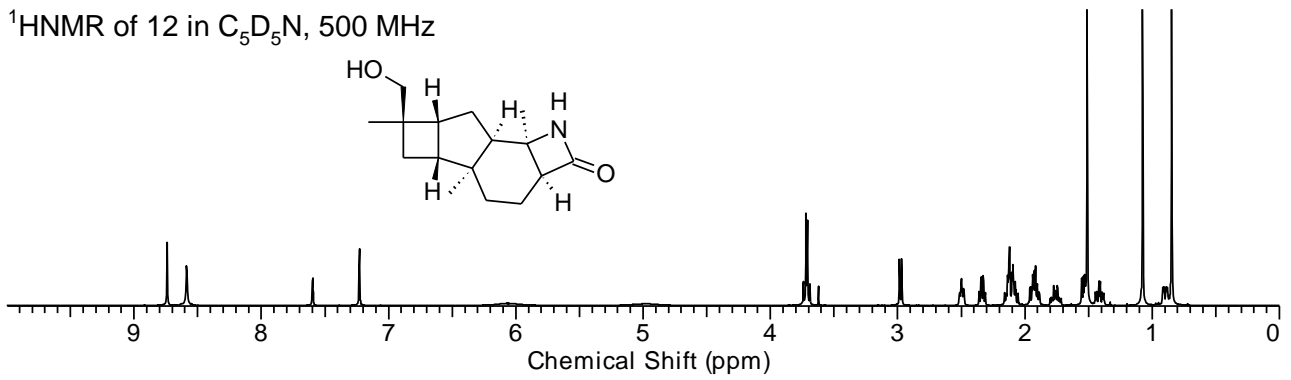


NOESY of 11

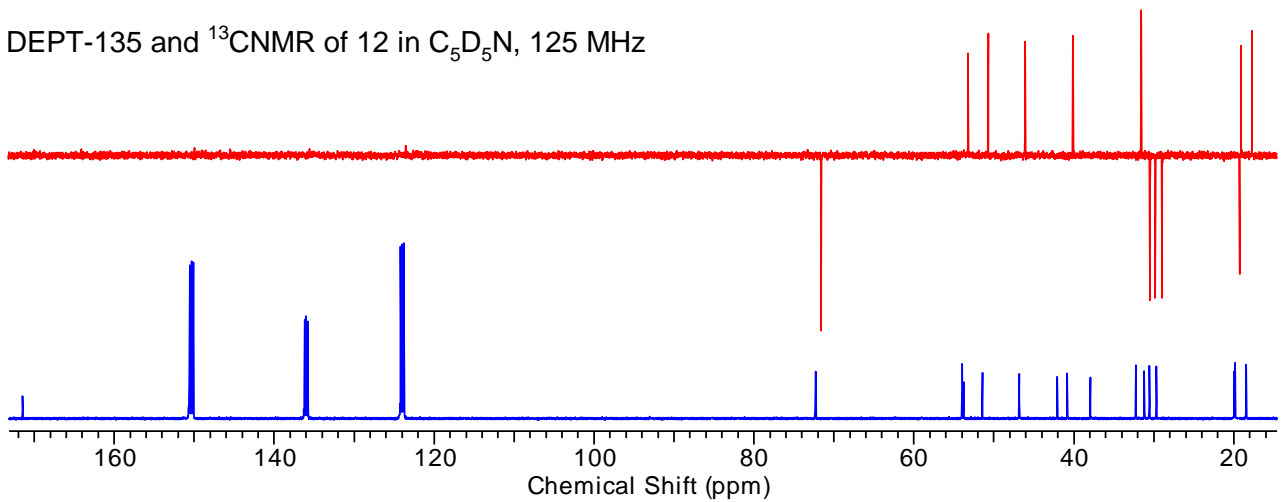


Compound 12

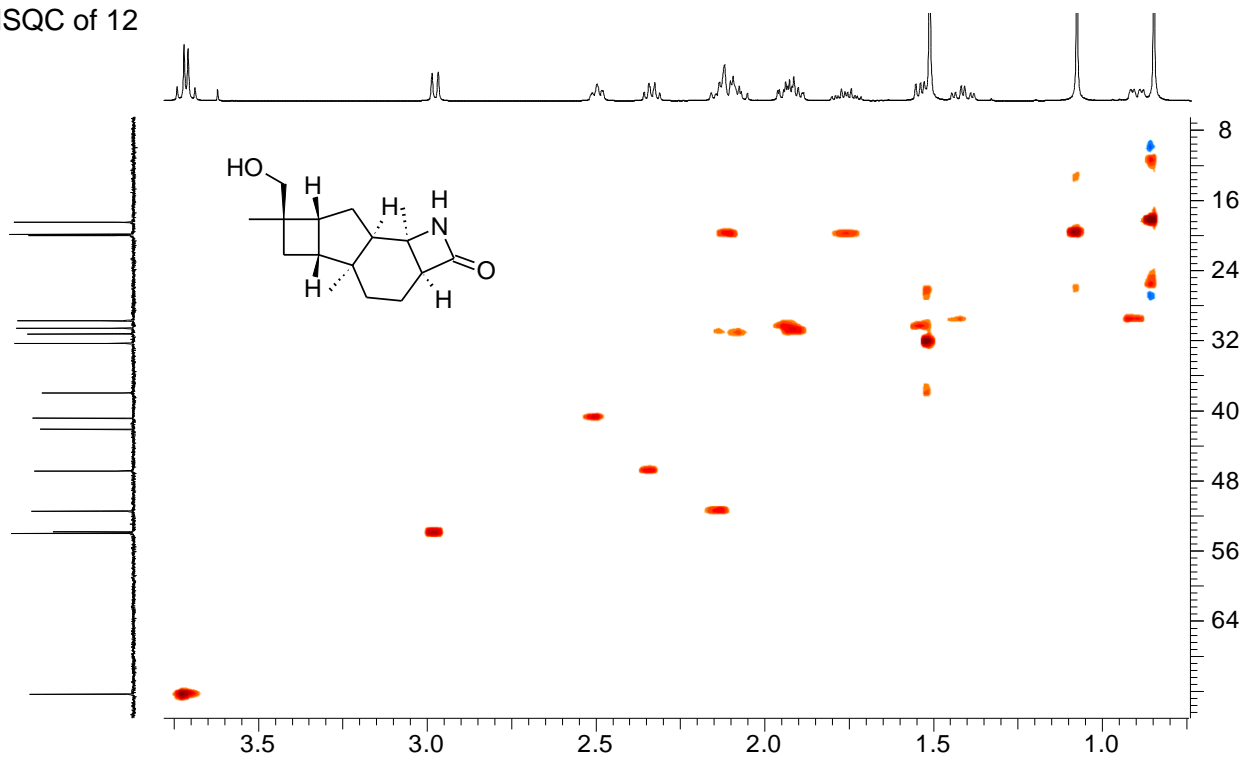
^1H NMR of 12 in $\text{C}_5\text{D}_5\text{N}$, 500 MHz



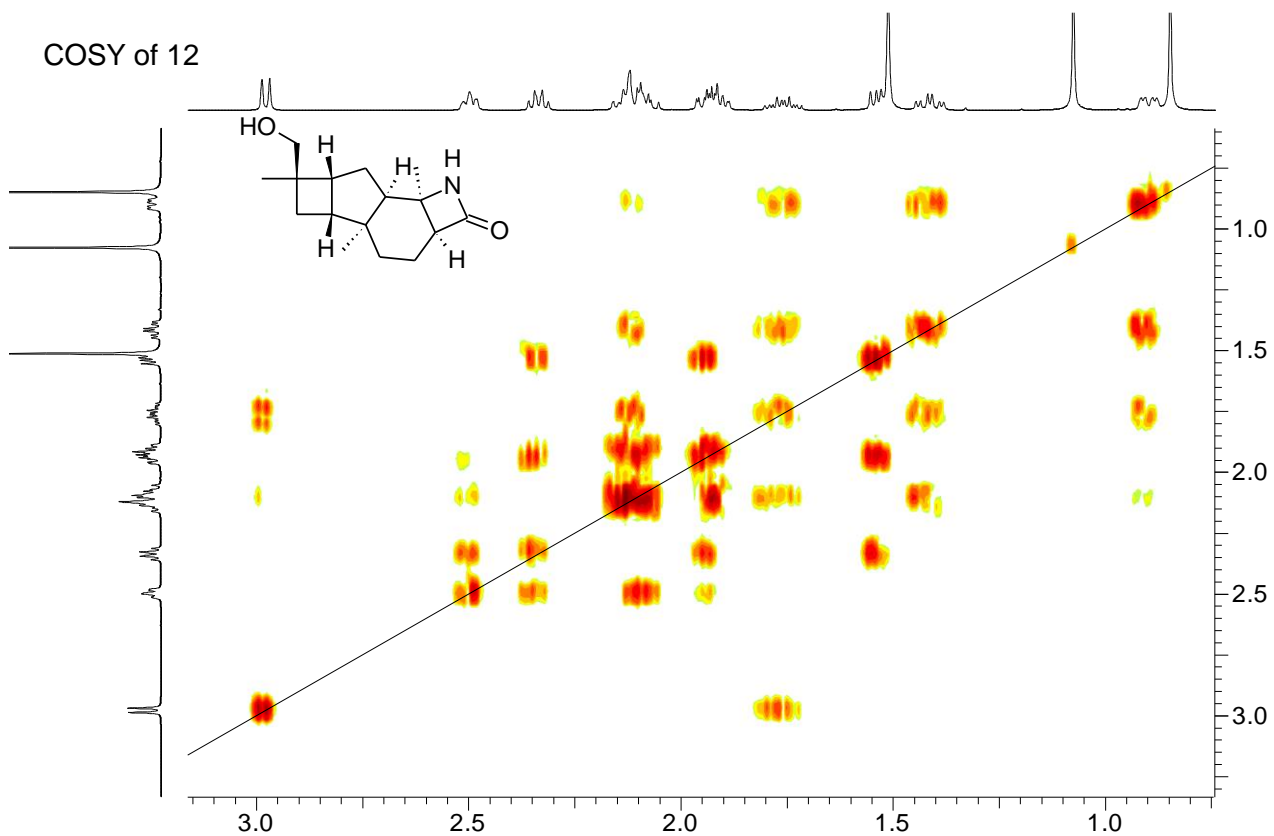
DEPT-135 and ^{13}C NMR of 12 in $\text{C}_5\text{D}_5\text{N}$, 125 MHz



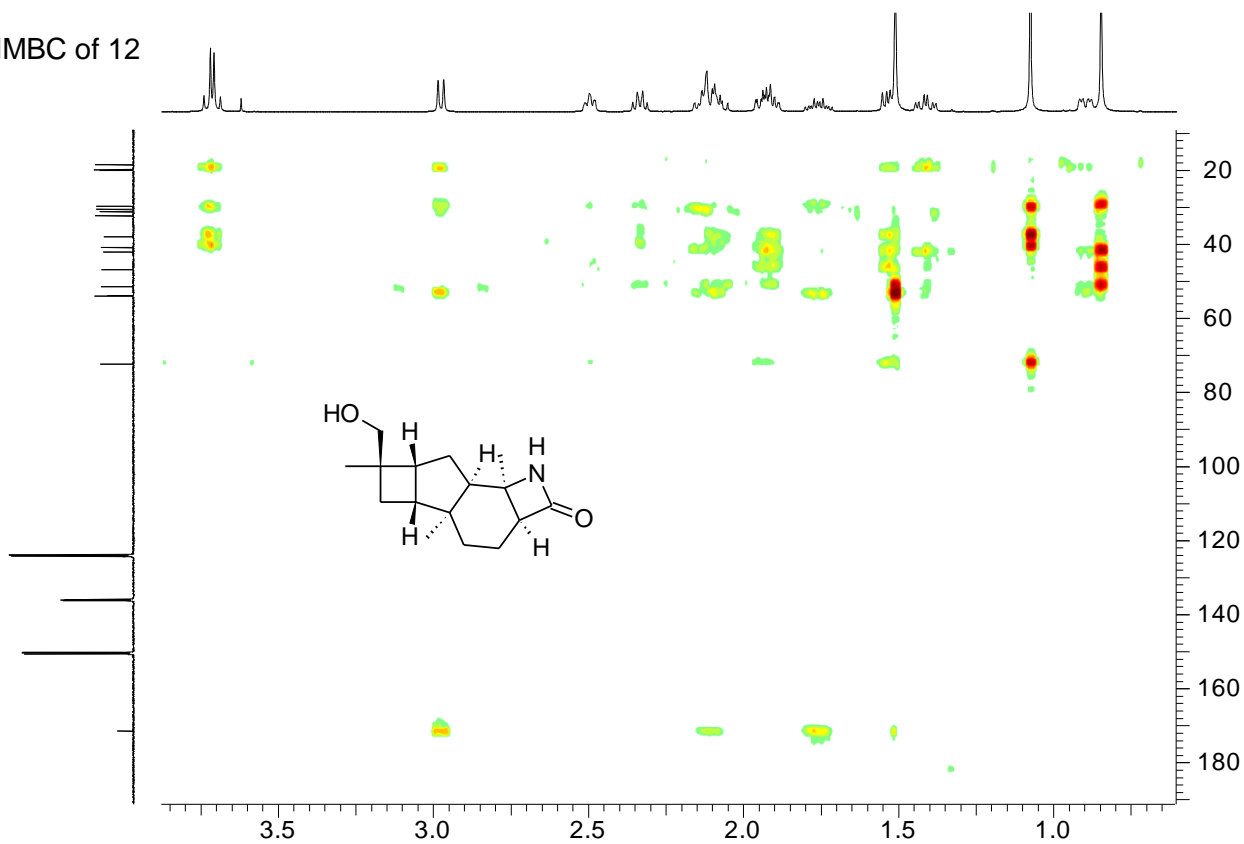
HSQC of 12



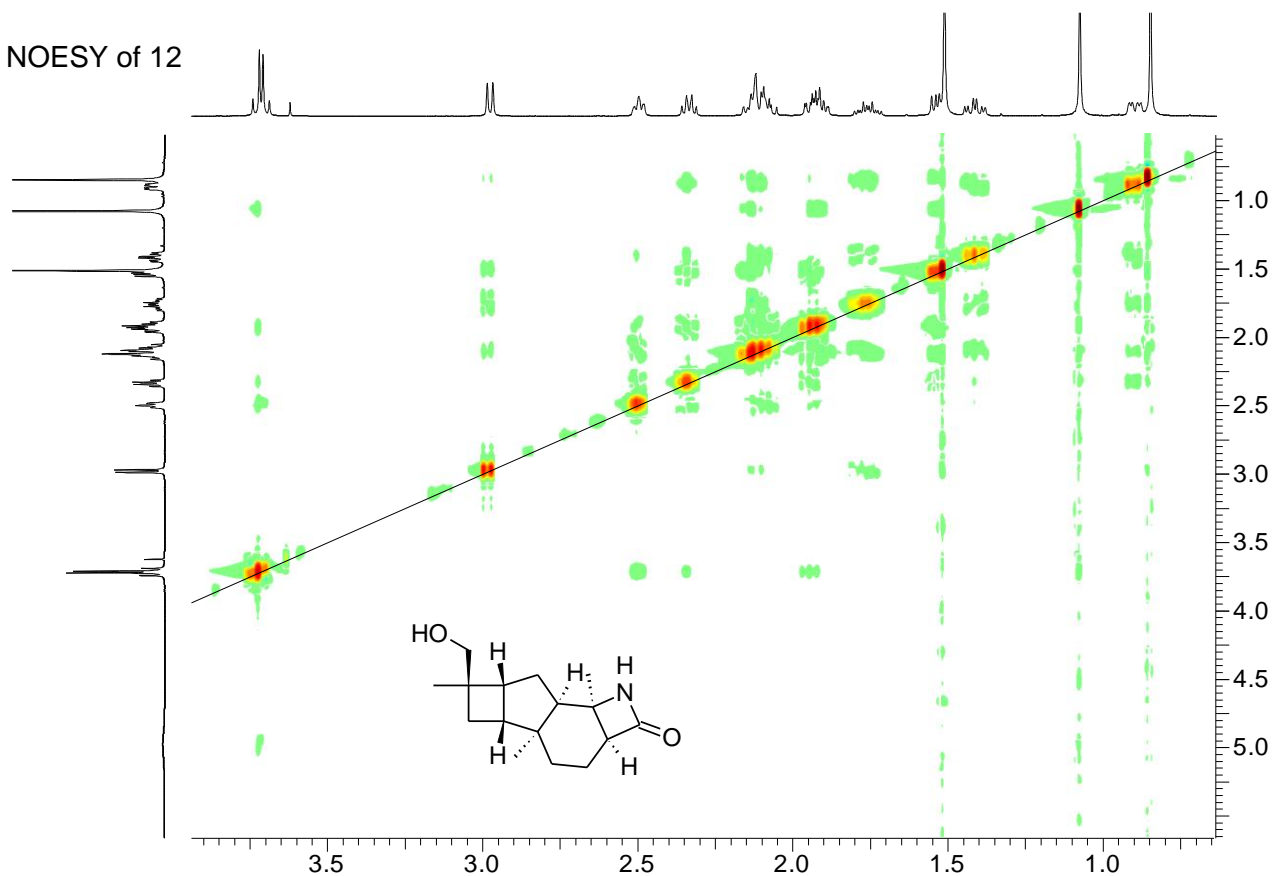
COSY of 12



HMBC of 12

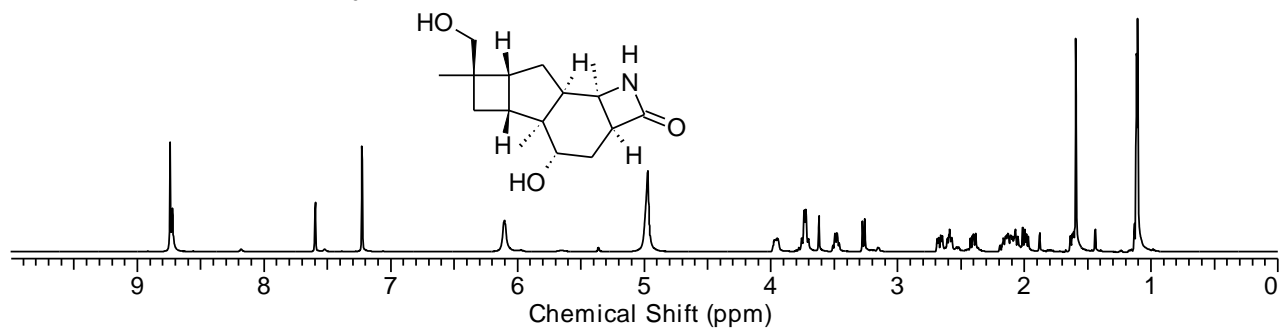


NOESY of 12

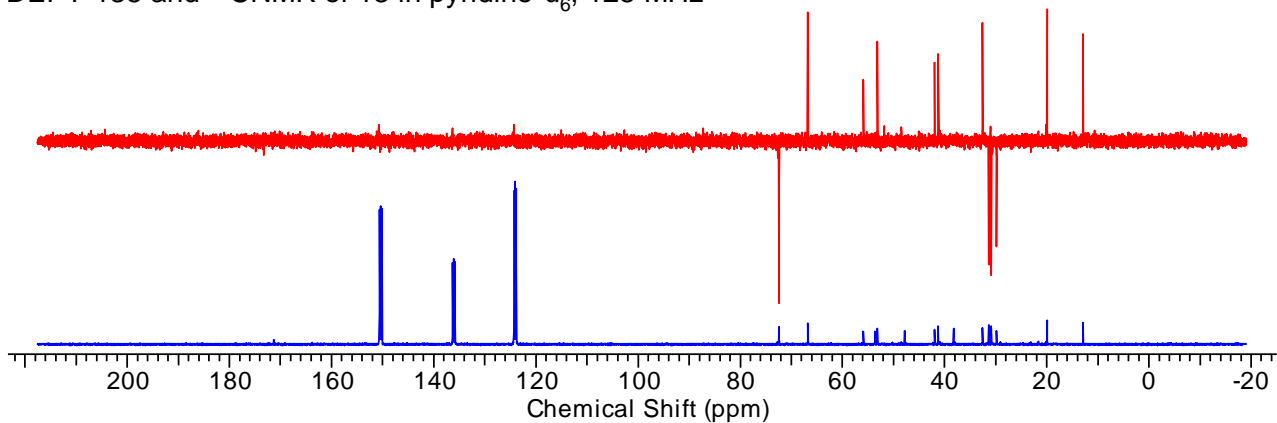


Compound 13

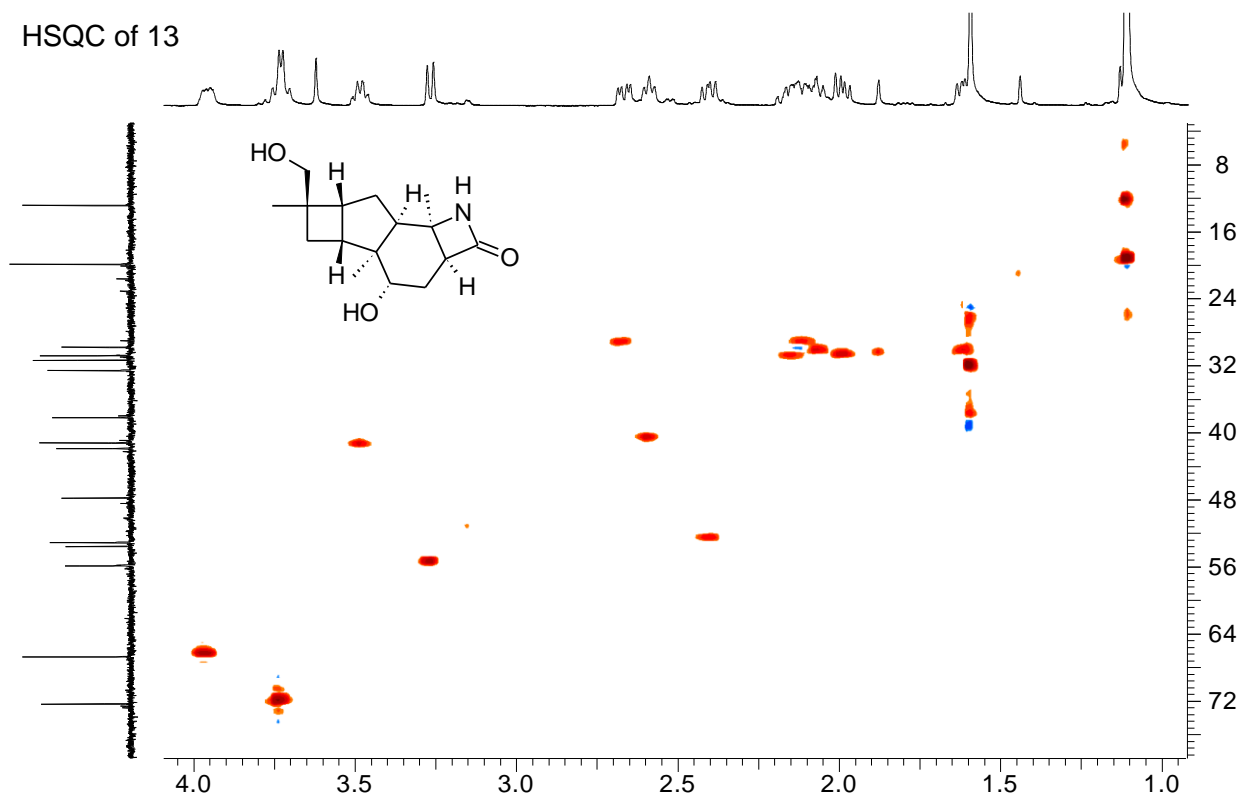
^1H NMR of 13 in pyridine- d_6 , 500 MHz



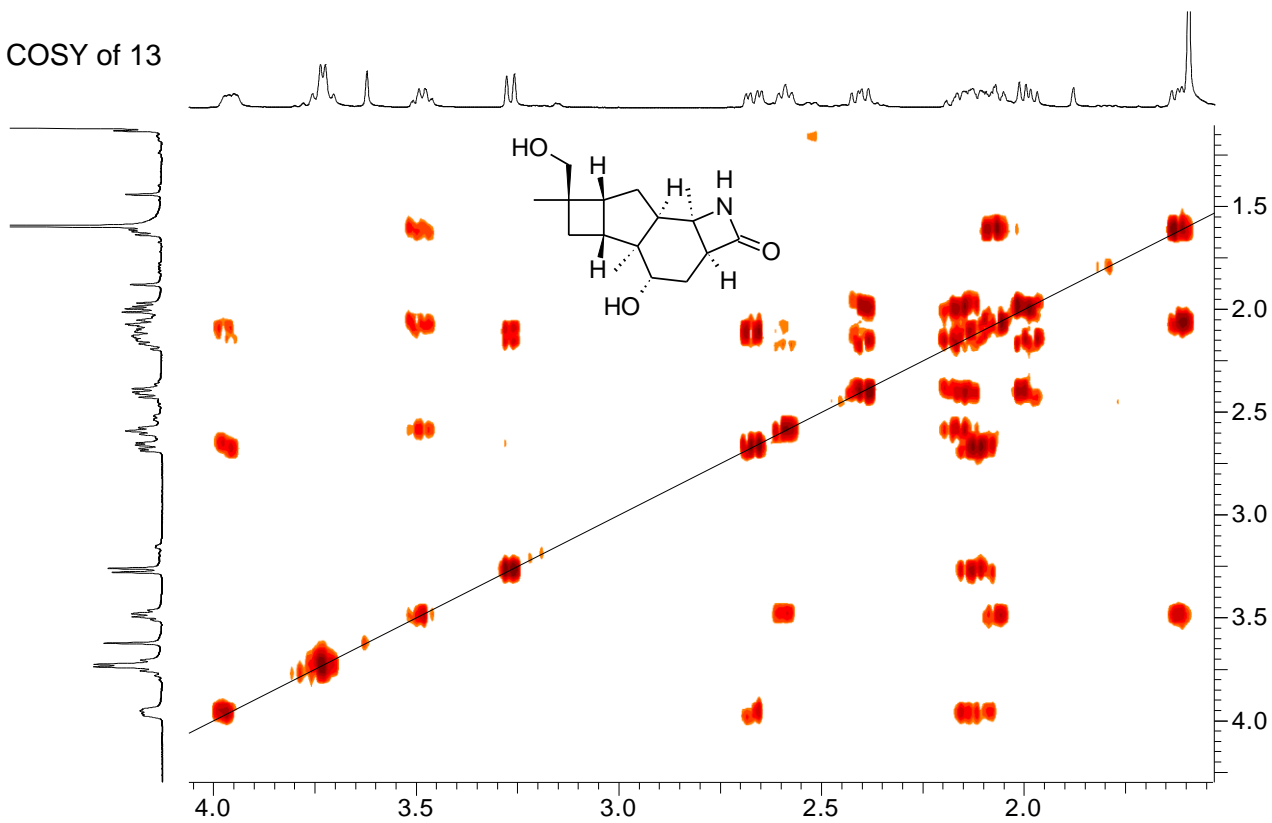
DEPT-135 and ^{13}C NMR of 13 in pyridine- d_6 , 125 MHz



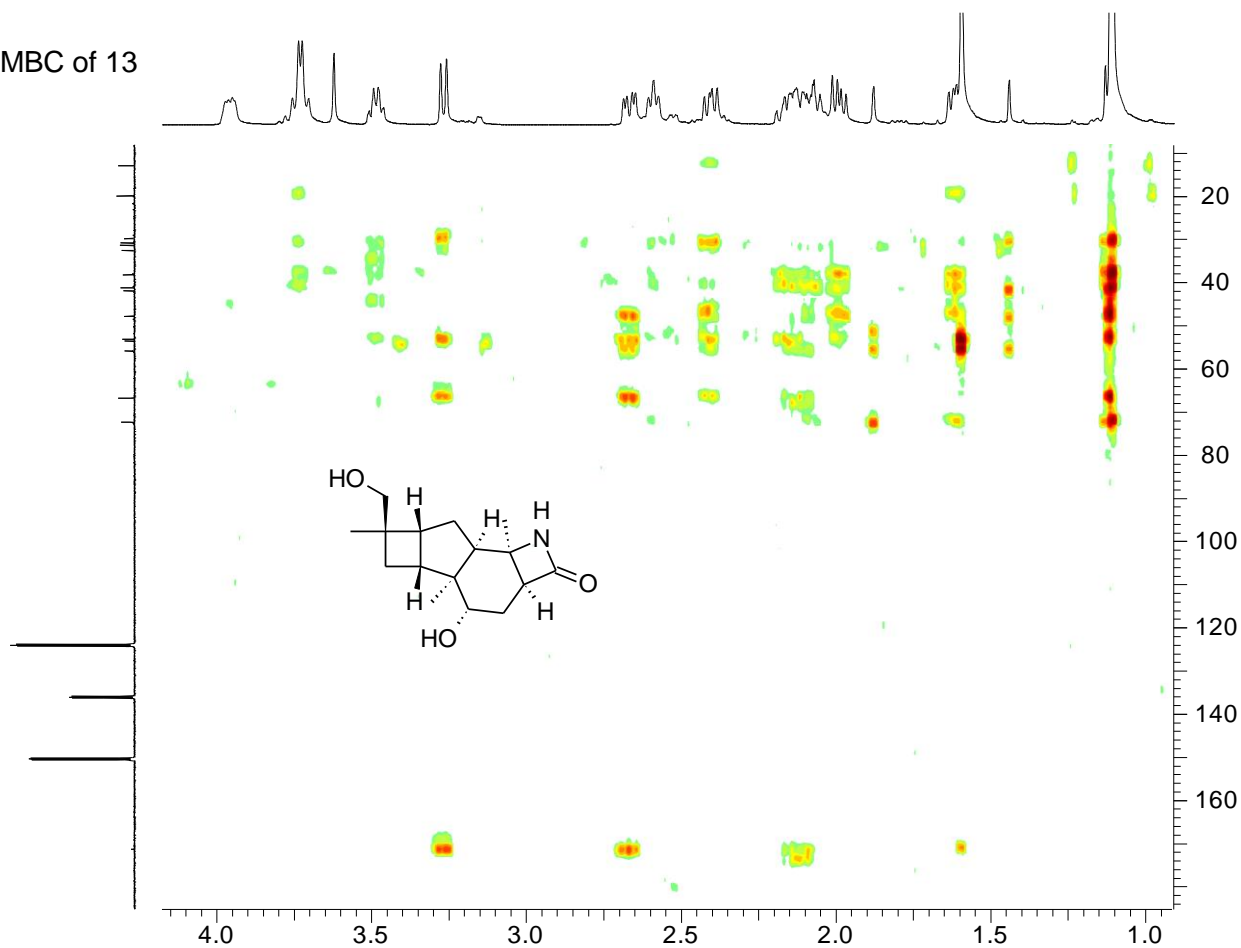
HSQC of 13



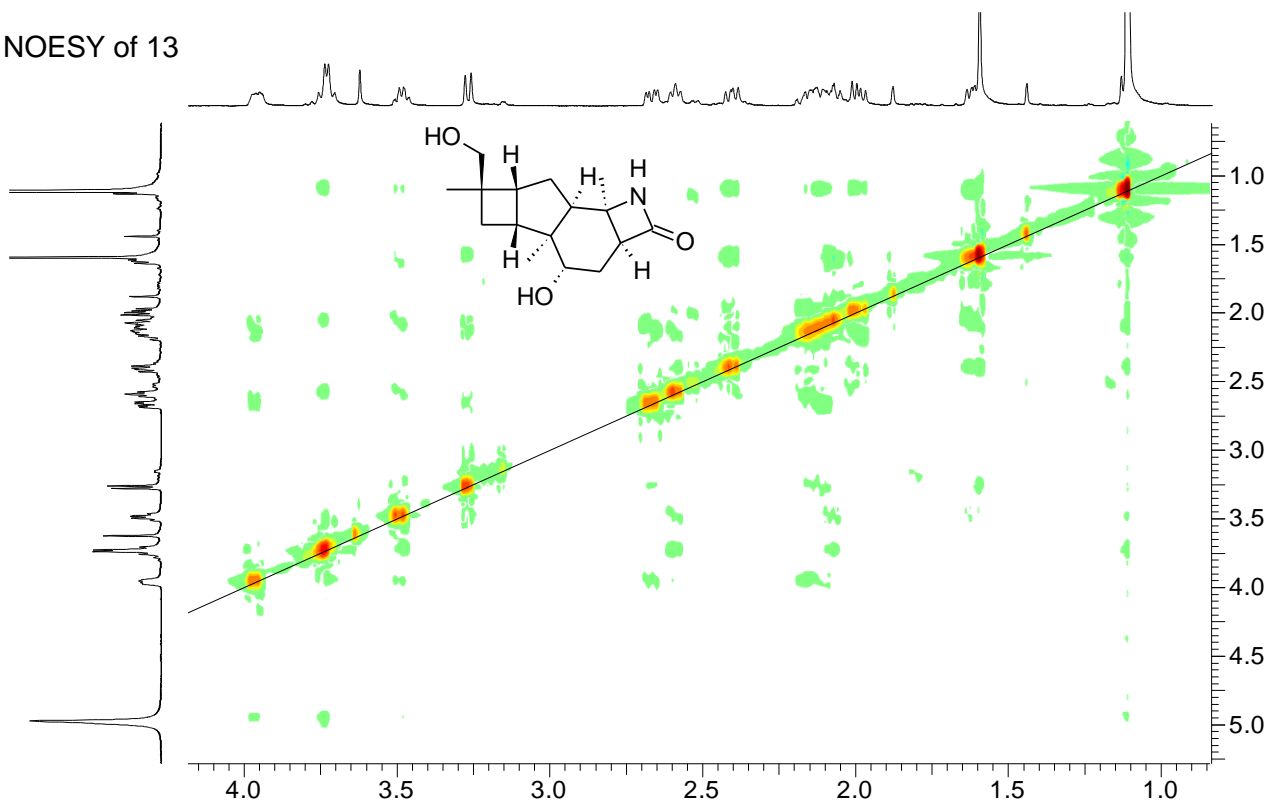
COSY of 13



HMBC of 13

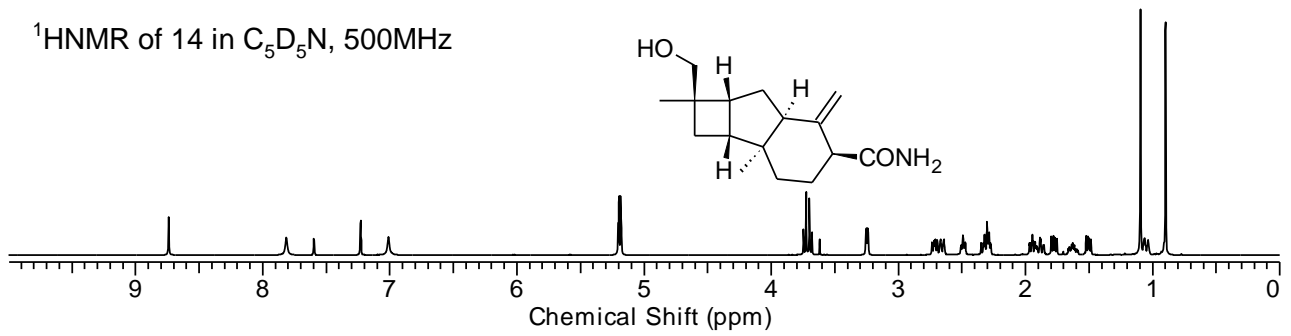


NOESY of 13

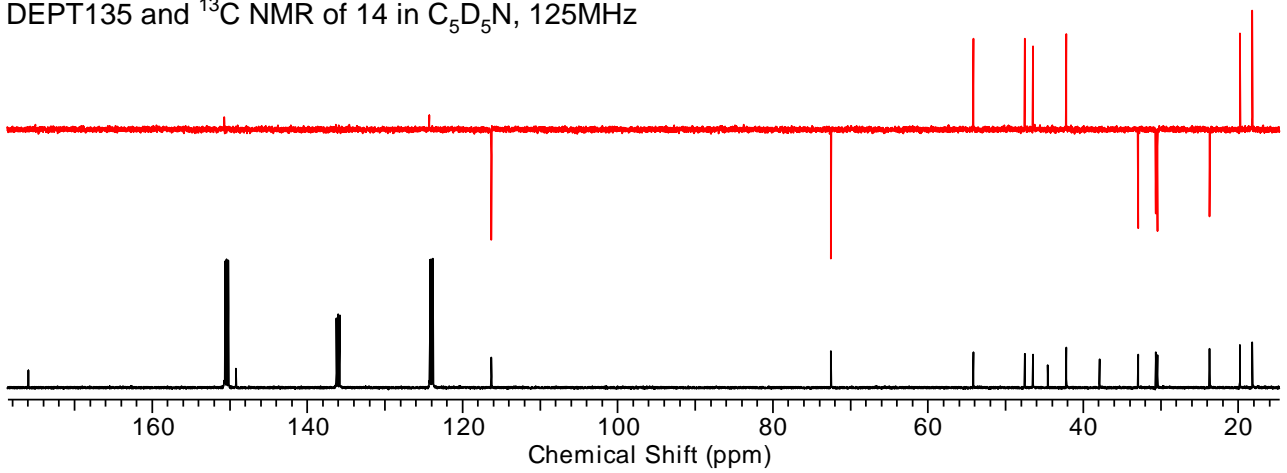


Compound 14

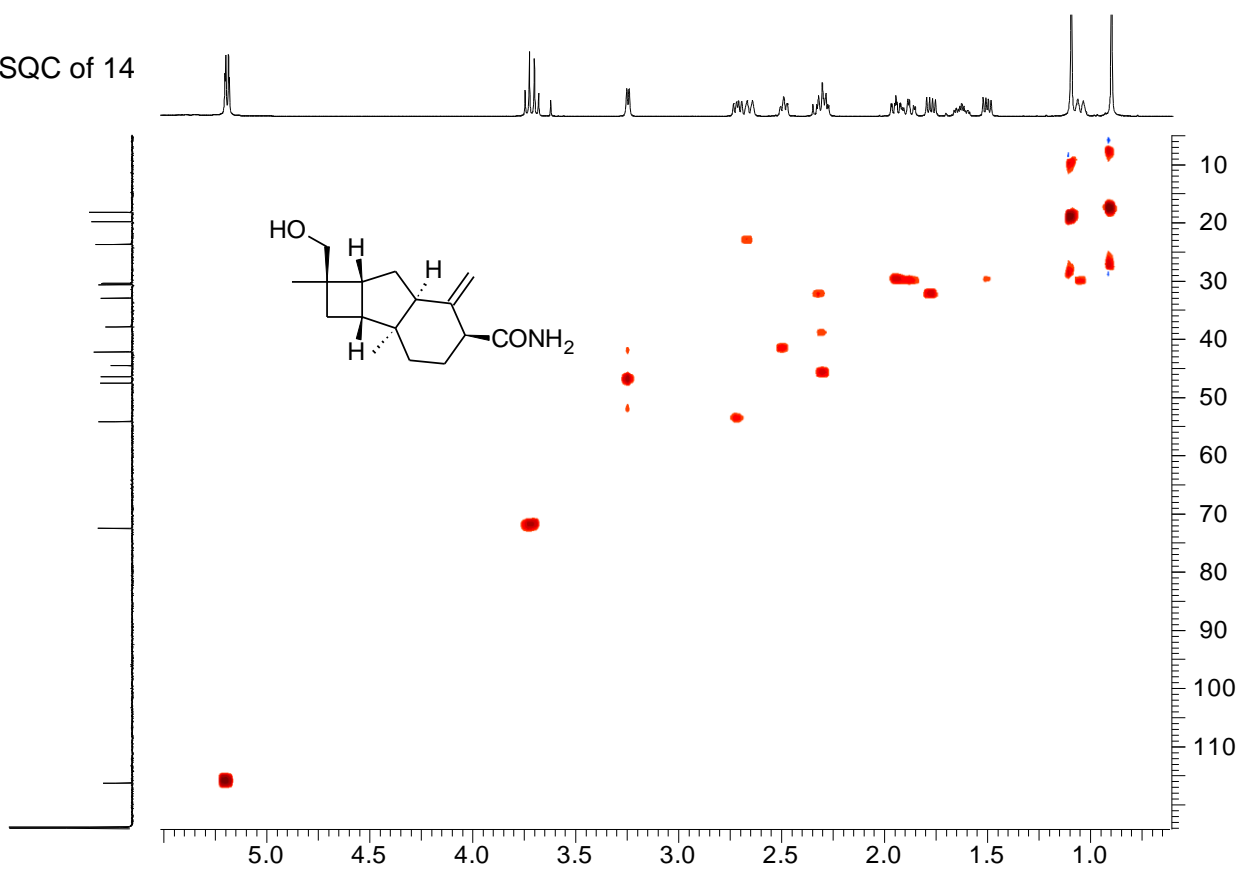
^1H NMR of 14 in $\text{C}_5\text{D}_5\text{N}$, 500MHz



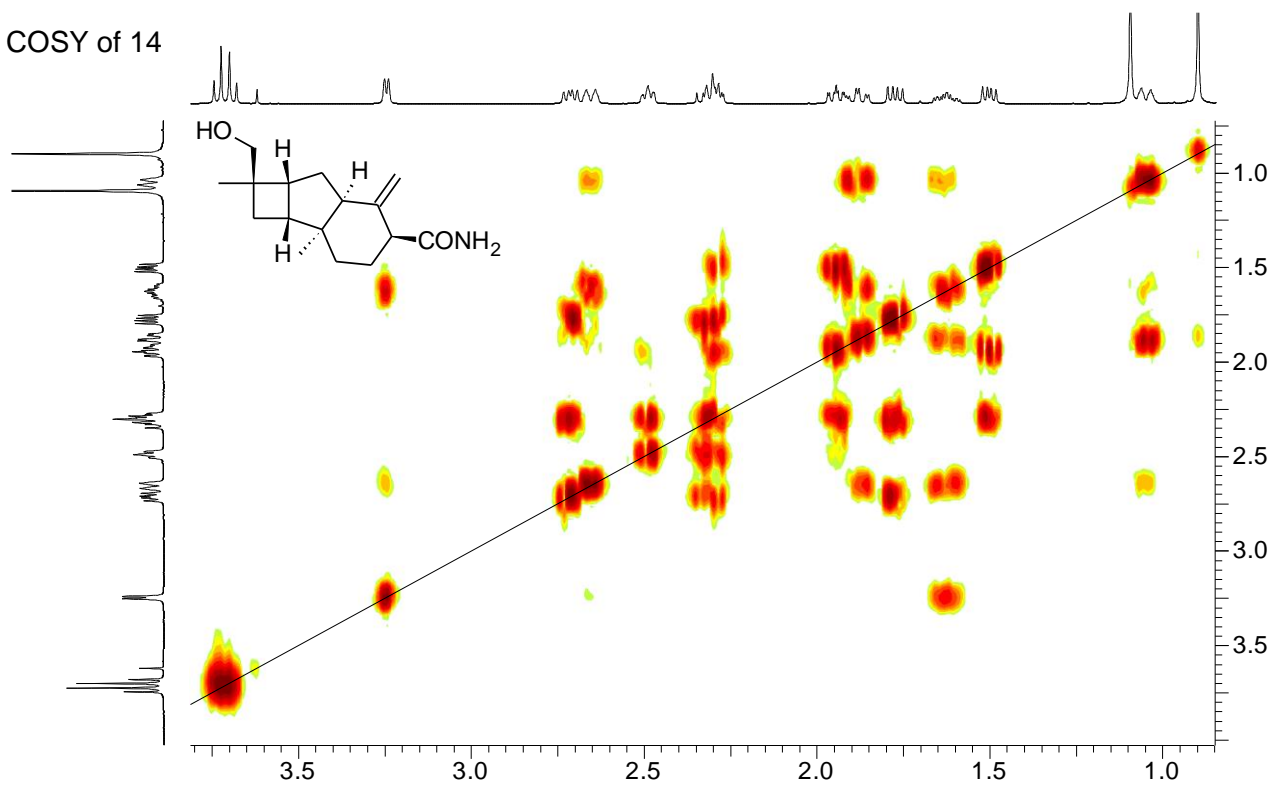
DEPT135 and ^{13}C NMR of 14 in $\text{C}_5\text{D}_5\text{N}$, 125MHz



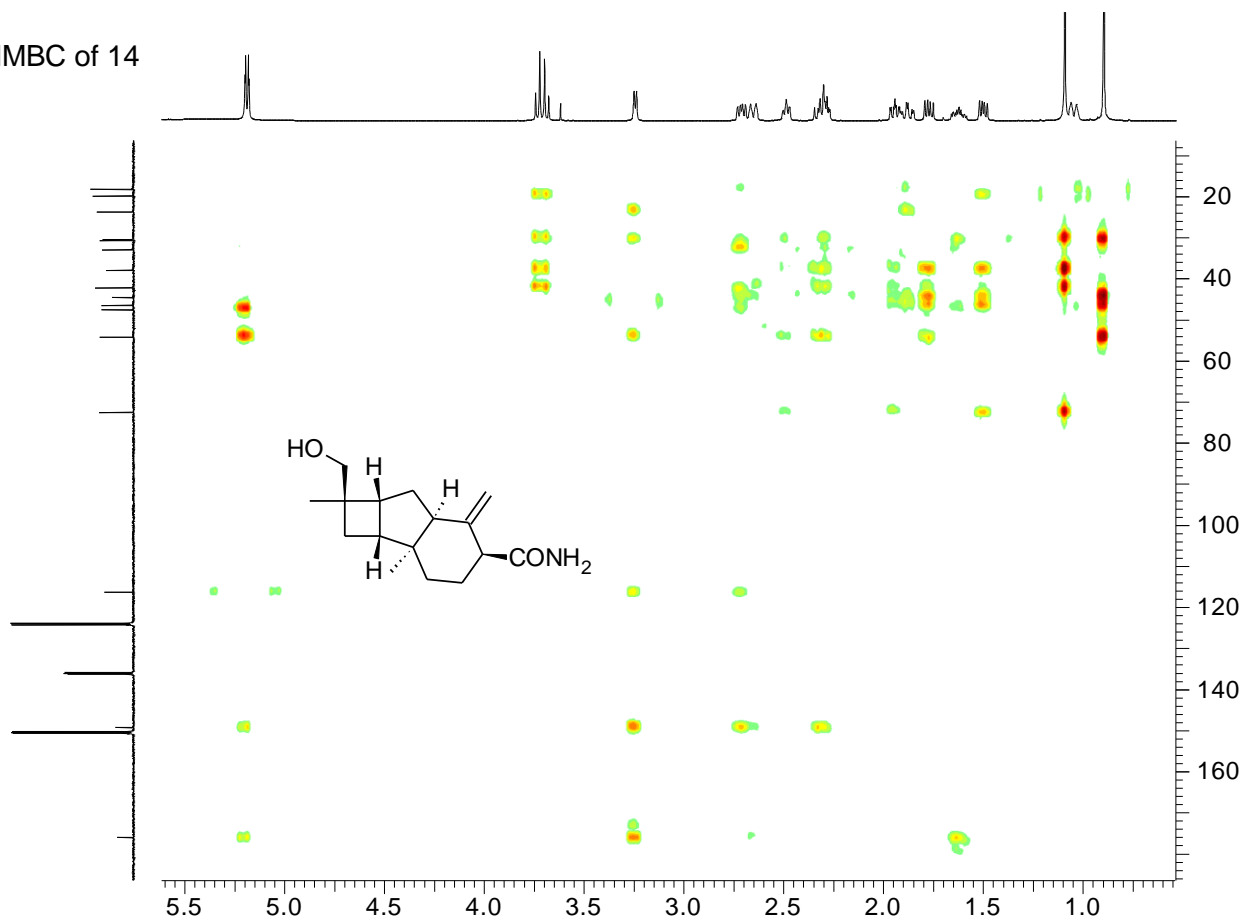
HSQC of 14



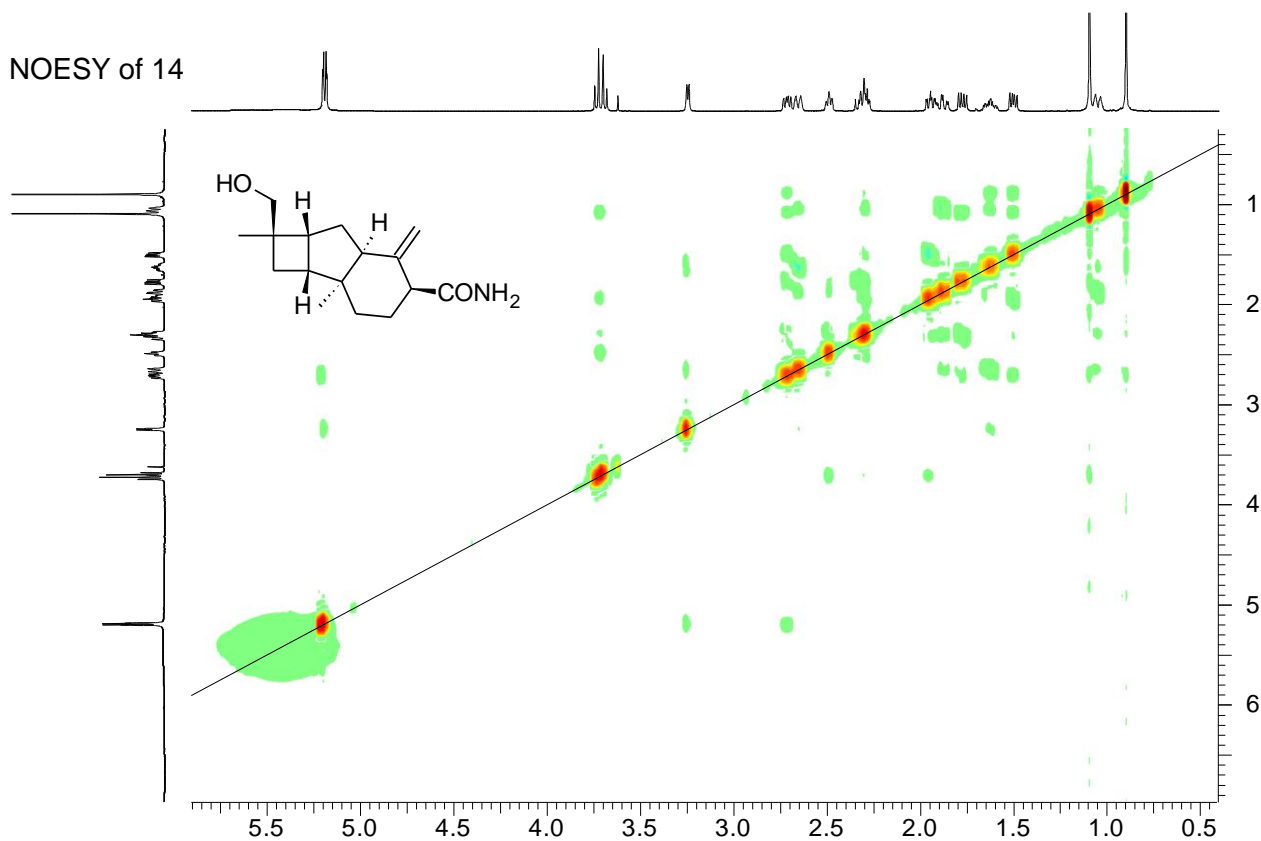
COSY of 14



HMBC of 14

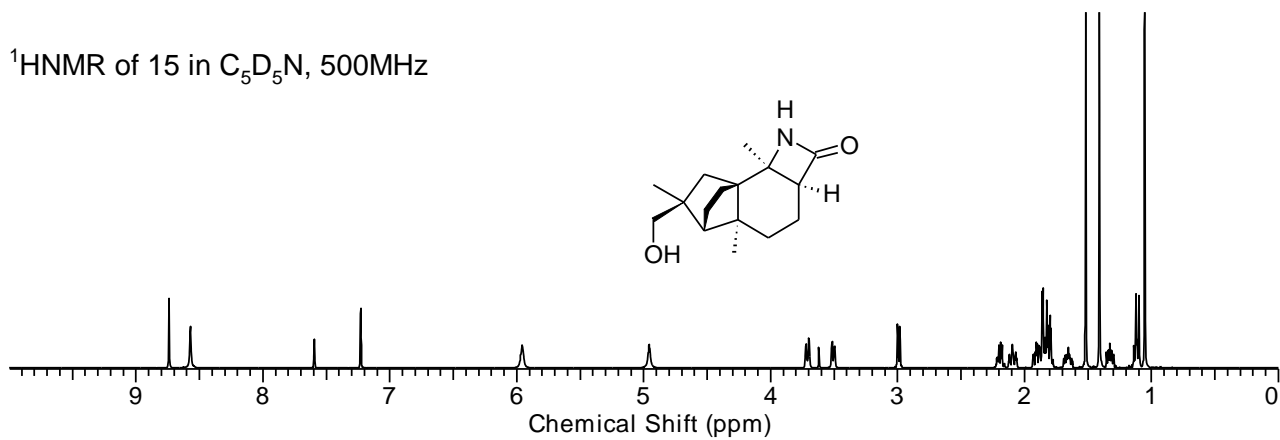


NOESY of 14

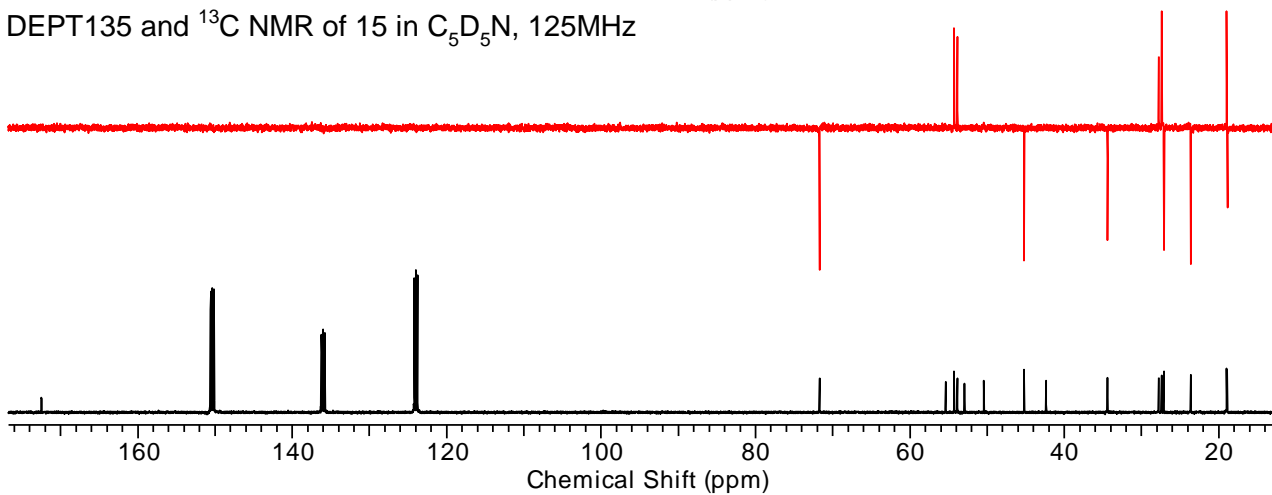


Compound 15

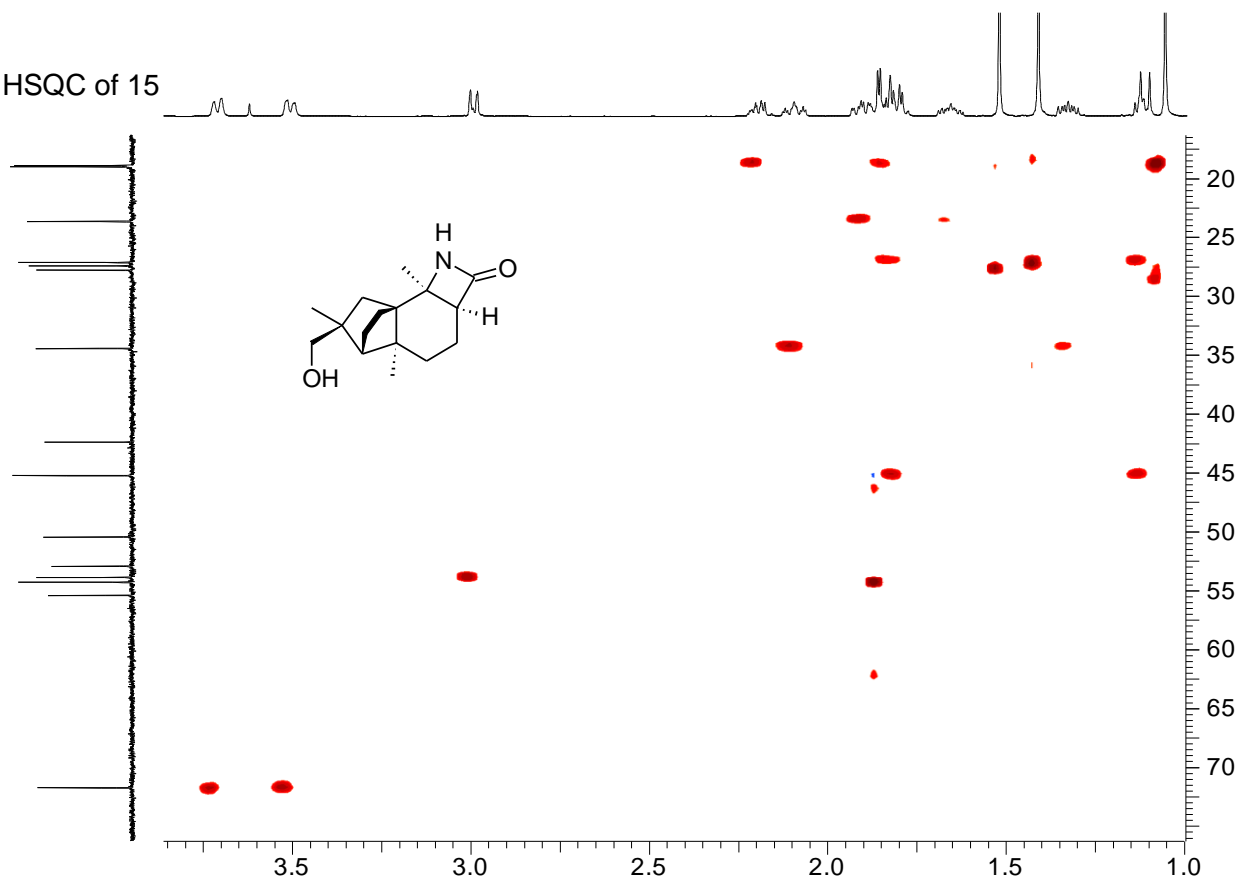
^1H NMR of 15 in $\text{C}_5\text{D}_5\text{N}$, 500MHz



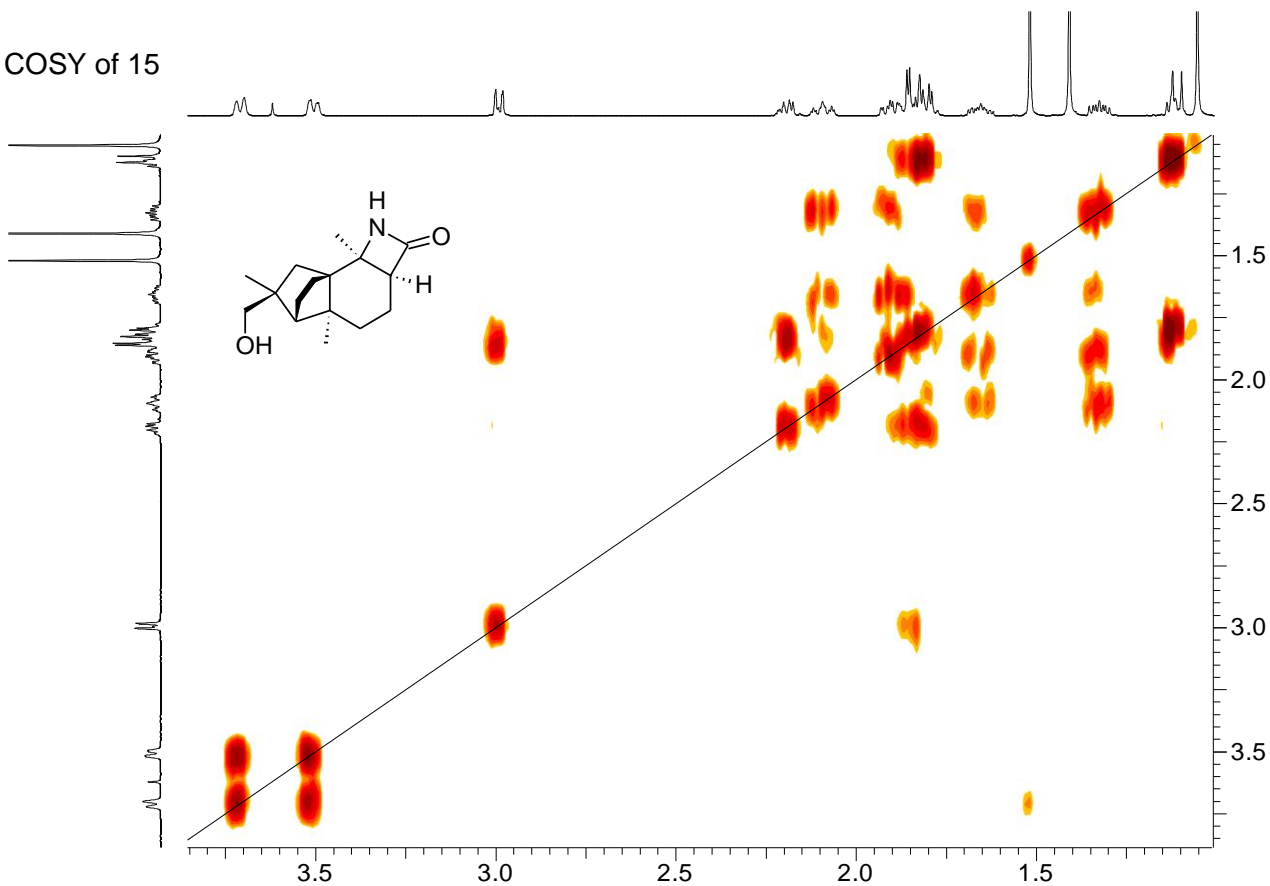
DEPT135 and ^{13}C NMR of 15 in $\text{C}_5\text{D}_5\text{N}$, 125MHz



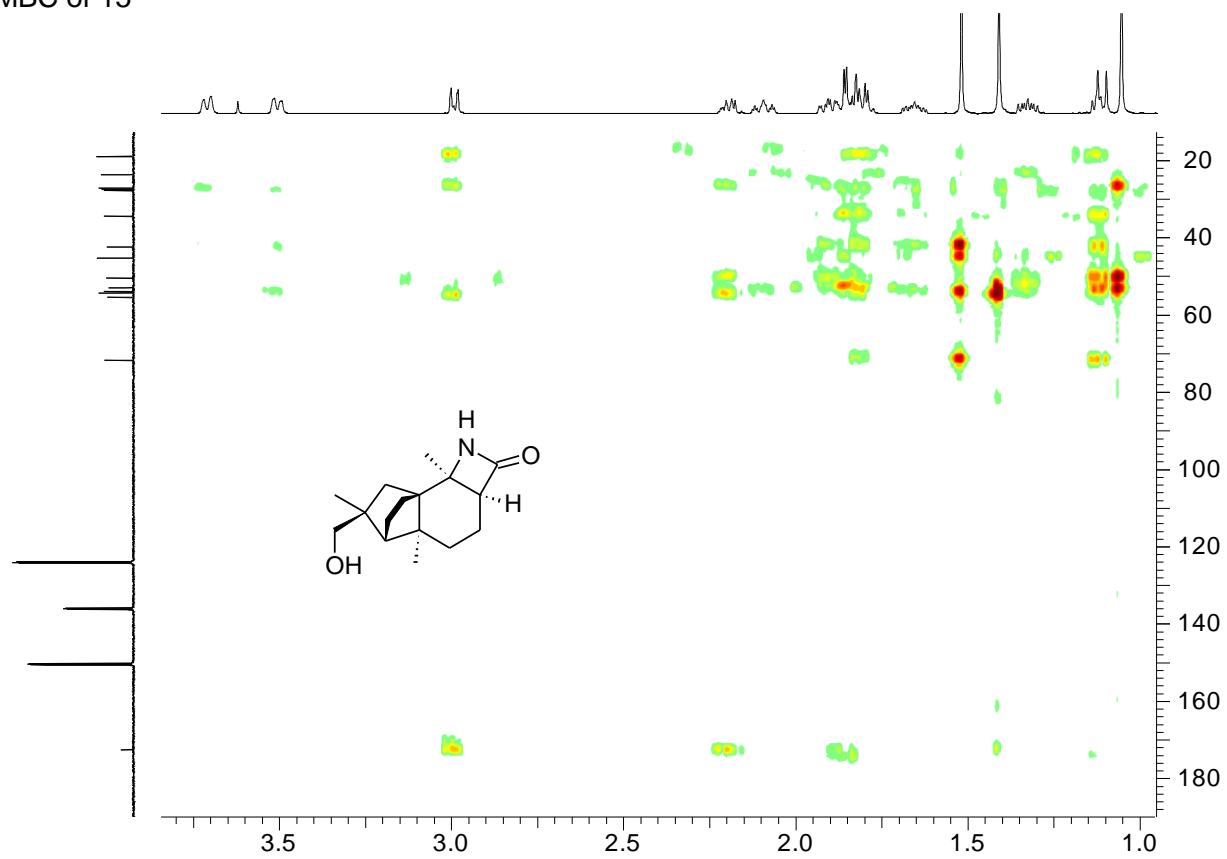
HSQC of 15



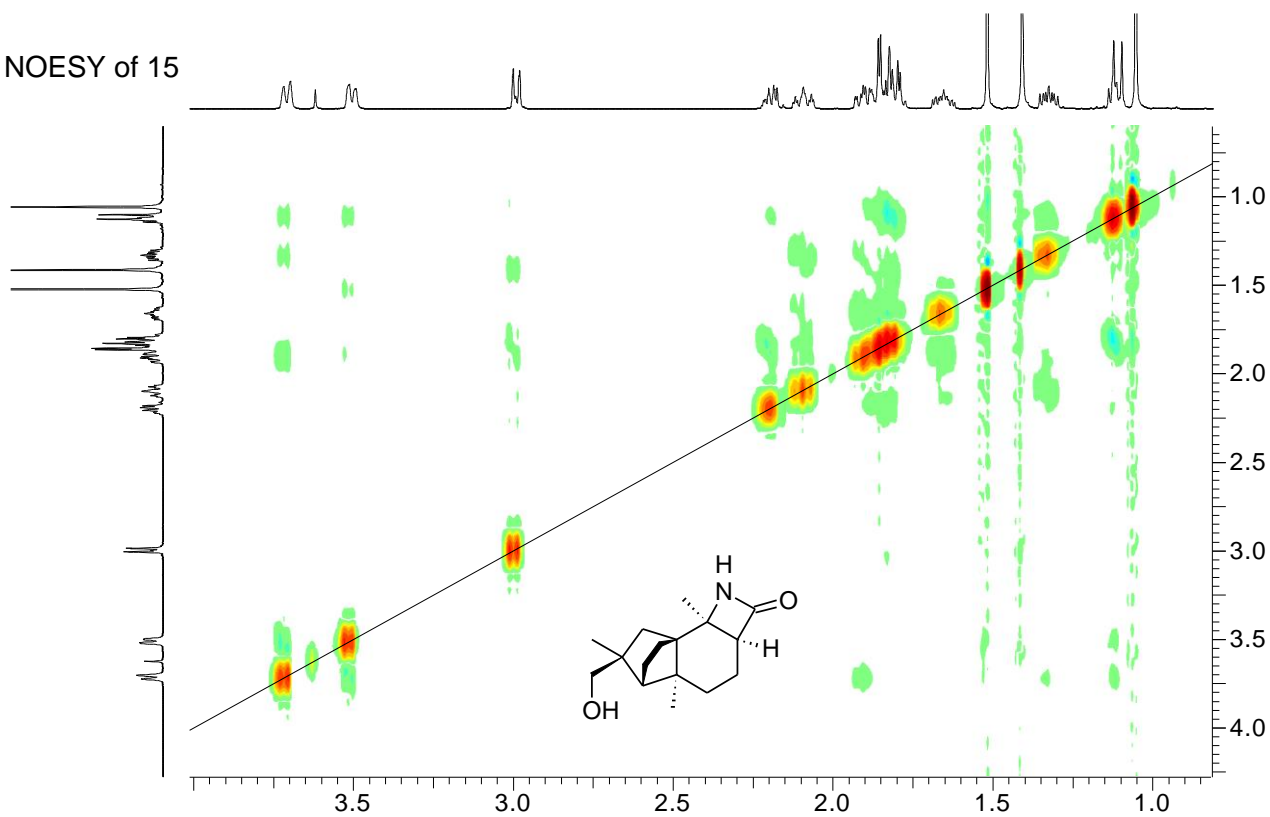
COSY of 15



HMBC of 15

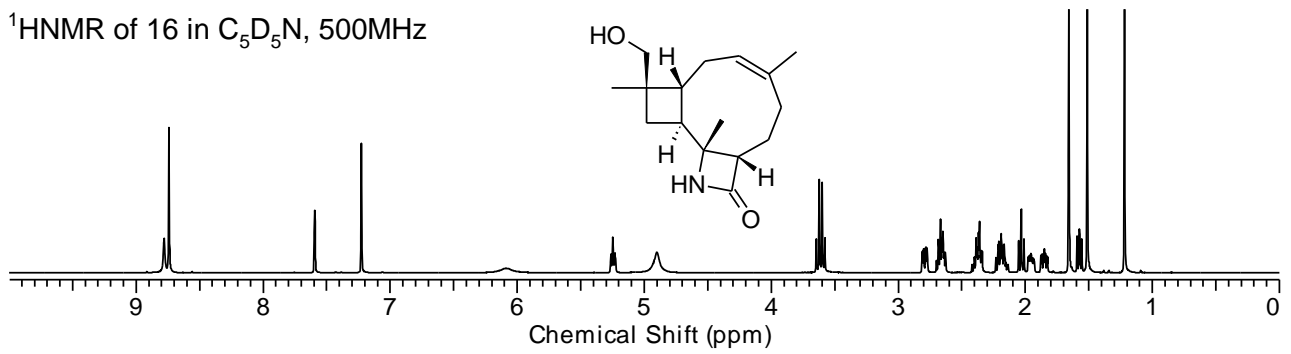


NOESY of 15

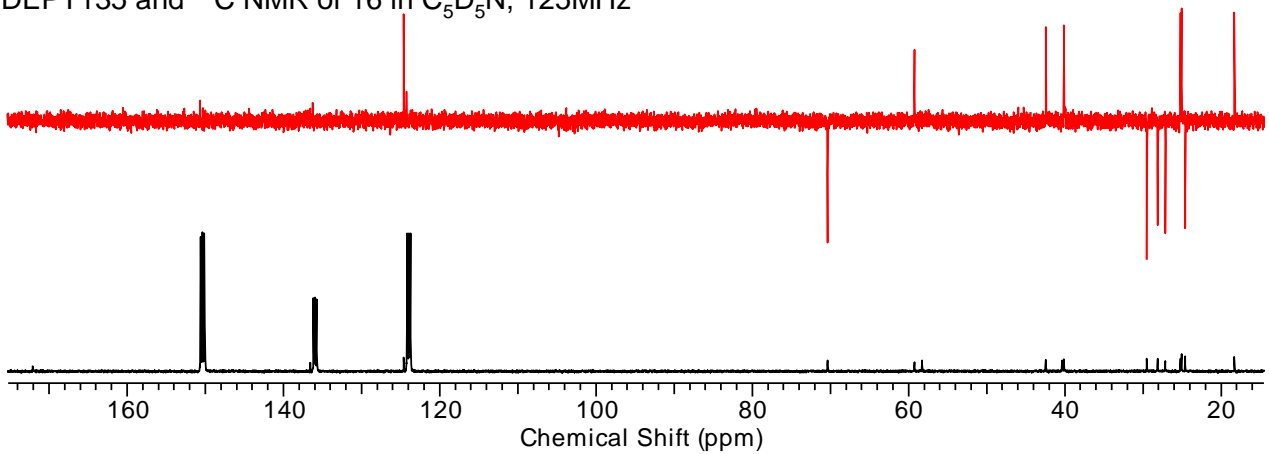


Compound 16

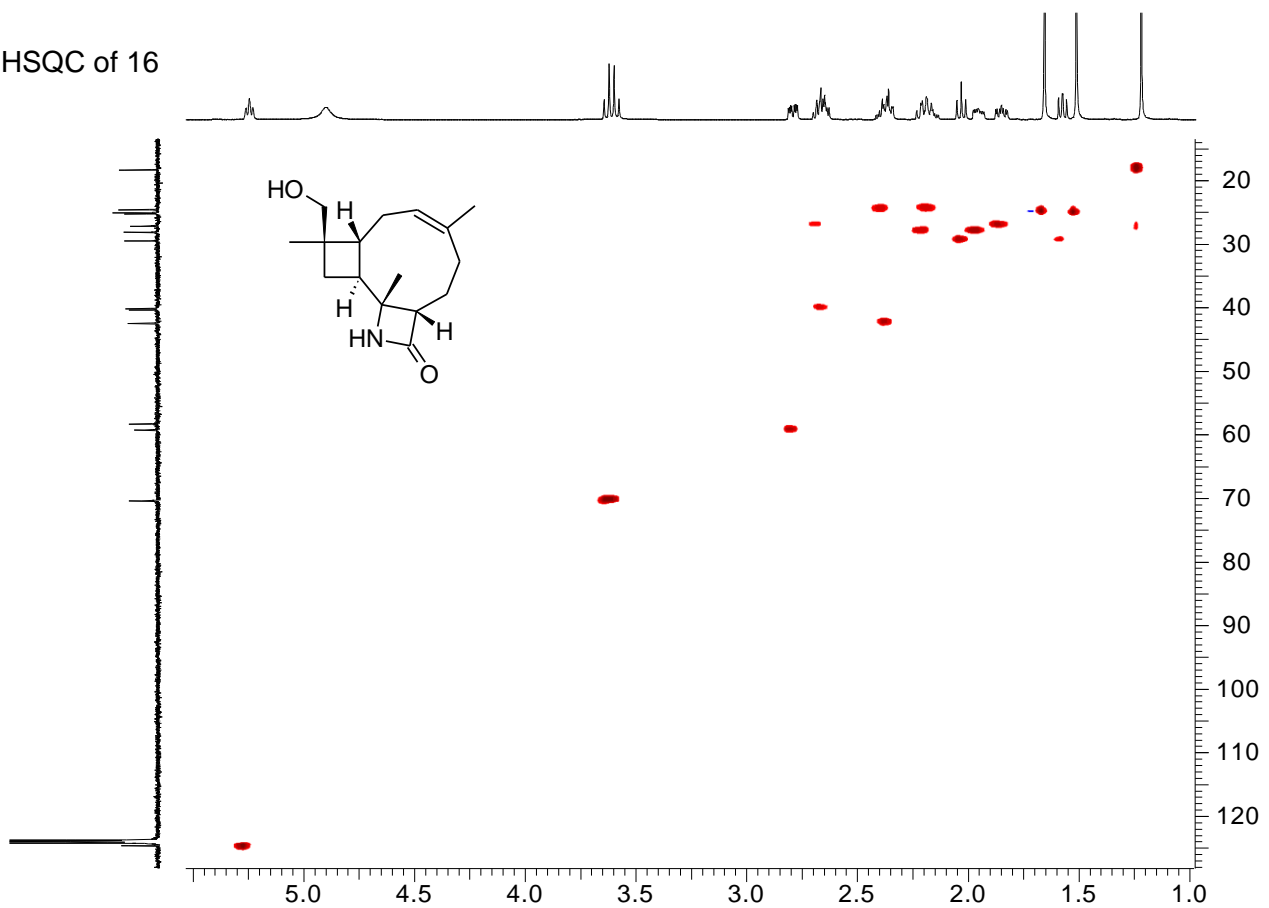
^1H NMR of 16 in $\text{C}_5\text{D}_5\text{N}$, 500MHz



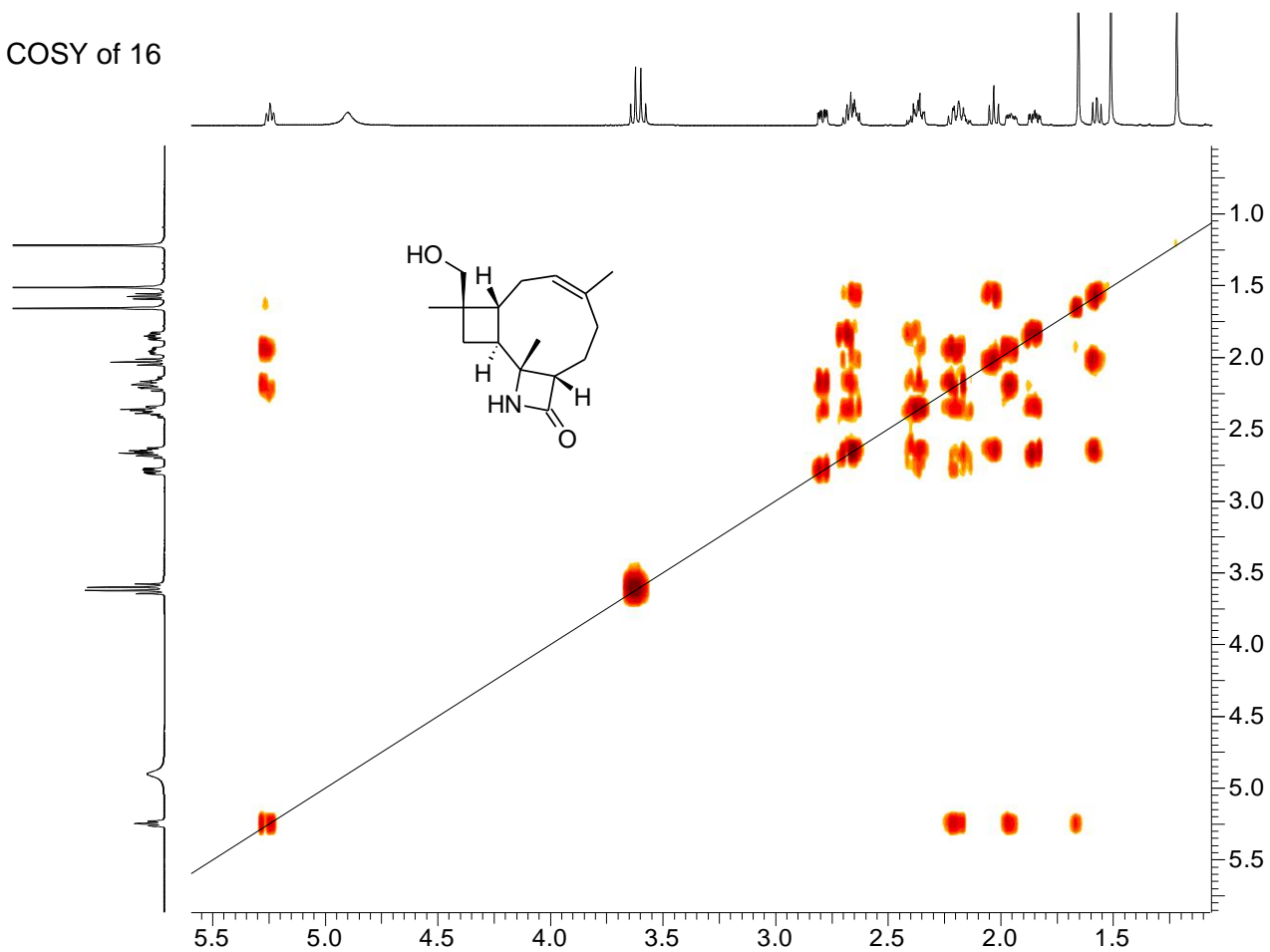
DEPT135 and ^{13}C NMR of 16 in $\text{C}_5\text{D}_5\text{N}$, 125MHz



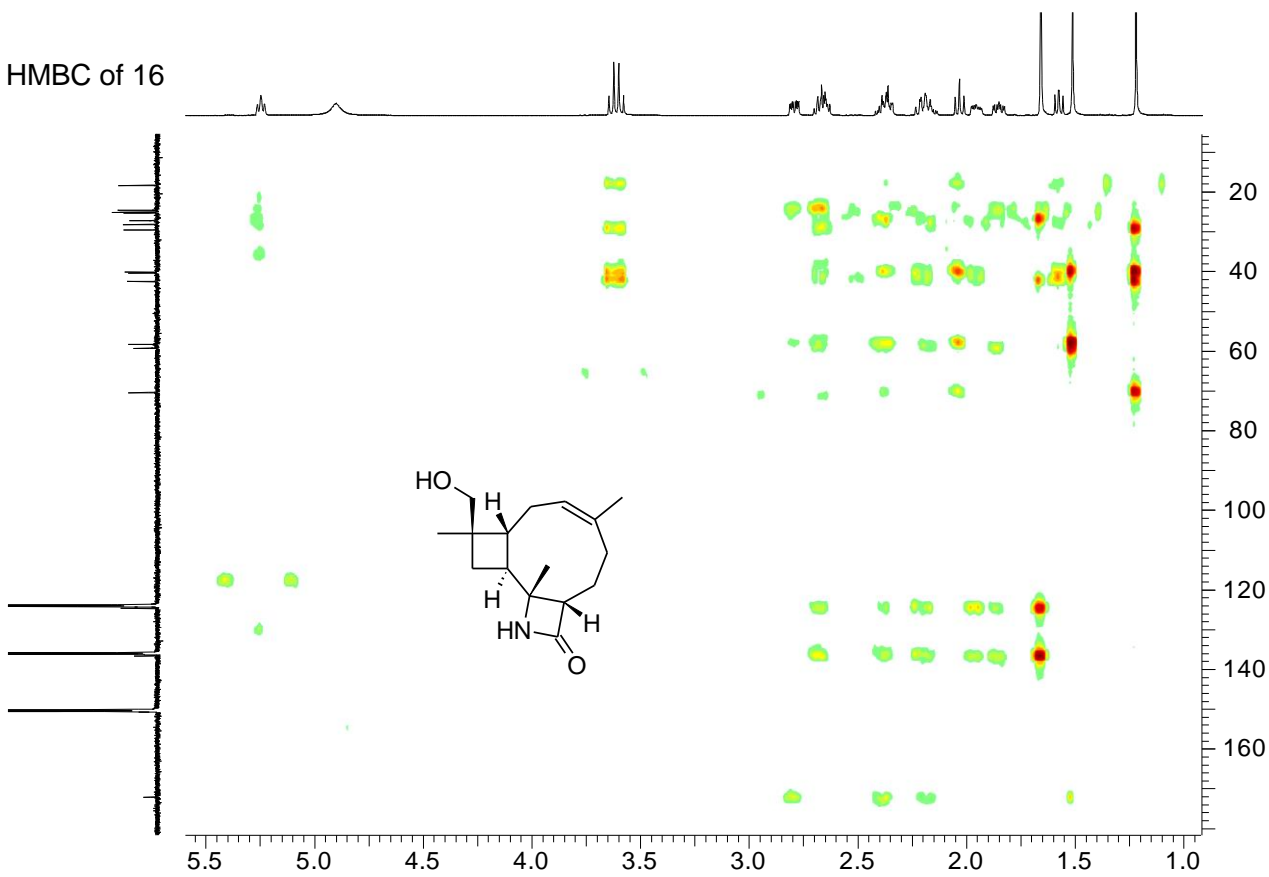
HSQC of 16



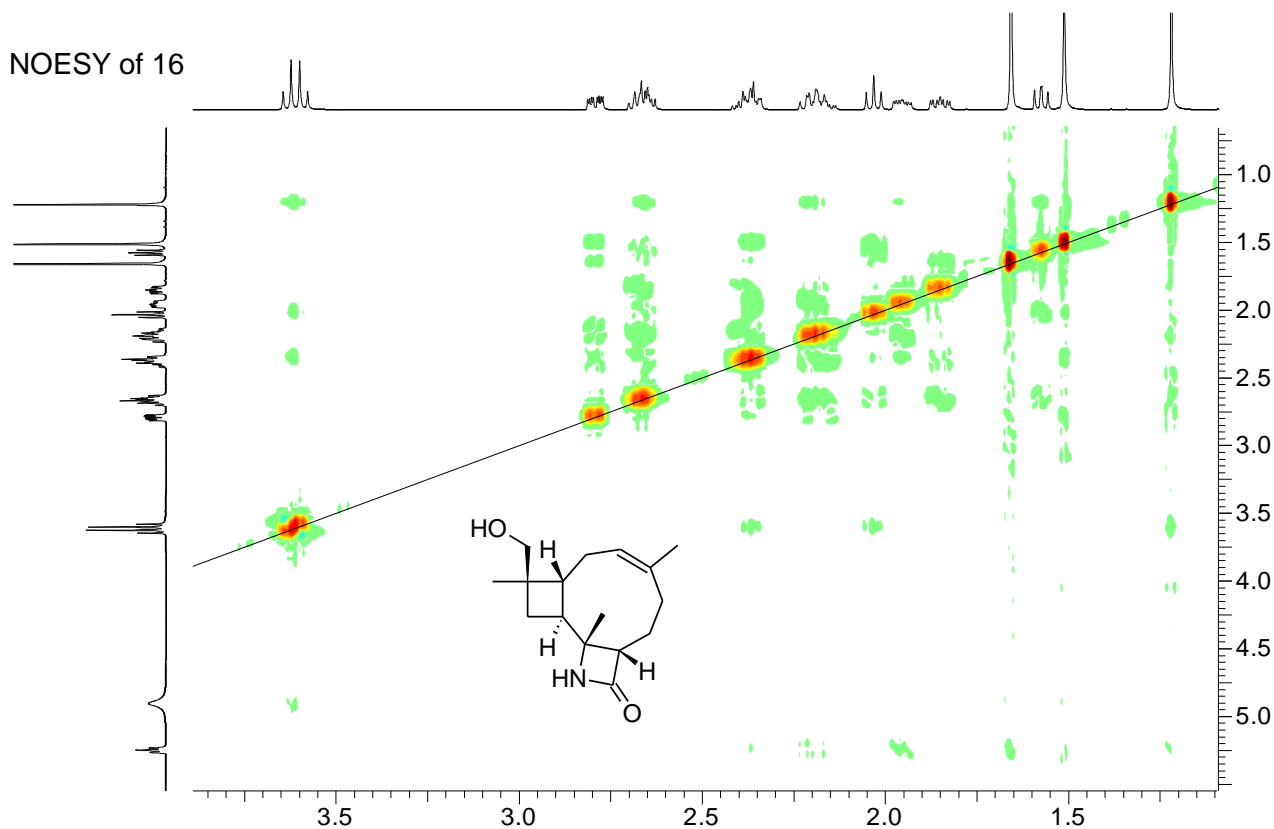
COSY of 16



HMBC of 16

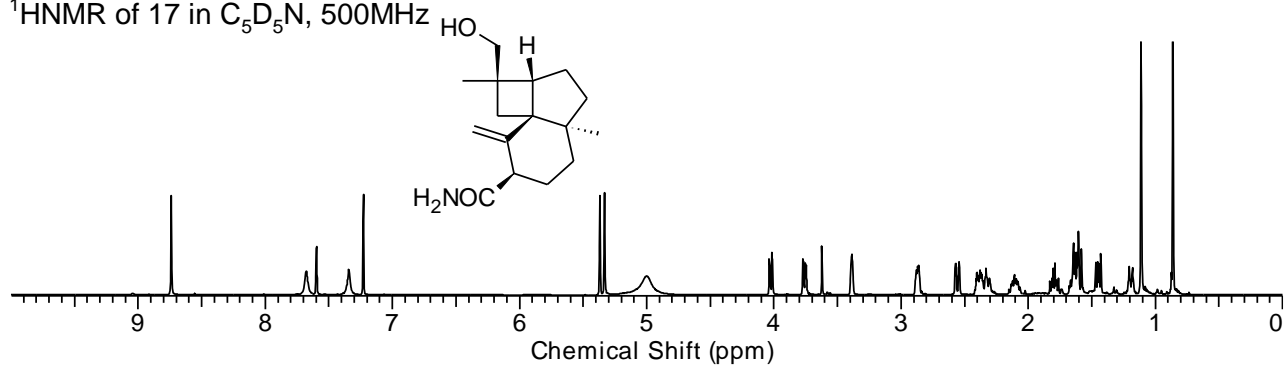


NOESY of 16

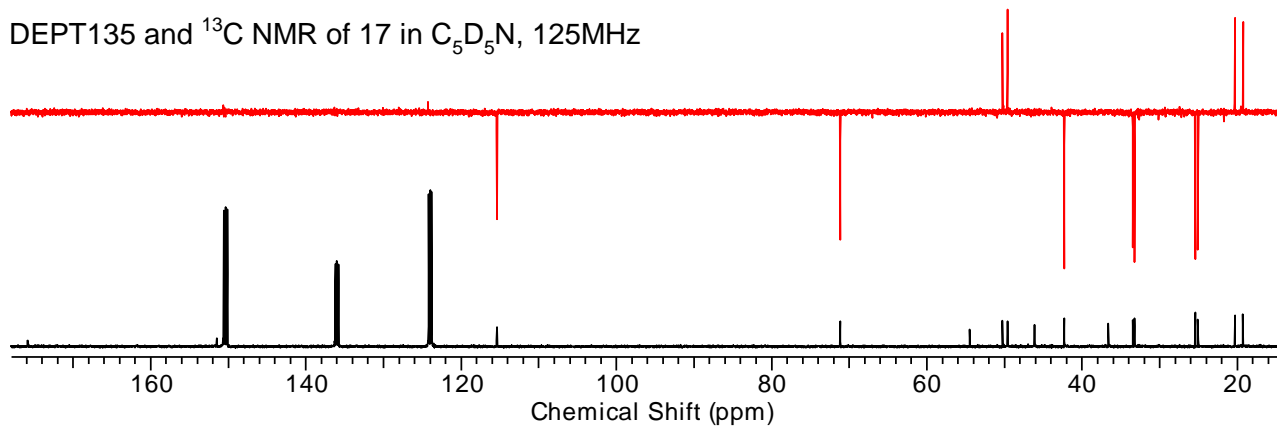


Compound 17

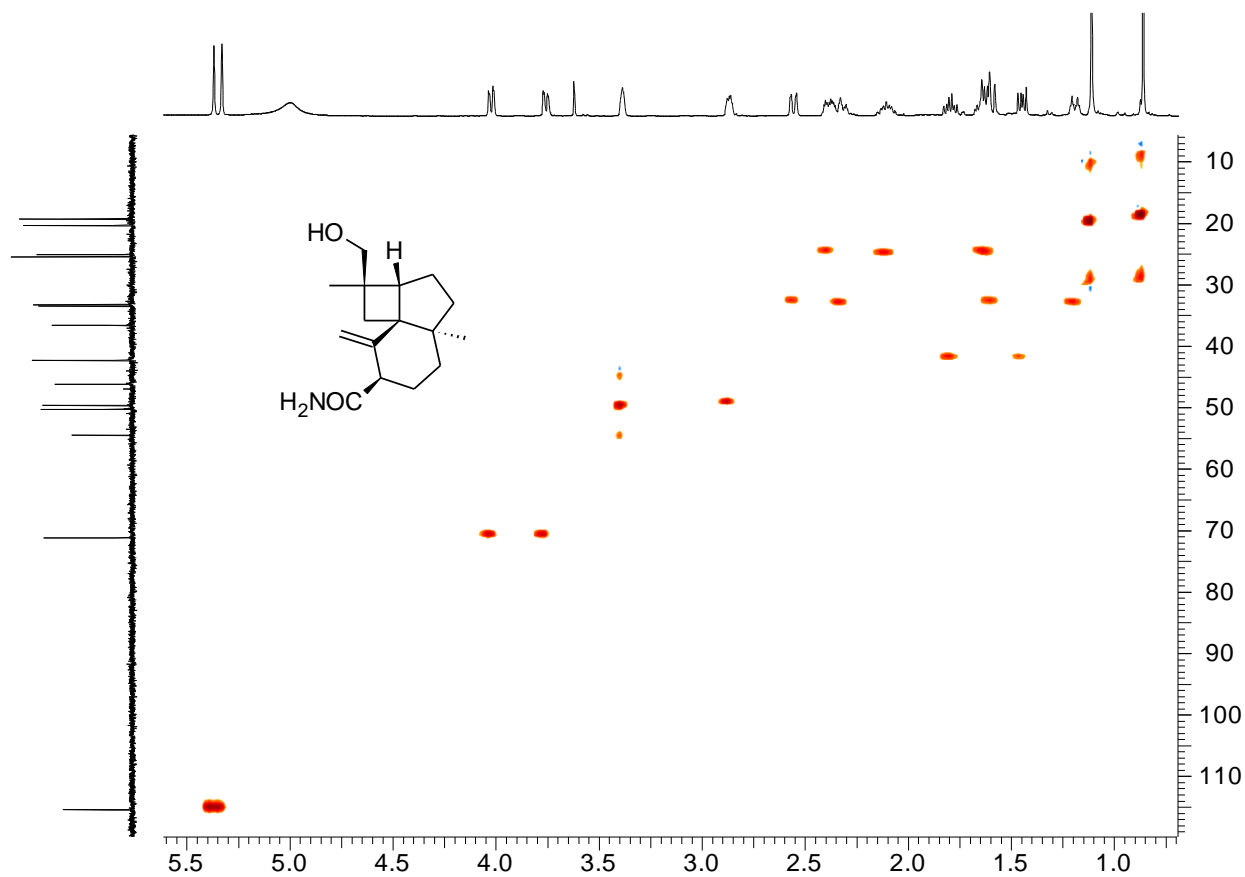
^1H NMR of 17 in $\text{C}_5\text{D}_5\text{N}$, 500MHz



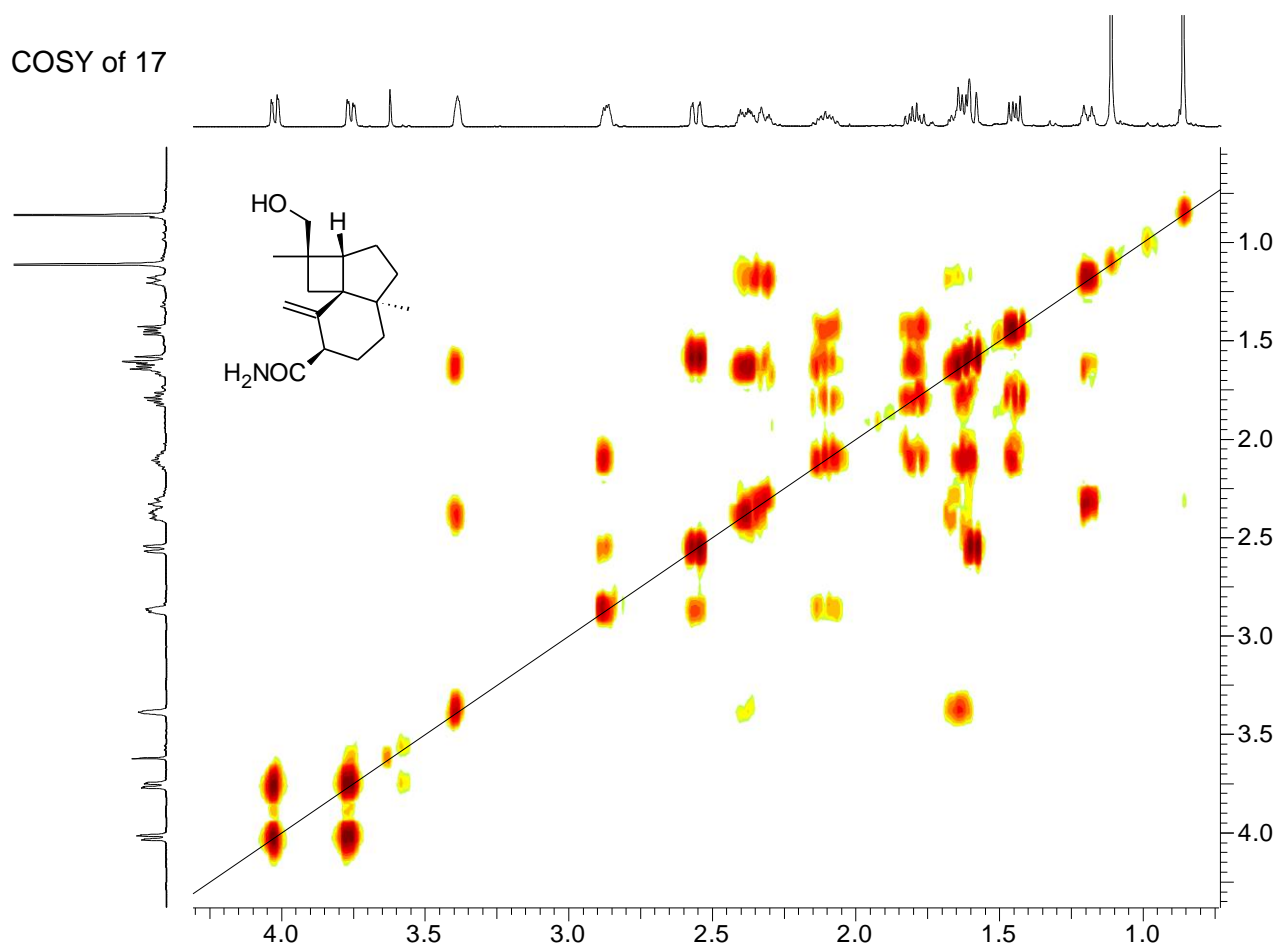
DEPT135 and ^{13}C NMR of 17 in $\text{C}_5\text{D}_5\text{N}$, 125MHz



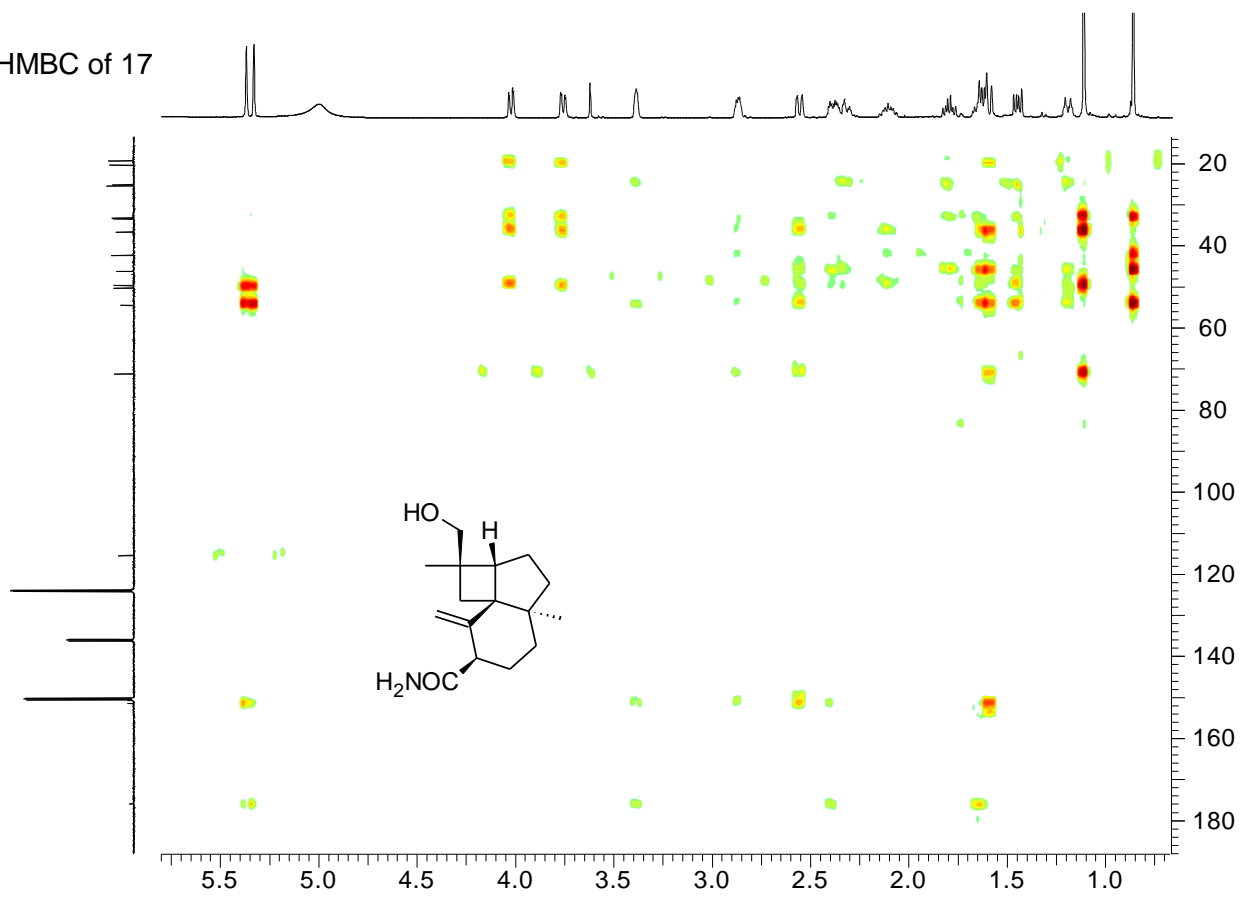
HSQC of 17



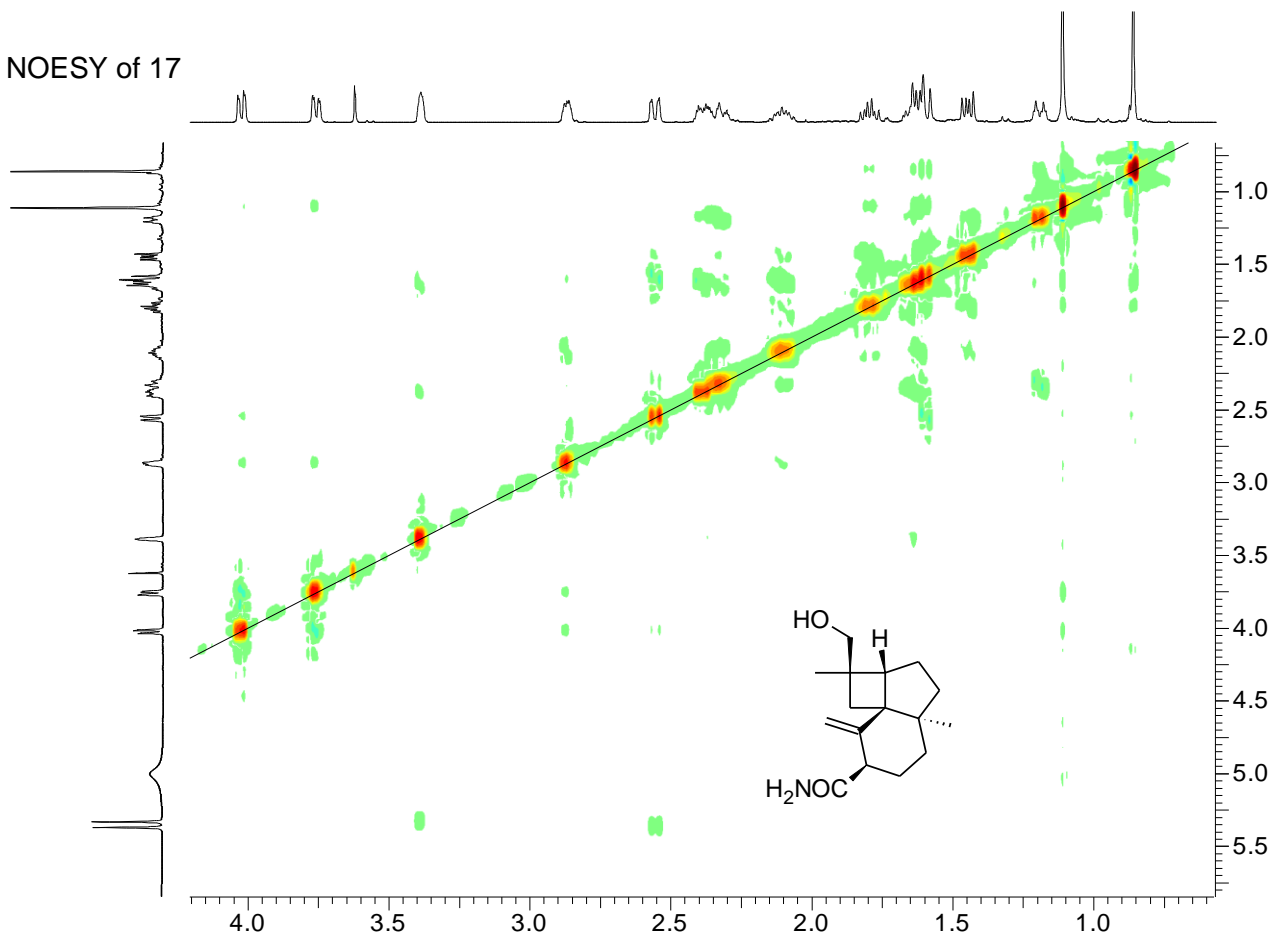
COSY of 17



HMBC of 17

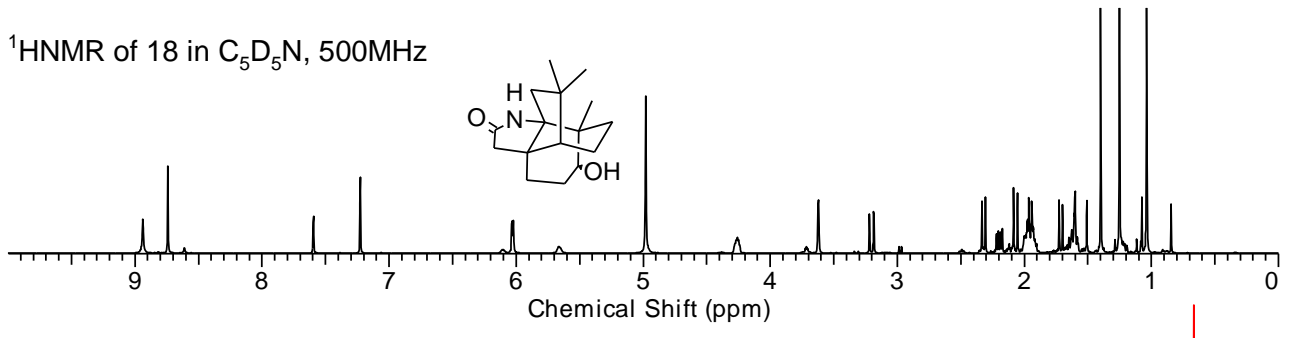


NOESY of 17

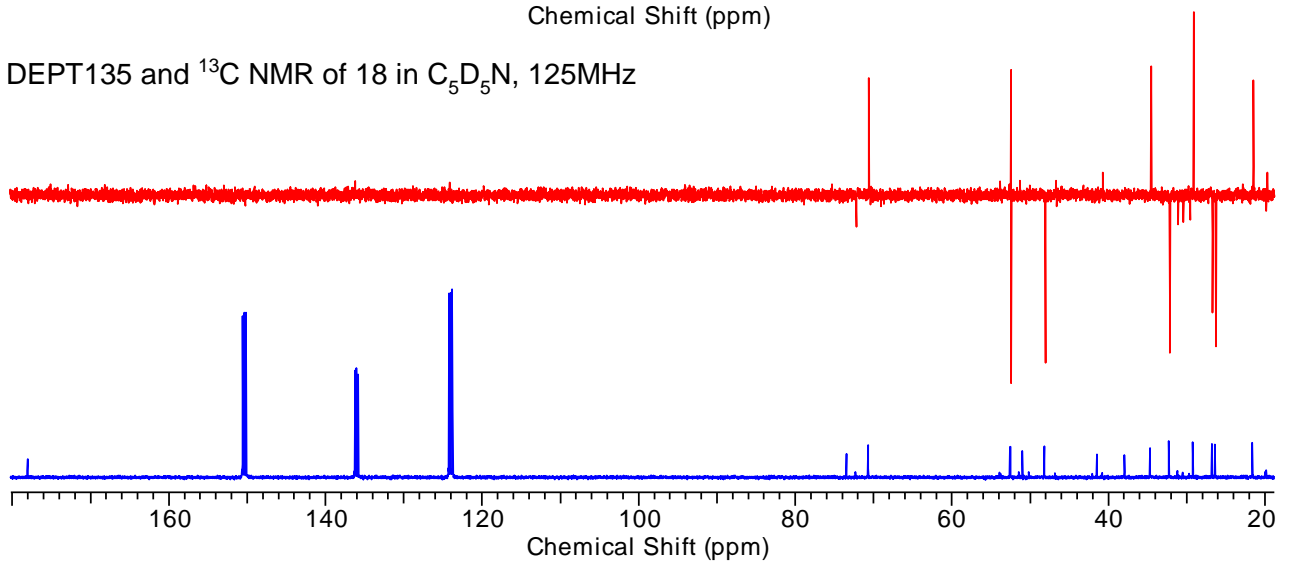


Compound 18

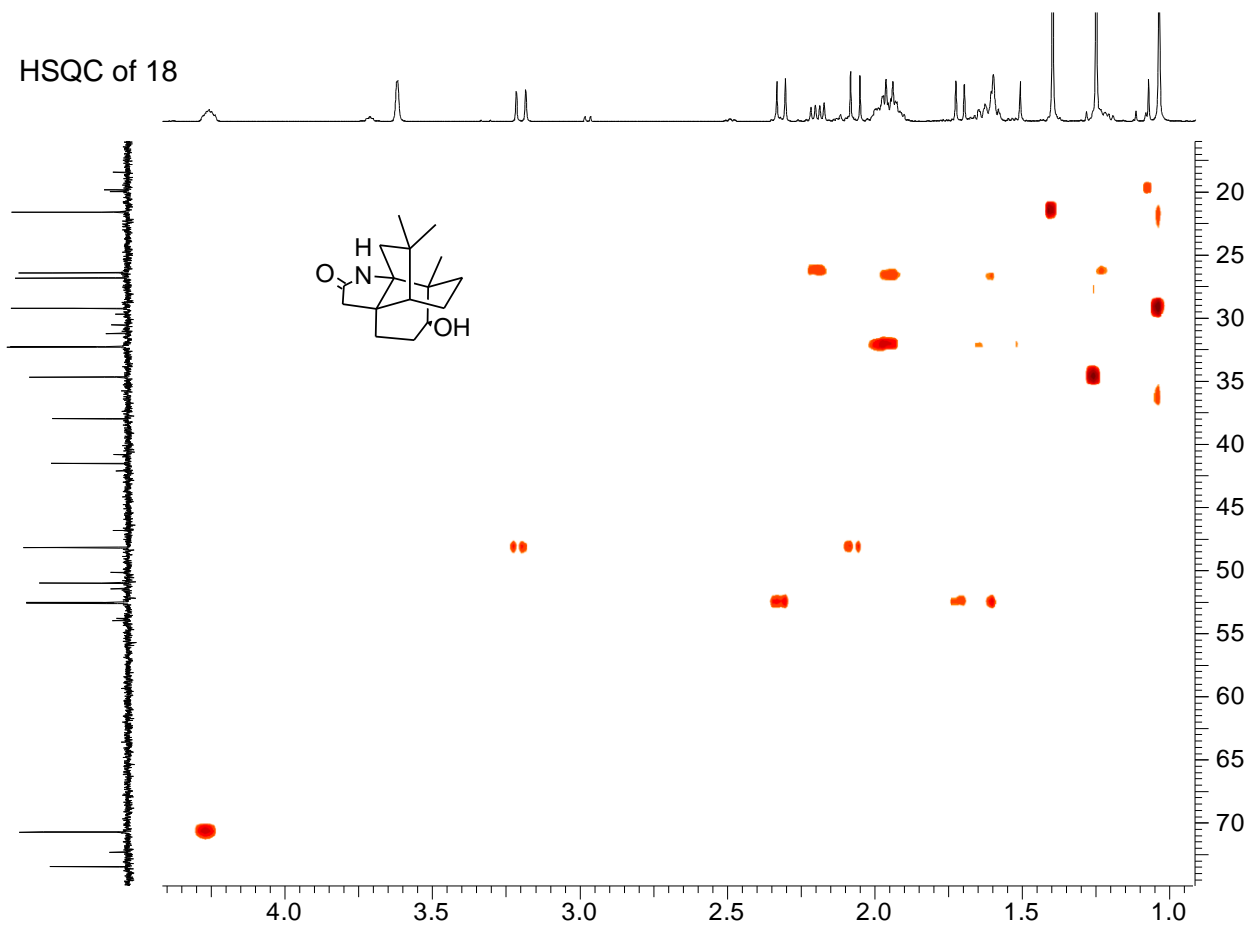
^1H NMR of 18 in $\text{C}_5\text{D}_5\text{N}$, 500MHz



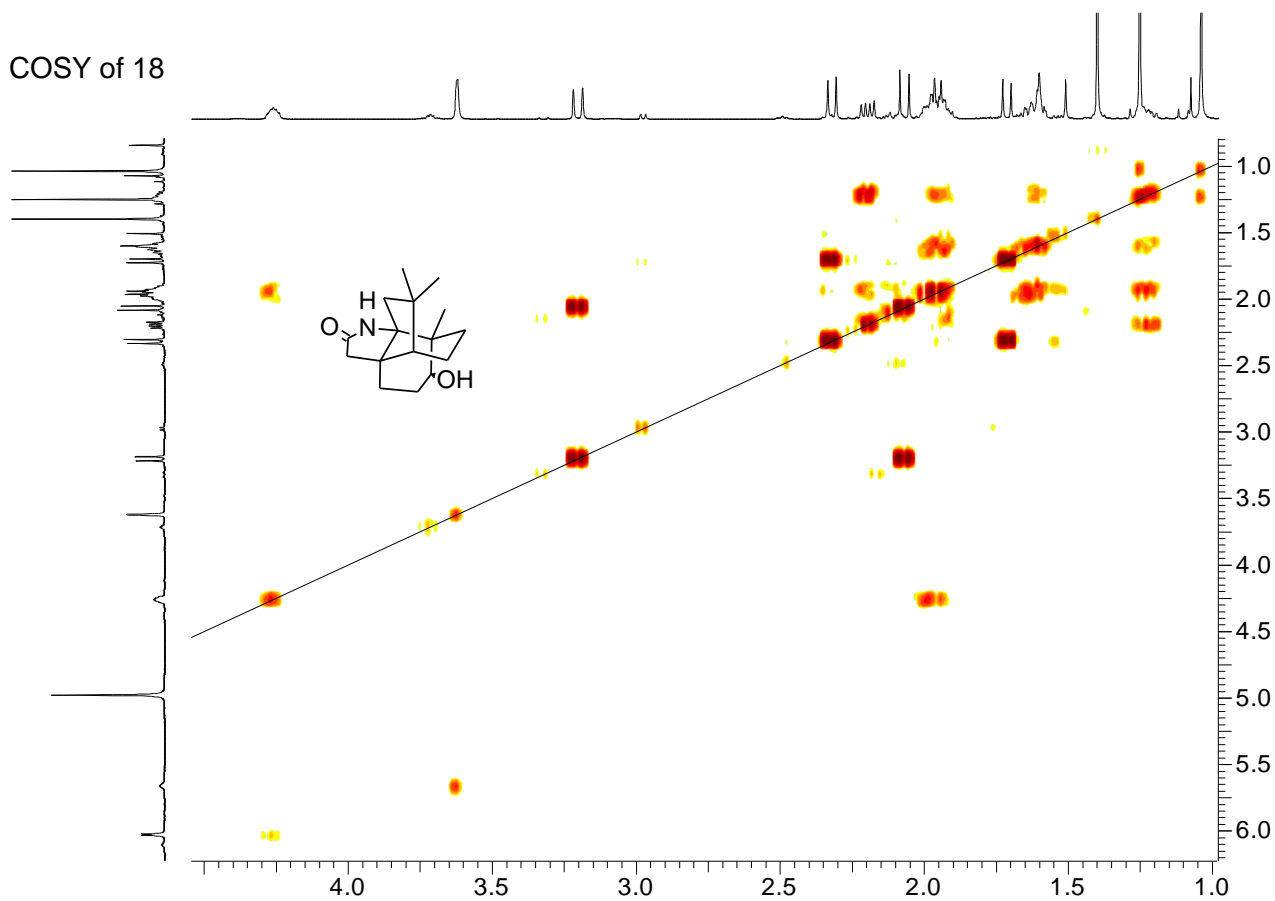
DEPT135 and ^{13}C NMR of 18 in $\text{C}_5\text{D}_5\text{N}$, 125MHz



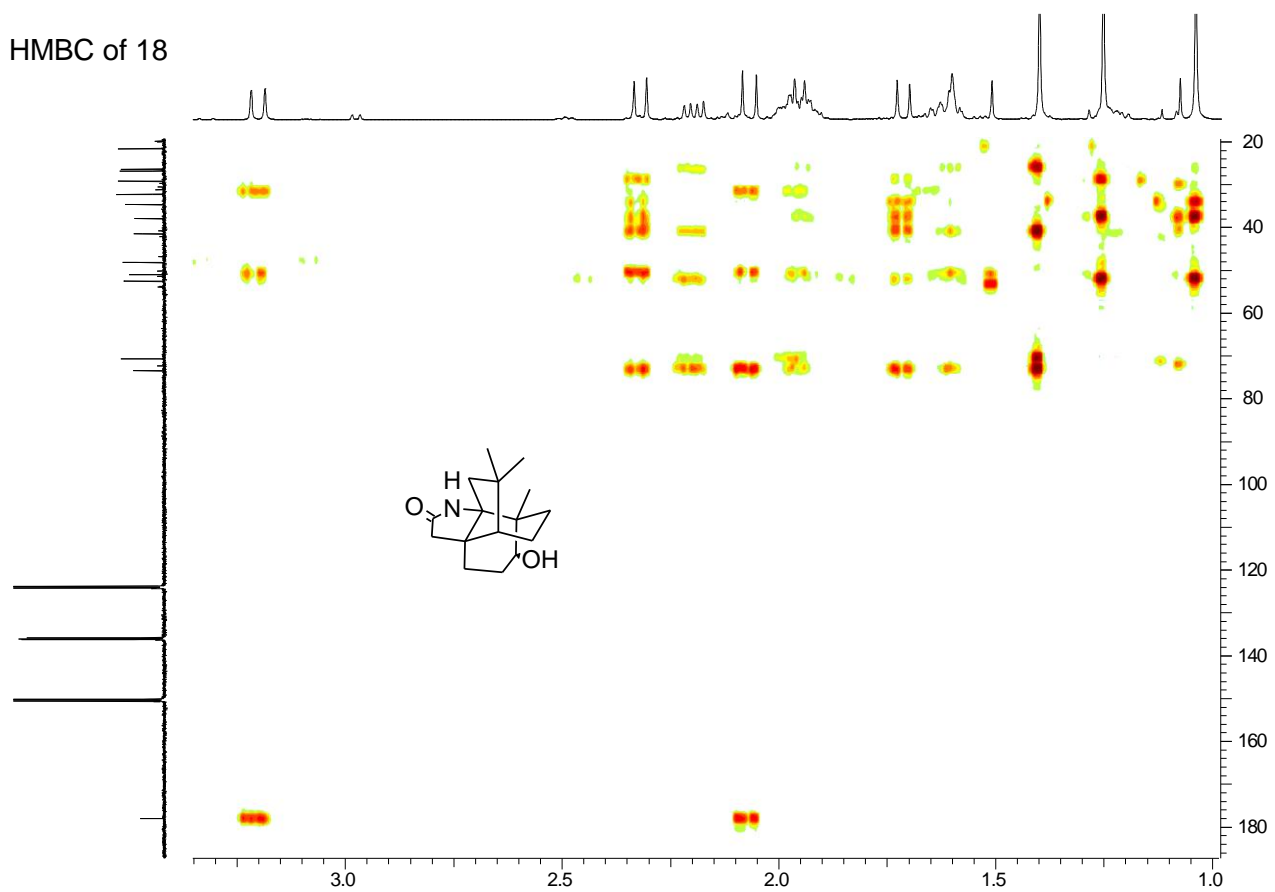
HSQC of 18

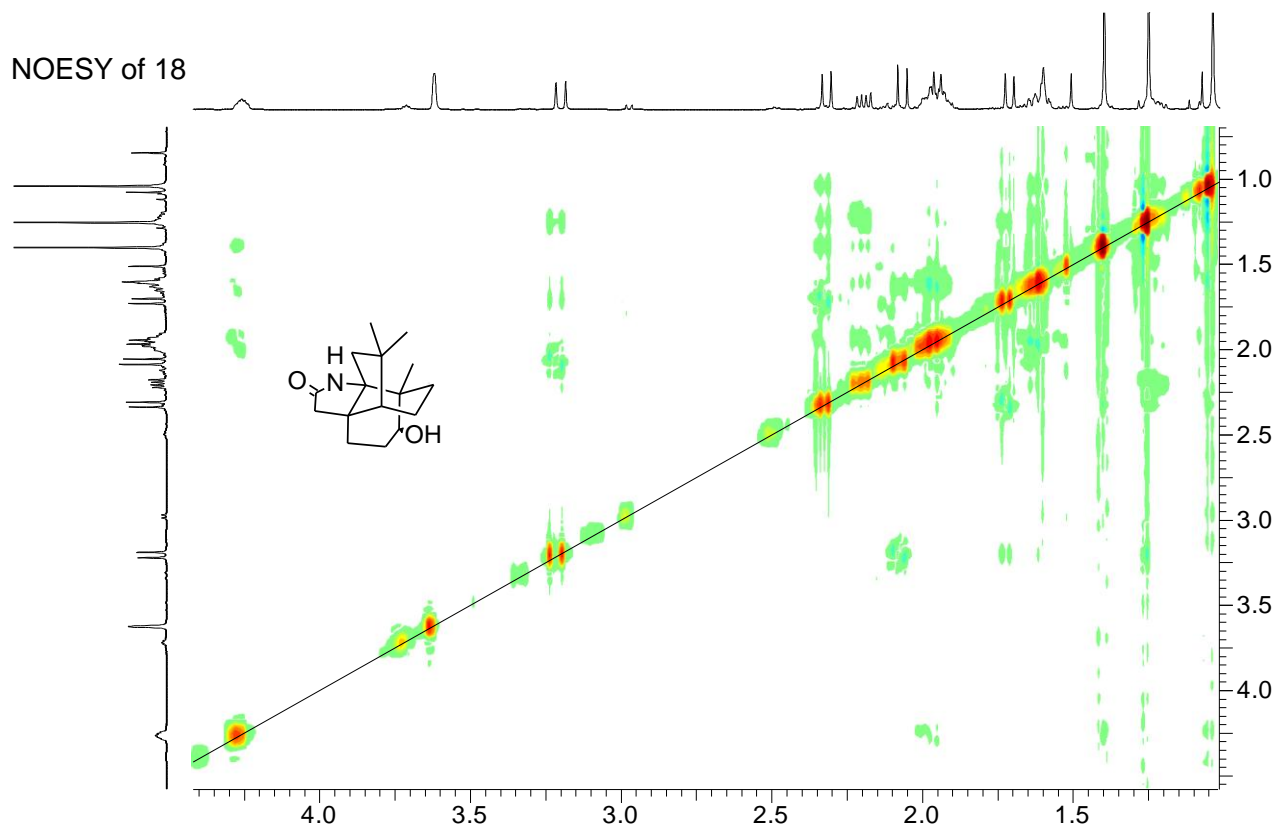


COSY of 18



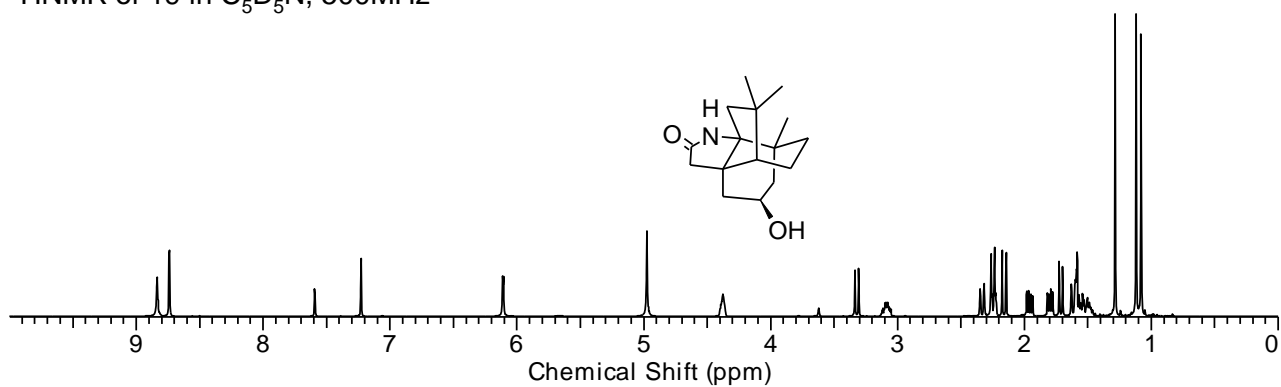
HMBC of 18



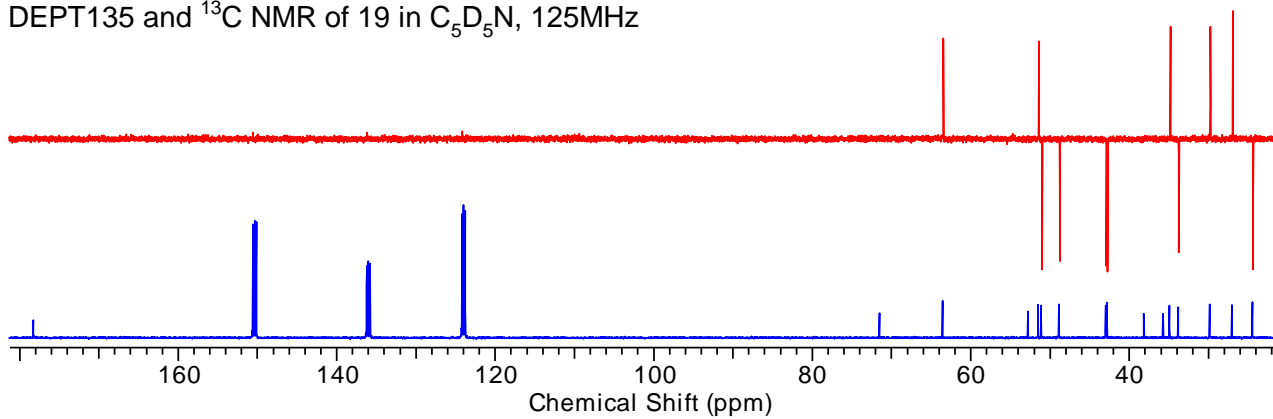


Compound 19

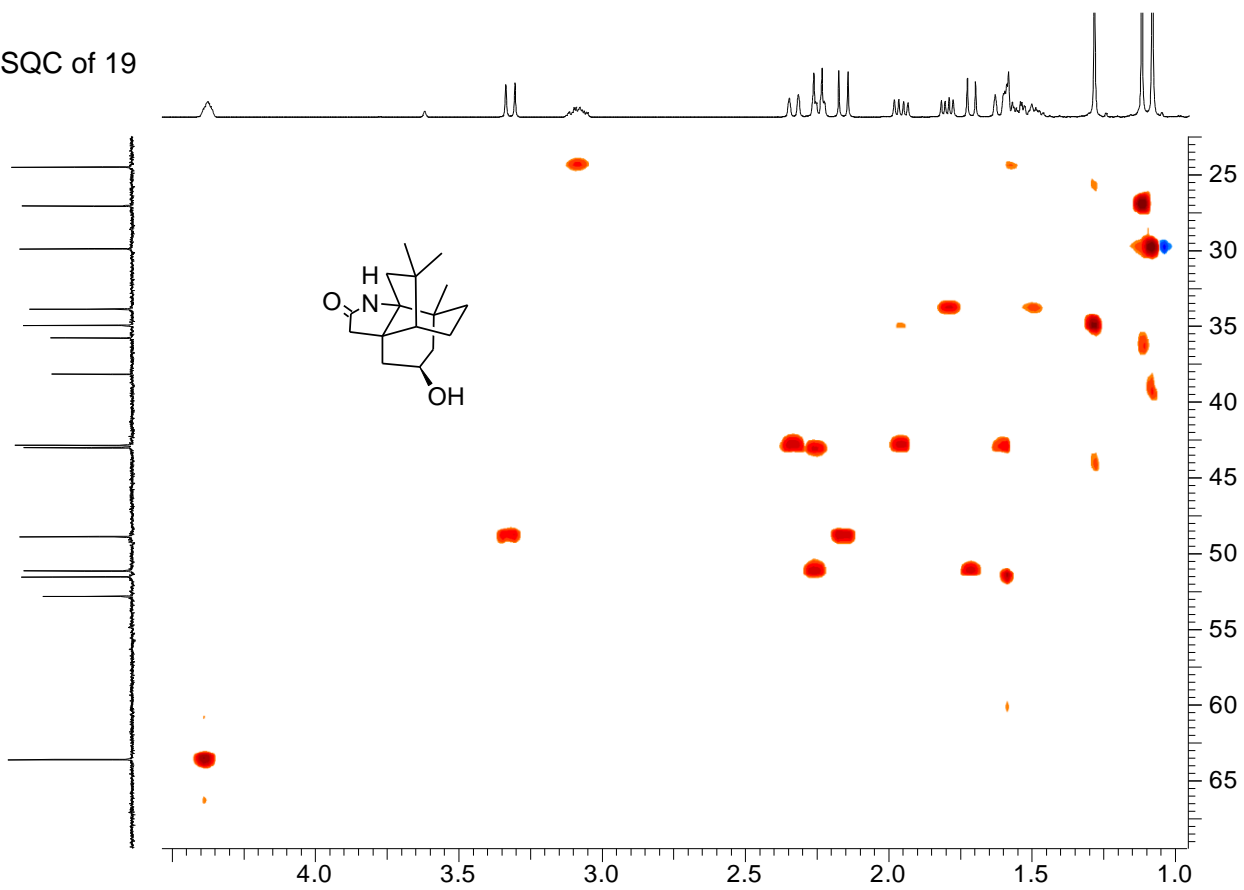
¹H NMR of 19 in C₅D₅N, 500MHz



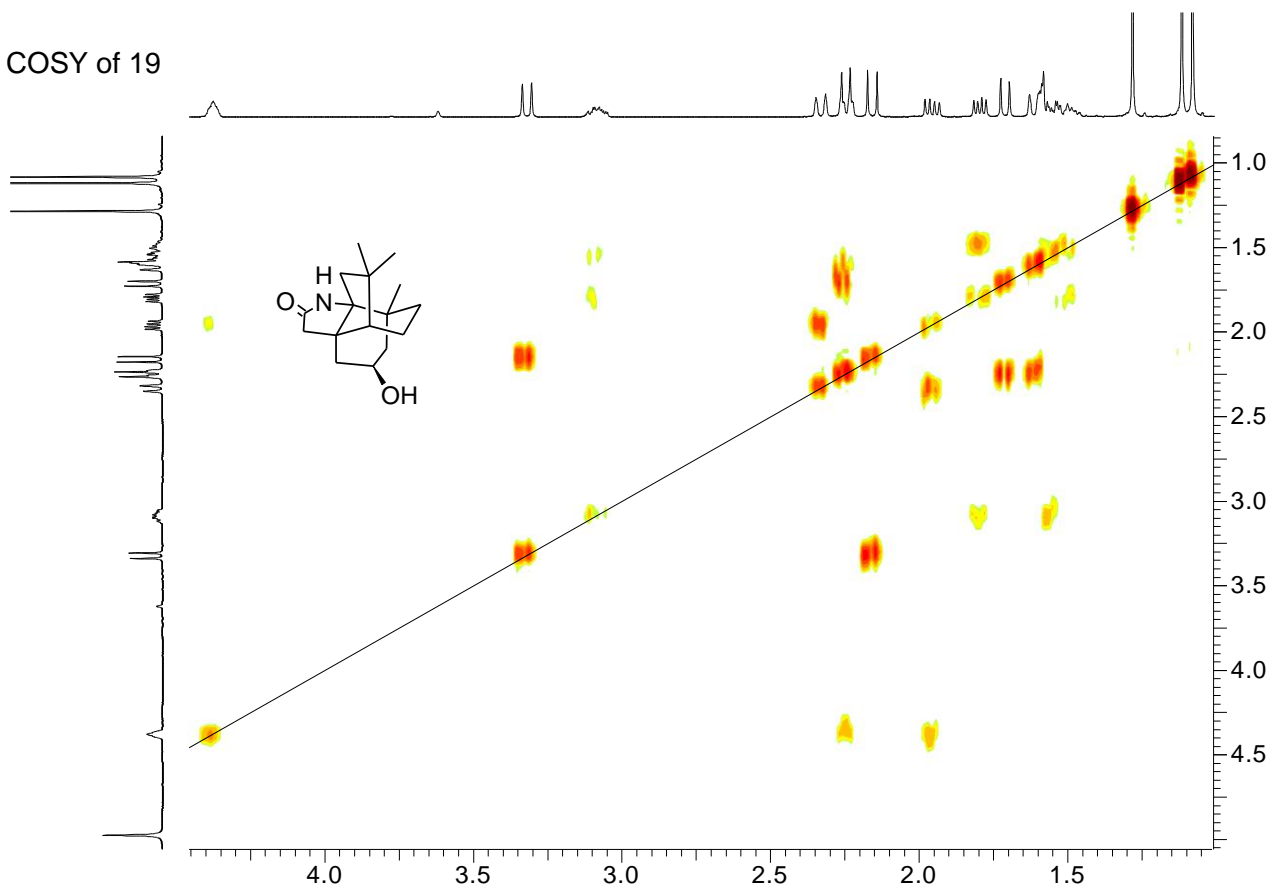
DEPT135 and ¹³C NMR of 19 in C₅D₅N, 125MHz



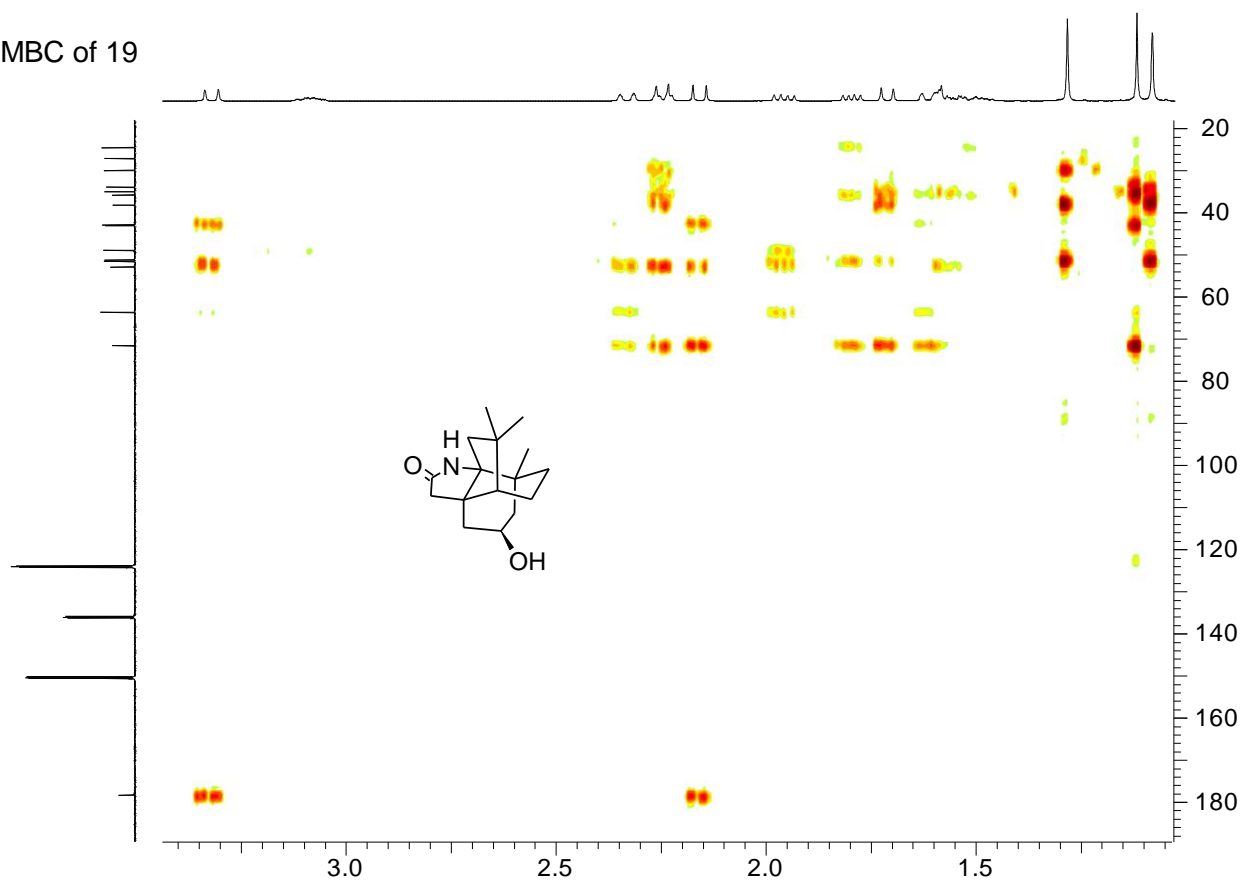
HSQC of 19



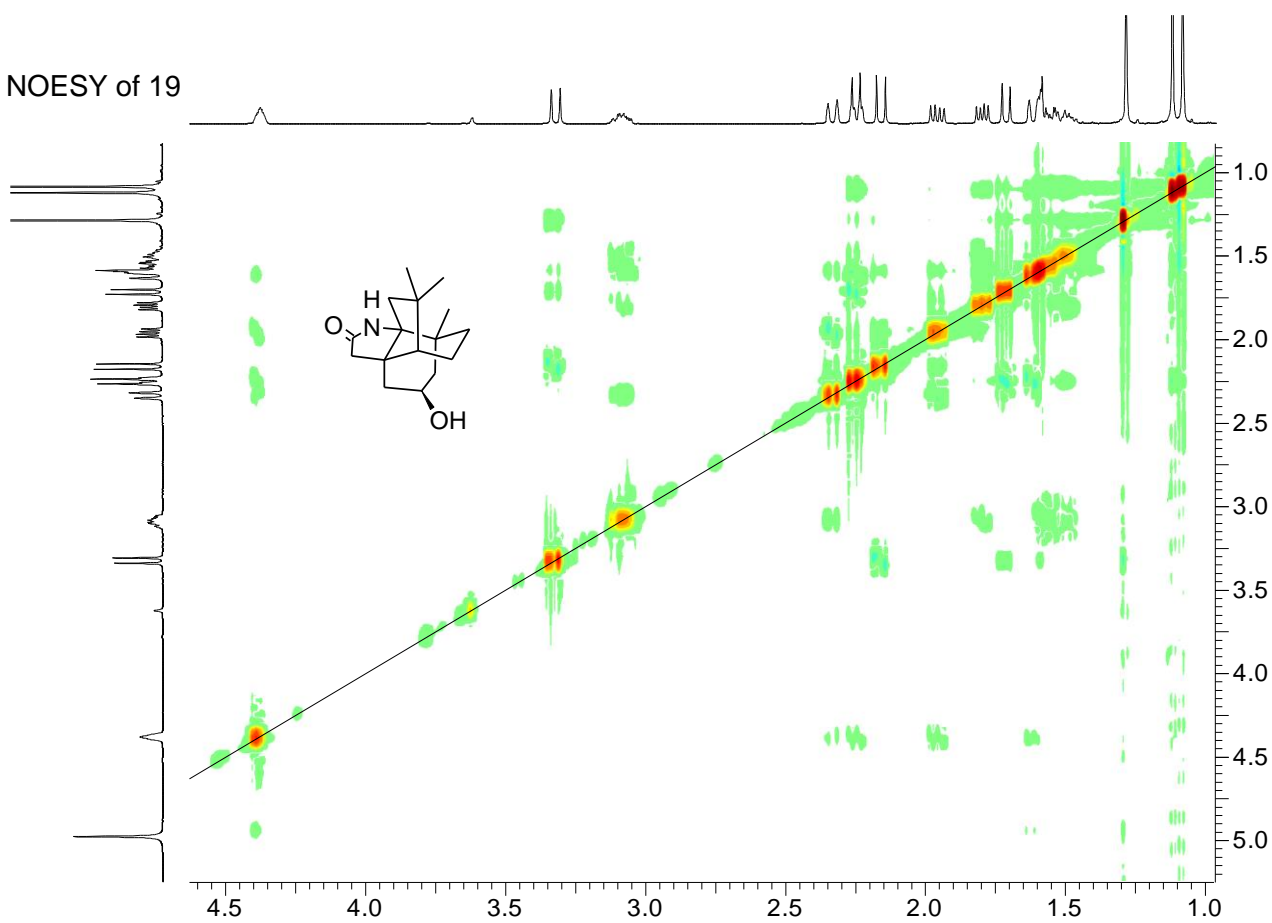
COSY of 19



HMBC of 19

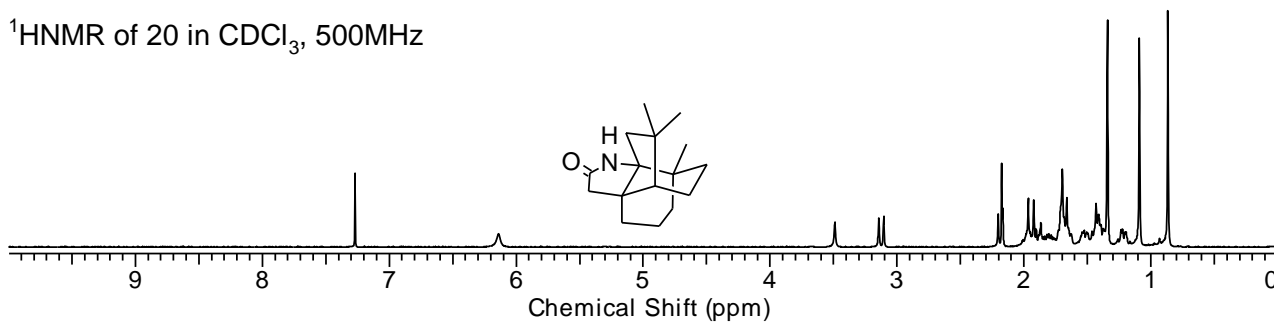


NOESY of 19

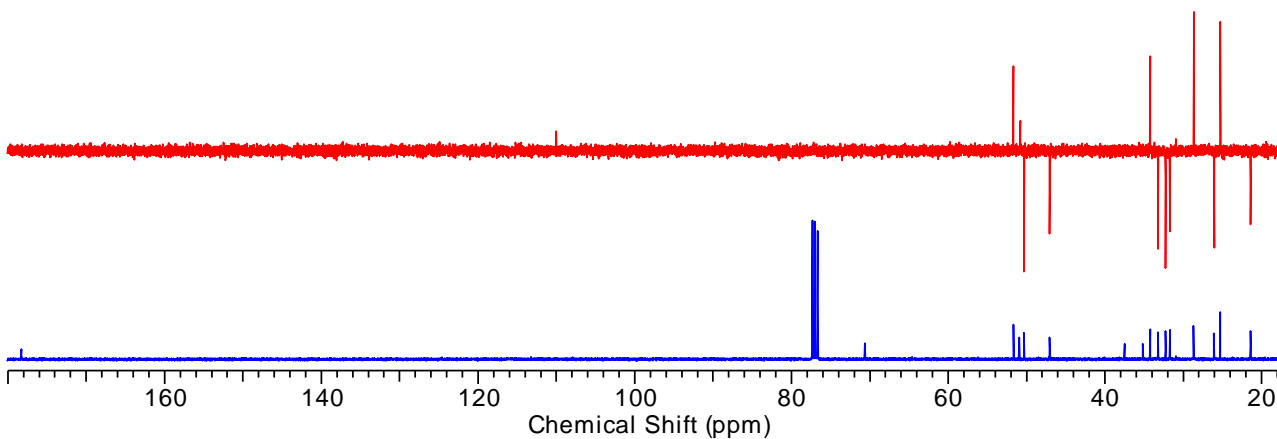


Compound 20

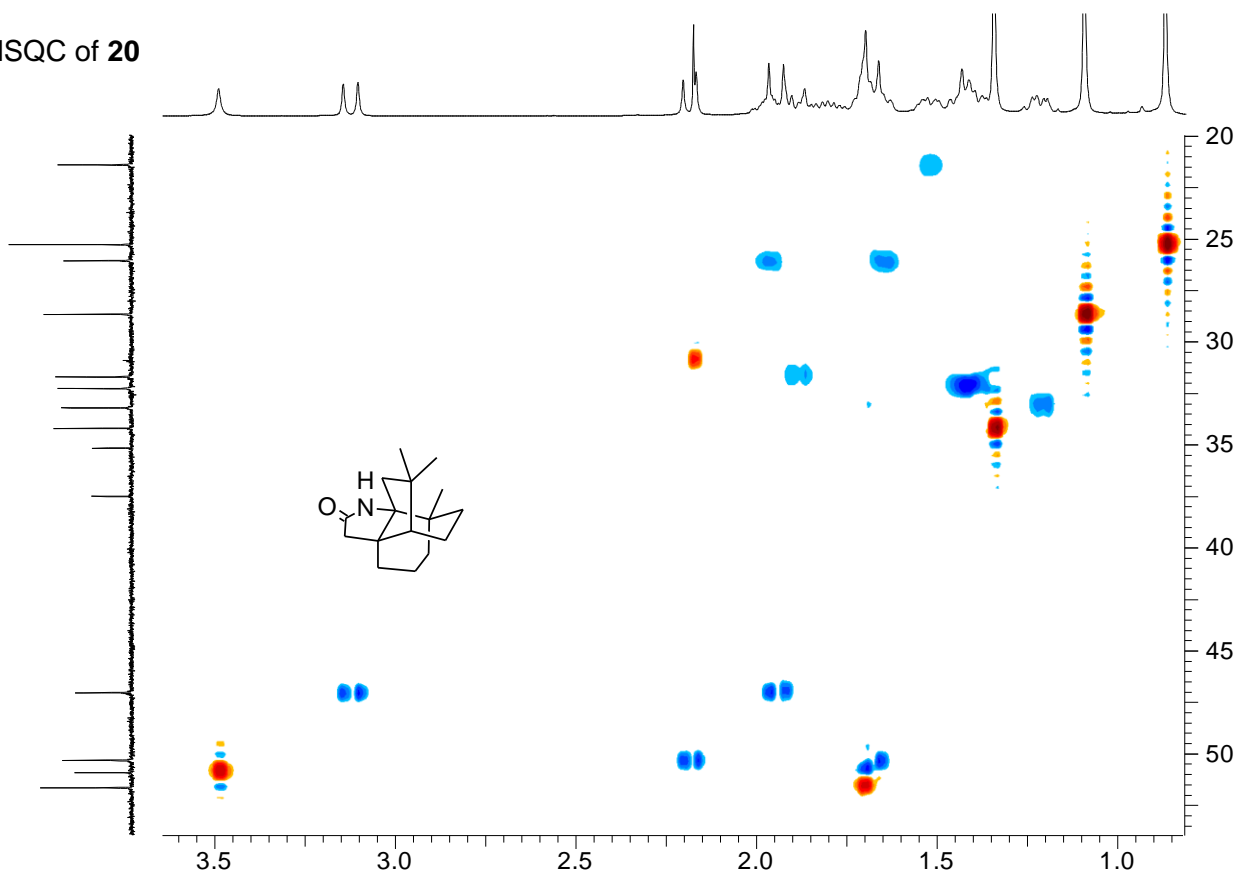
^1H NMR of 20 in CDCl_3 , 500MHz



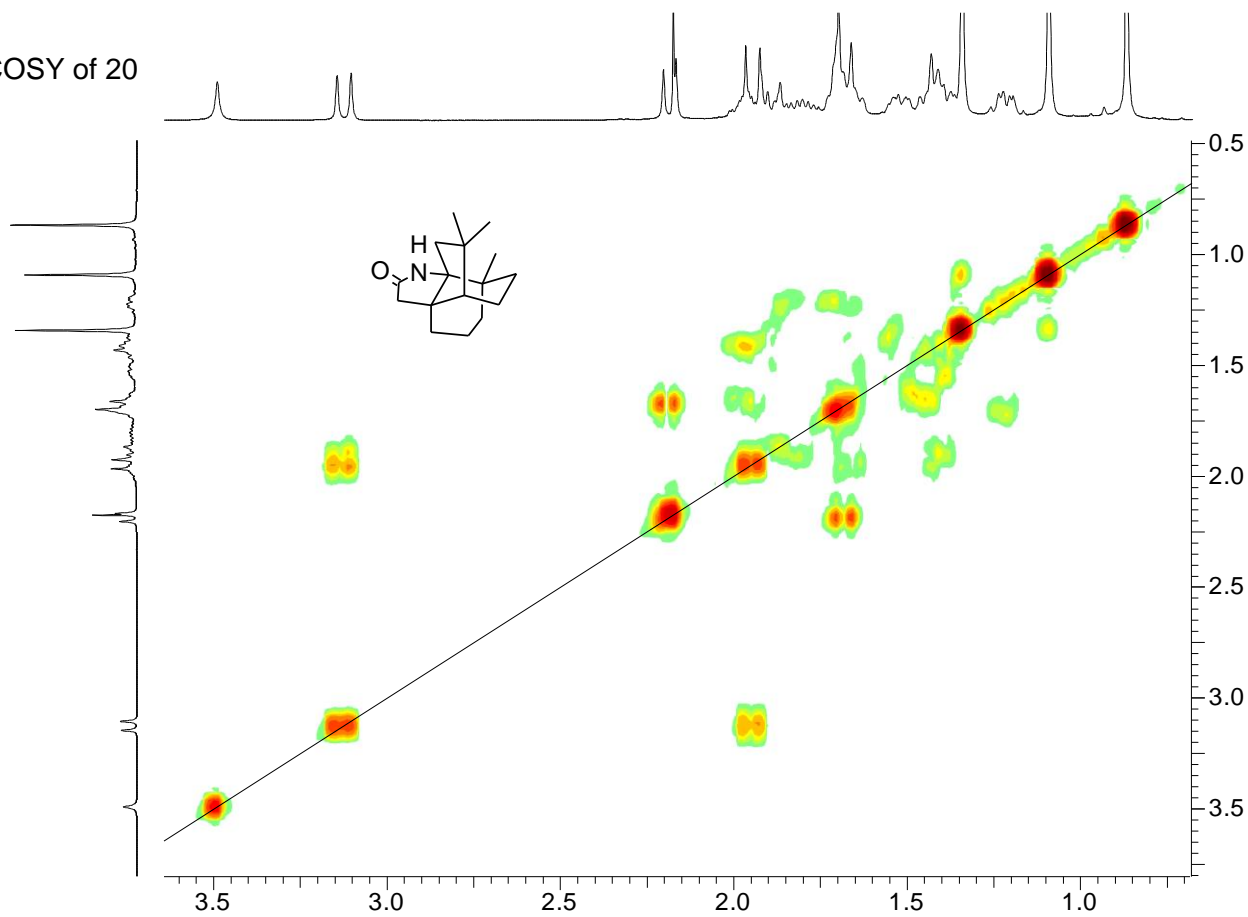
DEPT135 and ^{13}C NMR of 20 in $\text{C}_5\text{D}_5\text{N}$, 125MHz



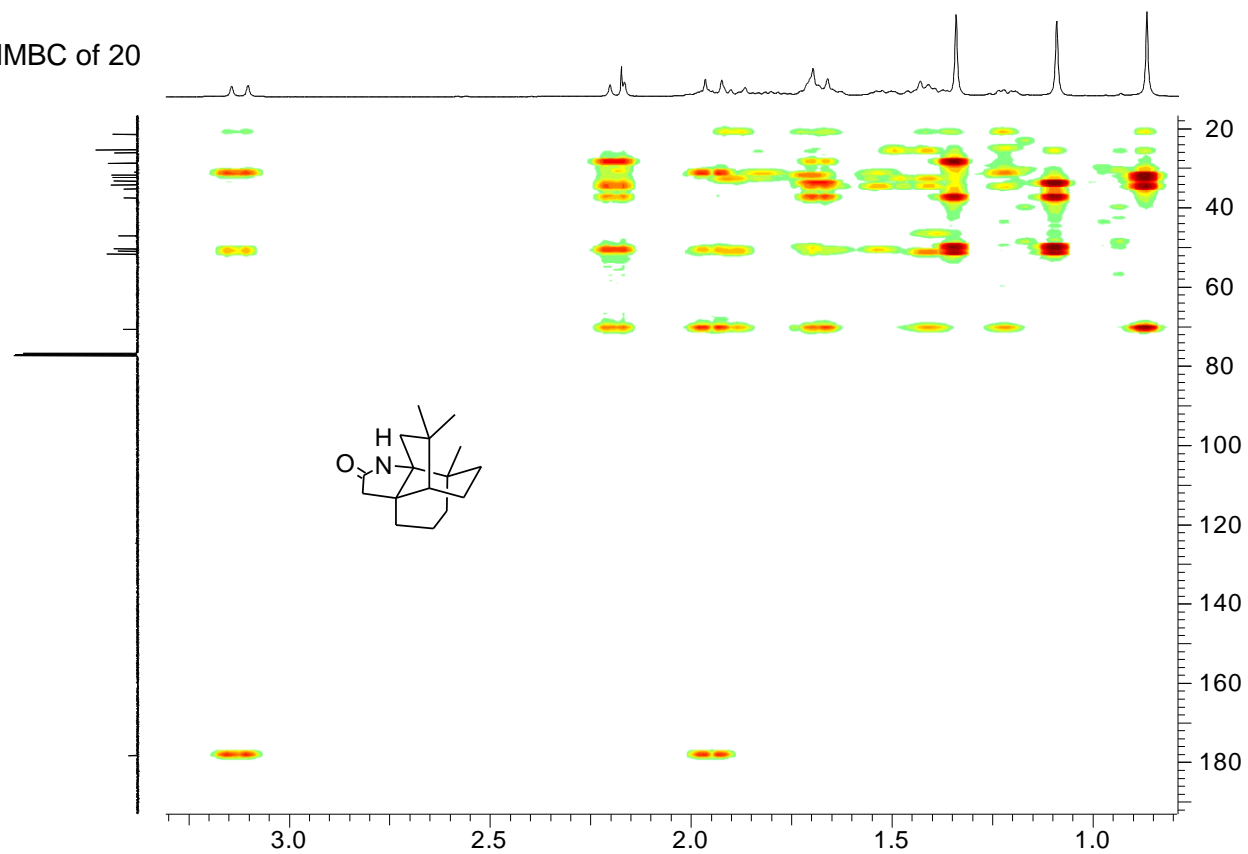
HSQC of 20



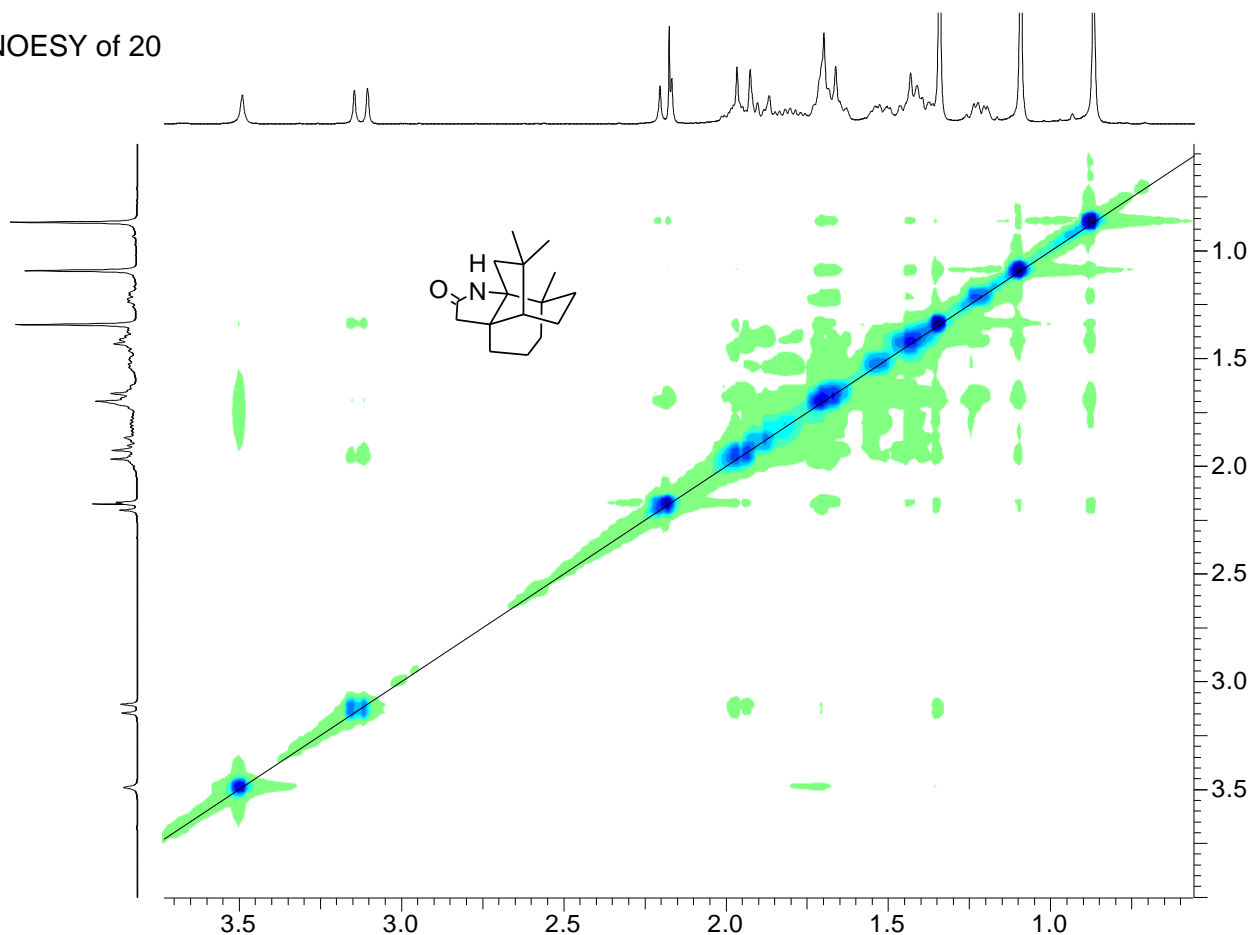
COSY of 20



HMBC of 20

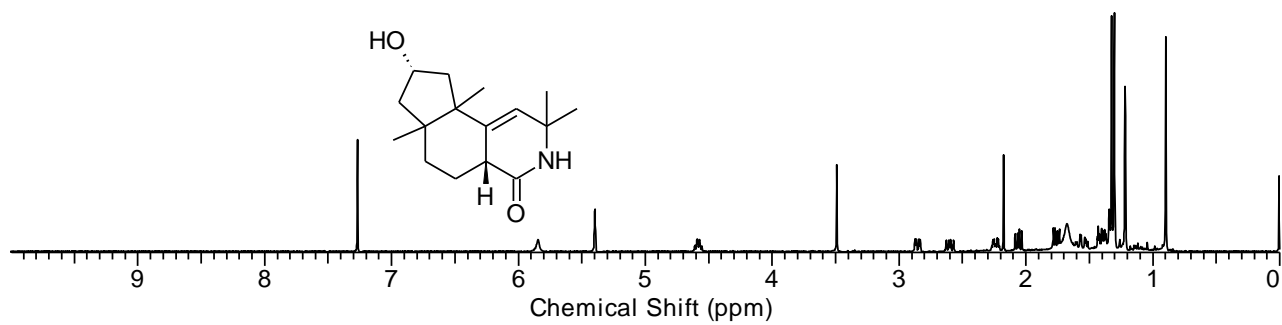


NOESY of 20

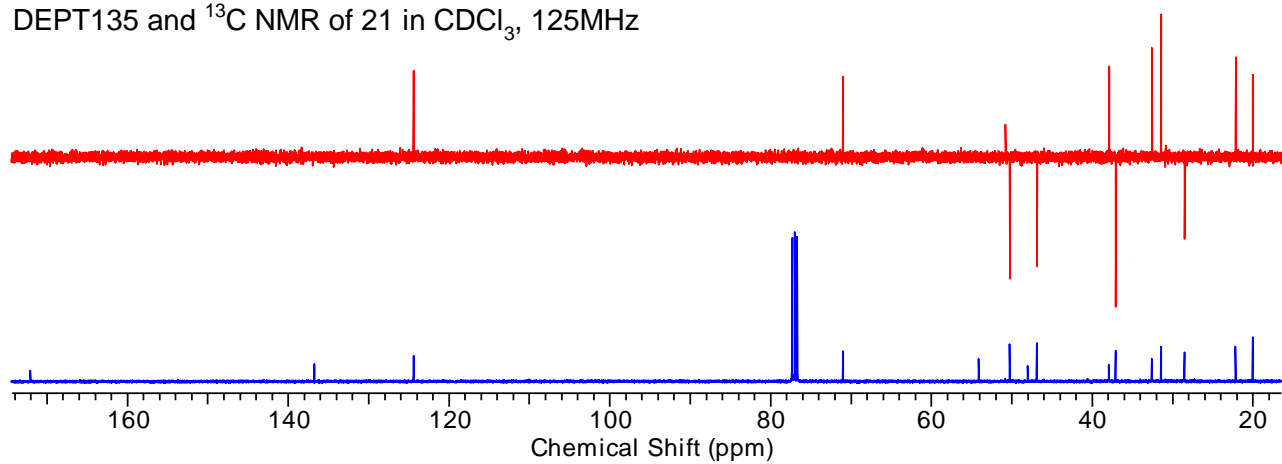


Compound 21

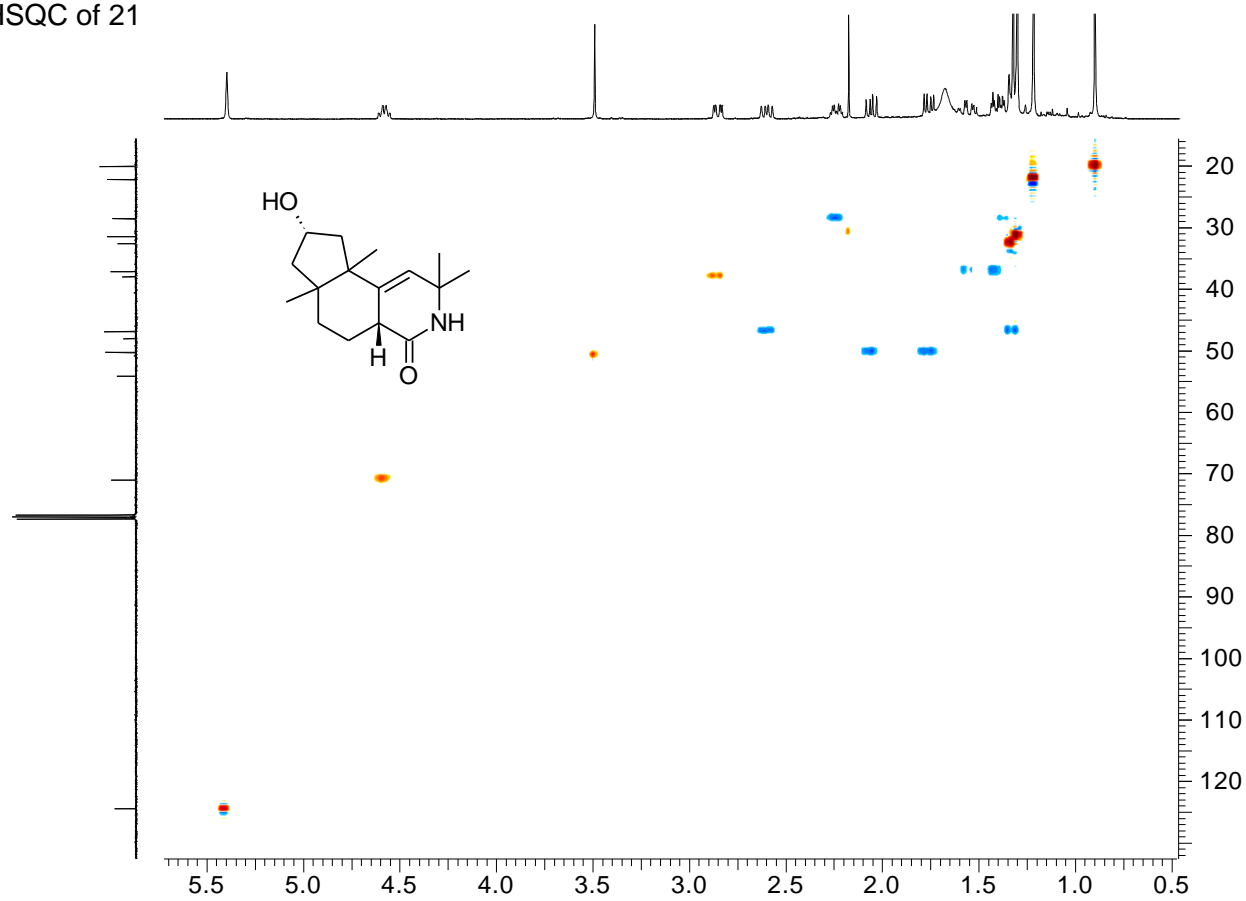
^1H NMR of 21 in CDCl_3 , 500MHz



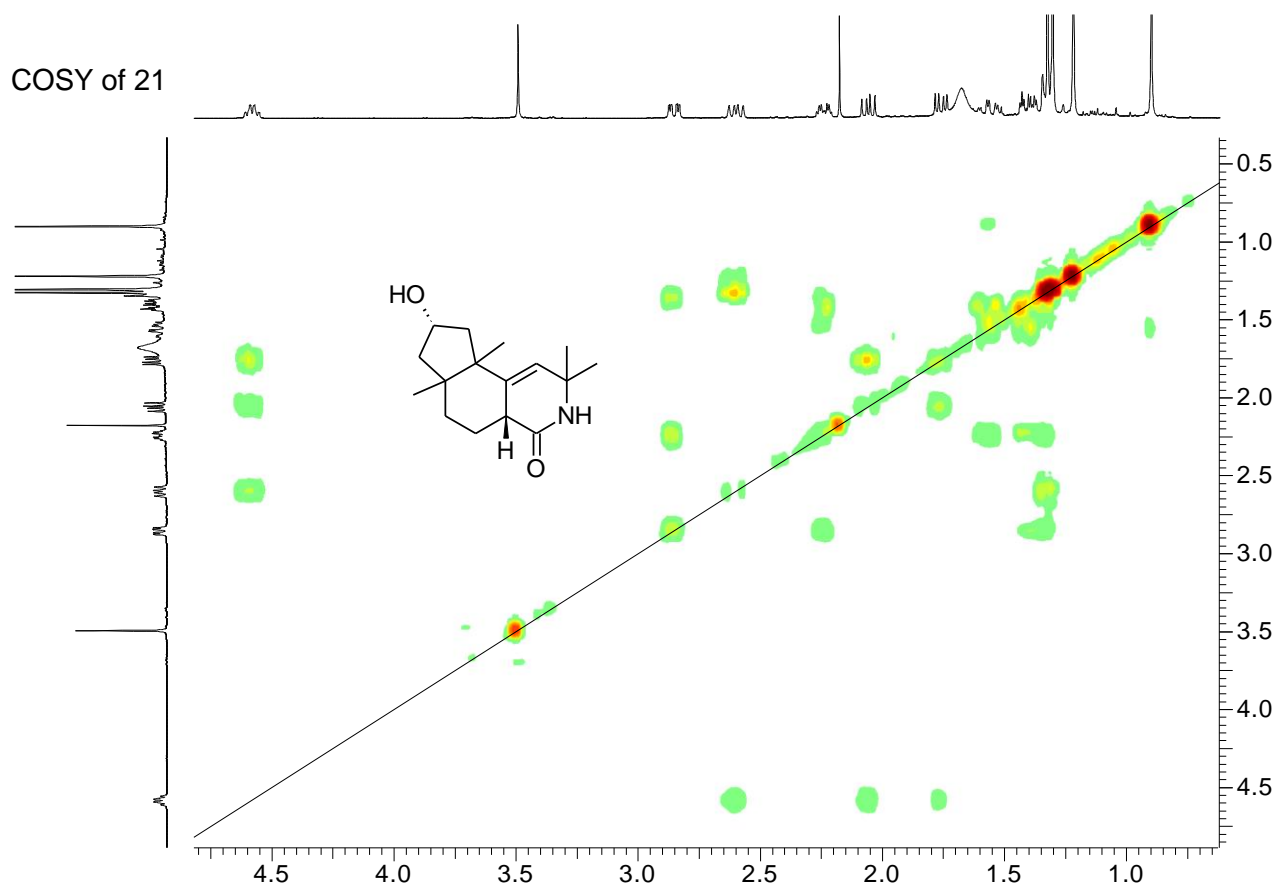
DEPT135 and ^{13}C NMR of 21 in CDCl_3 , 125MHz



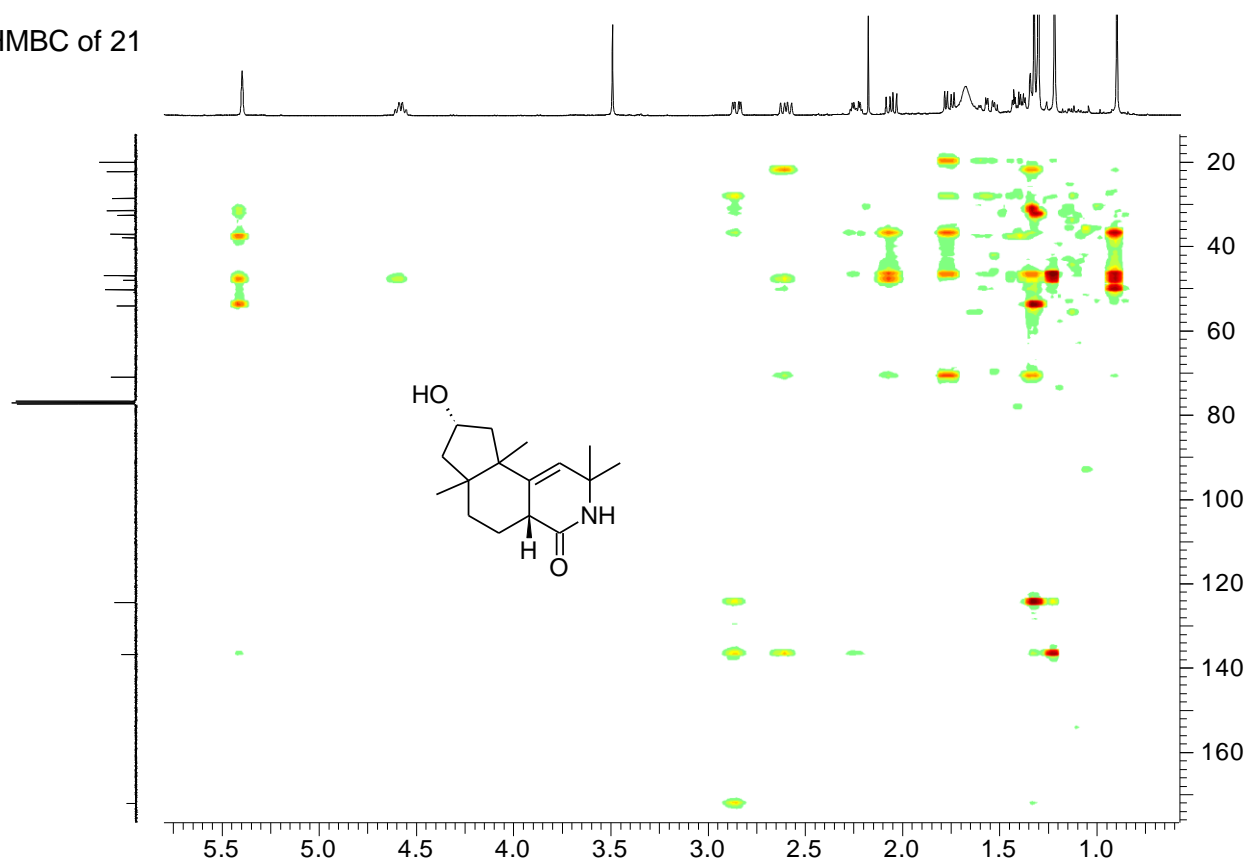
HSQC of 21



COSY of 21



HMBC of 21



NOESY of 21

