Supporting Information

Impacts of Steric Compression, Protonation, and Intramolecular Hydrogen-Bonding on the ^{15}N NMR spectroscopy of Norditerpenoid Alkaloids and Their Piperidine-Ring Analogues

Ziyu Zeng, Ashraf M. A. Qasem, Timothy J. Woodman, Michael G. Rowan, and Ian S. Blagbrough*

Department of Pharmacy and Pharmacology, University of Bath, Bath BA2 7AY, U.K.

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IR, MS, and NMR spectra

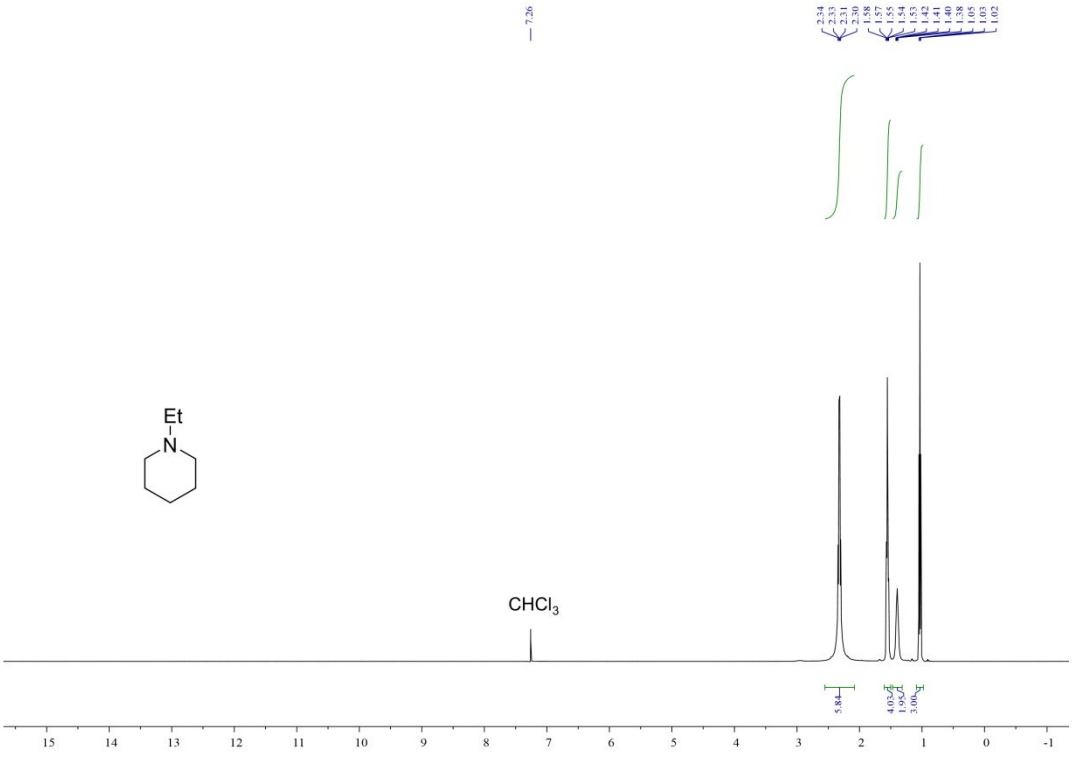


Figure S1. ^{1}H NMR spectrum of *N*-Et piperidine (**1**) in $CDCl_3$

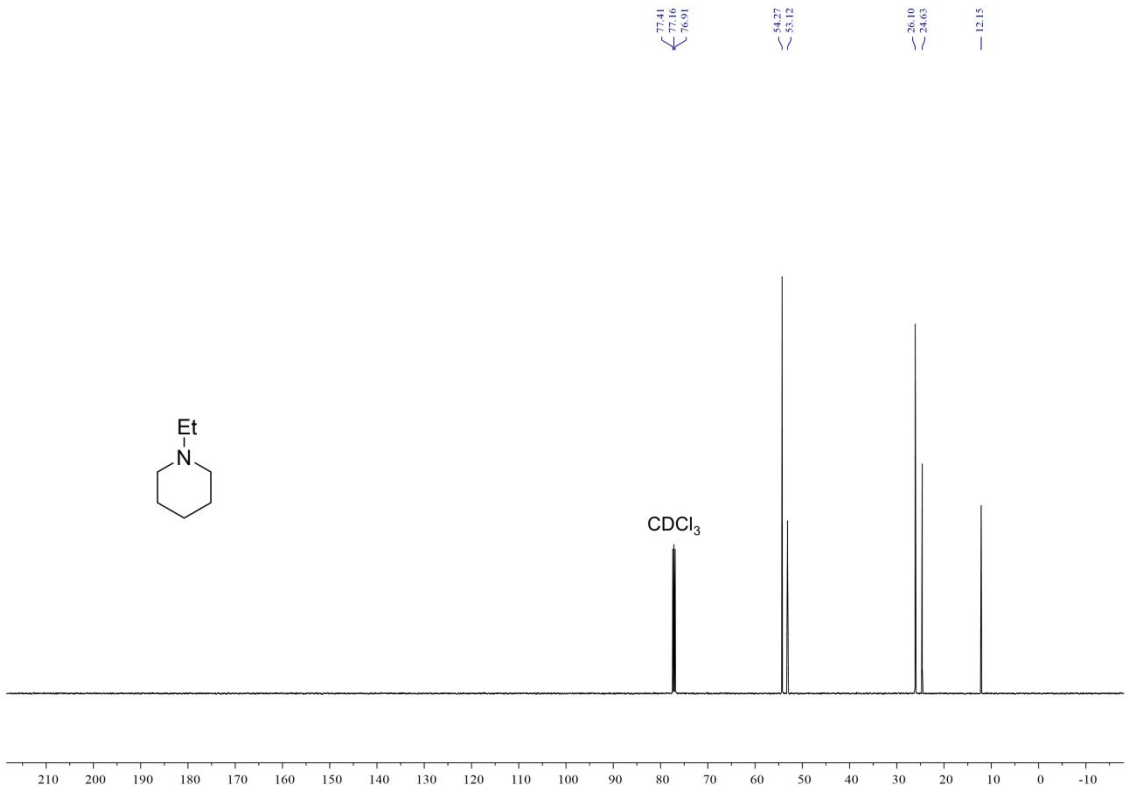


Figure S2. ^{13}C NMR spectrum of *N*-Et piperidine (**1**) in $CDCl_3$

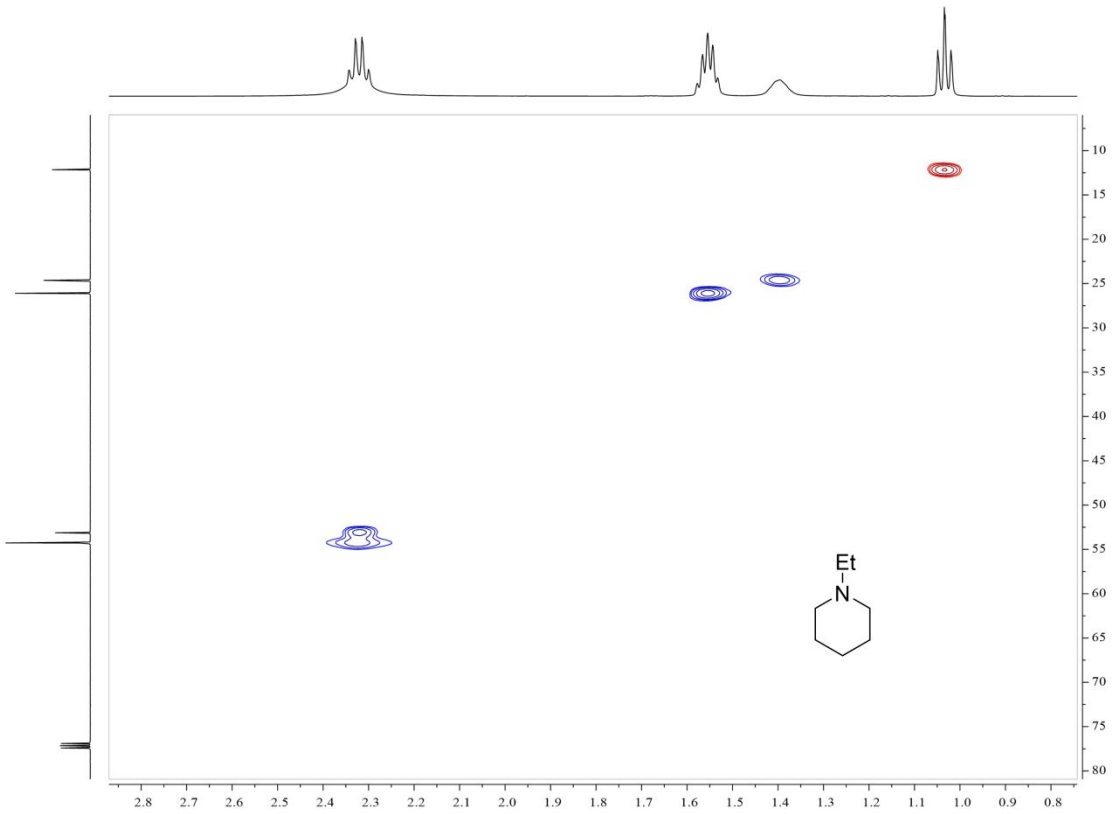


Figure S3. HSQC spectrum of *N*-Et piperidine (**1**) in $CDCl_3$

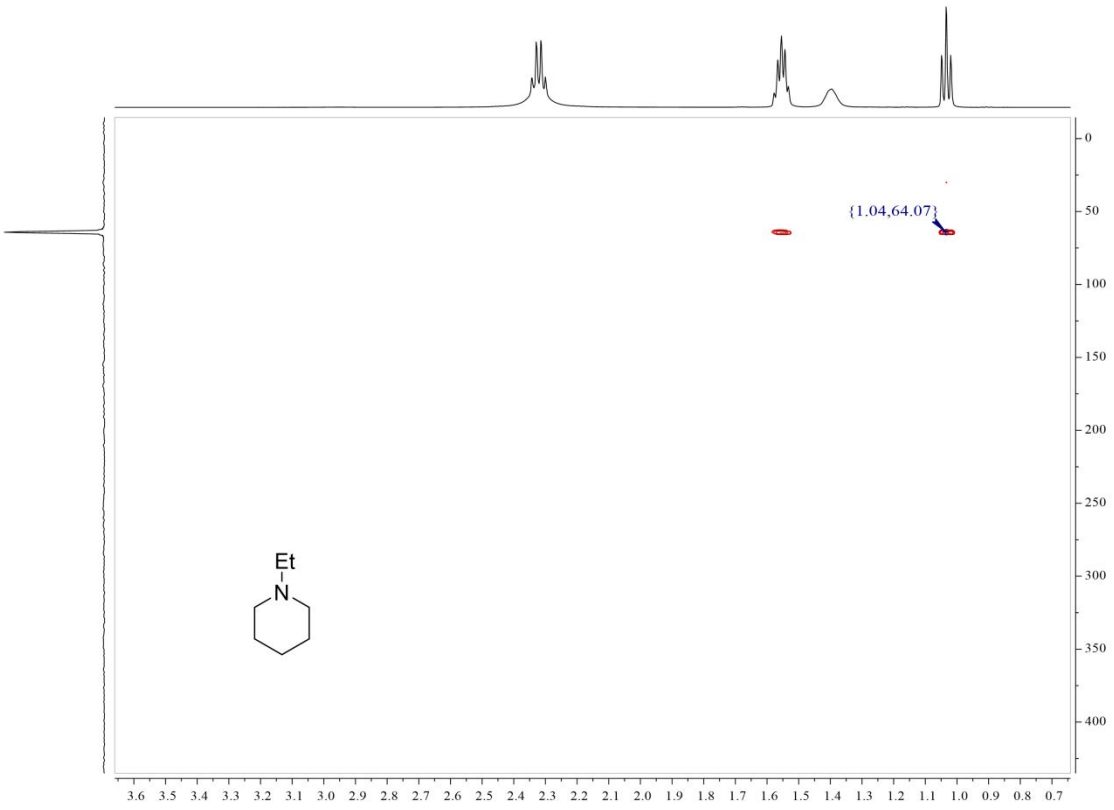
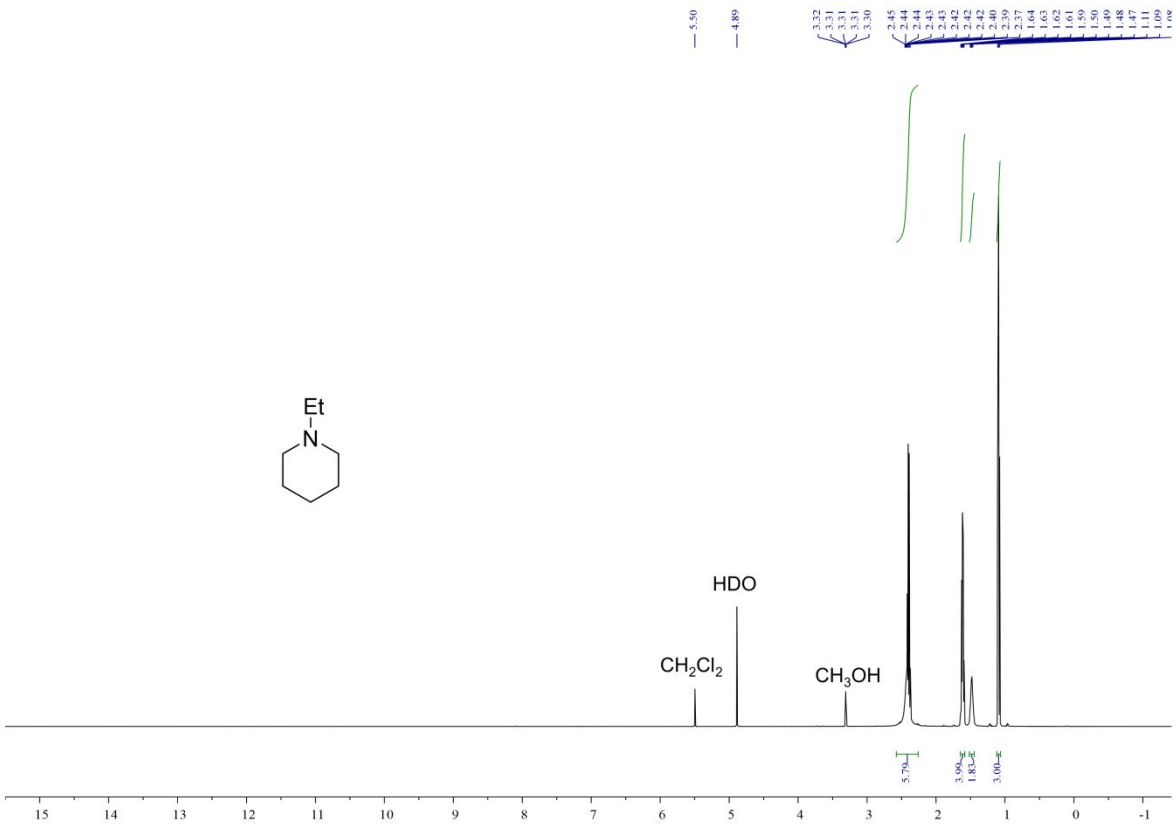


Figure S4. ^{1}H-^{15}N HMBC spectrum of *N*-Et piperidine (**1**) in $CDCl_3$



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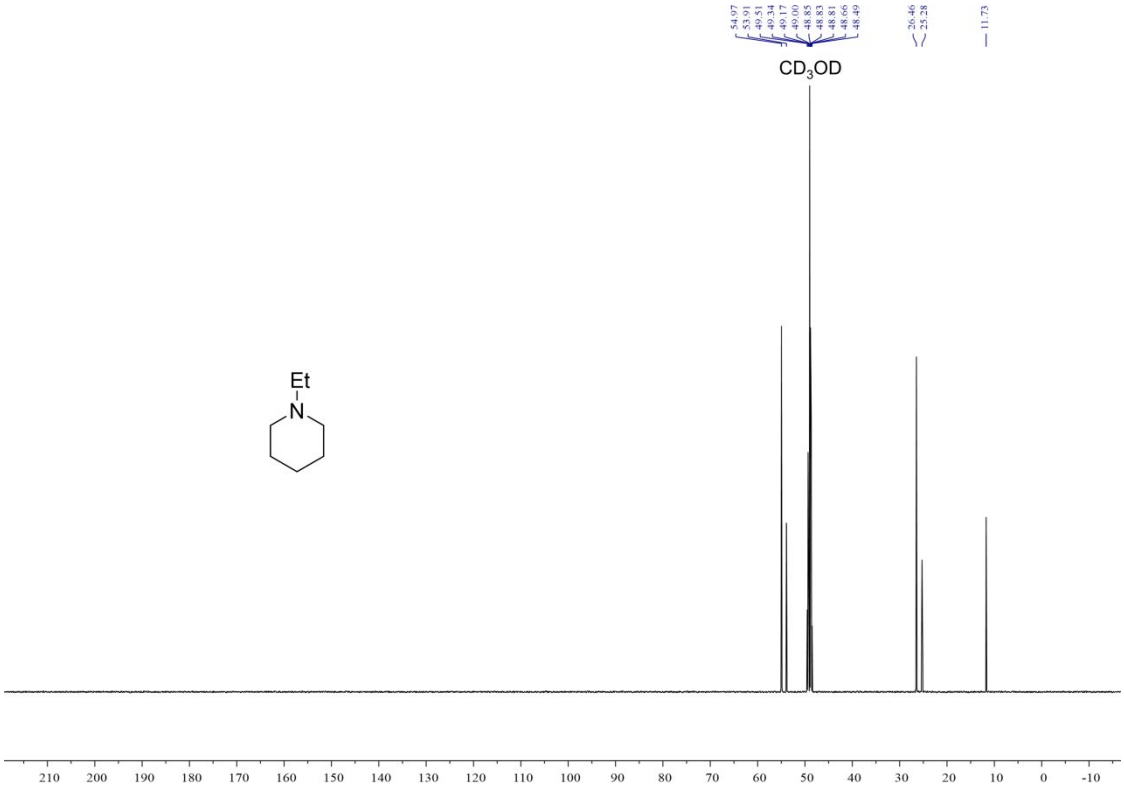


Figure S6. ^{13}C NMR spectrum of *N*-Et piperidine (**1**) in CD_3OD

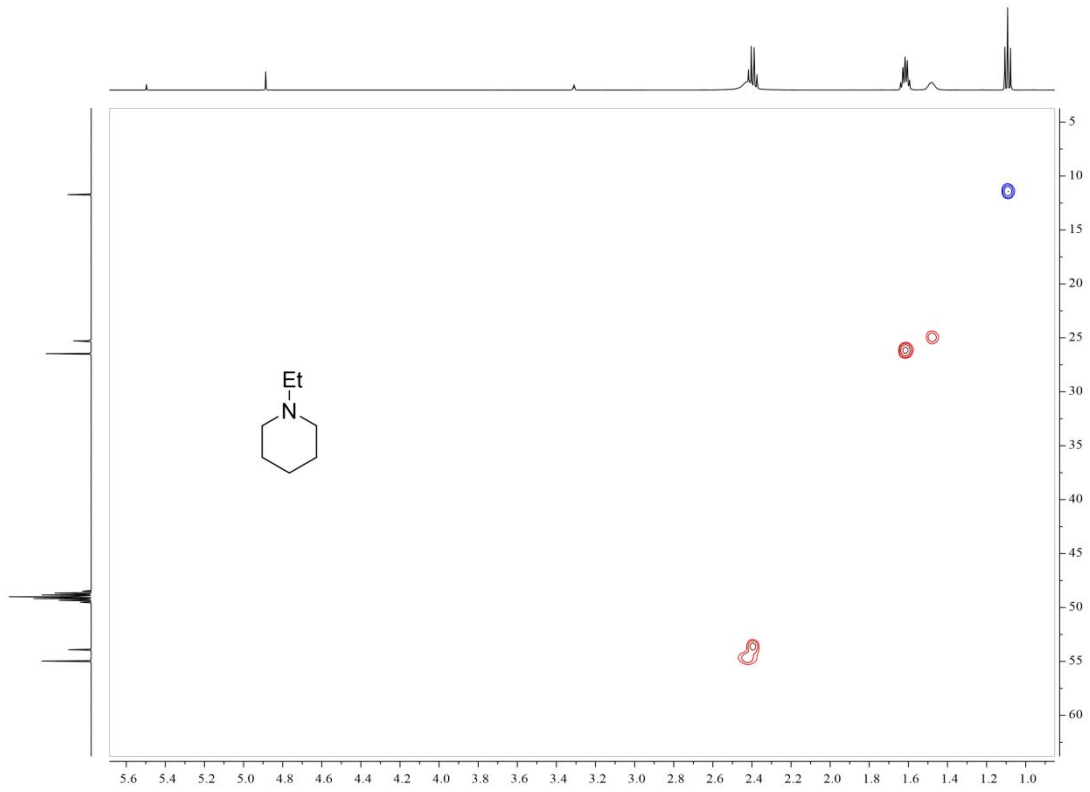


Figure S7. HSQC spectrum of *N*-Et piperidine (**1**) in CD_3OD

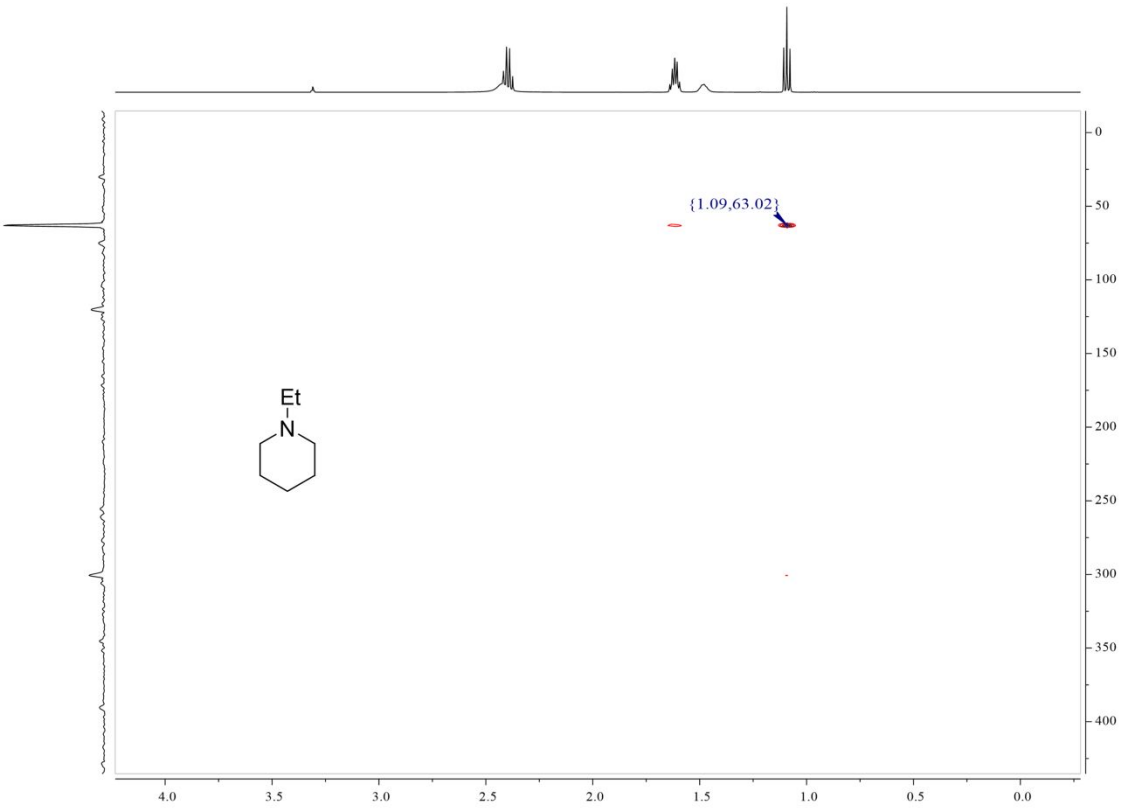


Figure S8. ^{1}H-^{15}N HMBC spectrum of *N*-Et piperidine (**1**) in CD_3OD

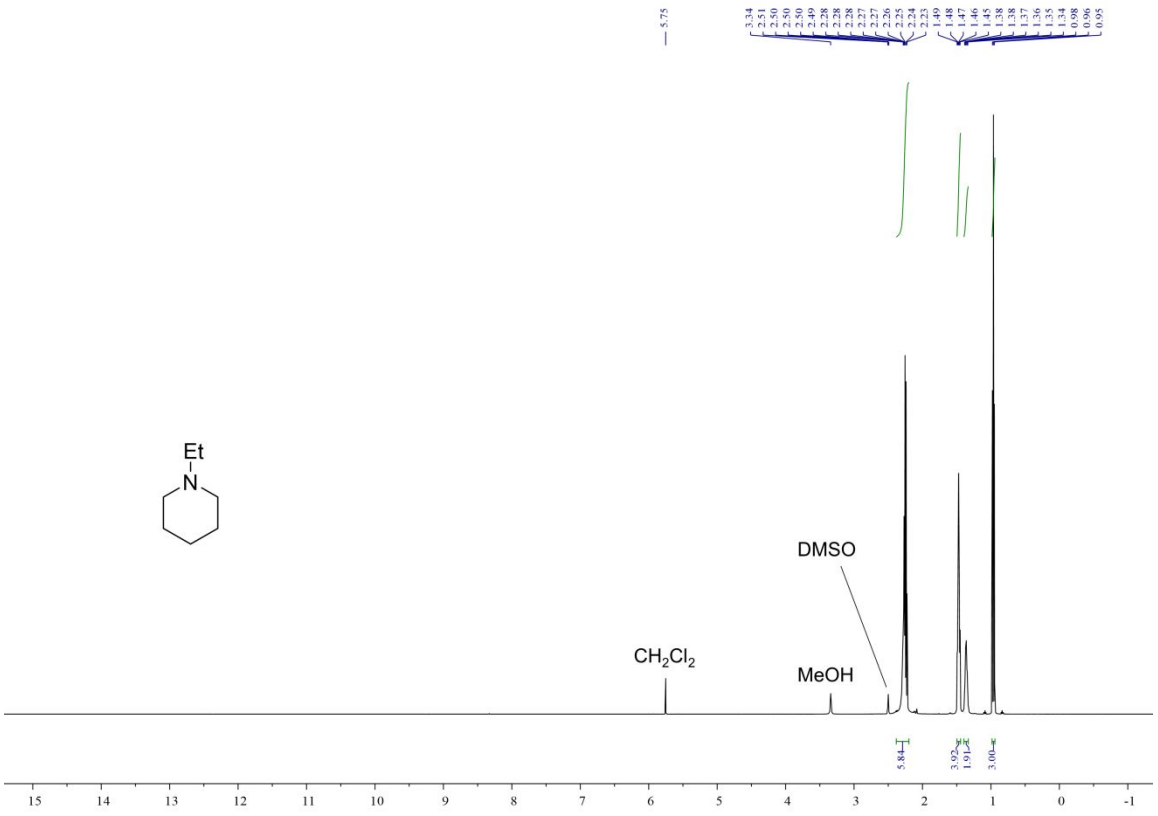


Figure S9. ^{1}H NMR spectrum of *N*-Et piperidine (**1**) in d_6-DMSO

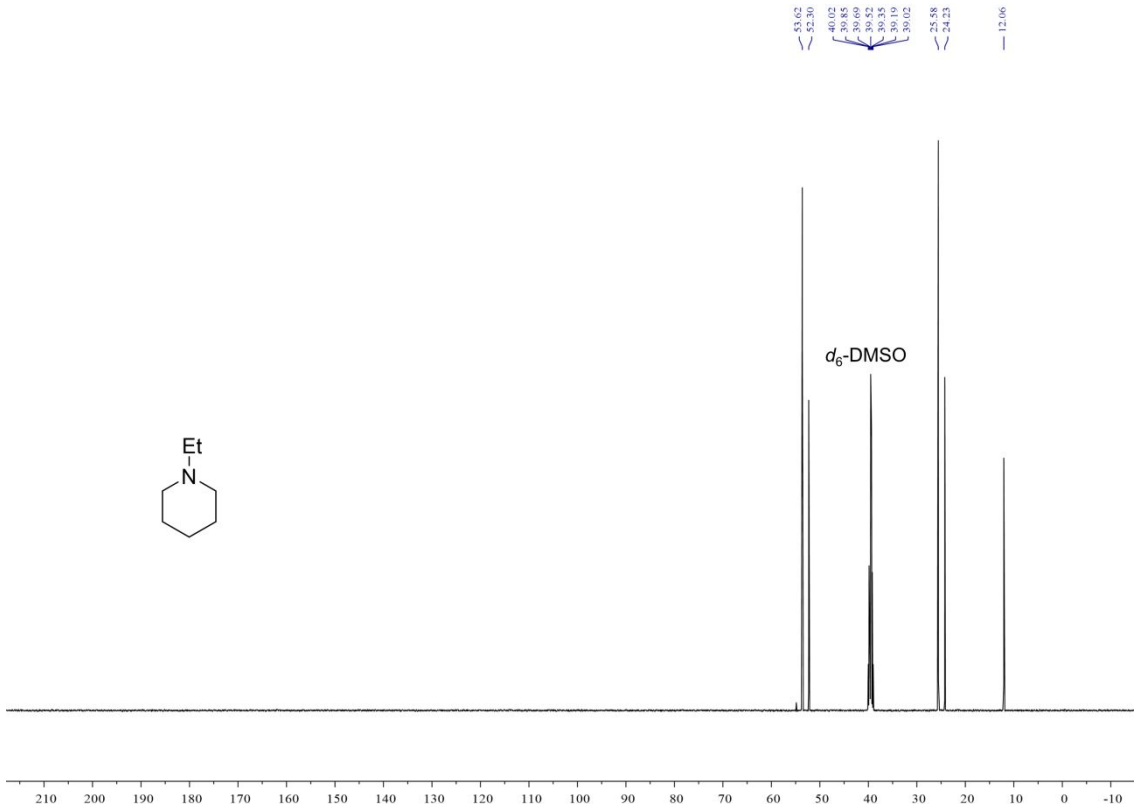


Figure S10. ^{13}C NMR spectrum of *N*-Et piperidine (**1**) in d_6-DMSO

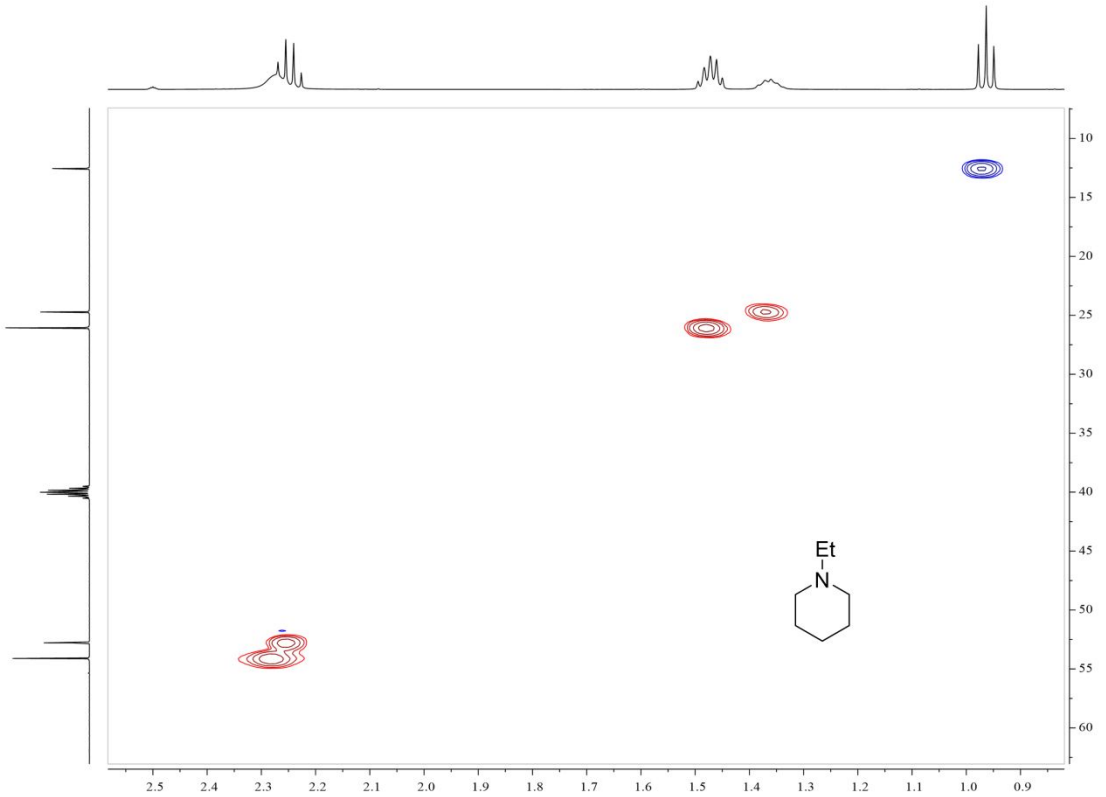
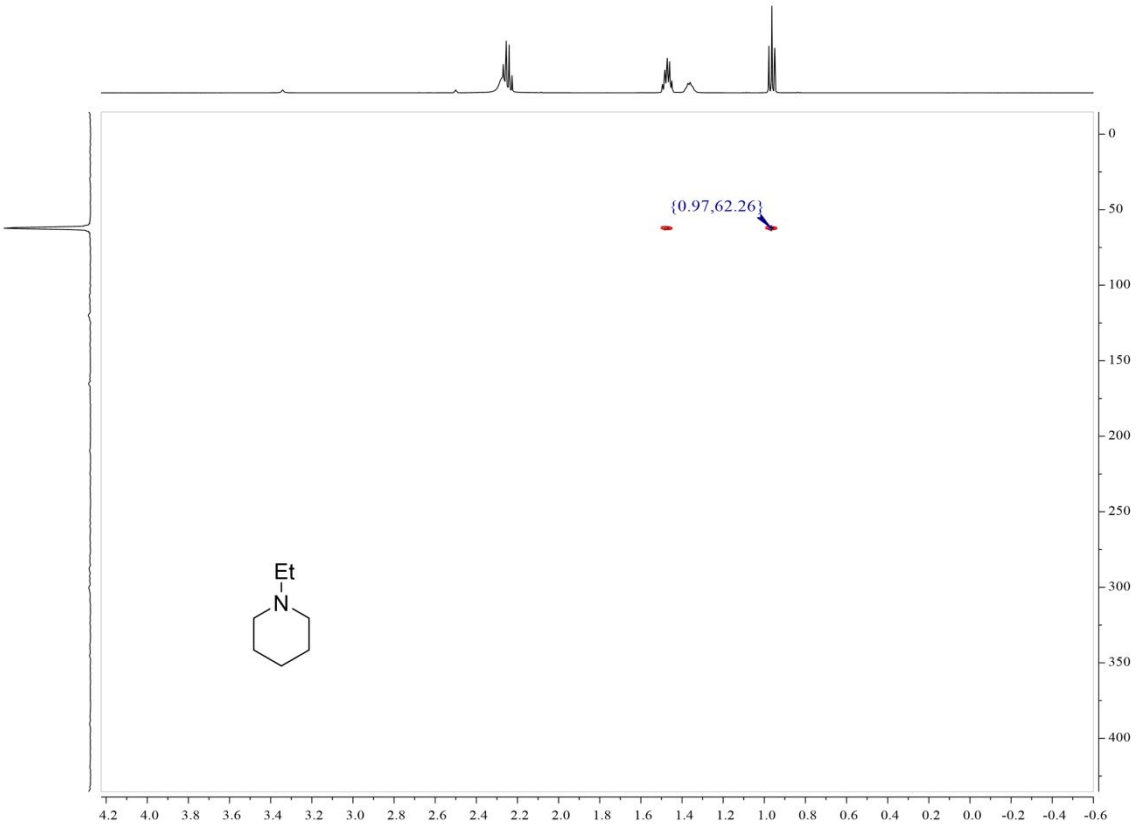


Figure S11. HSQC spectrum of *N*-Et piperidine (**1**) in d_6-DMSO



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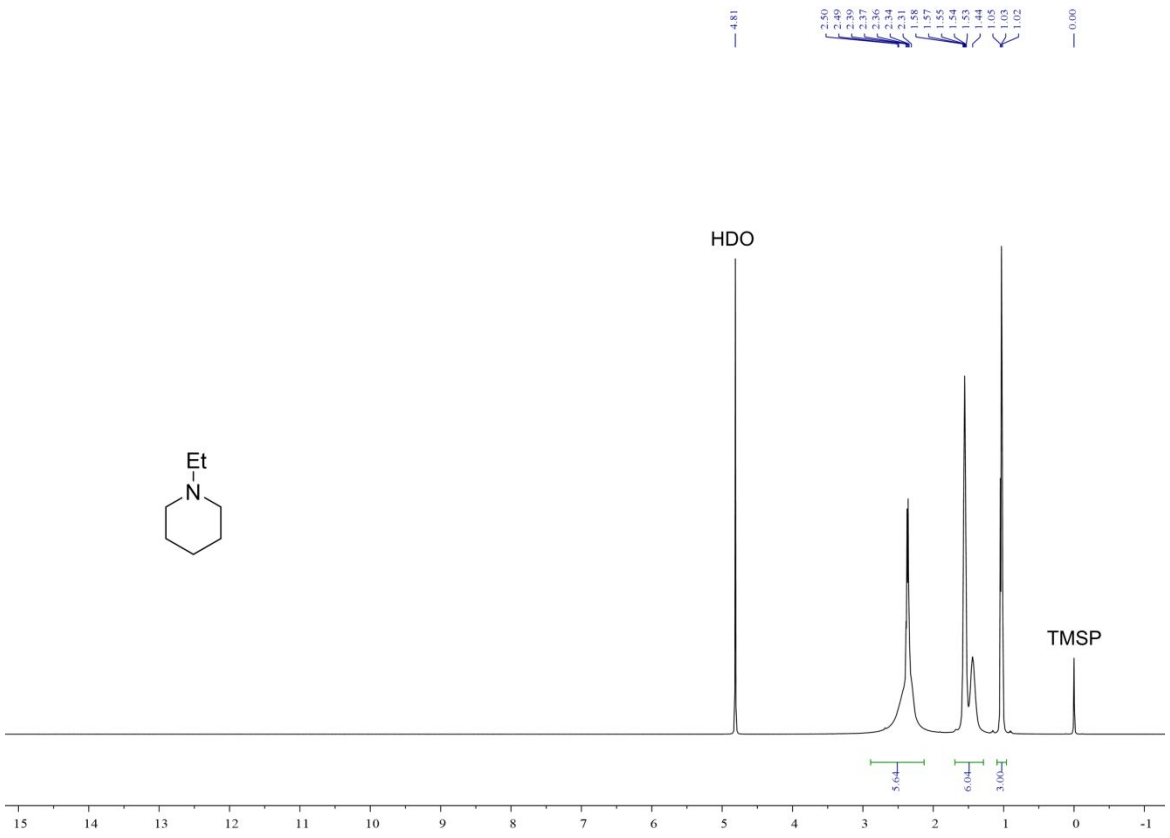


Figure S13. ^{1}H NMR spectrum of *N*-Et piperidine (**1**) in D_2O (with additional 2 drops of d_6-DMSO)

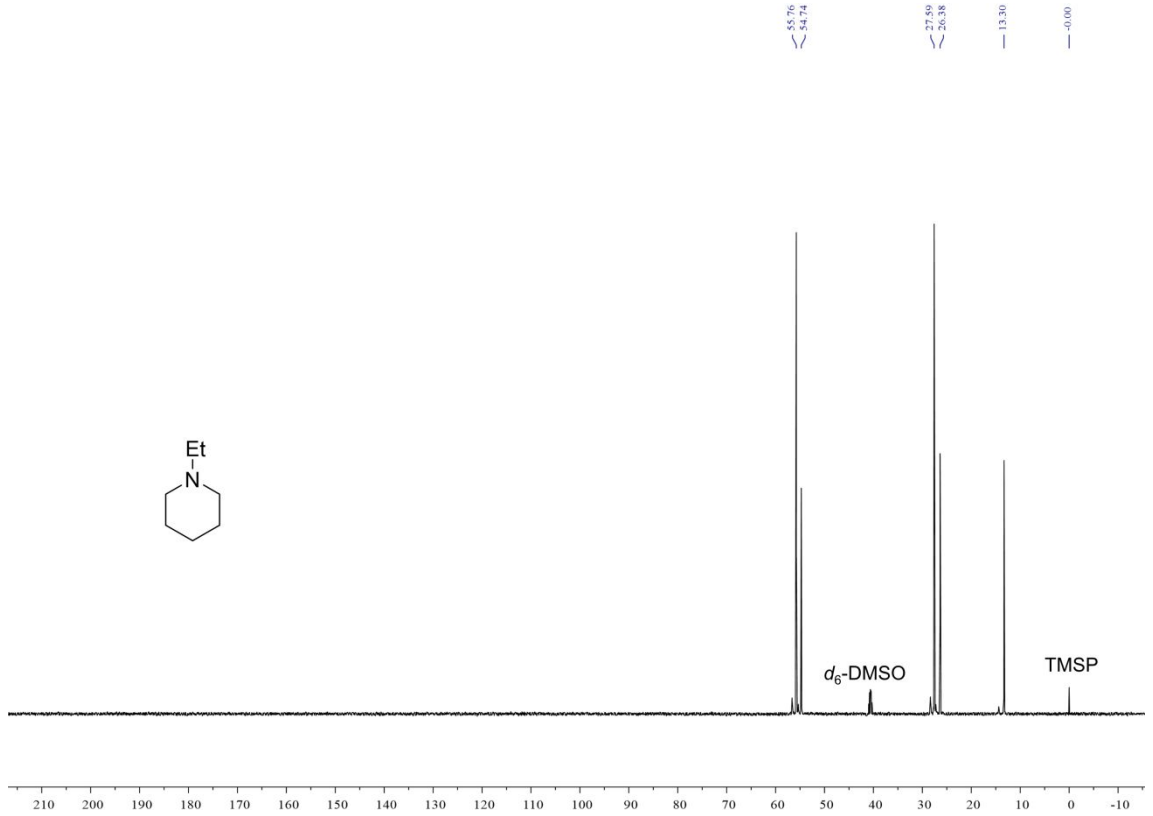


Figure S14. ^{13}C NMR spectrum of *N*-Et piperidine (**1**) in D_2O (with additional 2 drops of d_6-DMSO)

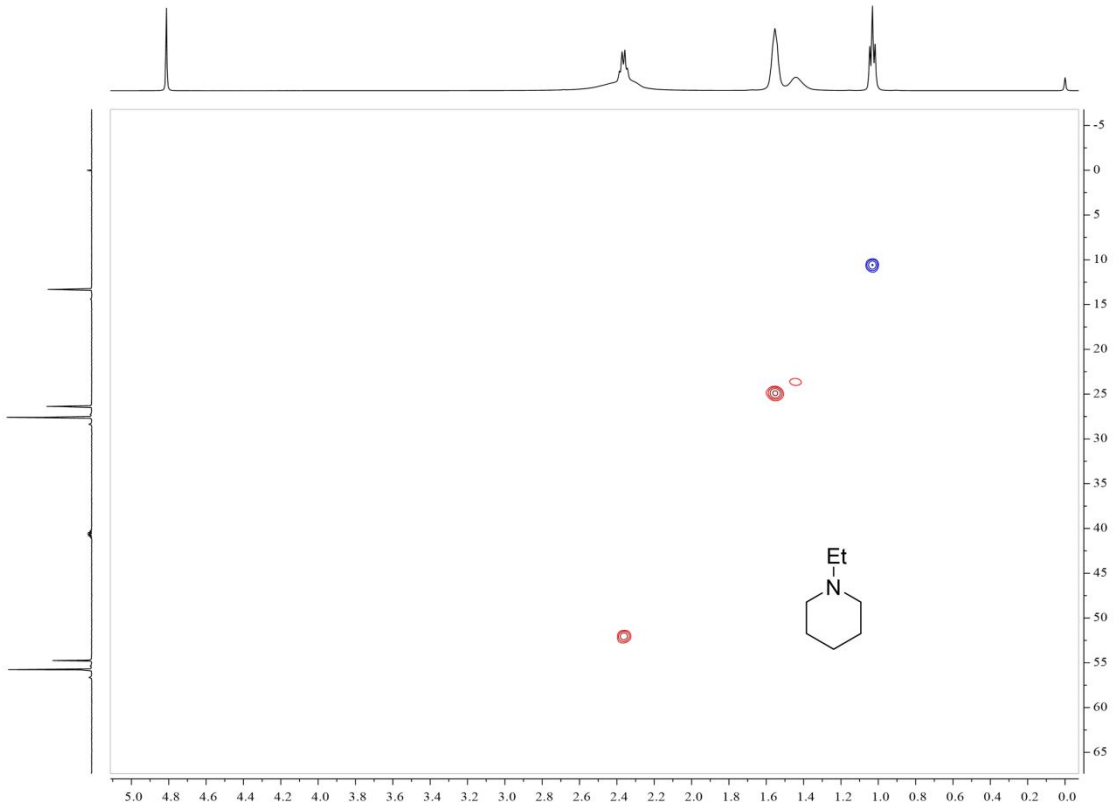


Figure S15. HSQC spectrum of *N*-Et piperidine (**1**) in D_2O (with additional 2 drops of d_6-DMSO)

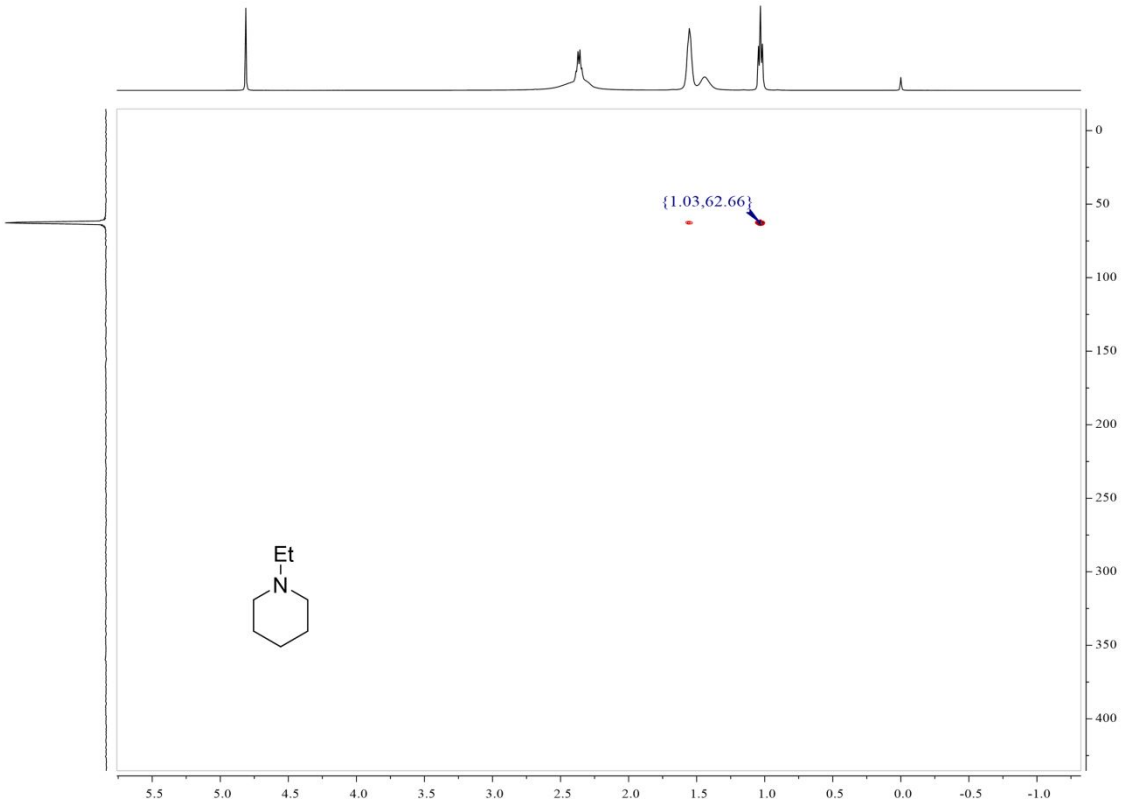


Figure S16. ^{1}H-^{15}N HMBC spectrum of *N*-Et piperidine (**1**) in D_2O (with additional 2 drops of d_6-DMSO)

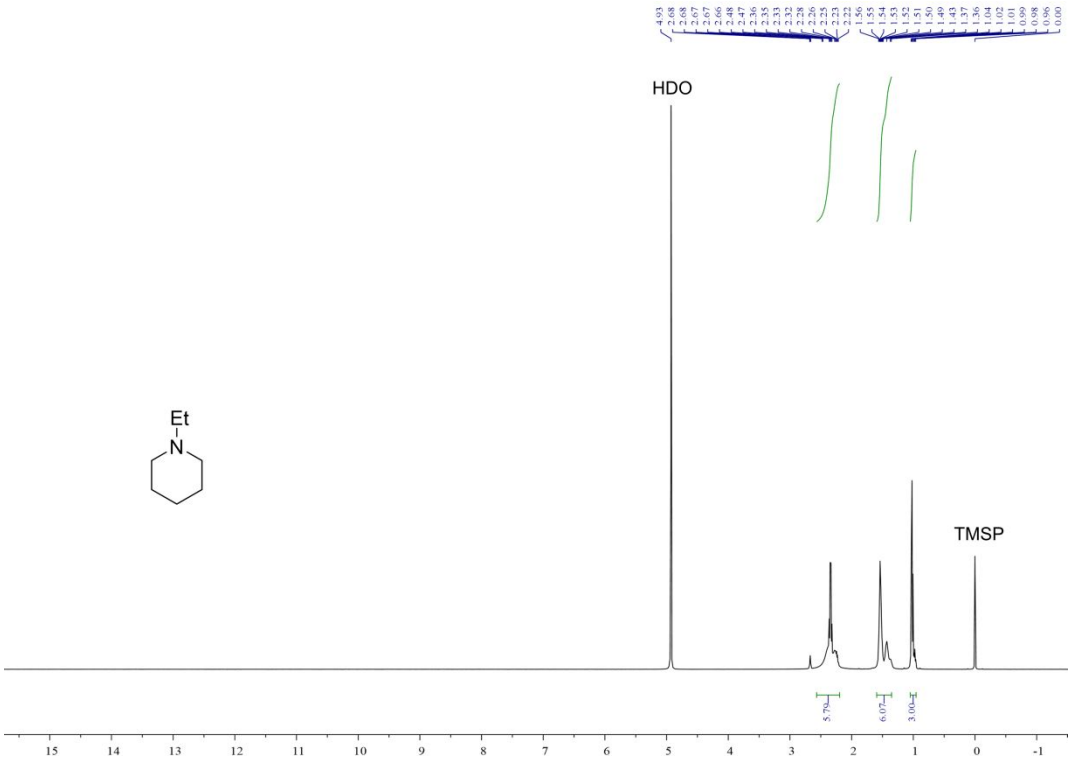


Figure S17. ^{1}H NMR spectrum of *N*-Et piperidine (**1**) in D_2O (with additional 2 drops of d_6-DMSO and drops of NaOD solution, 30% in D_2O, w/w, pD ~13)

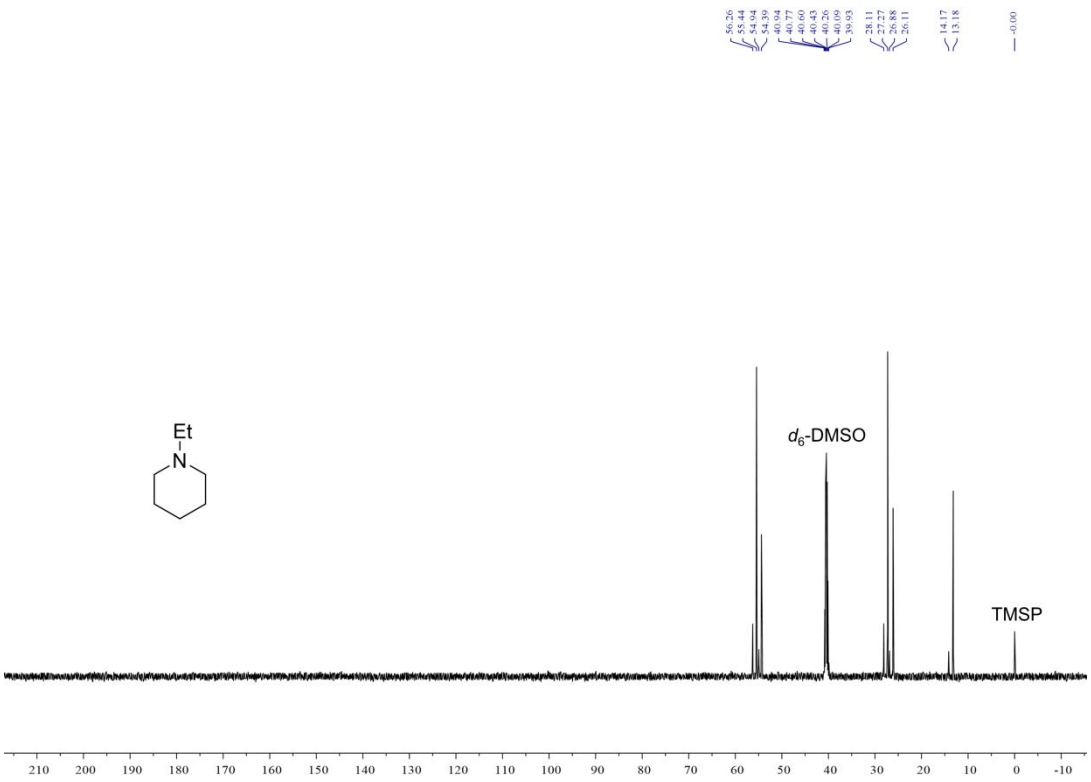


Figure S18. ^{13}C NMR spectrum of *N*-Et piperidine (**1**) in D_2O (with additional 2 drops of d_6-DMSO and drops of NaOD solution, 30% in D_2O, w/w, pD ~13)

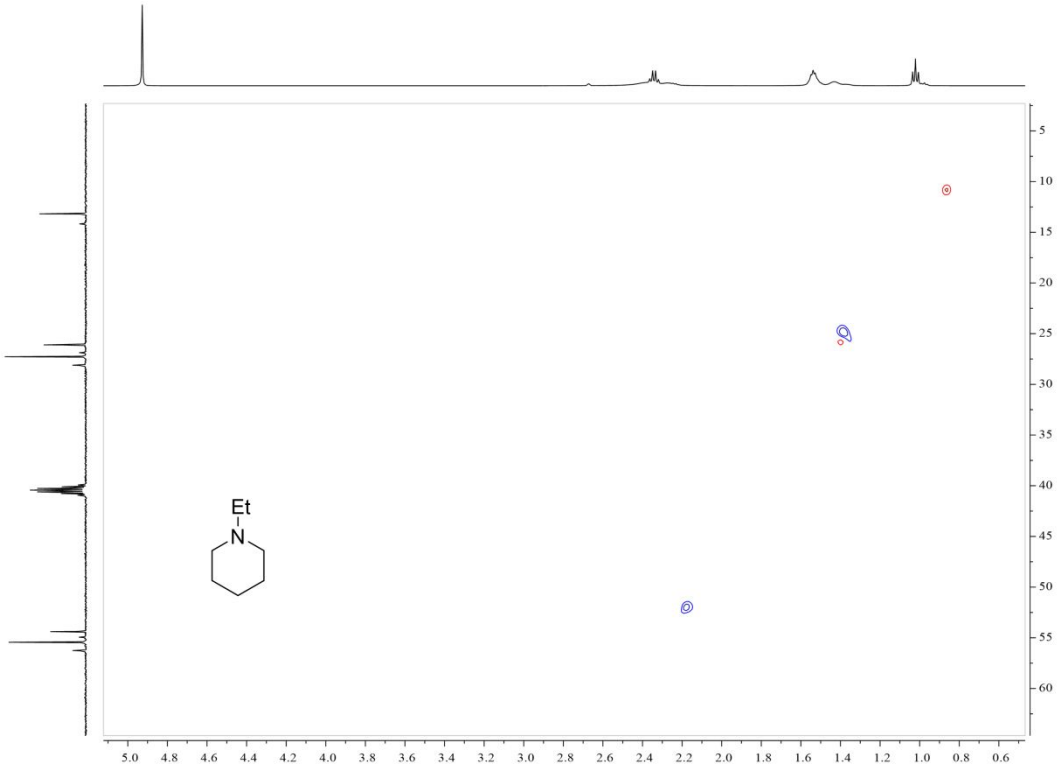


Figure S19. HSQC spectrum of *N*-Et piperidine (**1**) in D_2O (with additional 2 drops of d_6-DMSO and drops of NaOD solution, 30% in D_2O, w/w, pD ~13)

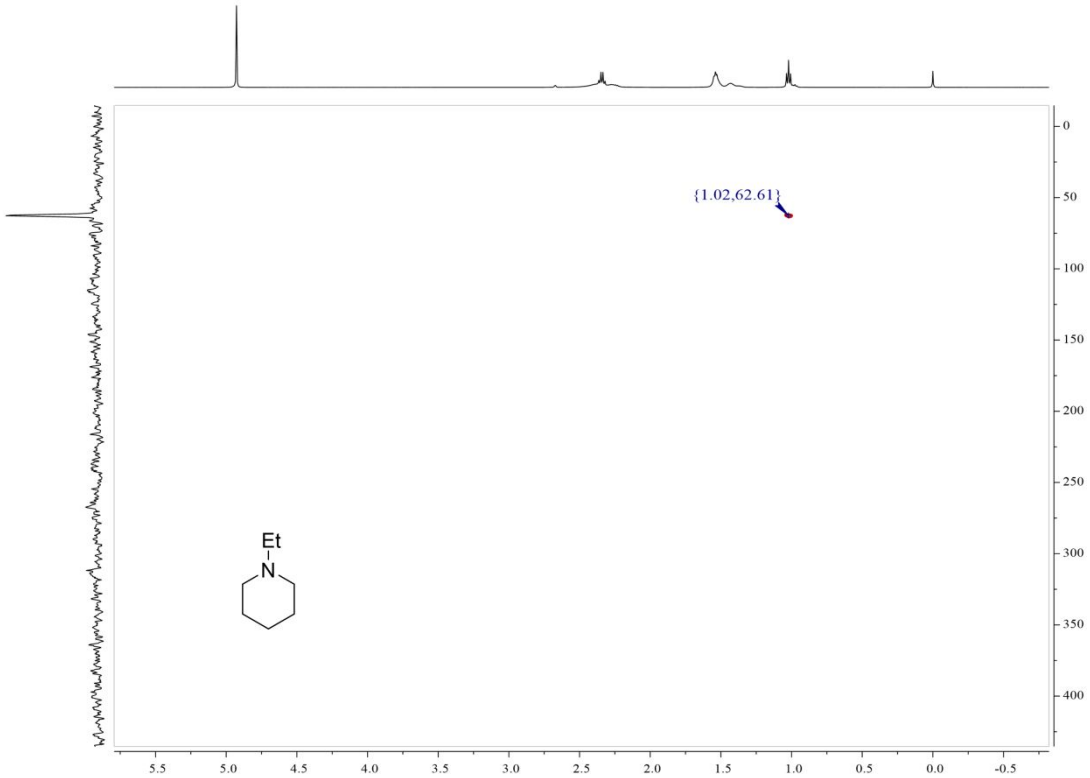


Figure S20. ^{1}H-^{15}N HMBC spectrum of *N*-Et piperidine (**1**) in D_2O (with additional 2 drops of d_6-DMSO and drops of NaOD solution, 30% in D_2O, w/w, pD ~13)

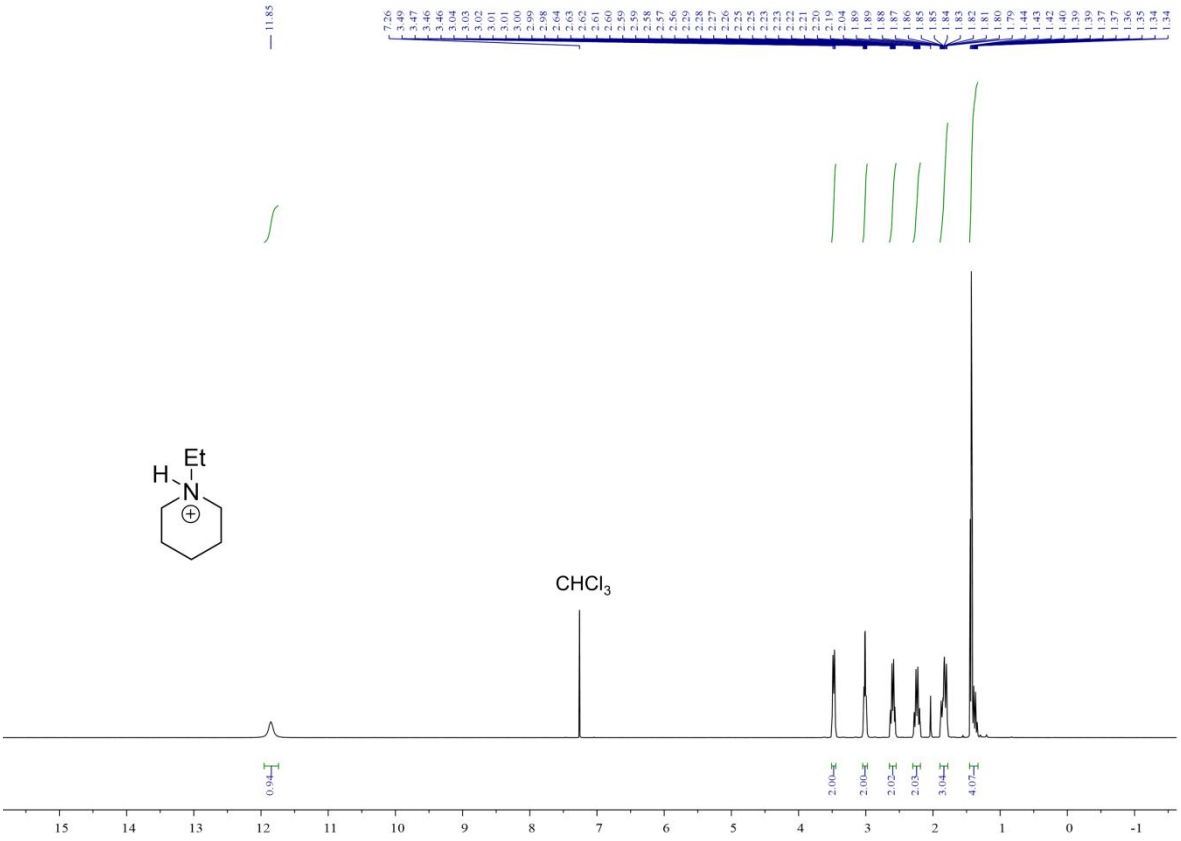


Figure S21. ^{1}H NMR spectrum of *N*-Et piperidine HCl salt (**1'**) in $CDCl_3$

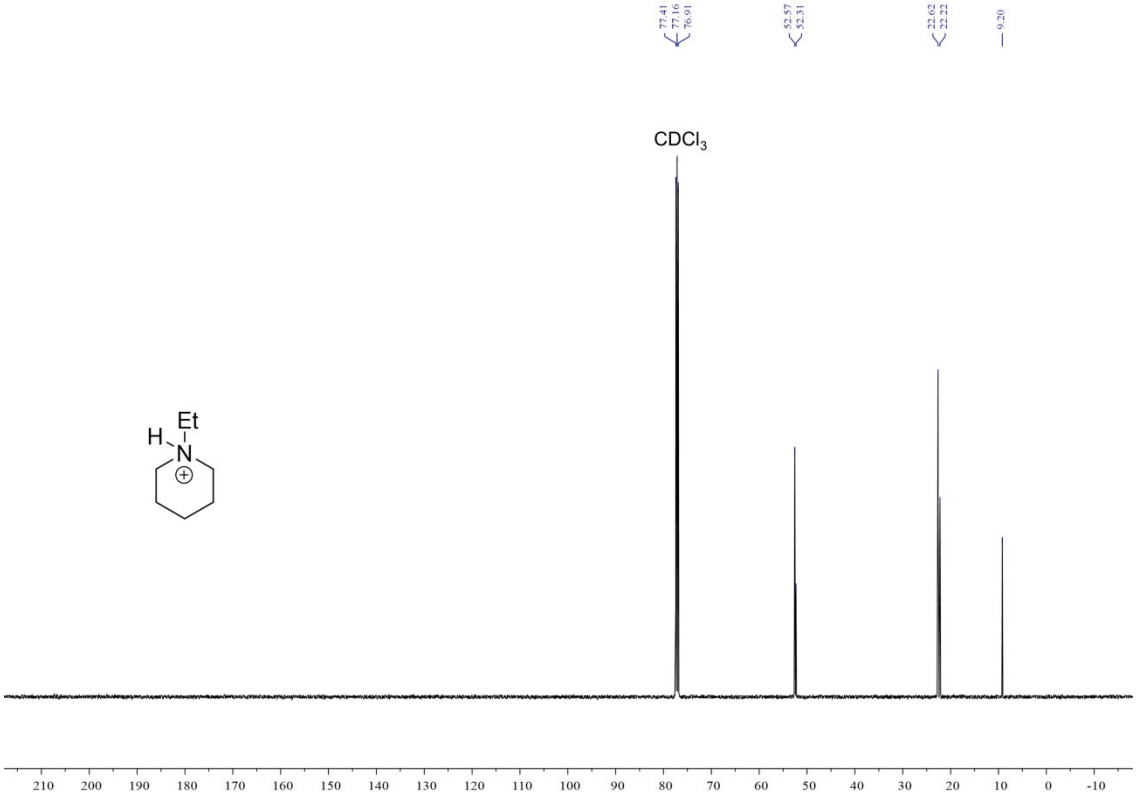


Figure S22. ^{13}C NMR spectrum of *N*-Et piperidine HCl salt (**1'**) in $CDCl_3$

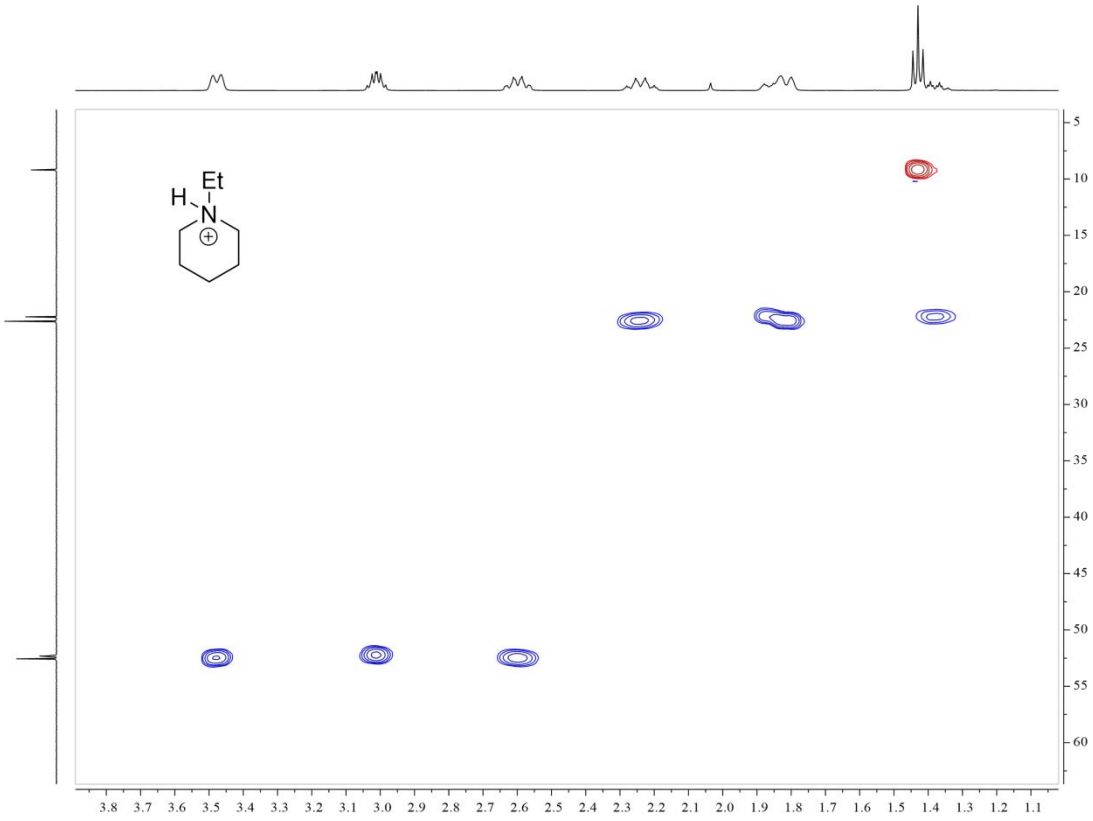


Figure S23. HSQC spectrum of *N*-Et piperidine HCl salt (**1'**) in $CDCl_3$

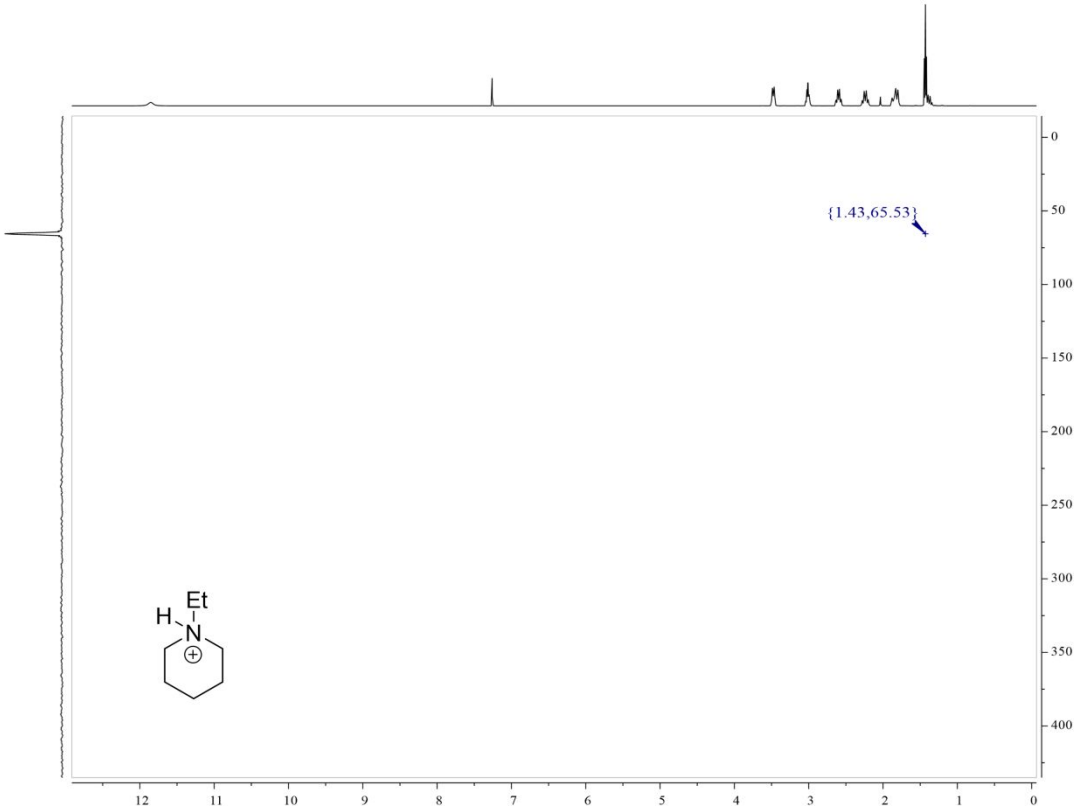


Figure S24. ^{1}H-^{15}N HMBC spectrum of *N*-Et piperidine HCl salt (**1'**) in $CDCl_3$

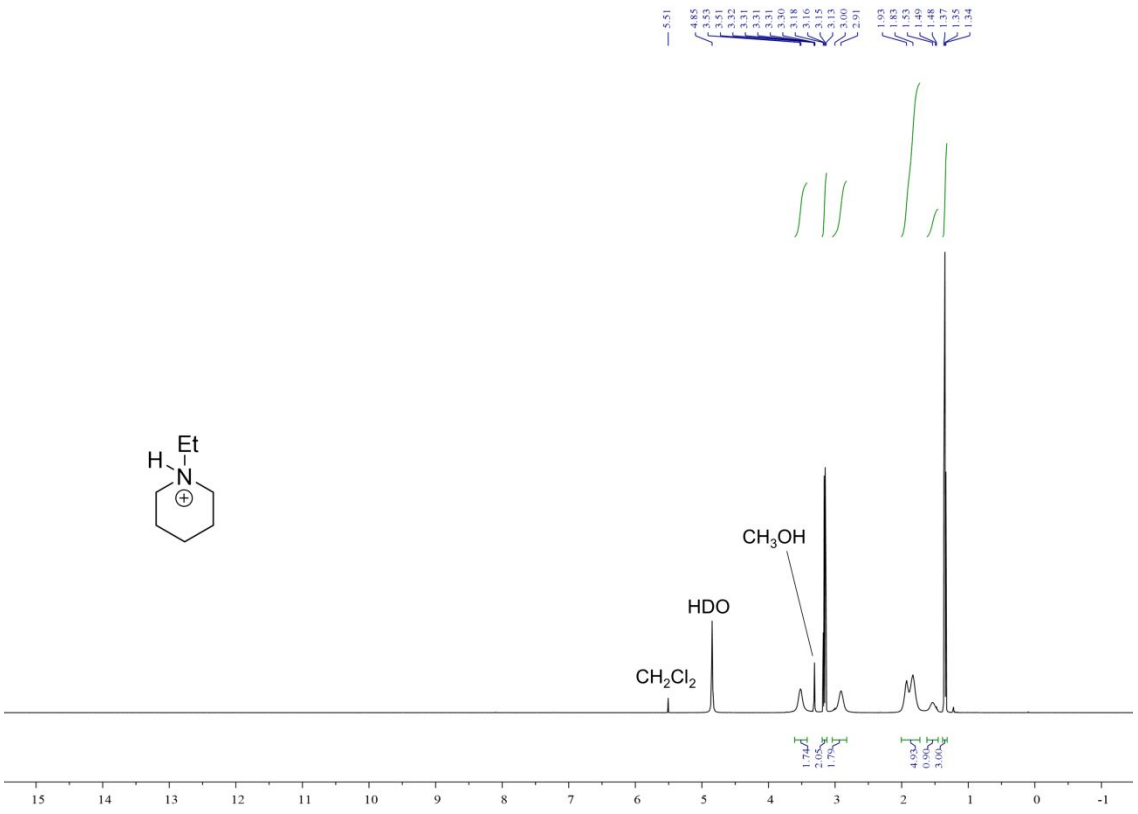


Figure S25. ^{1}H NMR spectrum of *N*-Et piperidine HCl salt (**1'**) in CD_3OD

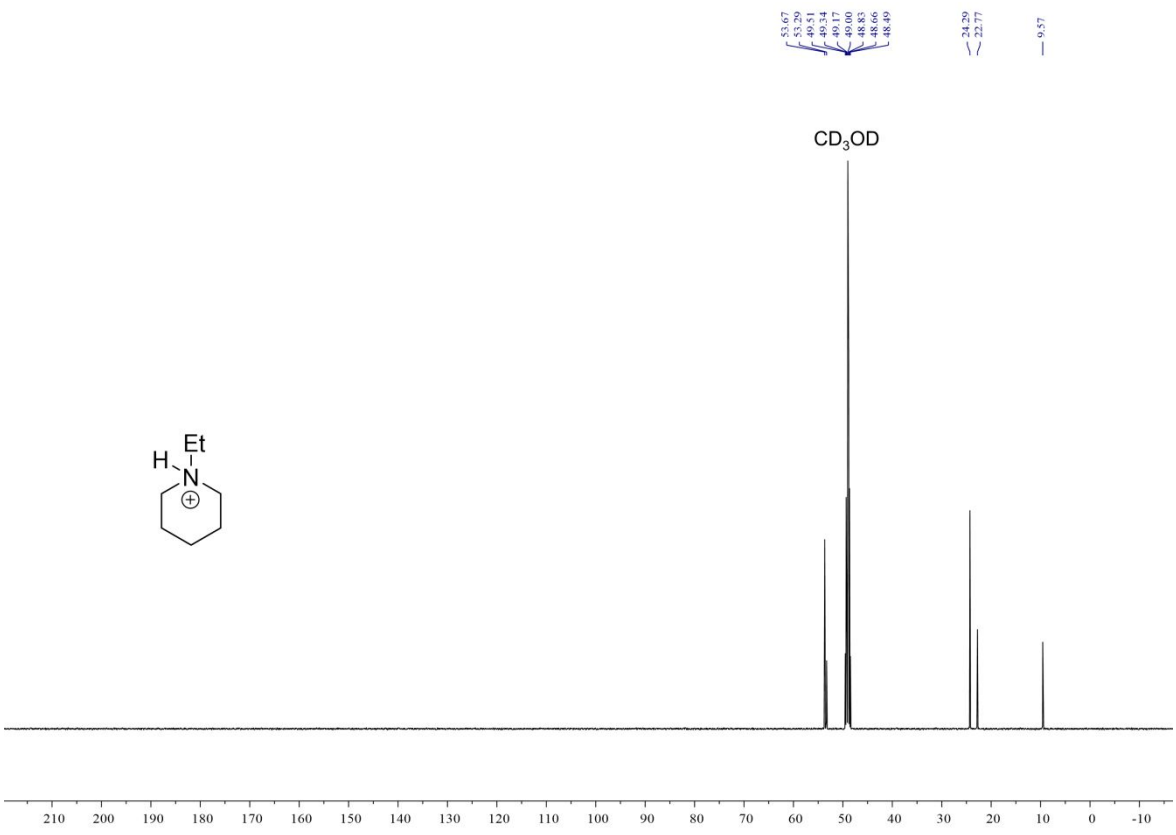


Figure S26. ^{13}C NMR spectrum of *N*-Et piperidine HCl salt (**1'**) in CD_3OD

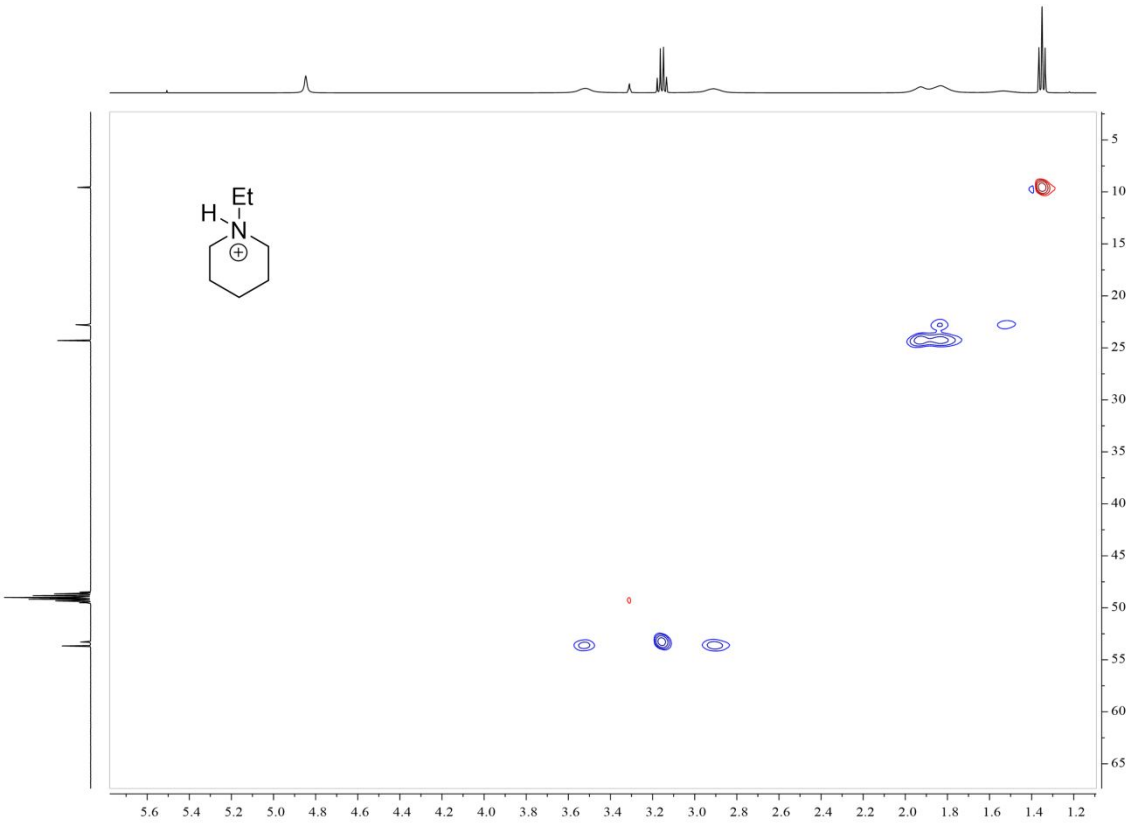
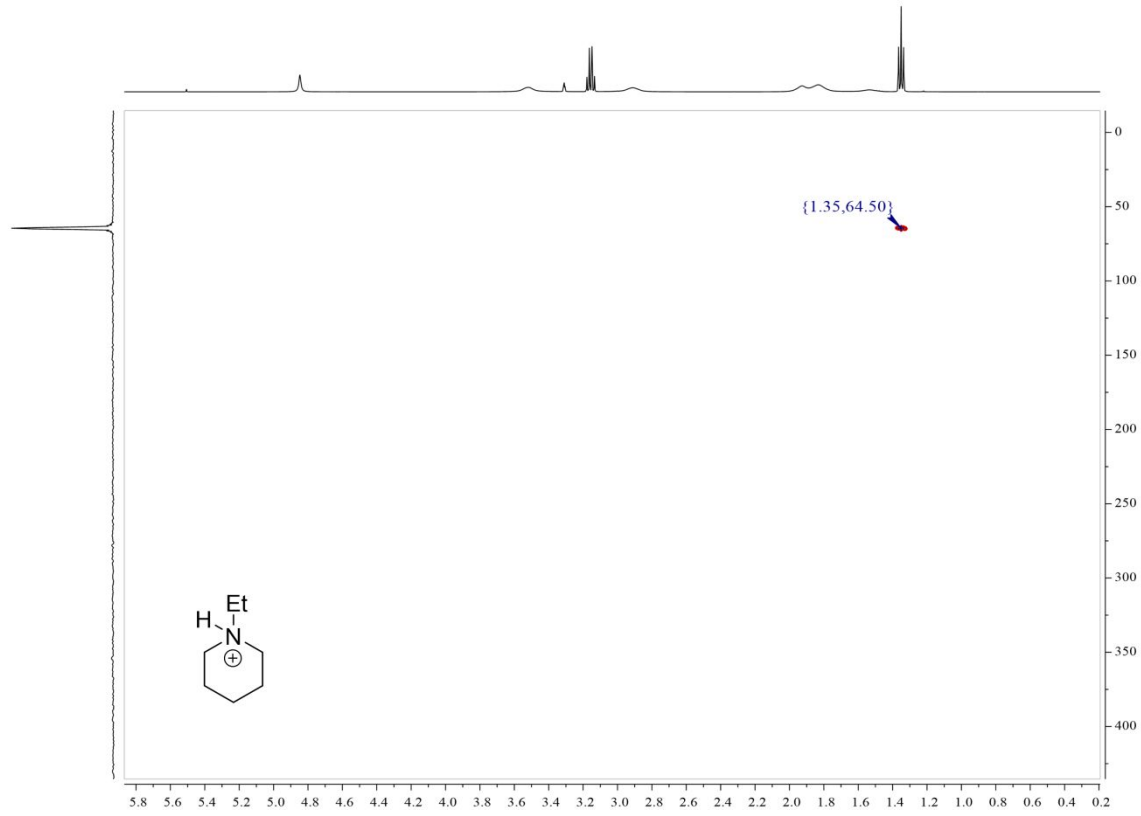


Figure S27. HSQC spectrum of *N*-Et piperidine HCl salt (**1'**) in CD_3OD



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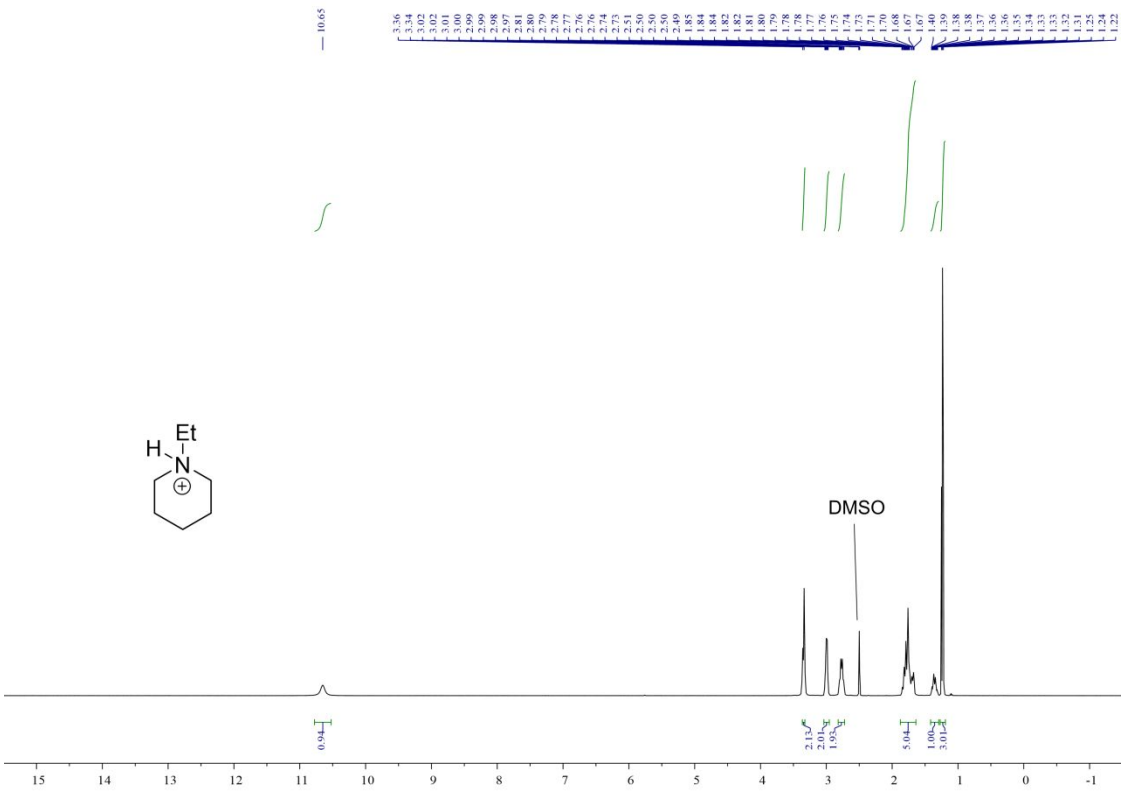


Figure S29. ^{1}H NMR spectrum of *N*-Et piperidine HCl salt (**1'**) in d_6-DMSO

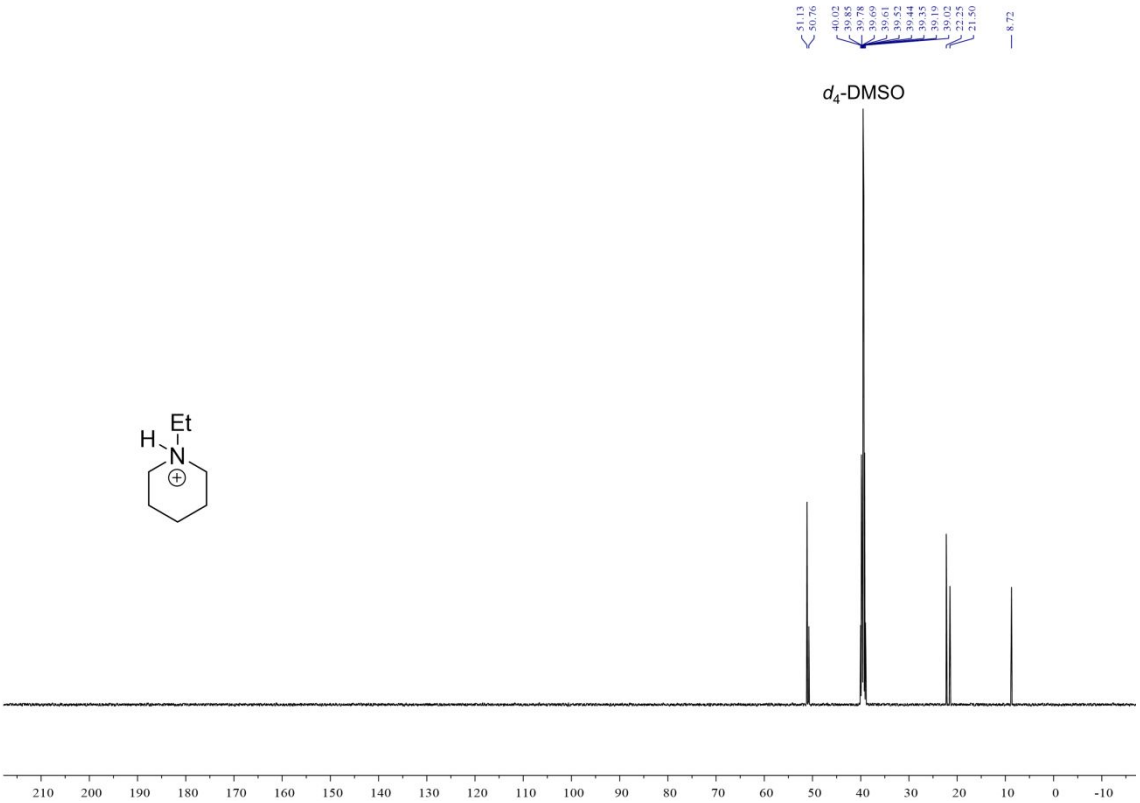


Figure S30. ^{13}C NMR spectrum of *N*-Et piperidine HCl salt (**1'**) in d_6-DMSO

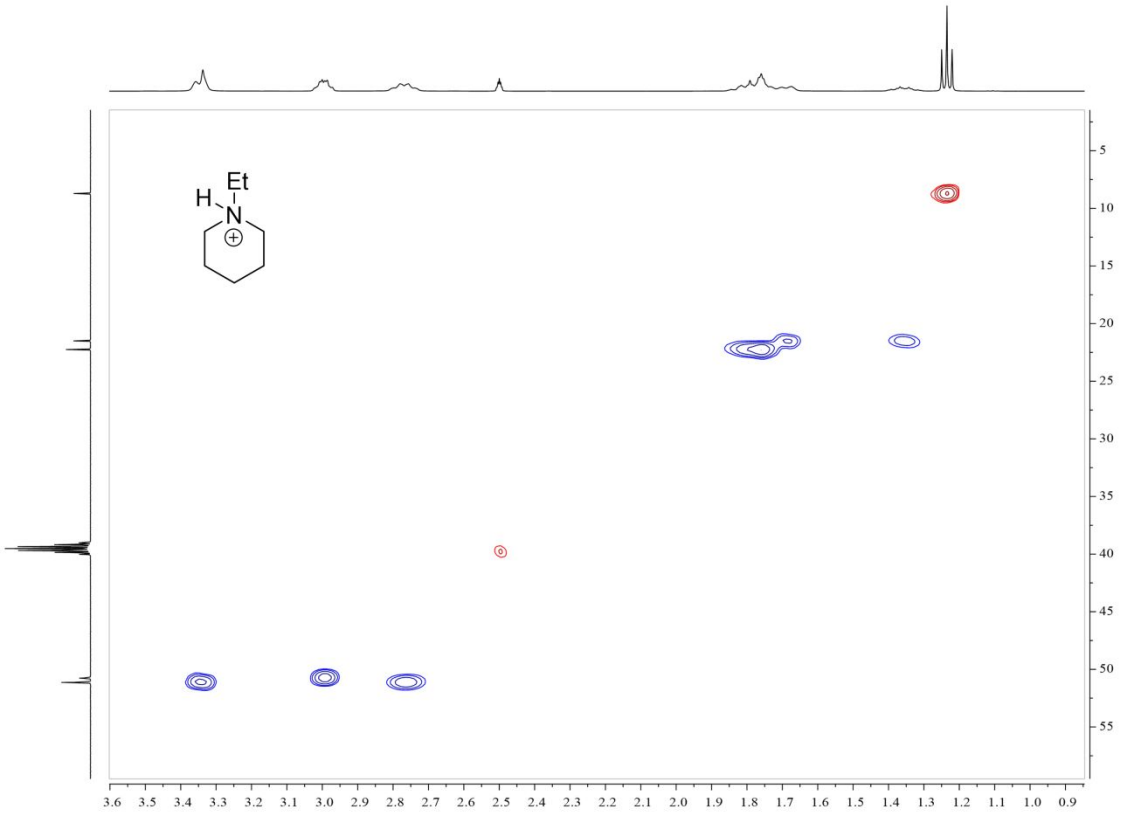


Figure S31. HSQC spectrum of *N*-Et piperidine HCl salt (**1'**) in d_6-DMSO

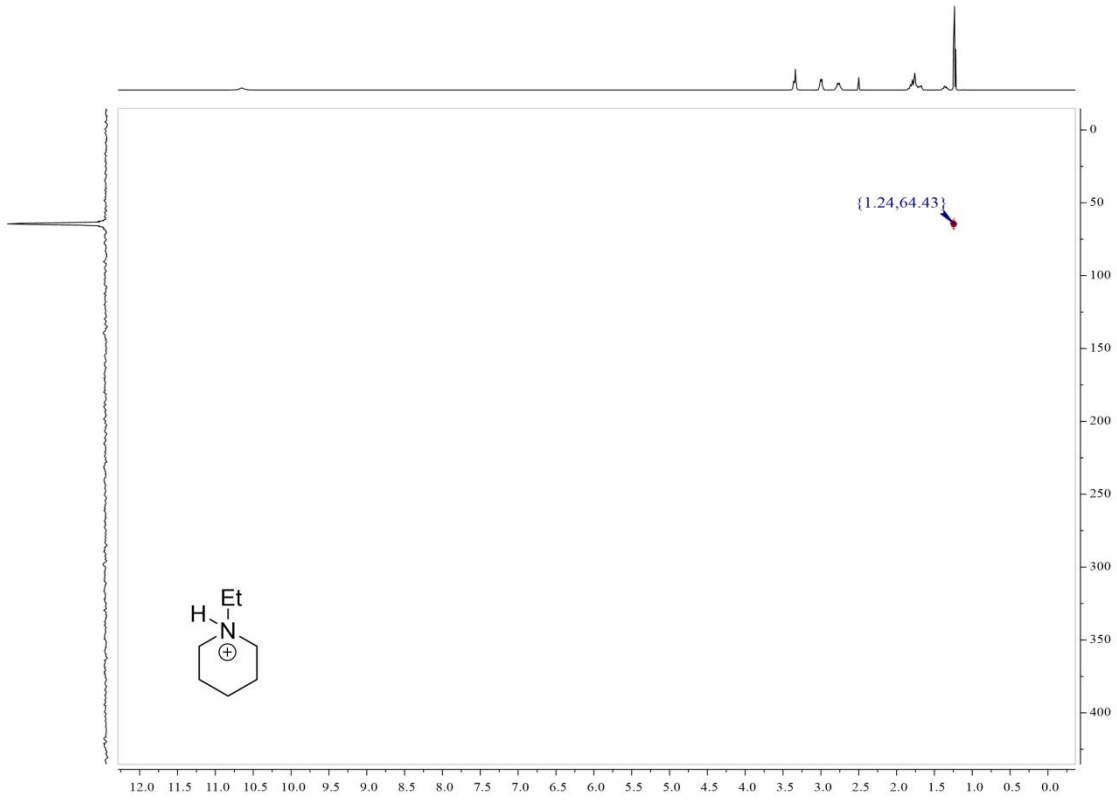


Figure S32. ^{1}H-^{15}N HMBC spectrum of *N*-Et piperidine HCl salt (**1'**) in d_6-DMSO

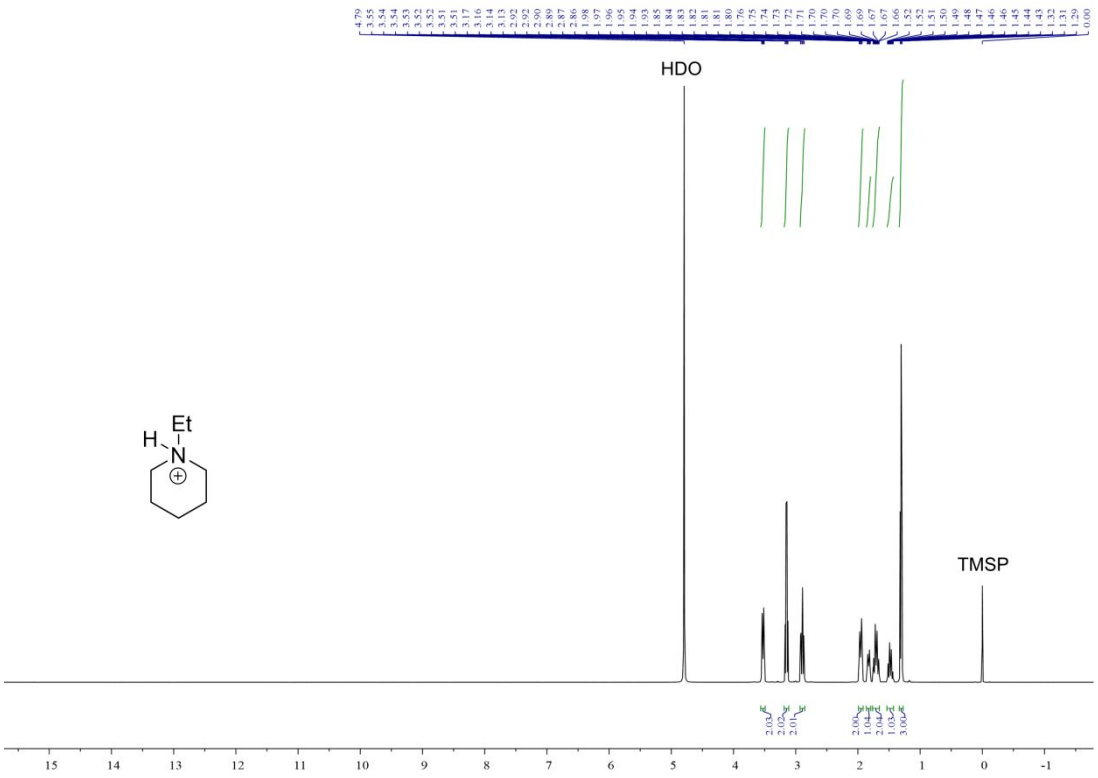


Figure S33. ^{1}H NMR spectrum of *N*-Et piperidine HCl salt (**1'**) in D_2O

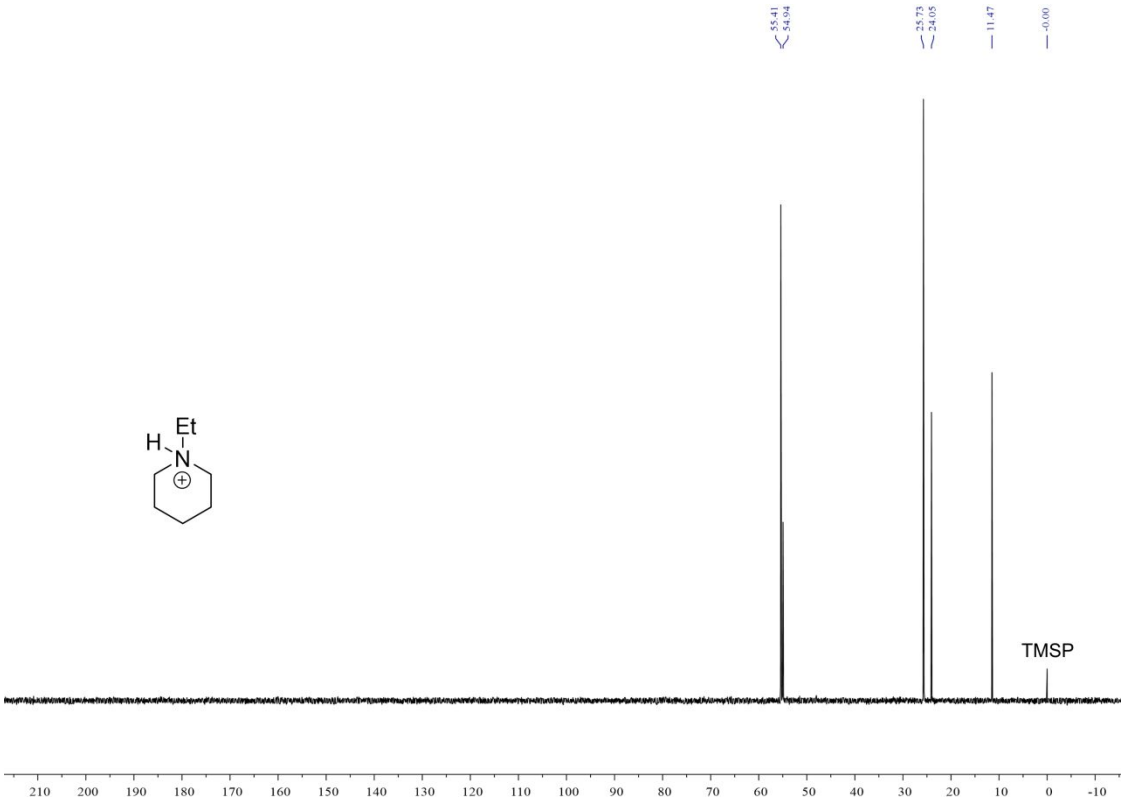


Figure S34. ^{13}C NMR spectrum of *N*-Et piperidine HCl salt (**1'**) in D_2O

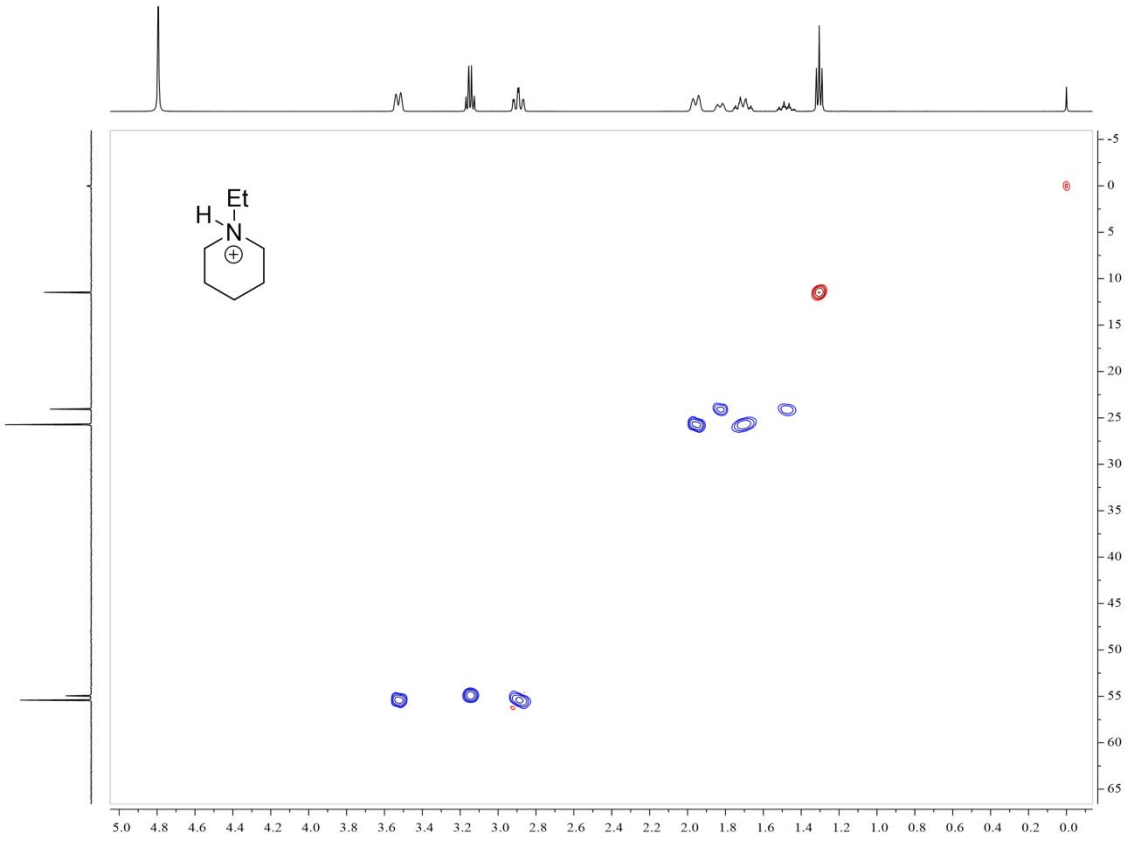


Figure S35. HSQC spectrum of *N*-Et piperidine HCl salt (**1'**) in D_2O

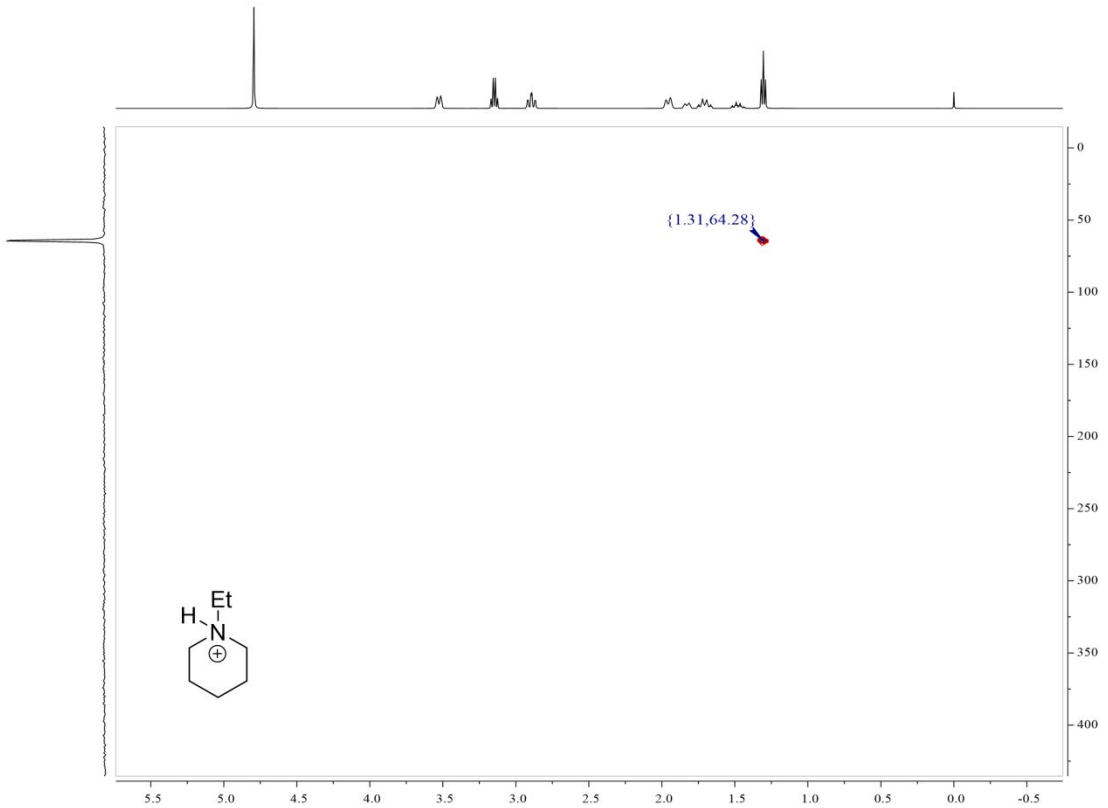


Figure S36. ^{1}H-^{15}N HMBC spectrum of *N*-Et piperidine HCl salt (**1'**) in D_2O

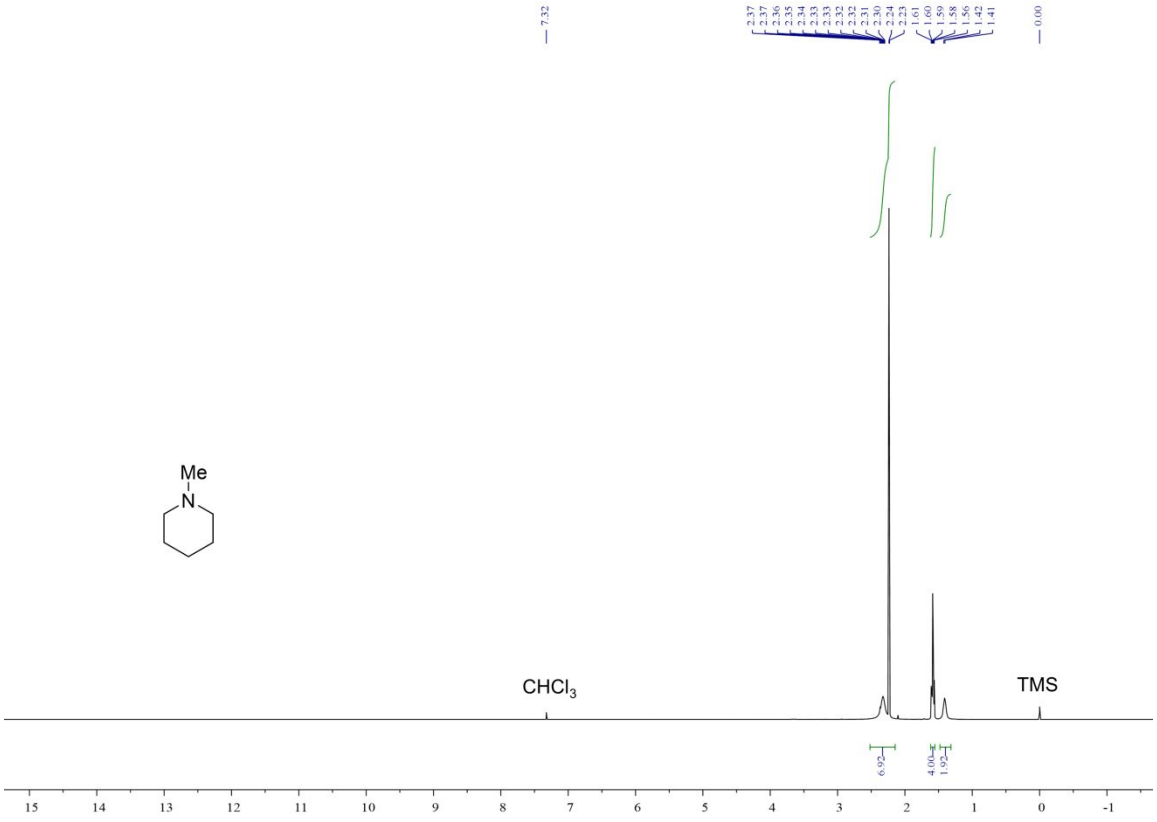


Figure S37. ^{1}H NMR spectrum of *N*-Me piperidine (**2**) in $CDCl_3$

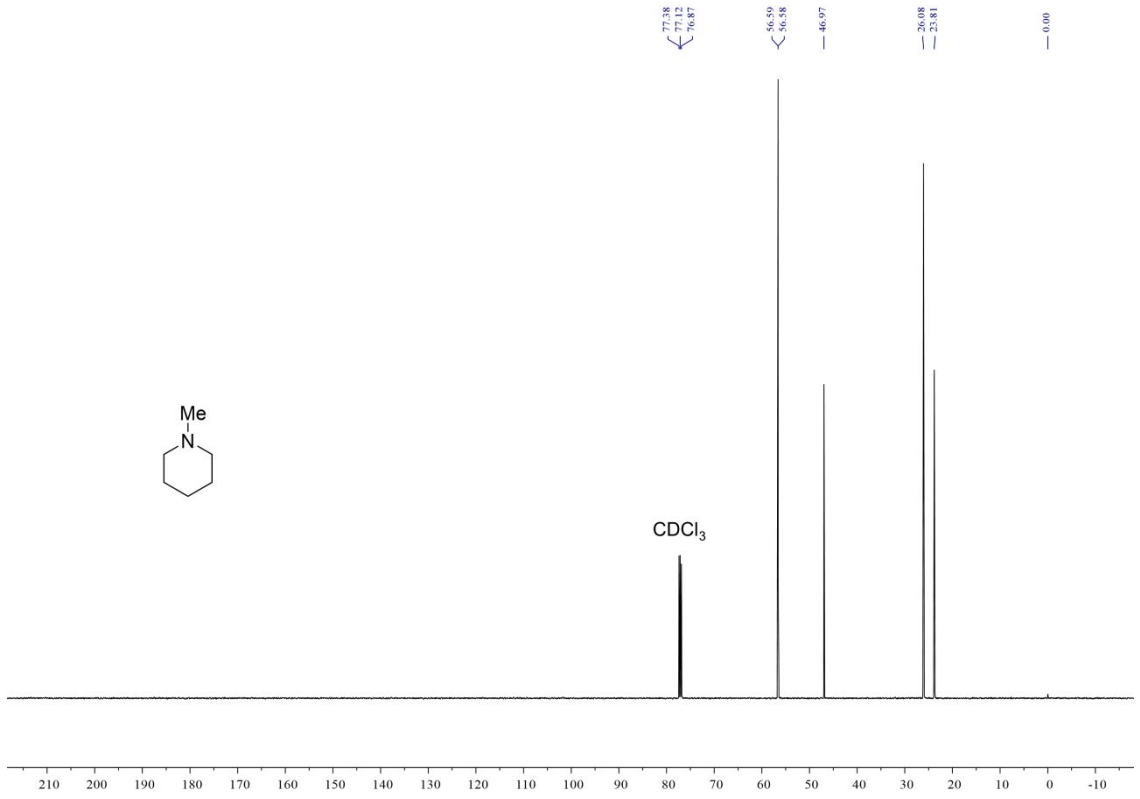


Figure S38. ^{13}C NMR spectrum of *N*-Me piperidine (**2**) in $CDCl_3$

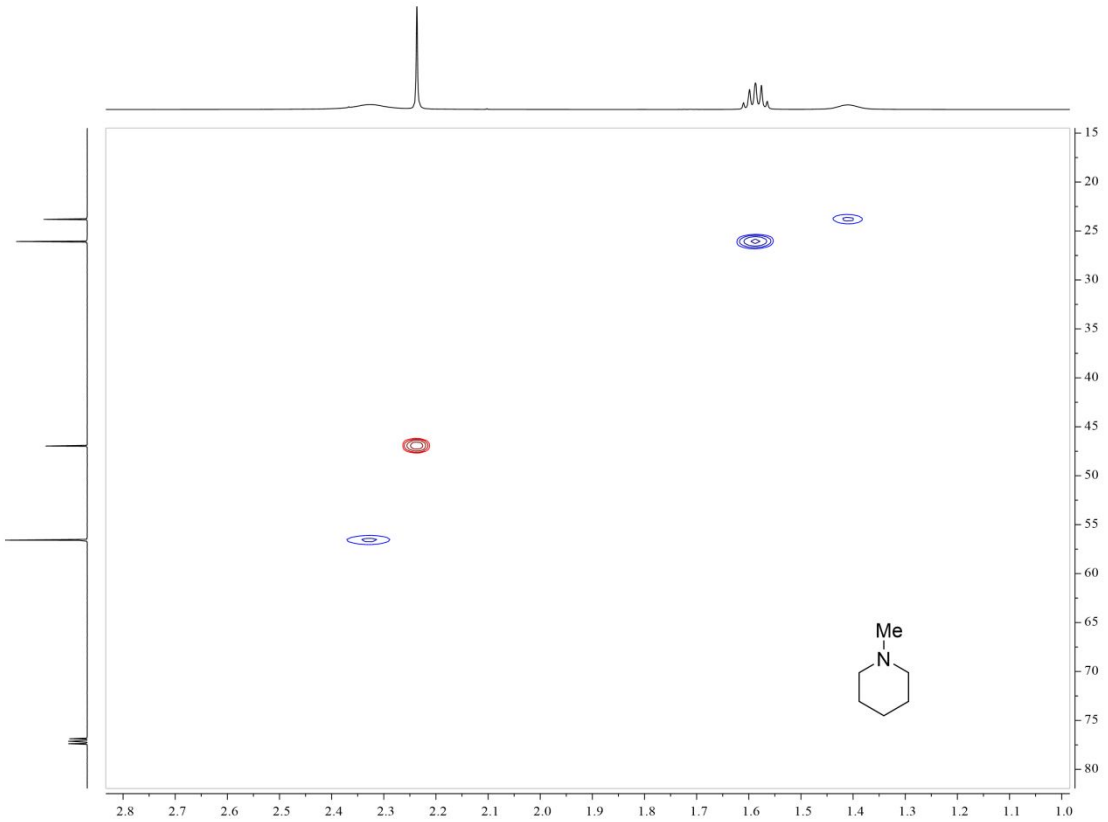


Figure S39. HSQC spectrum of *N*-Me piperidine (**2**) in $CDCl_3$

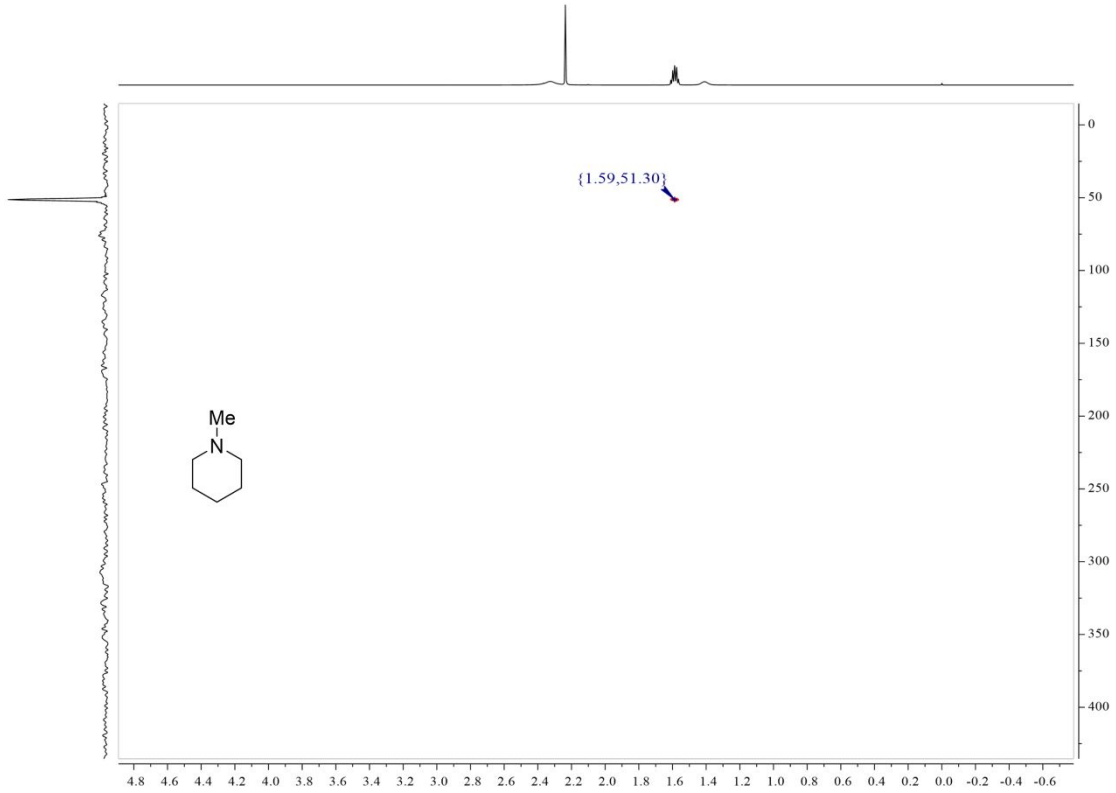


Figure S40. ^{1}H-^{15}N HMBC spectrum of *N*-Me piperidine (**2**) in $CDCl_3$

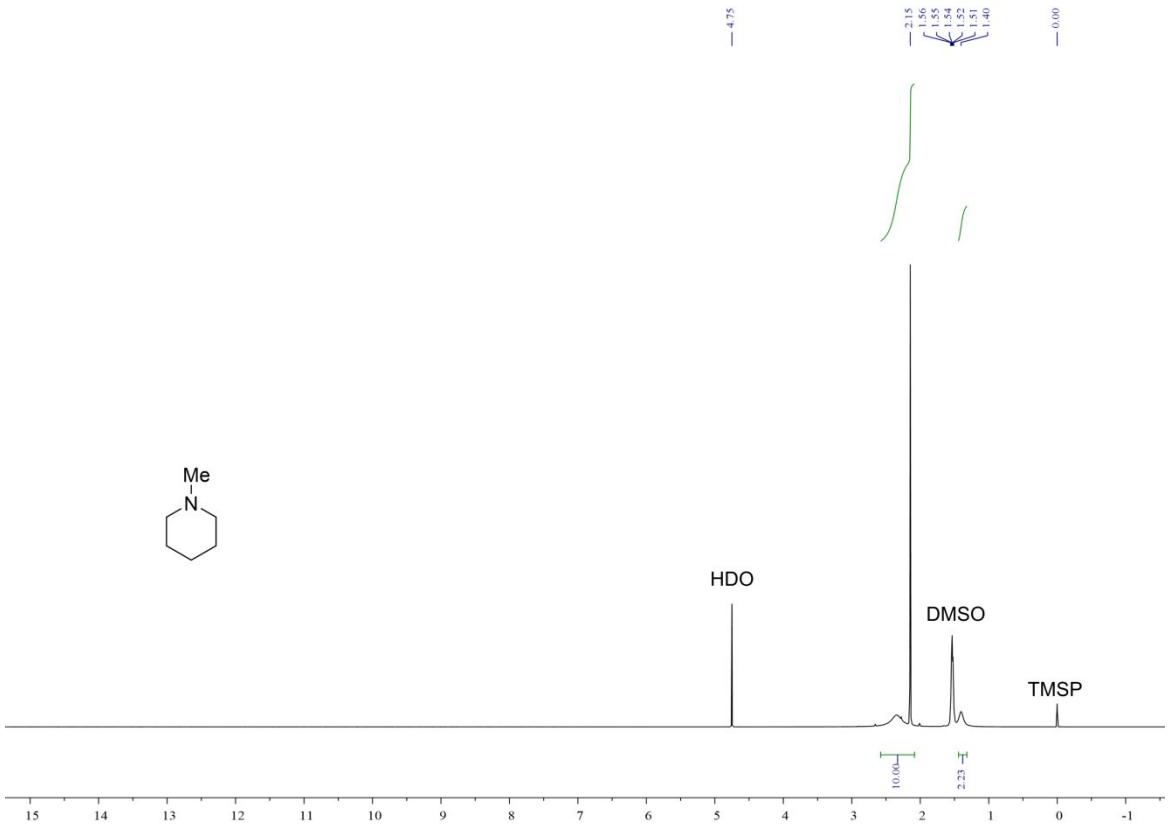


Figure S41. ^{1}H NMR spectrum of *N*-Me piperidine (**2**) in D_2O (with additional 2 drops of d_6-DMSO)

Figure S42. ^{13}C NMR spectrum of *N*-Me piperidine (**2**) in D_2O (with additional 2 drops of d_6-DMSO)

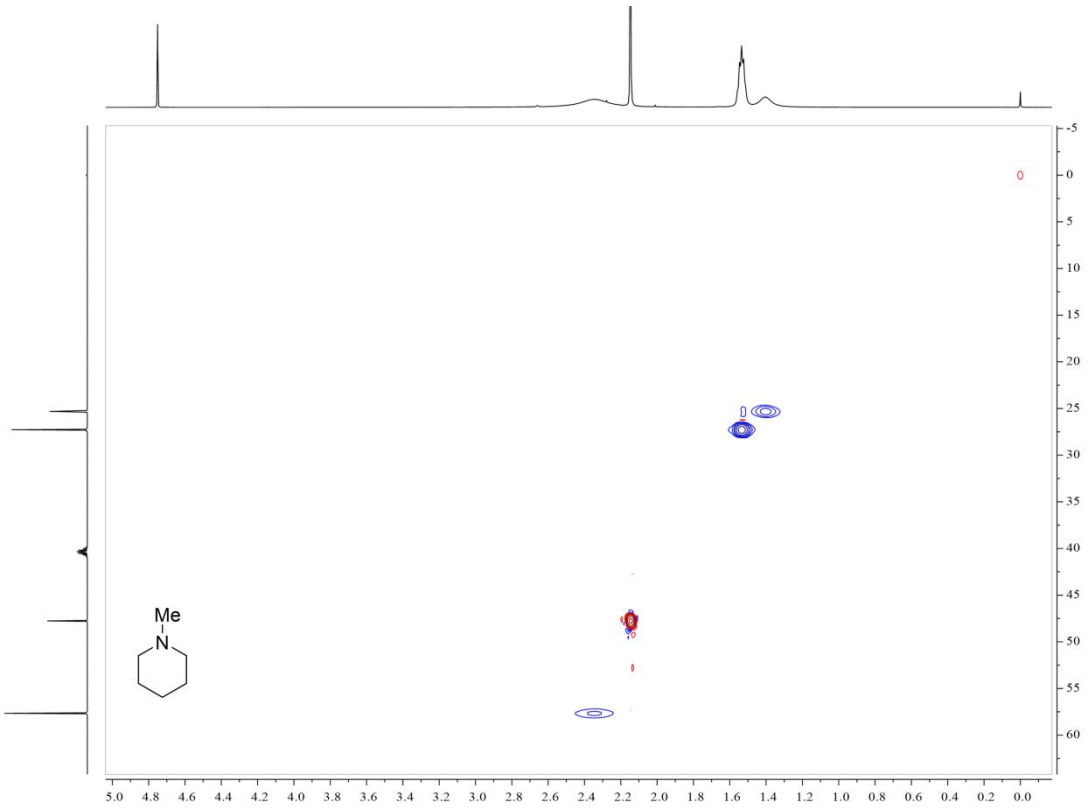


Figure S43. HSQC spectrum of *N*-Me piperidine (**2**) in D_2O (with additional 2 drops of d_6-DMSO)

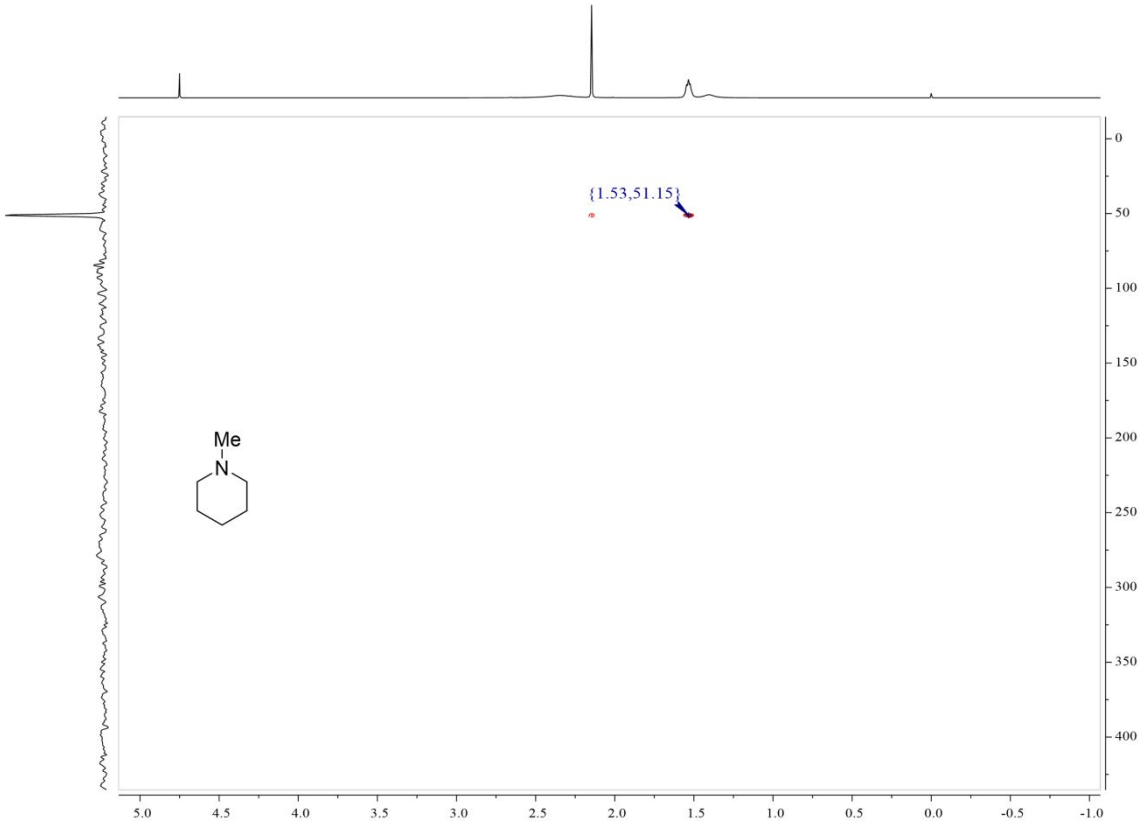


Figure S44. ^{1}H-^{15}N HMBC spectrum of *N*-Me piperidine (**2**) in D_2O (with additional 2 drops of d_6-DMSO)

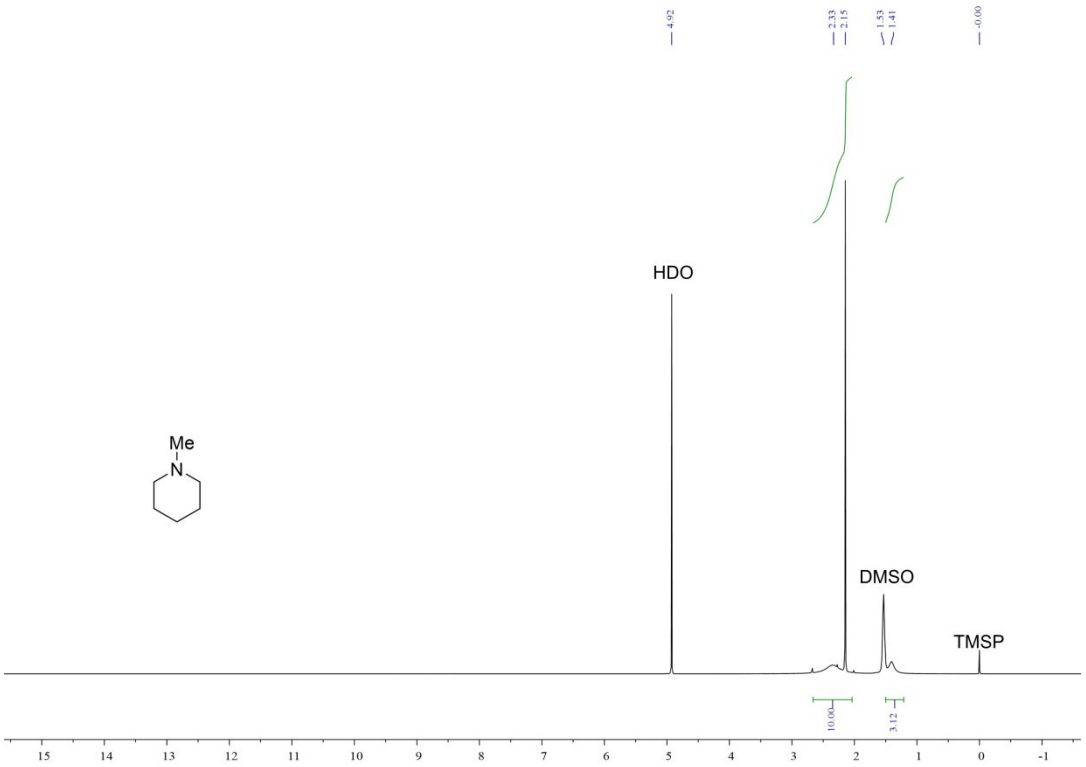


Figure S45. ^{1}H NMR spectrum of *N*-Me piperidine (**2**) in D_2O (with additional 2 drops of d_6-DMSO and drops of NaOD solution, 30% in D_2O, w/w, pD ~13)

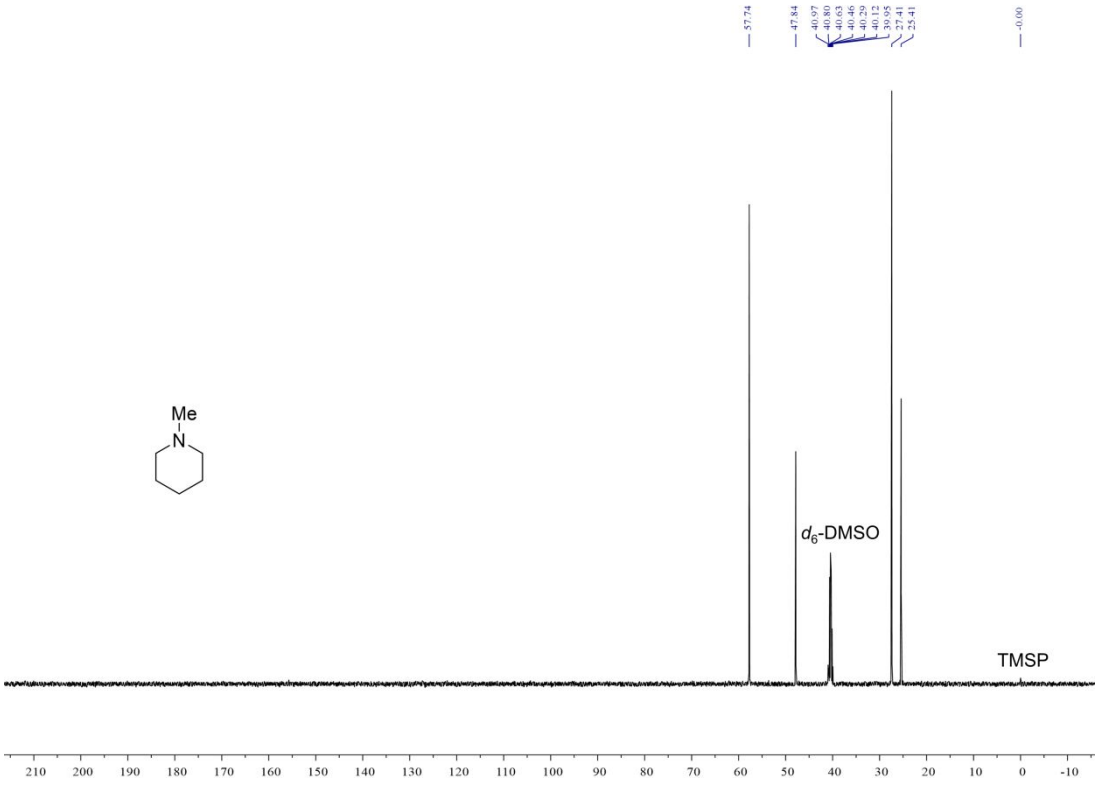


Figure S46. ^{13}C NMR spectrum of *N*-Me piperidine (**2**) in D_2O (with additional 2 drops of d_6-DMSO and drops of NaOD solution, 30% in D_2O, w/w, pD ~13)

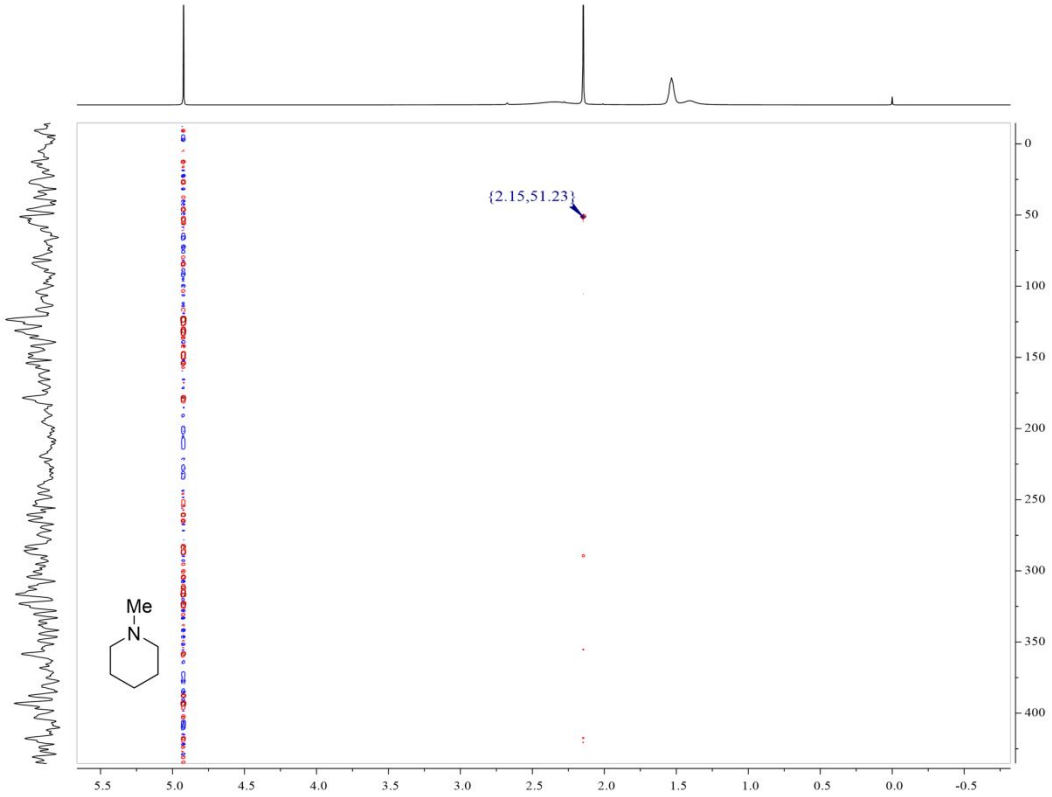


Figure S47. ^{1}H-^{15}N HMBC spectrum of *N*-Me piperidine (**2**) in D_2O (with additional 2 drops of d_6-DMSO and drops of NaOD solution, 30% in D_2O, w/w, pD ~13)

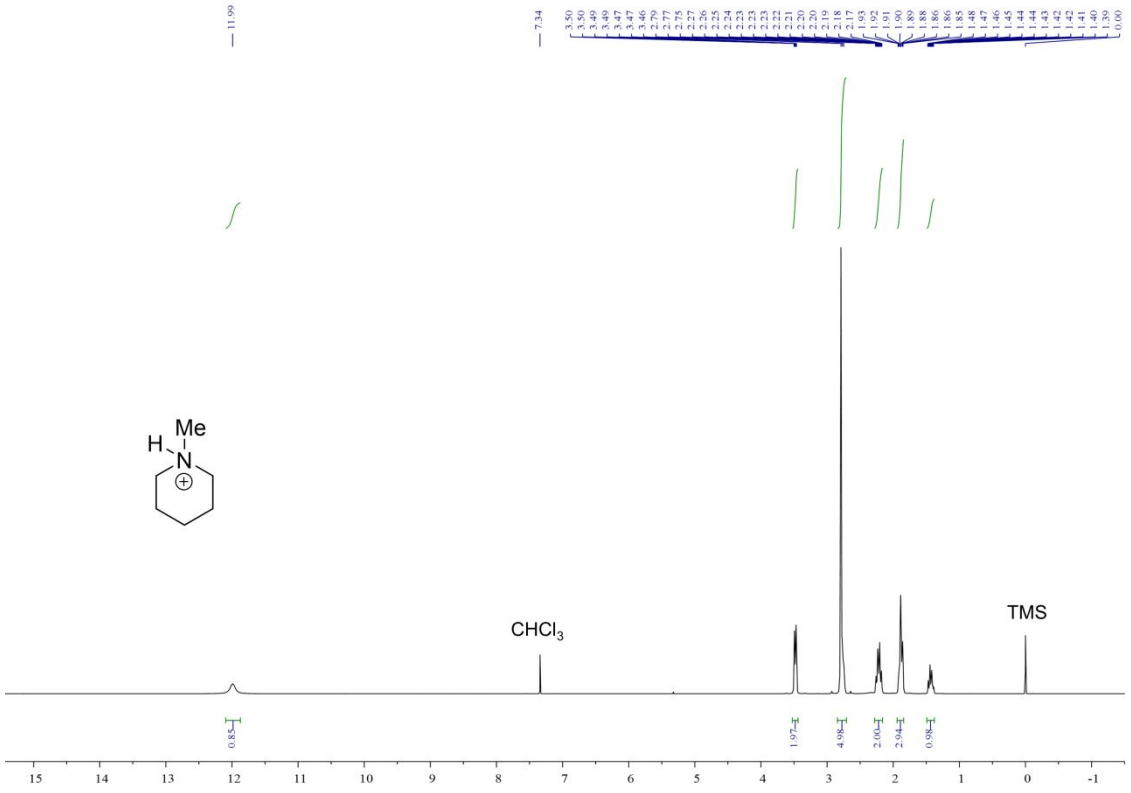


Figure S48. ^{1}H NMR spectrum of *N*-Me piperidine HCl salt (**2'**) in $CDCl_3$

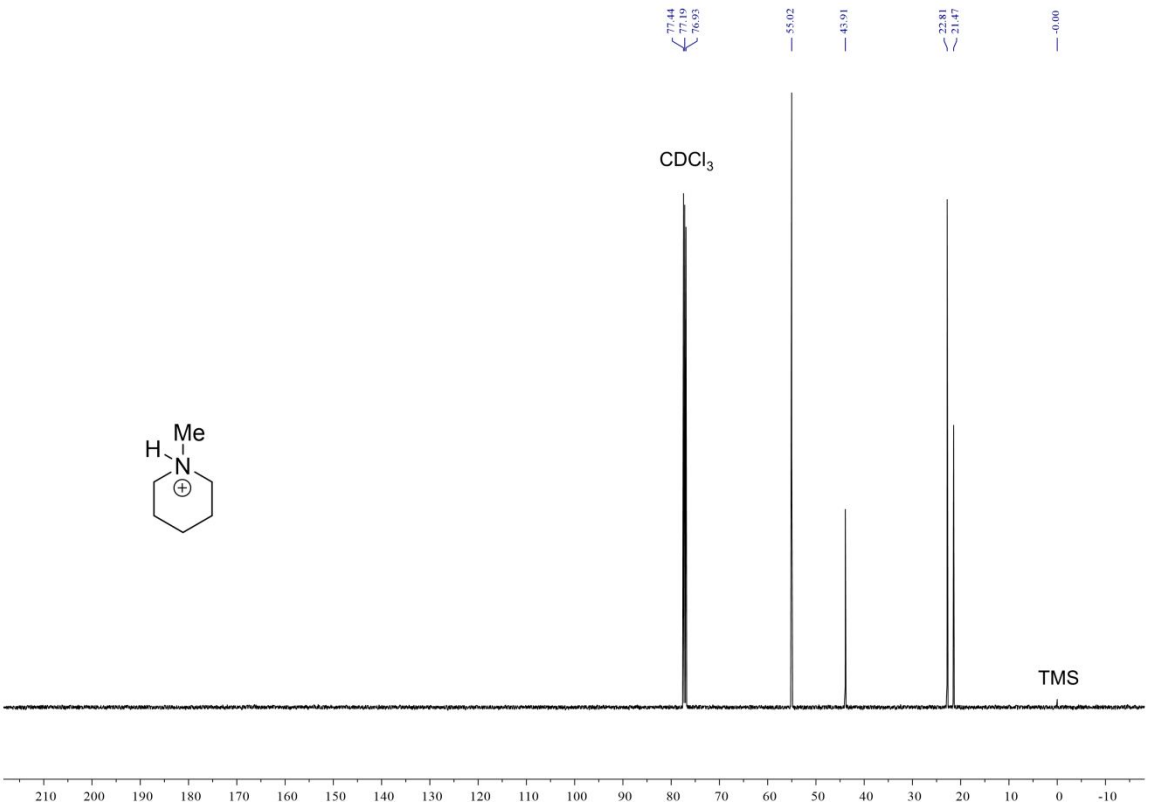


Figure S49. ^{13}C NMR spectrum of *N*-Me piperidine HCl salt (**2'**) in $CDCl_3$

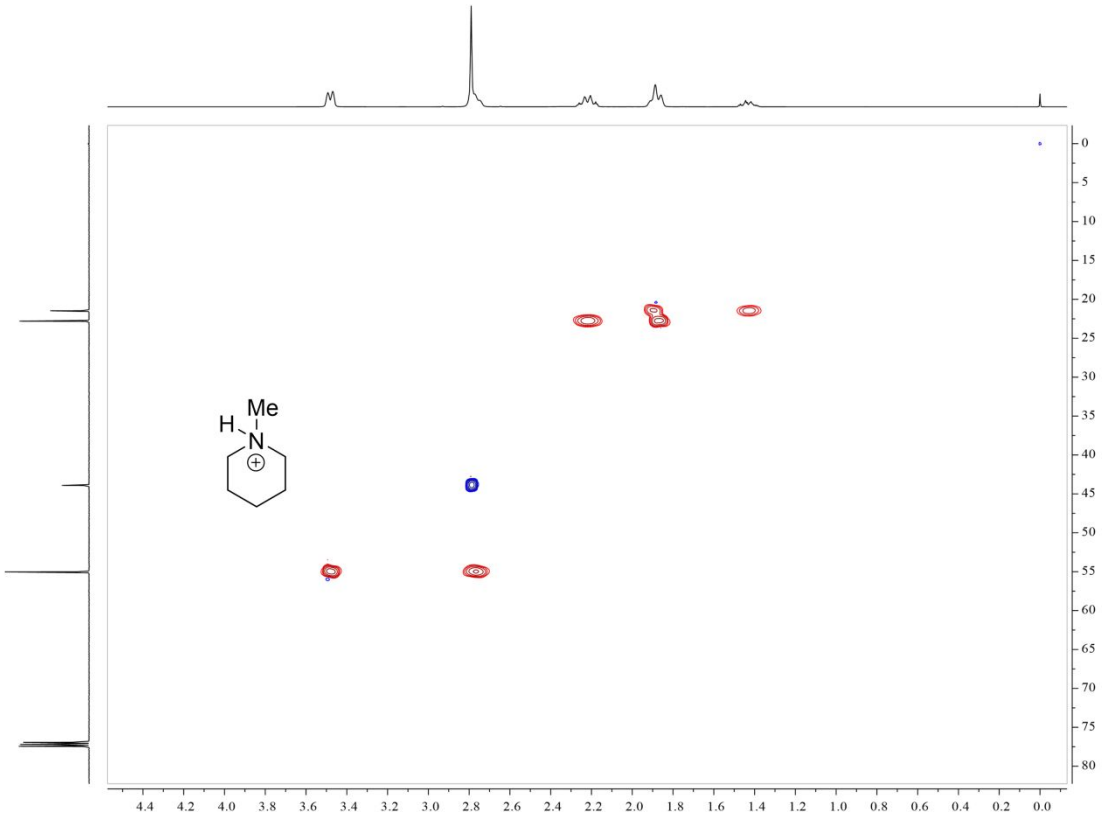


Figure S50. HSQC spectrum of *N*-Me piperidine HCl salt (**2'**) in $CDCl_3$

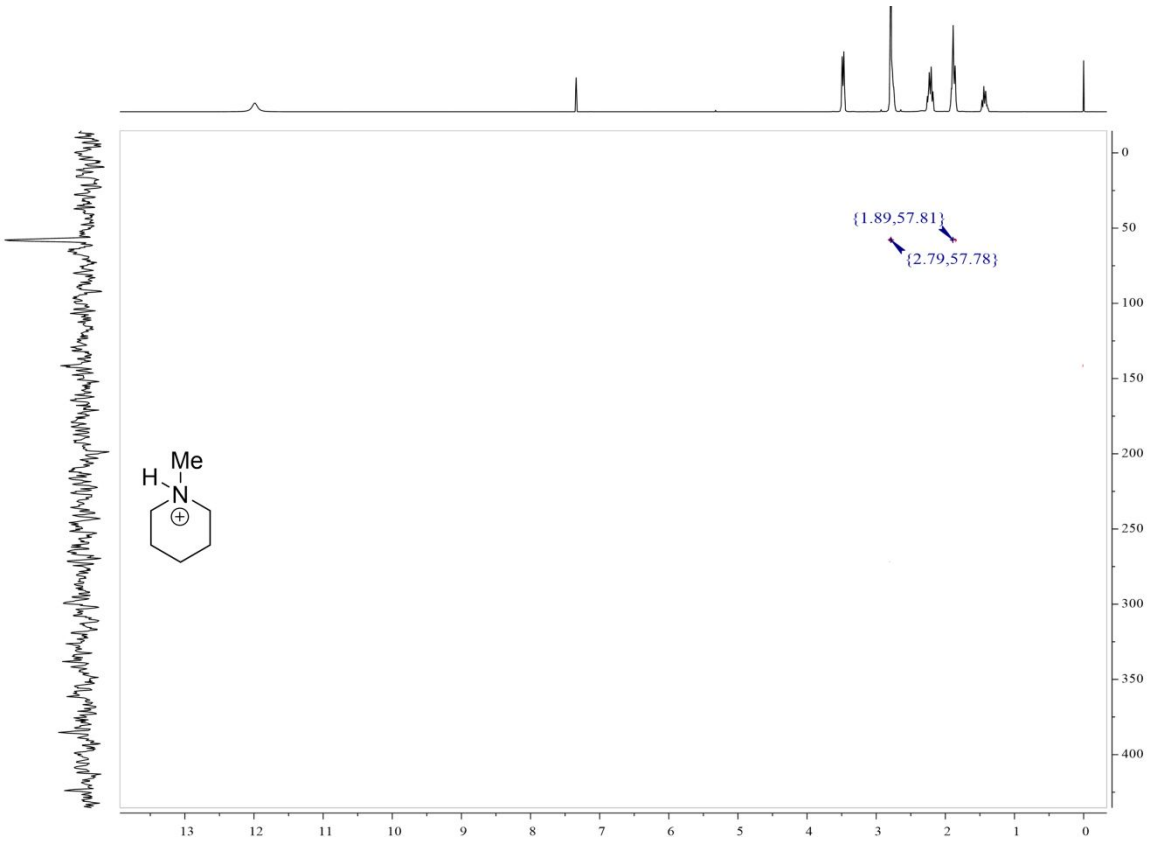


Figure S51. ^{1}H-^{15}N HMBC spectrum of *N*-Me piperidine HCl salt (**2'**) in $CDCl_3$

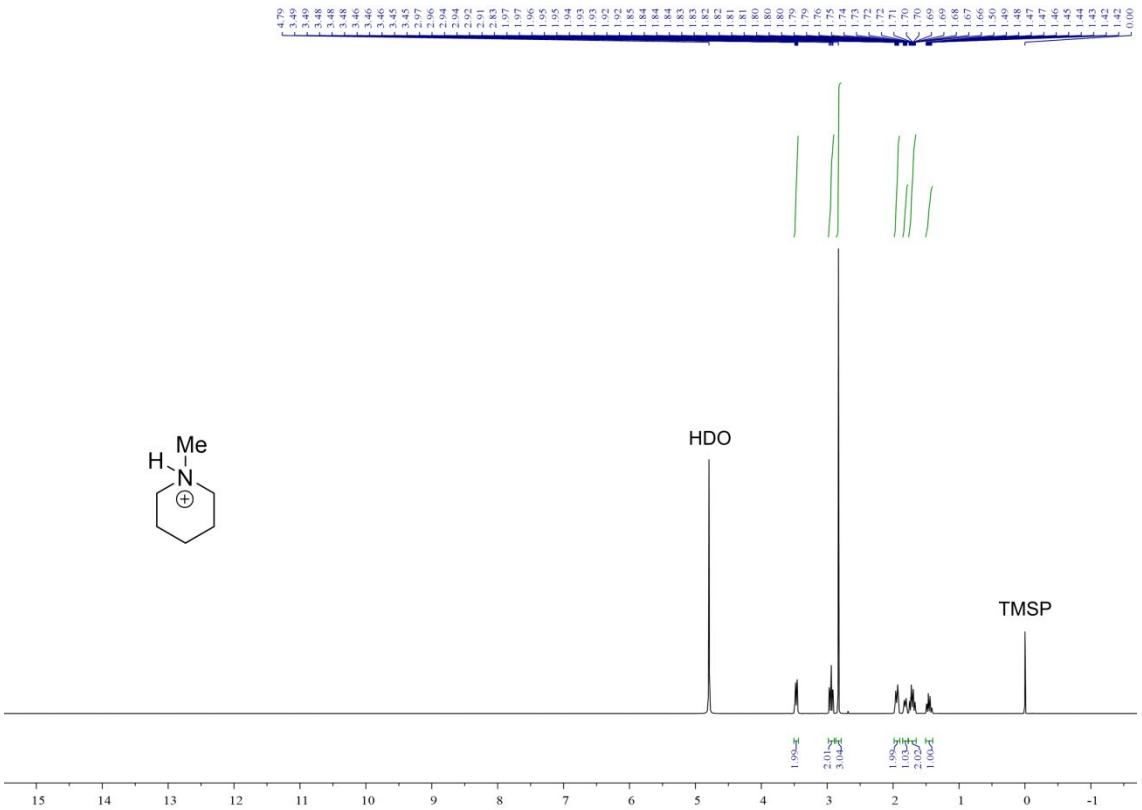


Figure S52. ^{1}H NMR spectrum of *N*-Me piperidine HCl salt (**2'**) in D_2O

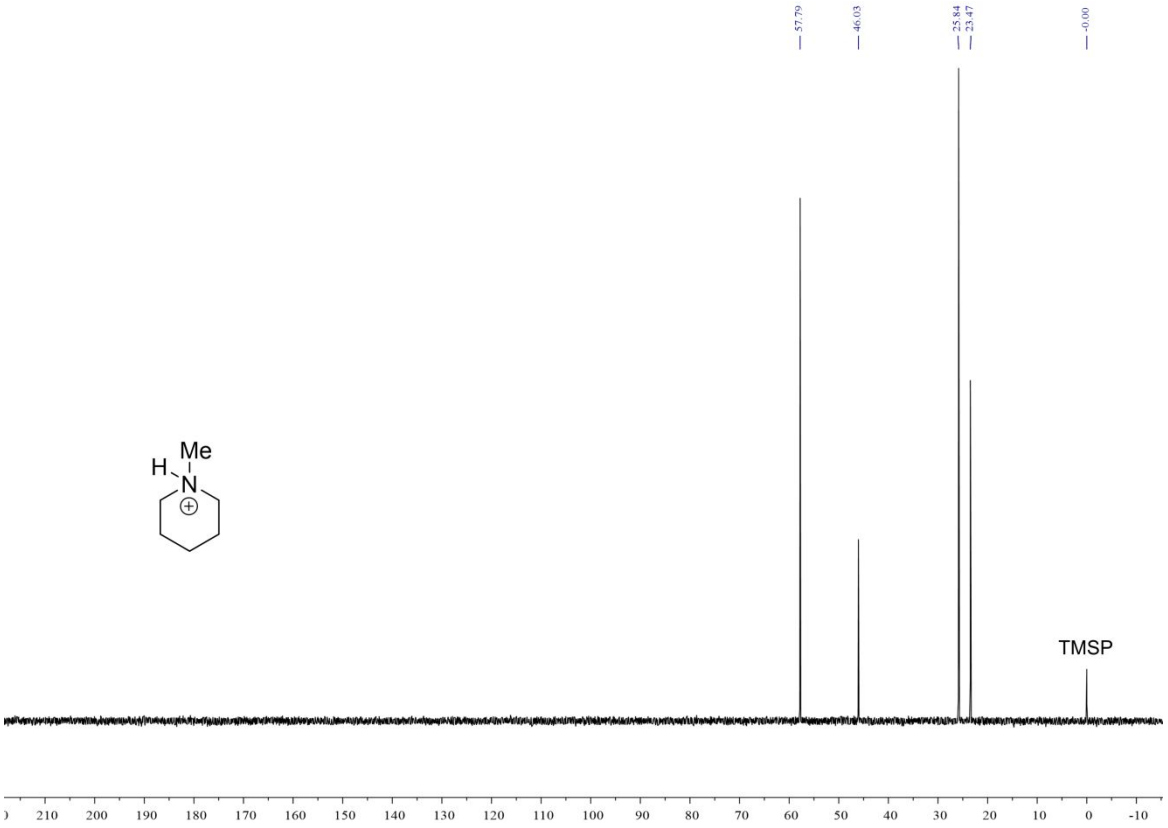


Figure S53. ^{13}C NMR spectrum of *N*-Me piperidine HCl salt (**2'**) in D_2O

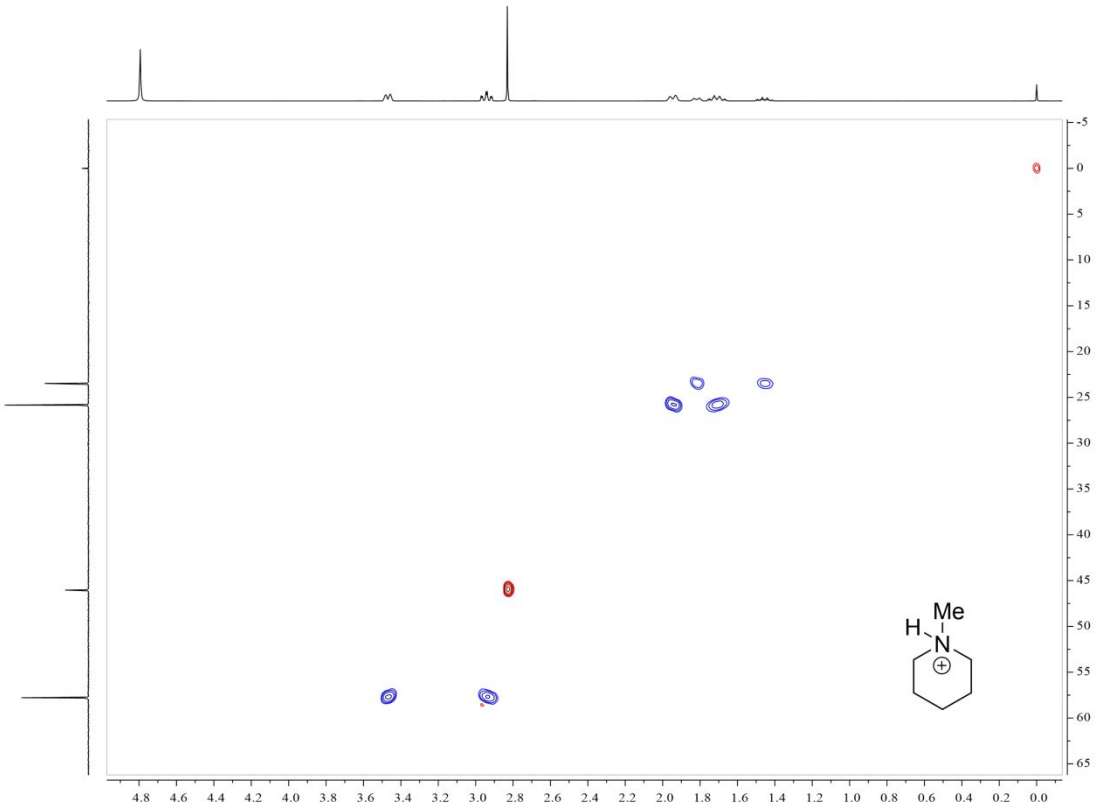


Figure S54. HSQC spectrum of *N*-Me piperidine HCl salt (**2'**) in D_2O

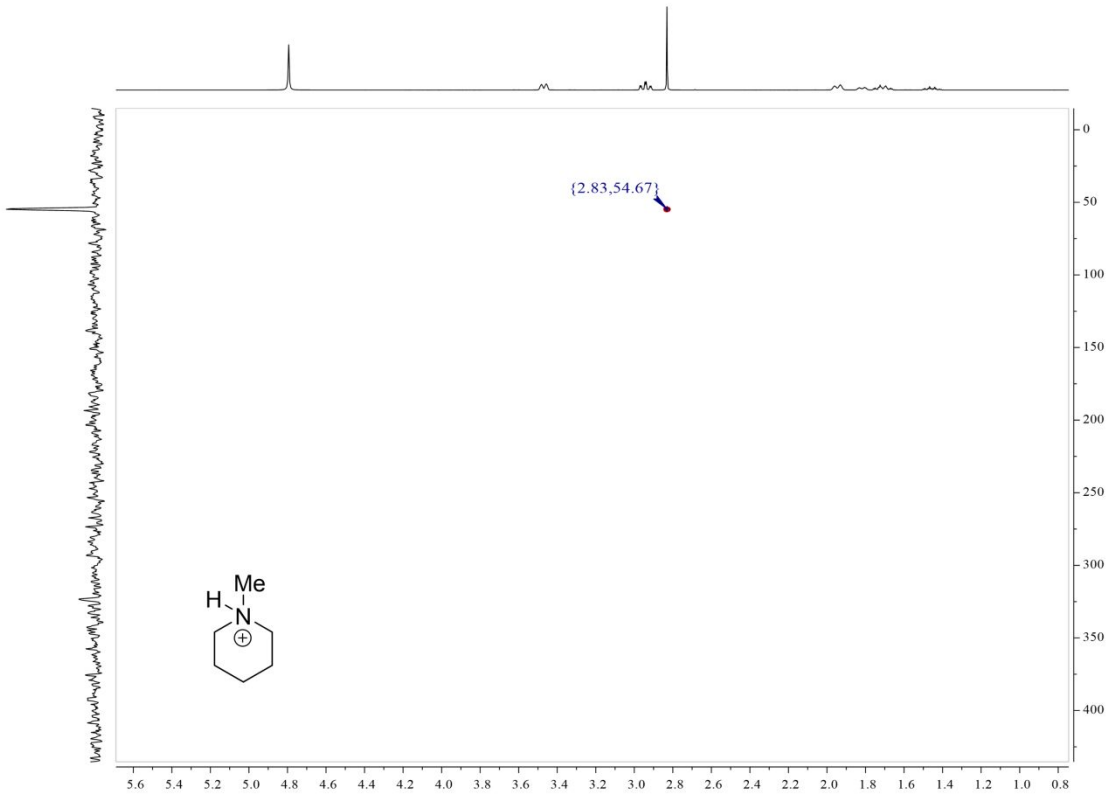


Figure S55. ^{1}H-^{15}N HMBC spectrum of *N*-Me piperidine HCl salt (**2'**) in D_2O

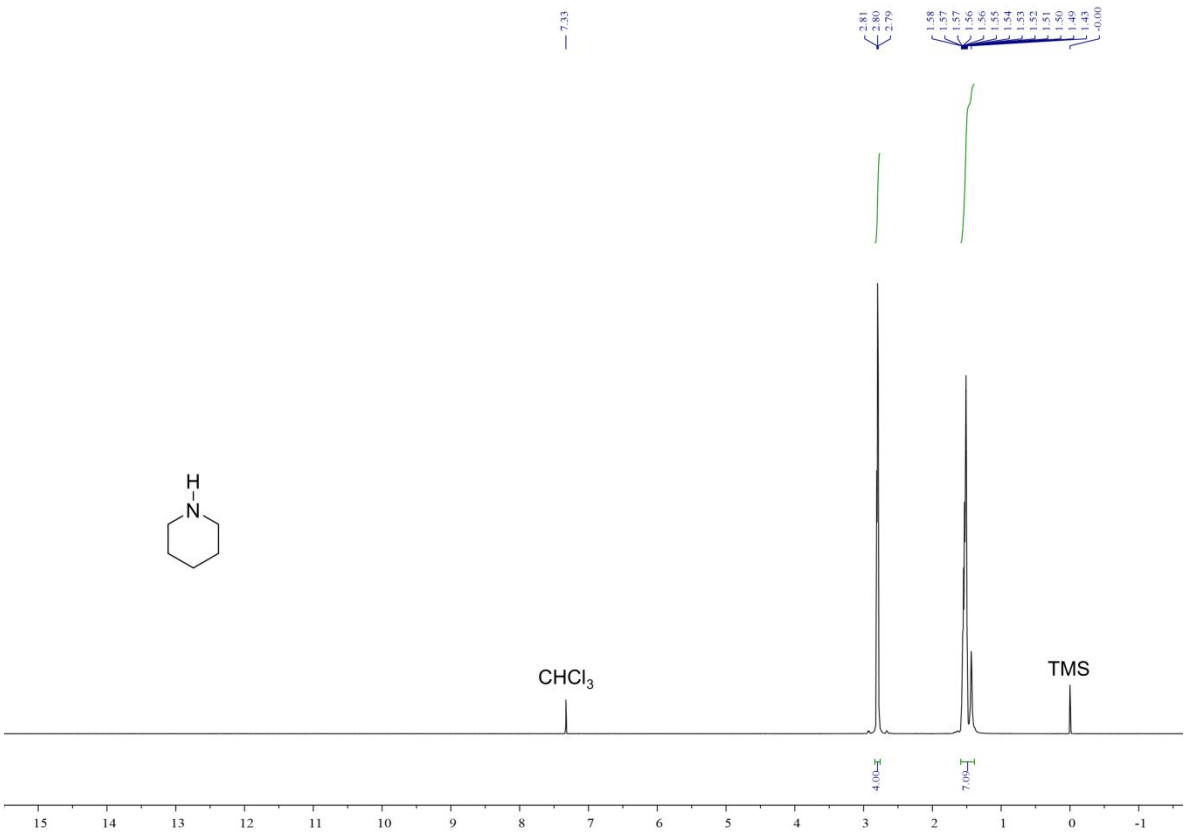


Figure S56. ^{1}H NMR spectrum of *N*-H piperidine (**3**) in $CDCl_3$

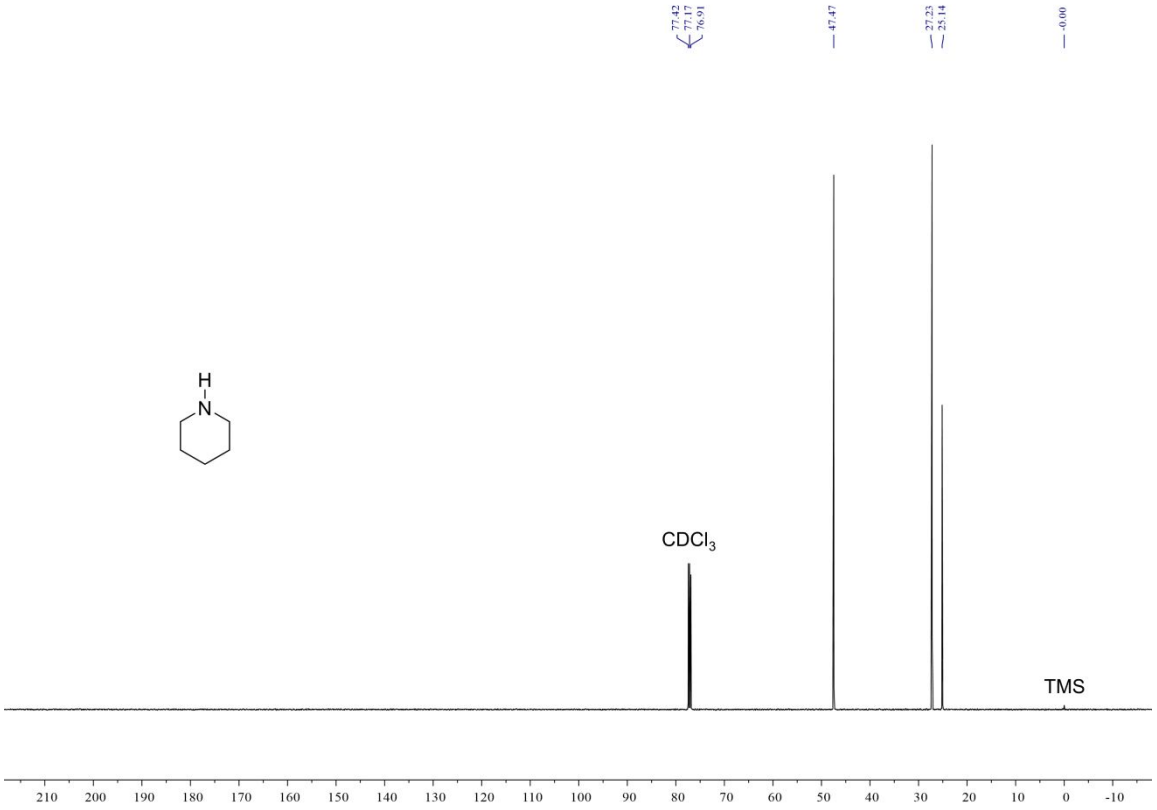


Figure S57. ^{13}C NMR spectrum of *N*-H piperidine (**3**) in $CDCl_3$

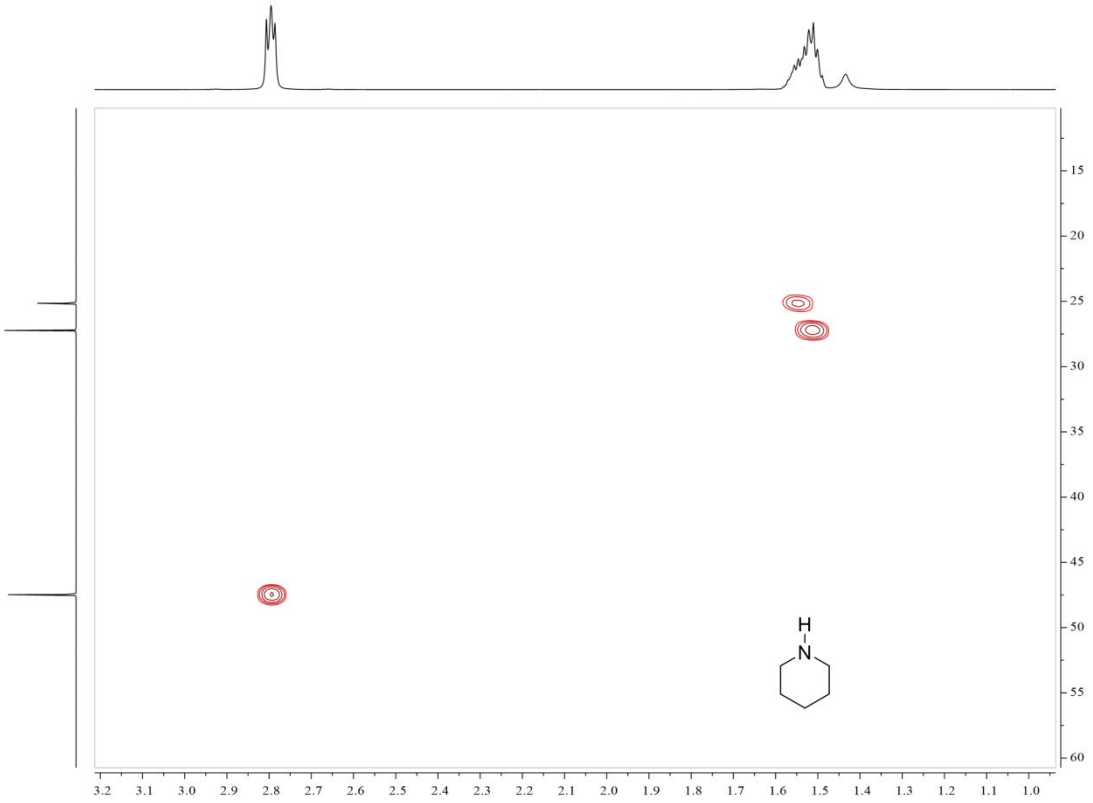


Figure S58. HSQC spectrum of *N*-H piperidine (**3**) in $CDCl_3$

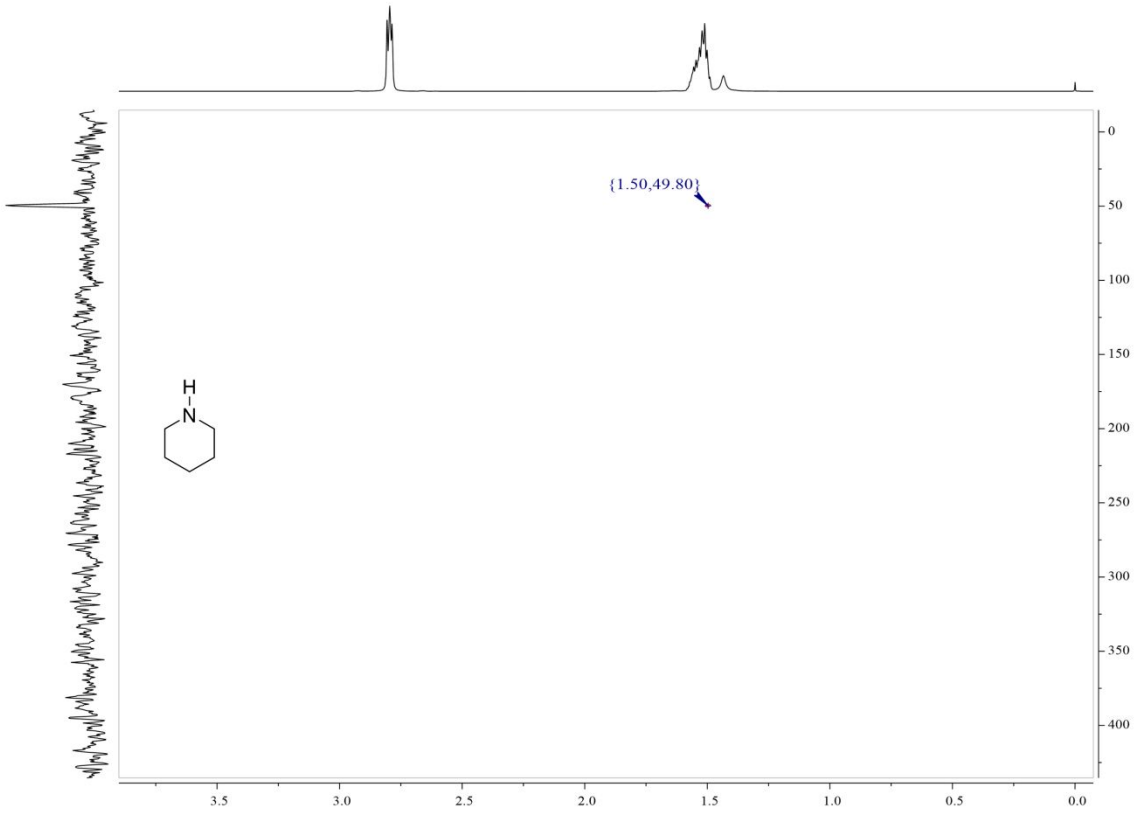


Figure S59. ^{1}H-^{15}N HMBC spectrum of *N*-H piperidine (**3**) in $CDCl_3$

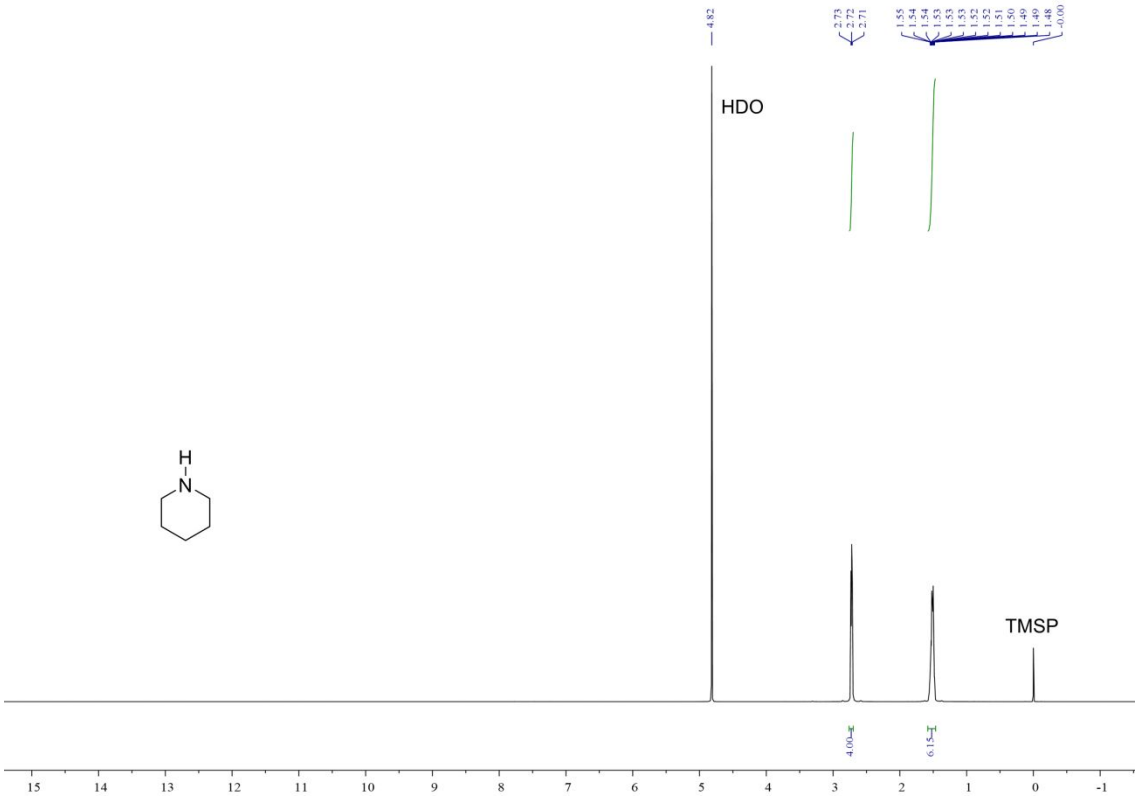


Figure S60. ^{1}H NMR spectrum of *N*-H piperidine (**3**) in D_2O

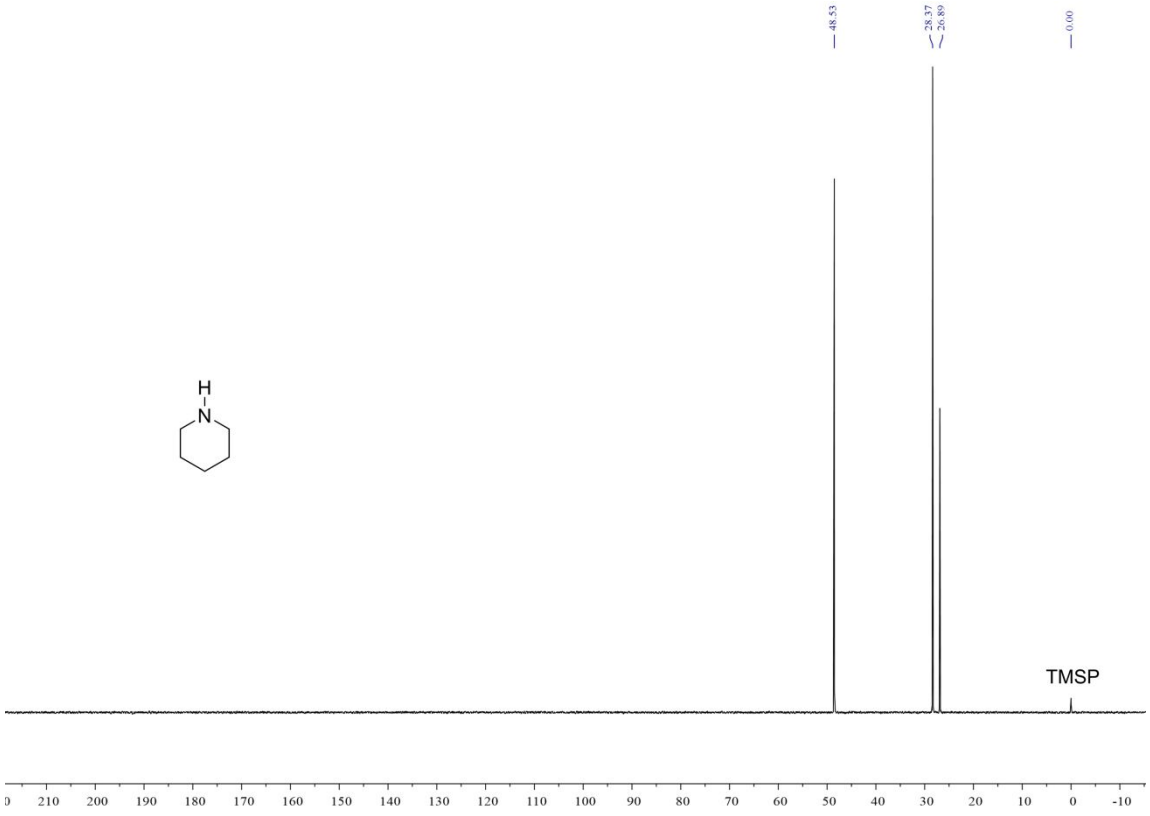


Figure S61. ^{13}C NMR spectrum of *N*-H piperidine (**3**) in D_2O

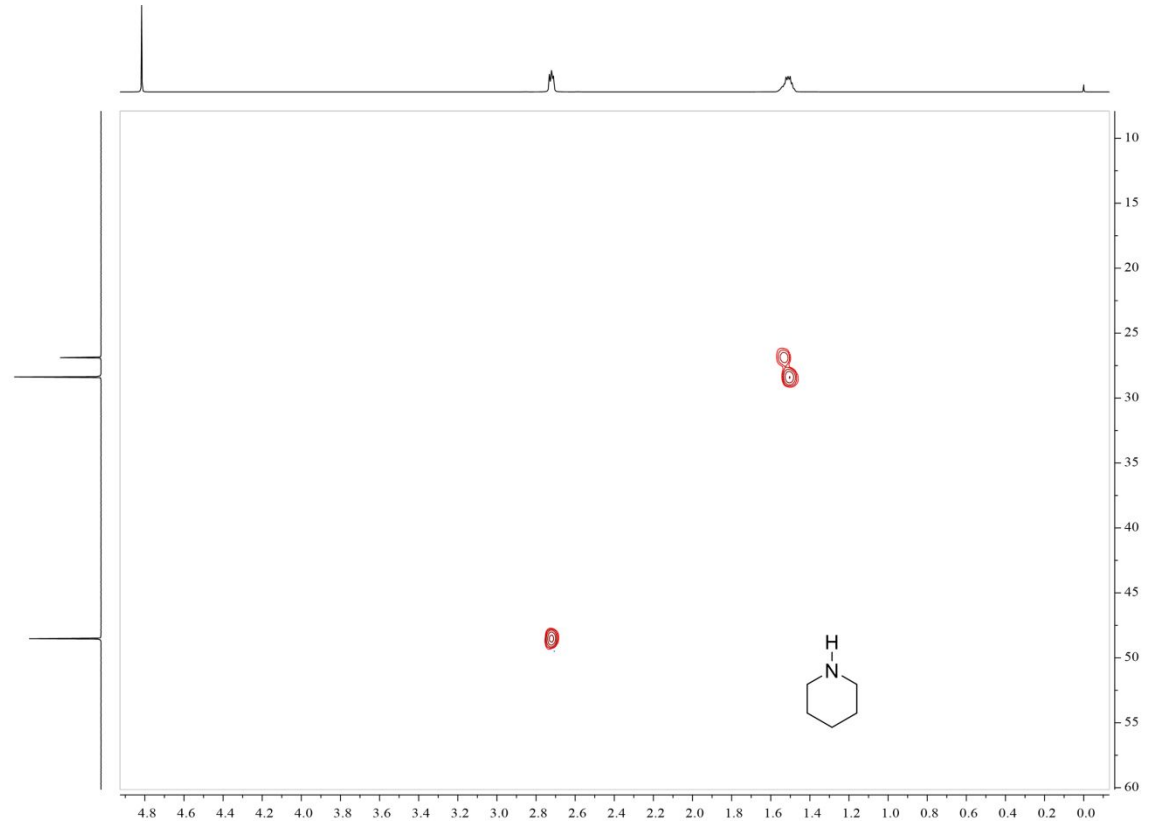


Figure S62. HSQC spectrum of *N*-H piperidine (**3**) in D_2O

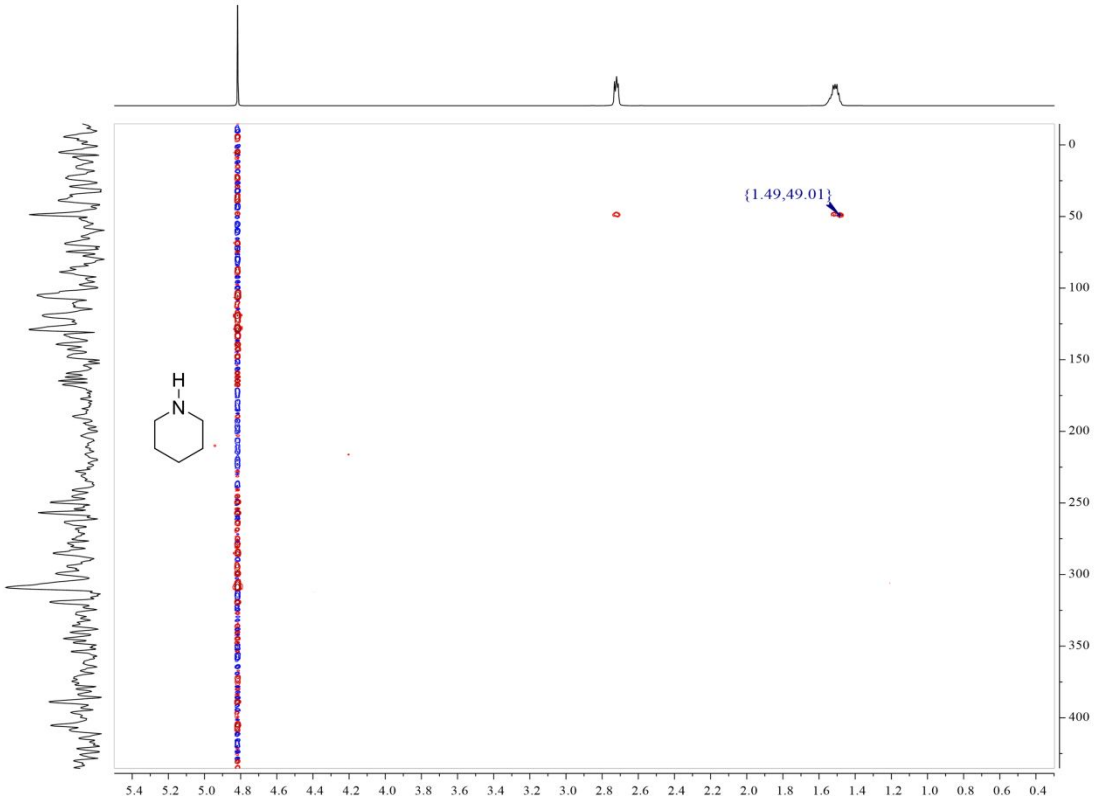


Figure S63. ^{1}H-^{15}N HMBC spectrum of *N*-H piperidine (**3**) in D_2O

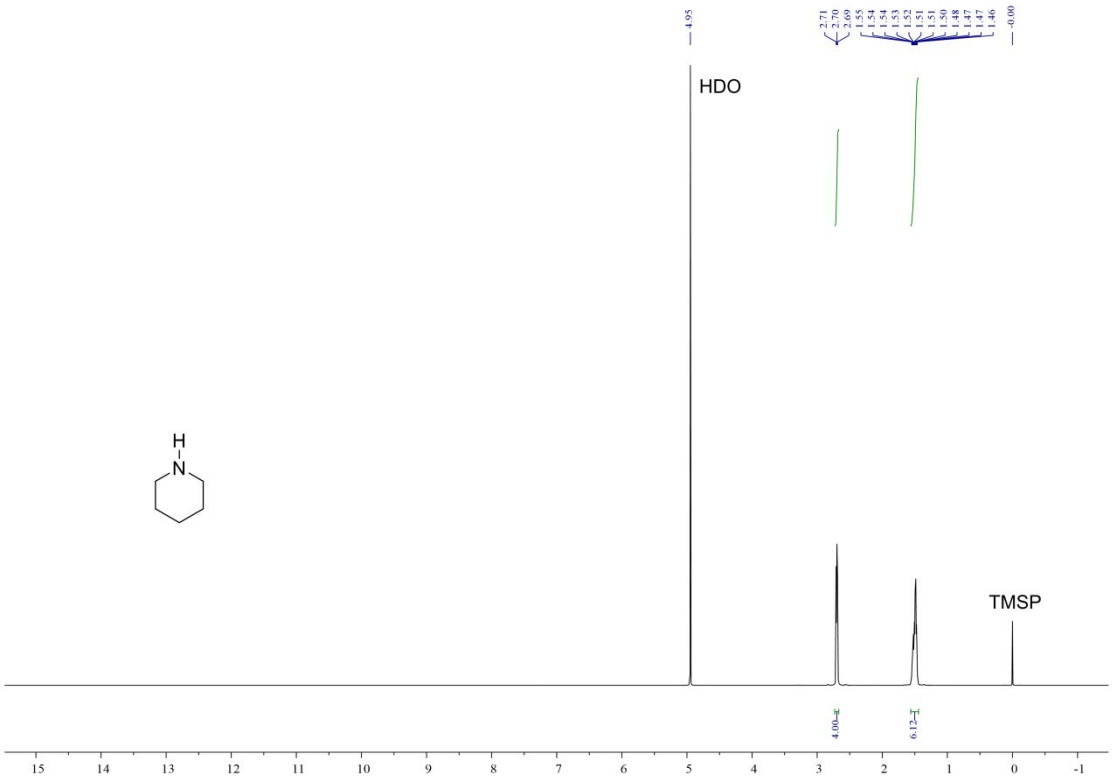


Figure S64. ^{1}H NMR spectrum of *N*-H piperidine (**3**) in D_2O (with additional drops of NaOD solution, 30% in D_2O, w/w, pD ~13)

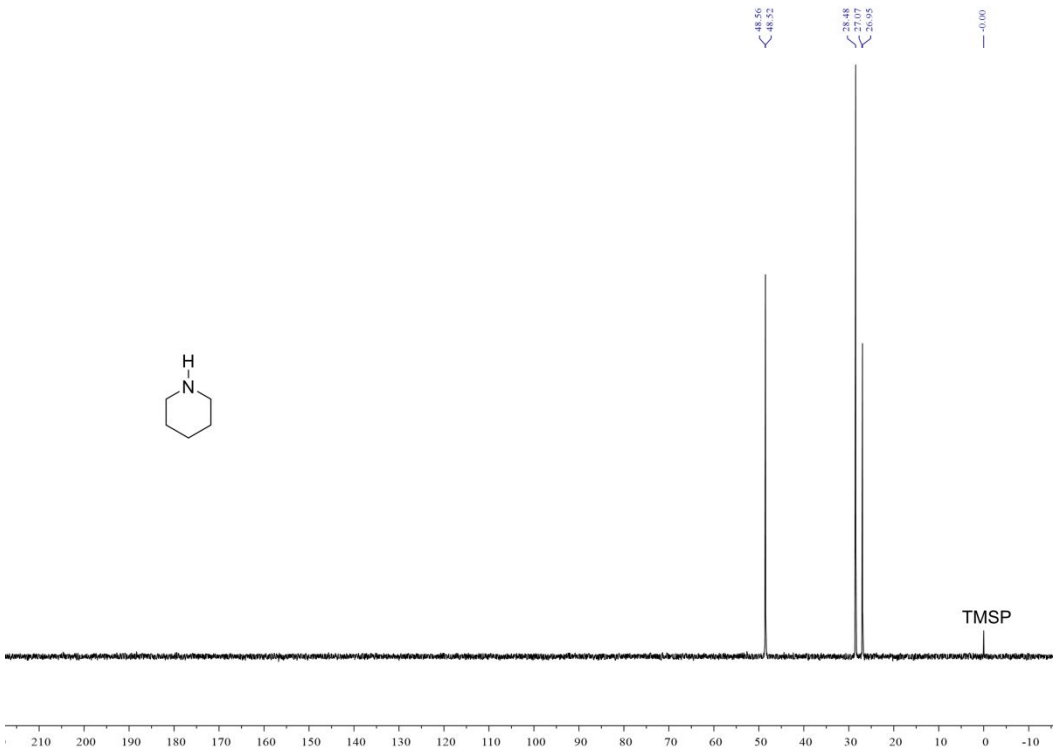


Figure S65. ^{13}C NMR spectrum of *N*-H piperidine (**3**) in D_2O (with additional drops of NaOD solution, 30% in D_2O, w/w, pD ~13)

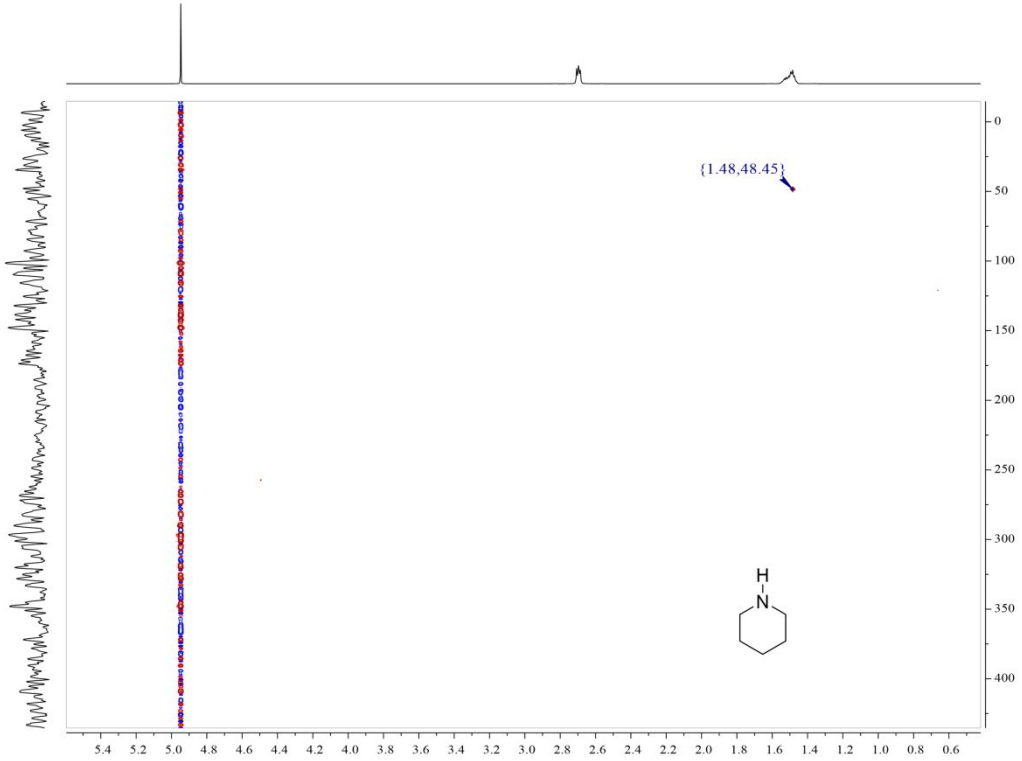


Figure S66. ^{1}H-^{15}N HMBC spectrum of *N*-H piperidine (**3**) in D_2O (with additional drops of NaOD solution, 30% in D_2O, w/w, pD ~13)

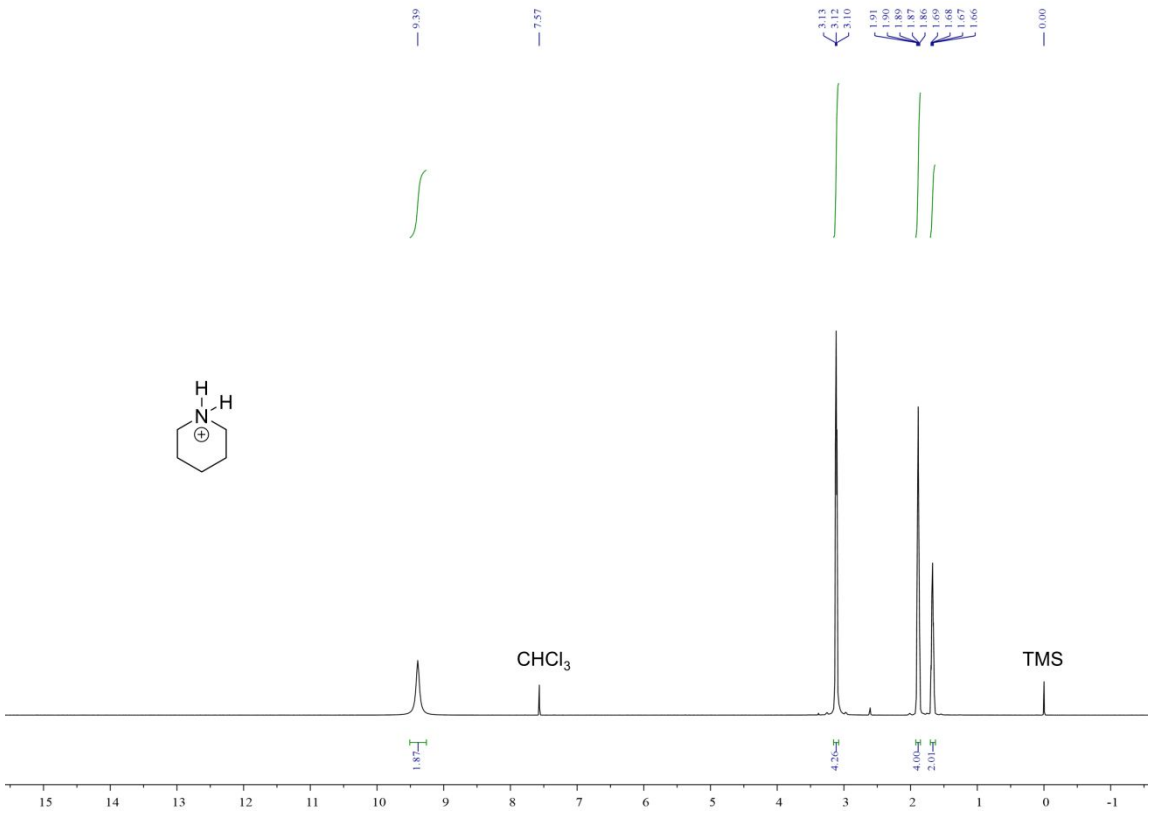


Figure S67. ^{1}H NMR spectrum of *N*-H piperidine HCl salt (**3'**) in $CDCl_3$ (with additional 2 drops of d_6-DMSO)

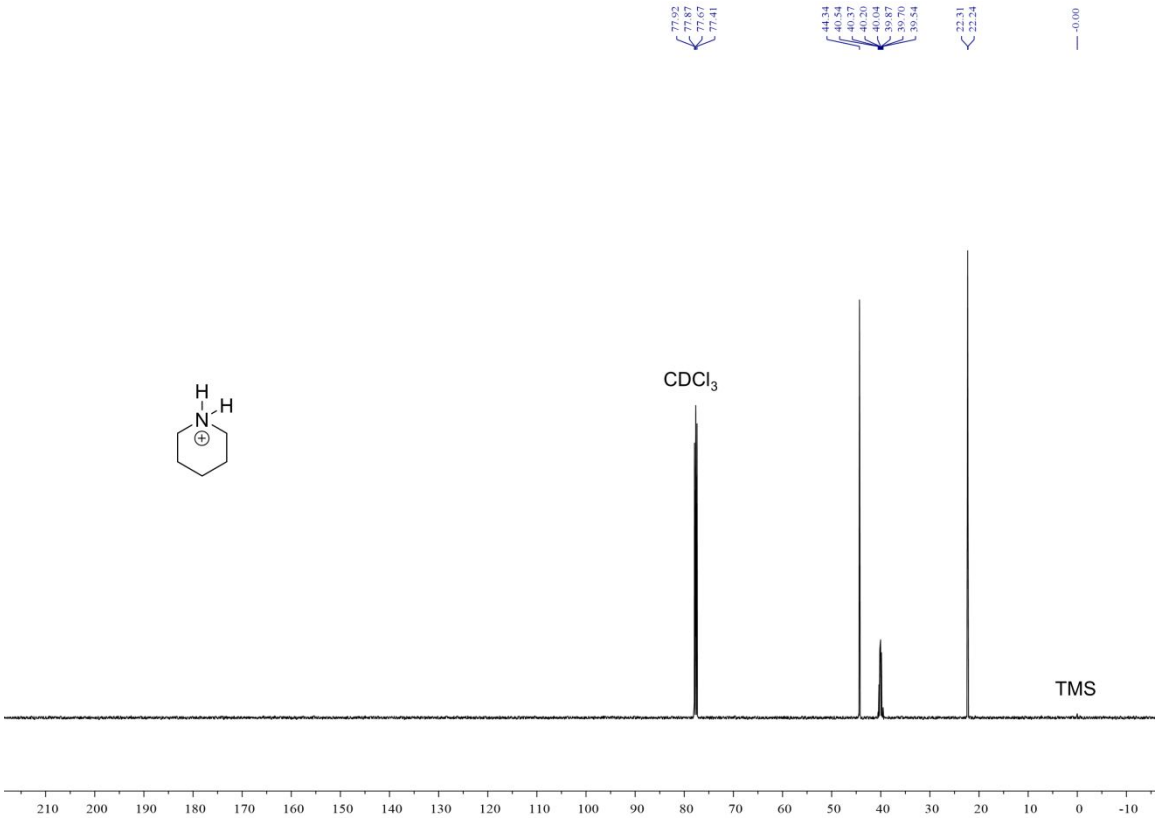


Figure S68. ^{13}C NMR spectrum of *N*-H piperidine HCl salt (**3'**) in $CDCl_3$ (with additional 2 drops of d_6-DMSO)

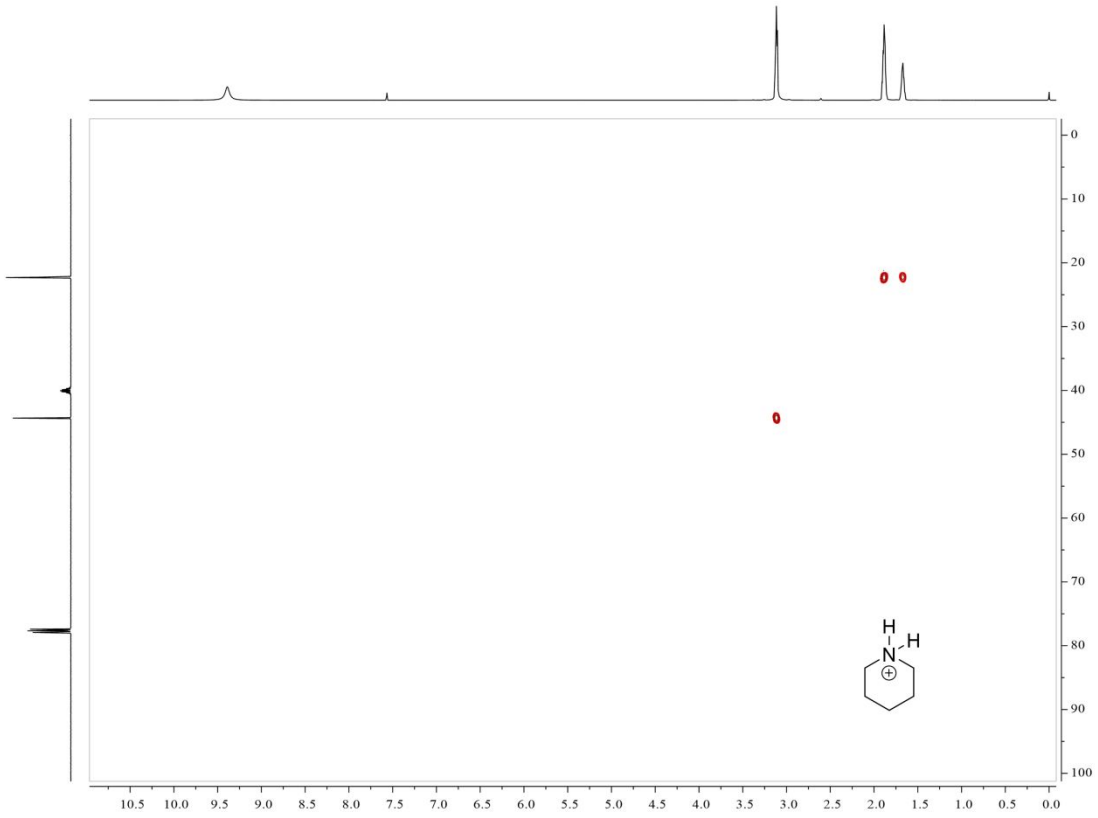


Figure S69. HSQC spectrum of *N*-H piperidine HCl salt (**3'**) in $CDCl_3$ (with additional 2 drops of d_6-DMSO)

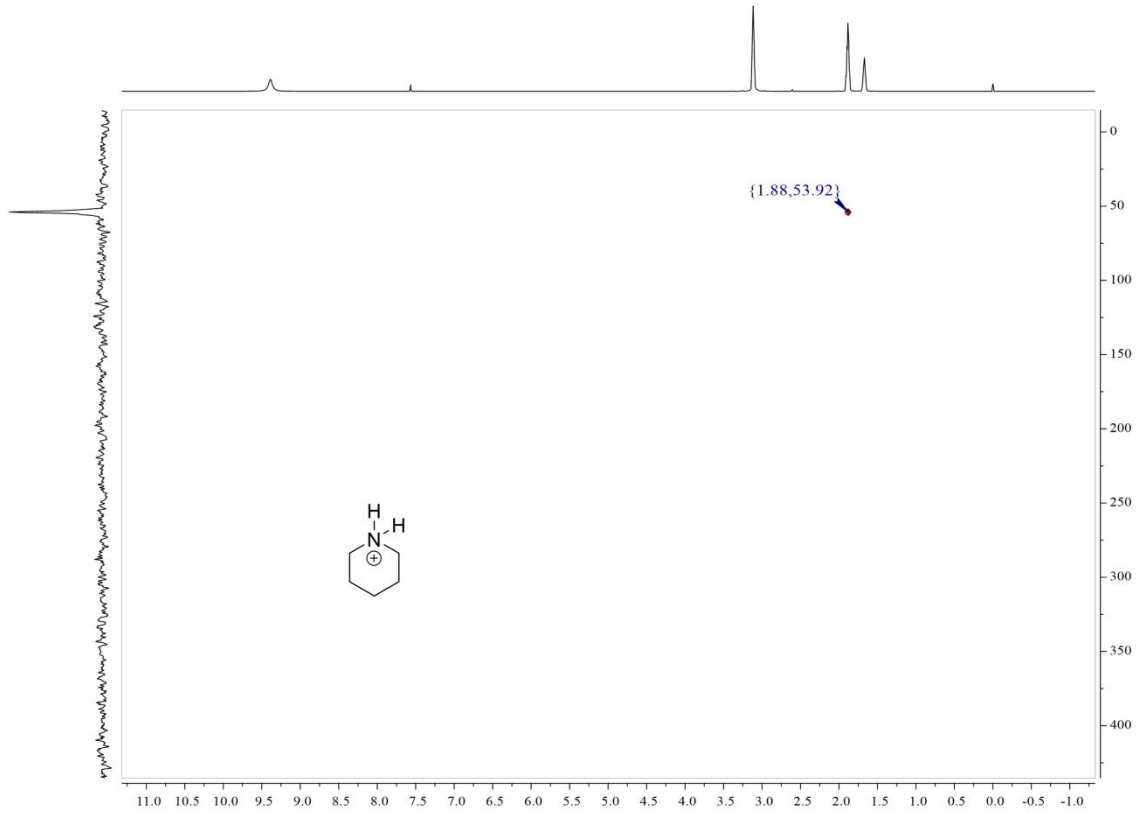


Figure S70. ^{1}H-^{15}N HMBC spectrum of *N*-H piperidine HCl salt (**3'**) in $CDCl_3$ (with additional 2 drops of d_6-DMSO)

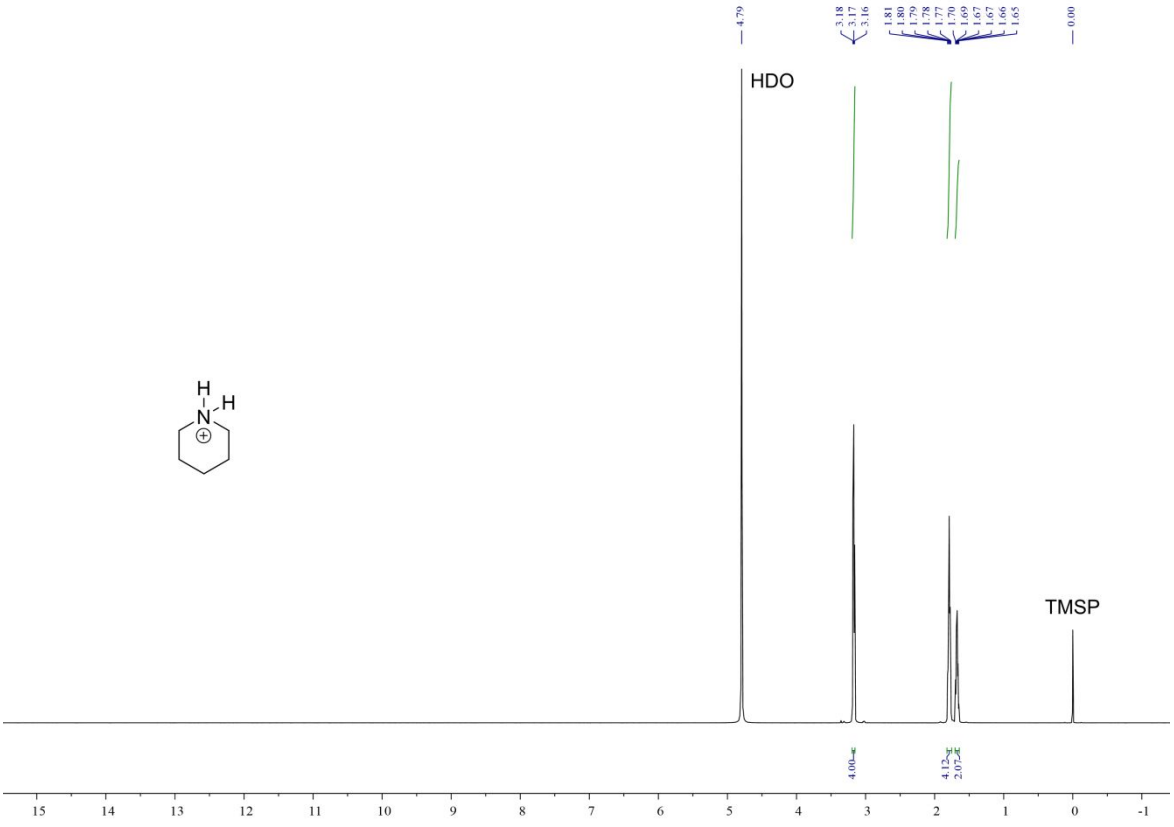


Figure S71. ^{1}H NMR spectrum of *N*-H piperidine HCl salt (**3'**) in D_2O

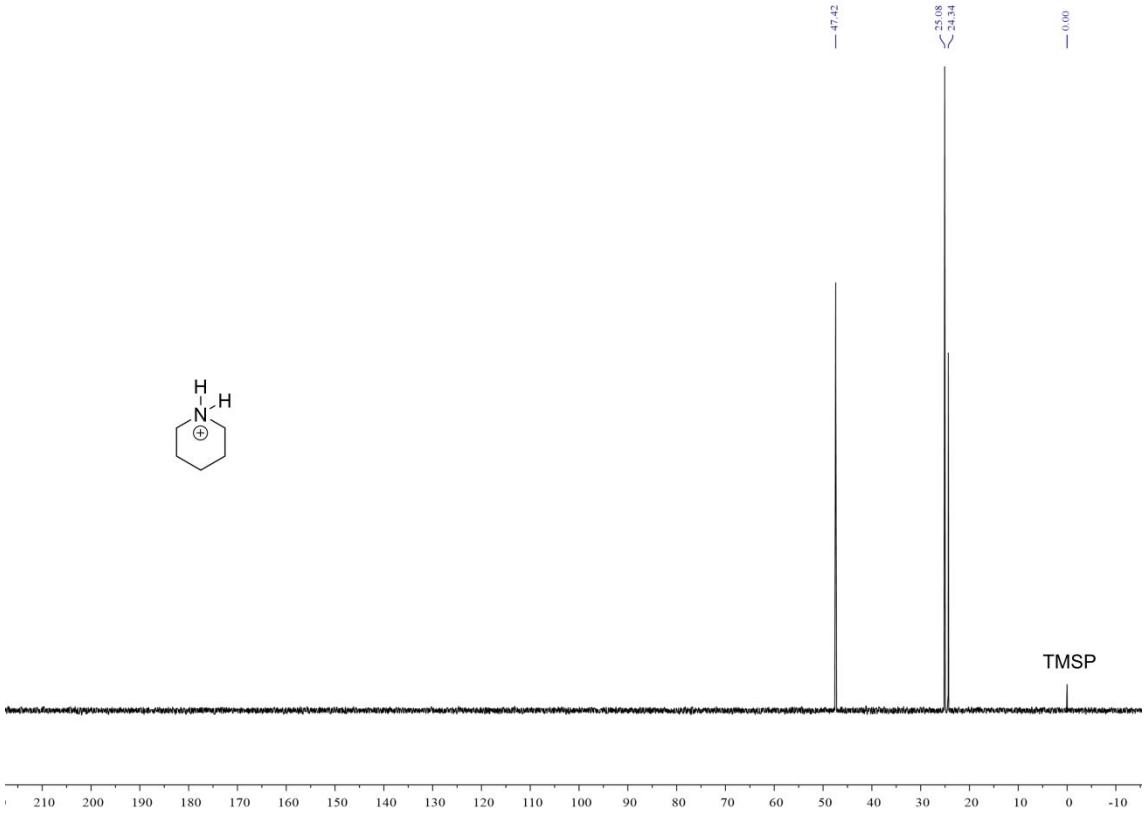


Figure S72. ^{13}C NMR spectrum of *N*-H piperidine HCl salt (**3'**) in D_2O

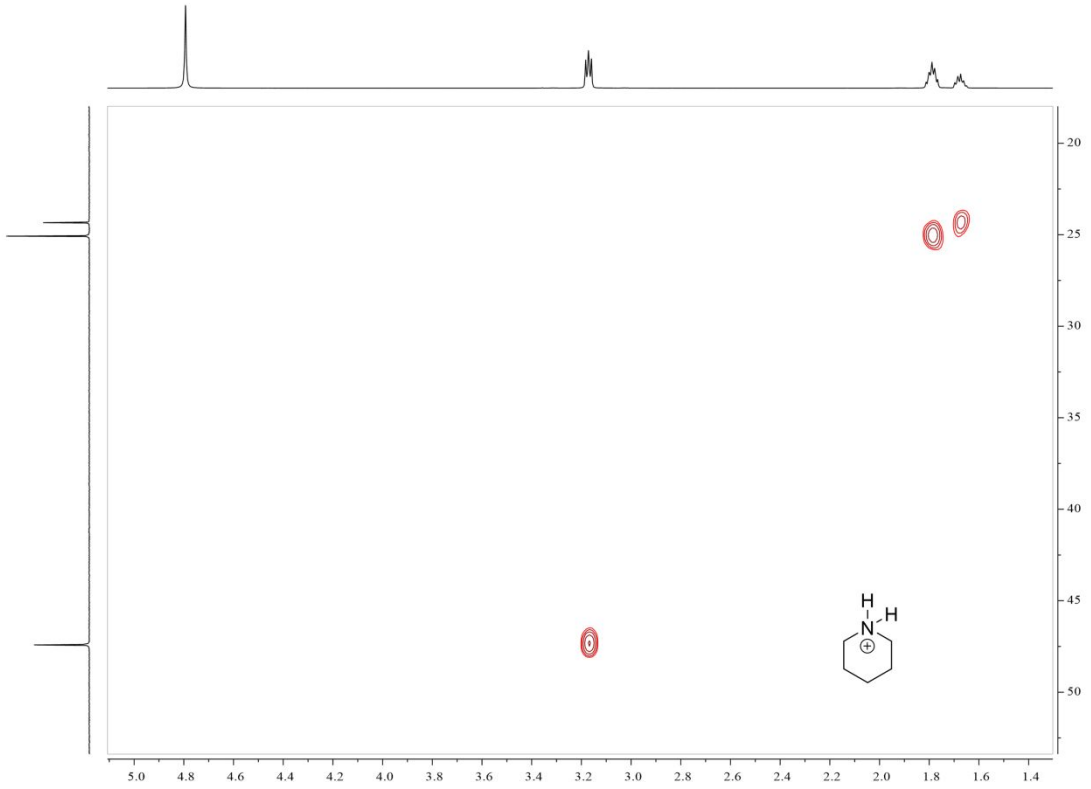


Figure S73. HSQC spectrum of *N*-H piperidine HCl salt (**3'**) in D_2O

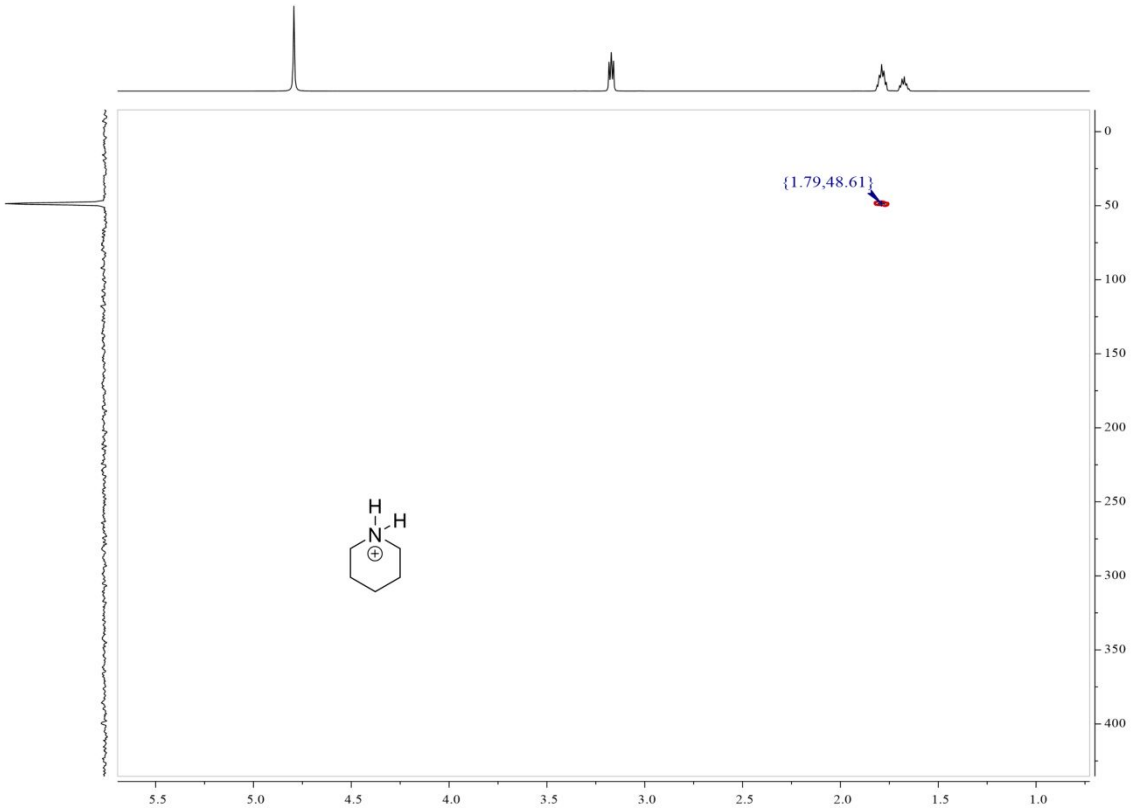


Figure S74. ^{1}H-^{15}N HMBC spectrum of *N*-H piperidine HCl salt (**3'**) in D_2O

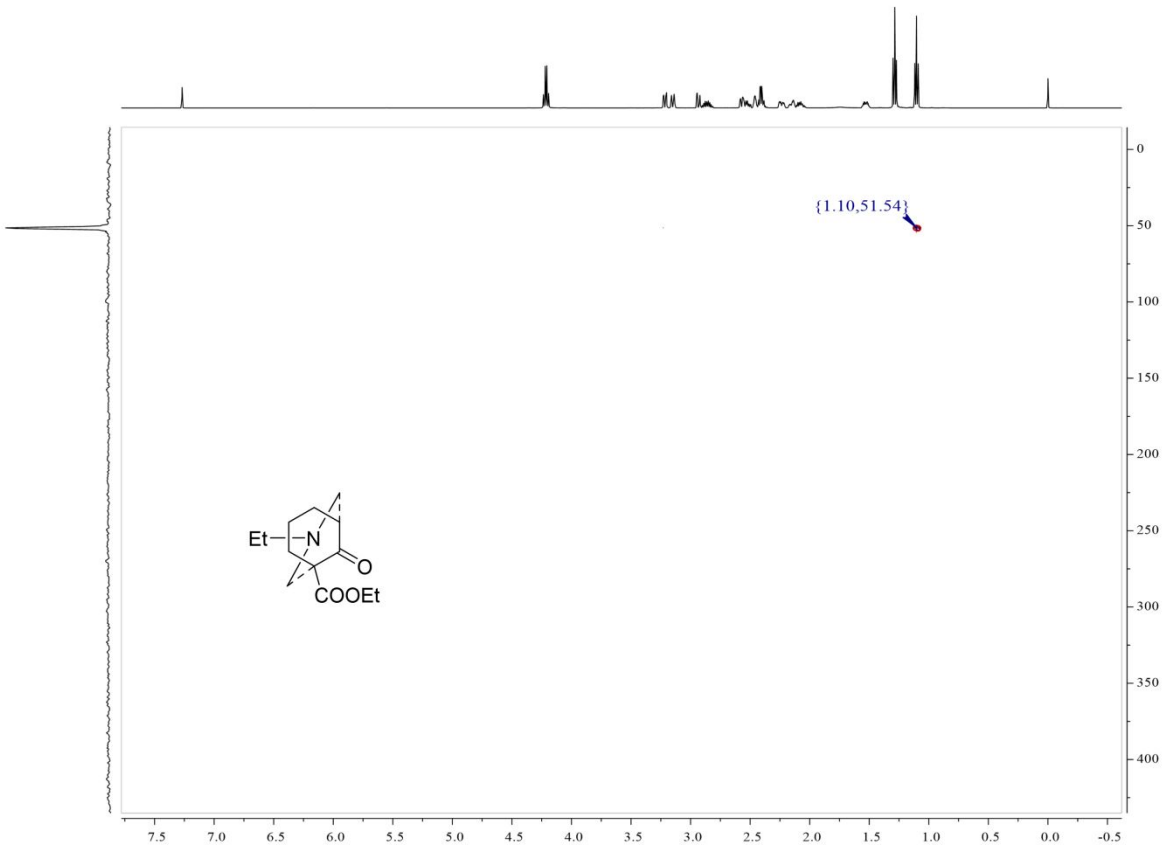


Figure S75. ^{1}H-^{15}N HMBC spectrum of *N*-Et [3.3.1]azabicycle (**5**) in $CDCl_3$

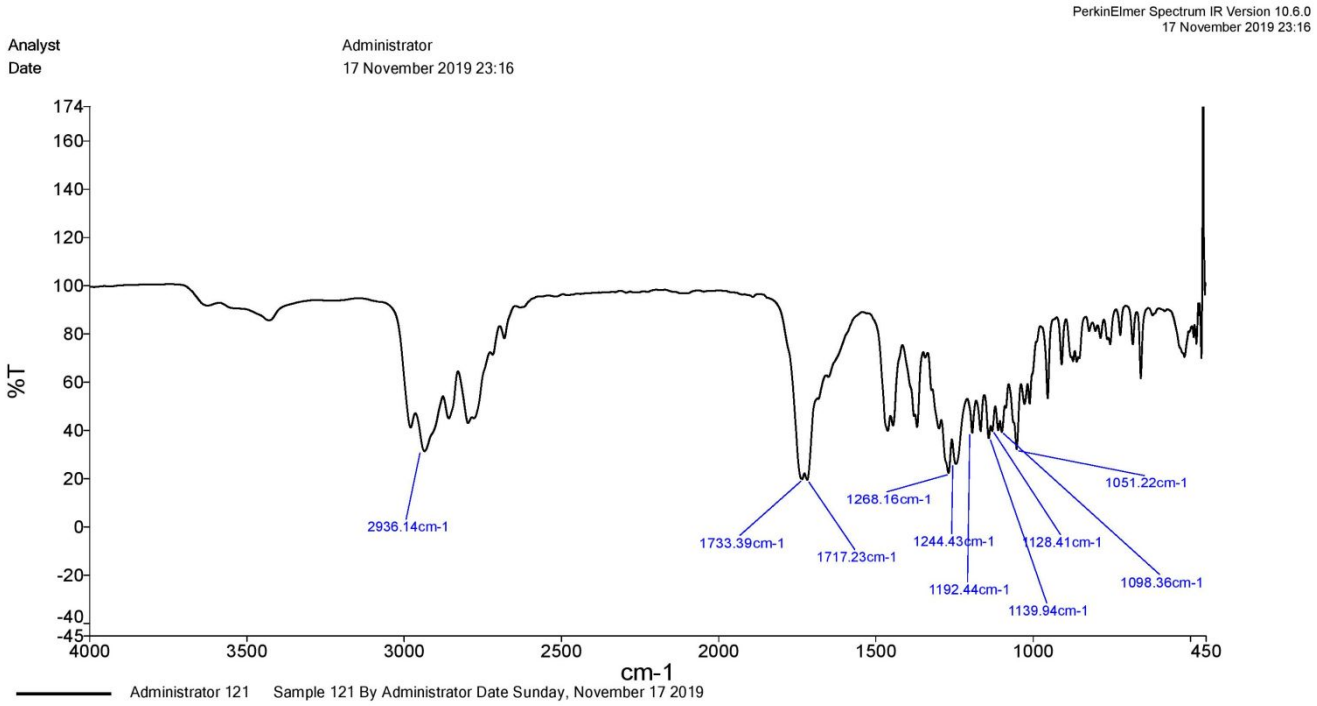


Figure S76. IR data of *N*-Me [3.3.1]azabicycle (**6**)

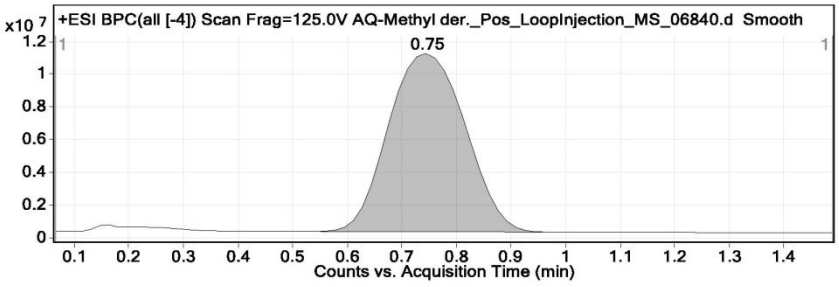
Walkup Analysis Report

Data Filename	AQ-Methyl der._Pos_LoopInjection_MS_06840.d	**Sample Name**	AQ-Methyl der.
Sample Type	Sample	**Position**	P1-A1
Instrument Name	6545 QTof	**User Name**	Ashraf Qasem
Acq Method	Pos_LoopInjection_MS.m	**Acquired Time**	8/6/2019 6:25:43 PM
IRM Calibration Status	Success	**DA Method**	Pos_LoopInjection_MS.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description		**Walkup Method**	Pos_LoopInjection_MS
Formula	C12H19NO3	**Walkup Method Description**	Positive mode ionization using loop injection
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

User Chromatograms

Fragmentor Voltage 125 **Collision Energy** 0 **Ionization Mode** ESI

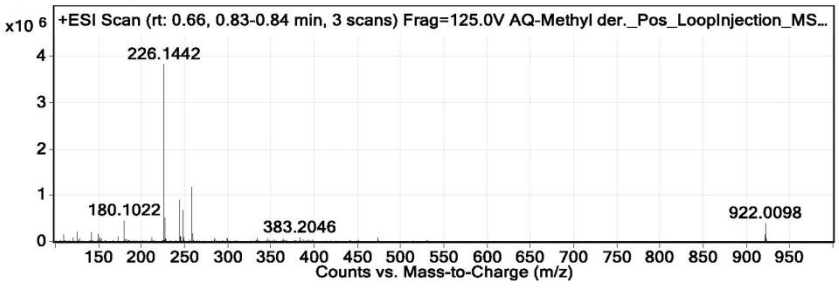


Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	0.49	0.75	1.08	10530759	106650548	100

User Spectra

Spectrum Source	**Fragmentor Voltage**	**Collision Energy**	**Ionization Mode**
Peak (1) in "+ BPC(all [-4]) Scan"	125	0	ESI



Peak List

m/z	z	Abund
125.9864	1	216205.68
141.9587		209535.34
180.1022	1	477595.58
226.1442	1	4117693.9
226.2041		238089.05
227.1478	1	521067.41
244.1548	1	898850.12
248.1261	1	680643.15

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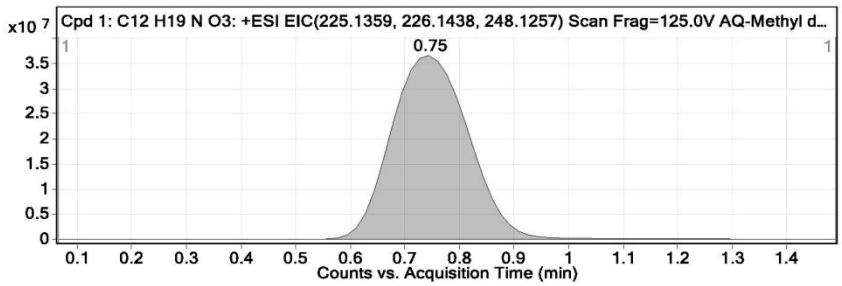
Figure S77. MS data of *N*-Me [3.3.1]azabicycle (**6**) (part 1)

Walkup Analysis Report

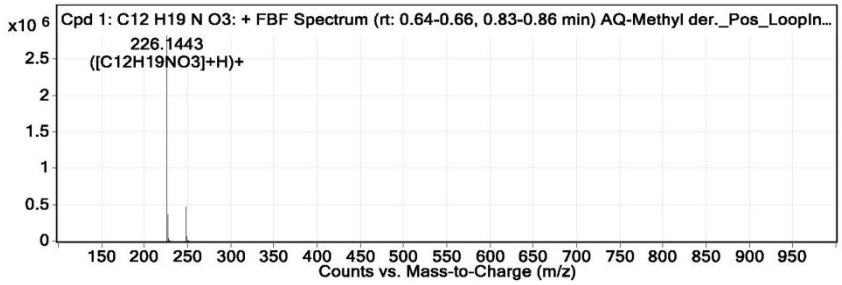
258.1703	1	1196526.36
922.0098	1	407661.15

Compounds



Integration Peak List

Start	RT	End	Height	Area
0.49	0.75	1.47	35229636	362359831



Peak List

m/z	z	Abund	Formula	Ion
226.1443	1	2824311.5	C12H19NO3	(M+H)+
227.1478	1	358342.16	C12H19NO3	(M+H)+
228.1498	1	37712.87	C12H19NO3	(M+H)+
229.1501	1	5251.61	C12H19NO3	(M+H)+
230.141	1	2468.59	C12H19NO3	(M+H)+
248.1262	1	469635.25	C12H19NO3	(M+Na)+
249.1294	1	60601.92	C12H19NO3	(M+Na)+
250.1331	1	6829.82	C12H19NO3	(M+Na)+
251.1273	1	3046.43	C12H19NO3	(M+Na)+
252.1276	1	1597.46	C12H19NO3	(M+Na)+

--- End Of Report ---

Figure S78. MS data of *N*-Me [3.3.1]azabicycle (**6**) (part 2)

Walkup MS Report

Data File	AQ-Methyl der._Pos_LoopInjection_MS_06840.d	**Sample Name**	AQ-Methyl der.
Sample Type	Sample	**Position**	P1-A1
Instrument Name	6545 QTof	**User Name**	Ashraf Qasem
Acq Method	Pos_LoopInjection_MS.m	**Acquired Time**	8/6/2019 6:25:43 PM
IRM Calibration Status	Success	**DA Method**	Pos_LoopInjection_MS.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description		**Walkup Method**	Pos_LoopInjection_MS
Formula	C12H19NO3	**Walkup Method Description**	Positive mode ionization using loop injection
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

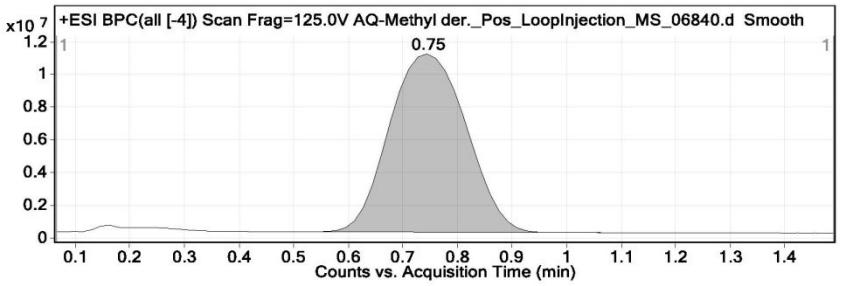


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.75	106650548	100.00	100.00	226.1442	0.180

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)
Cpd 1: C12 H19 N O3	0.75	248.1262	225.1370	225.1365	2.18	99.26

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

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Figure S79. MS data of *N*-Me [3.3.1]azabicycle (**6**) (part 3)

Walkup MS Report

Compound specific information

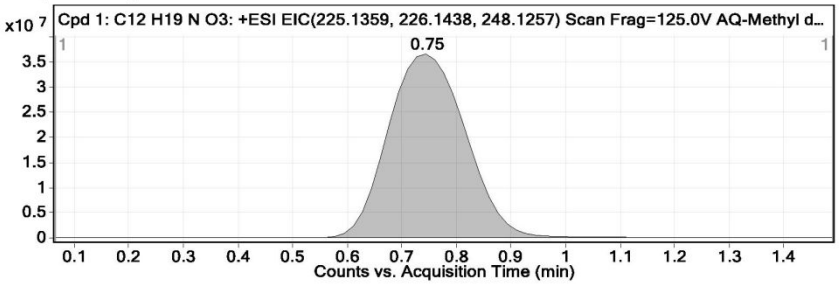

Figure: Extracted ion chromatogram (EIC) of compound.

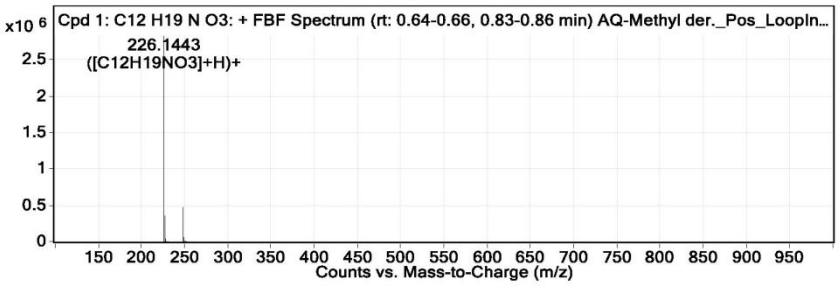

Figure: Full range view of Compound spectra and potential adducts.

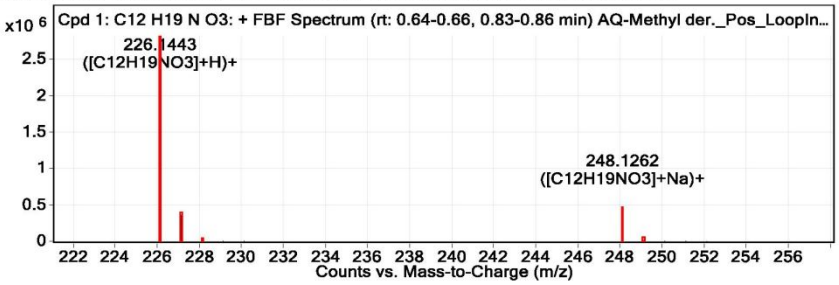

Figure: Zoomed Compound spectra view
(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
226.1443	1	2824311.5	C12H19NO3	(M+H)+
227.1478	1	358342.2	C12H19NO3	(M+H)+
228.1498	1	37712.9	C12H19NO3	(M+H)+
229.1501	1	5251.6	C12H19NO3	(M+H)+
230.1410	1	2468.6	C12H19NO3	(M+H)+
248.1262	1	469635.3	C12H19NO3	(M+Na)+
249.1294	1	60601.9	C12H19NO3	(M+Na)+
250.1331	1	6829.8	C12H19NO3	(M+Na)+
251.1273	1	3046.4	C12H19NO3	(M+Na)+
252.1276	1	1597.5	C12H19NO3	(M+Na)+

--- End Of Report ---

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Figure S80. MS data of *N*-Me [3.3.1]azabicycle (**6**) (part 4)

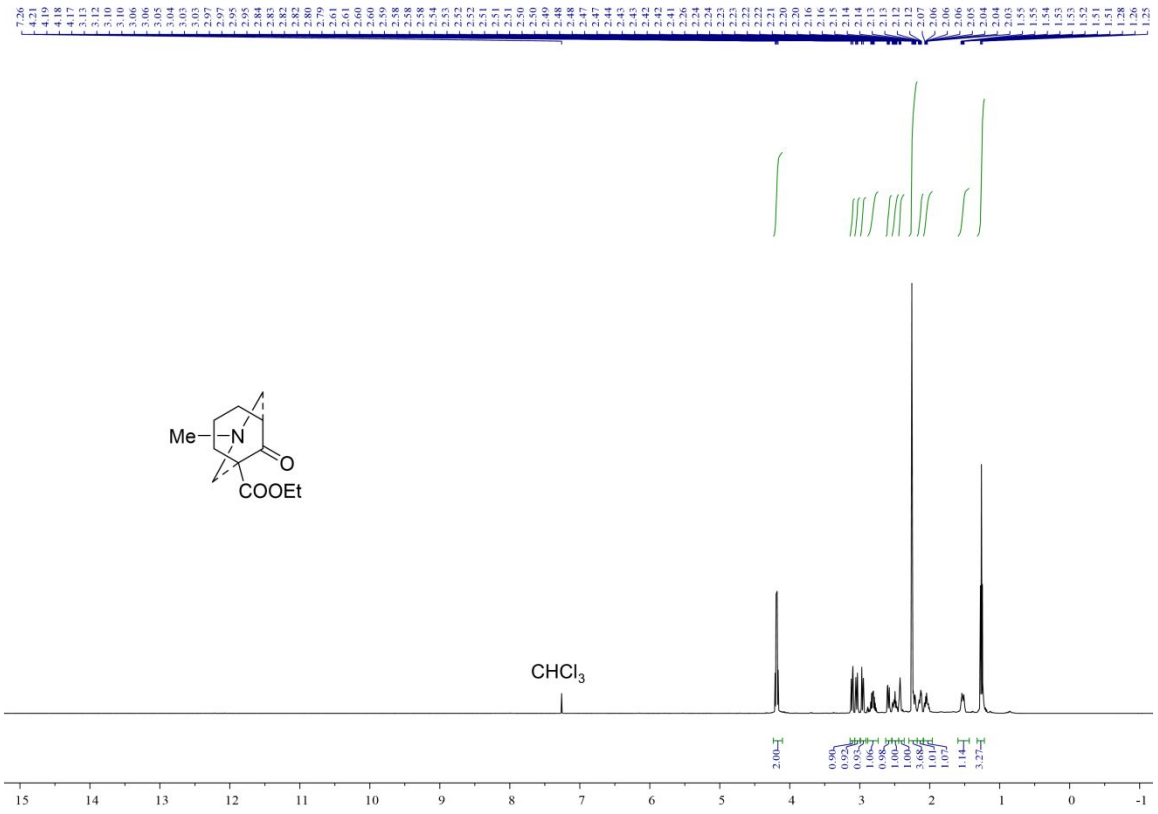

Figure S81. ^{1}H NMR spectrum of *N*-Me [3.3.1]azabicycle (**6**) in $CDCl_3$

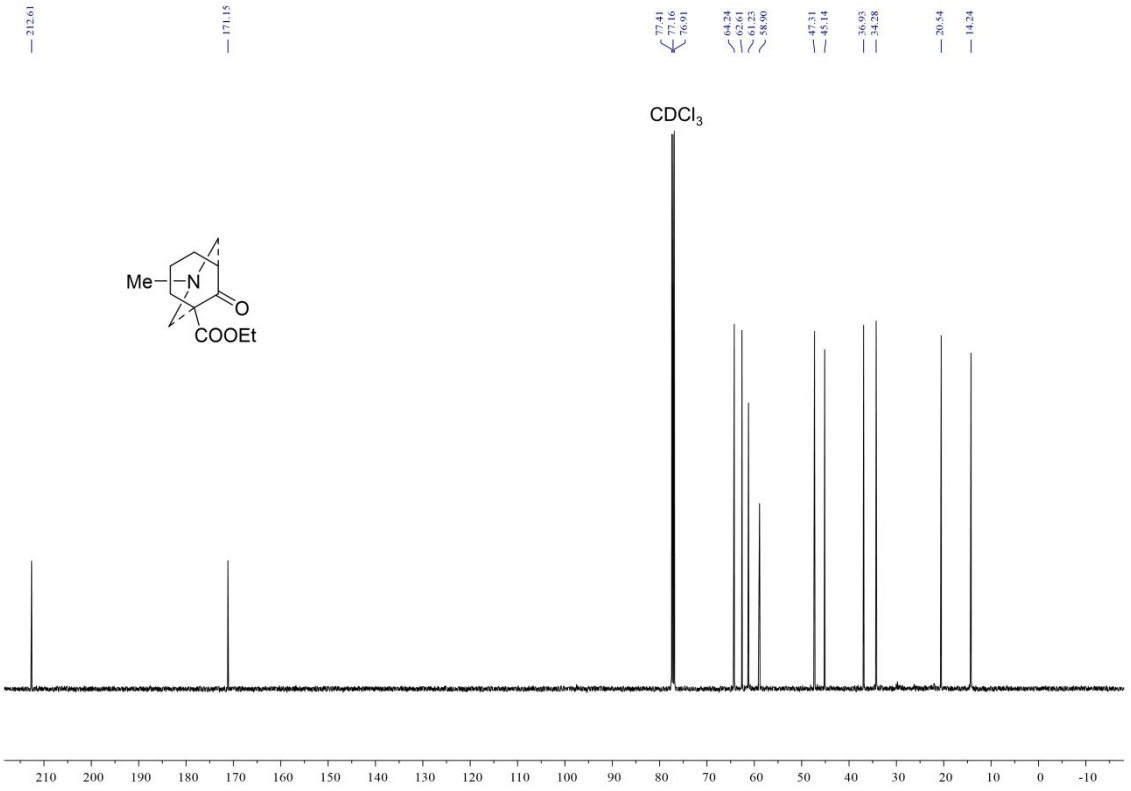

Figure S82. ^{13}C NMR spectrum of *N*-Me [3.3.1]azabicycle (**6**) in $CDCl_3$

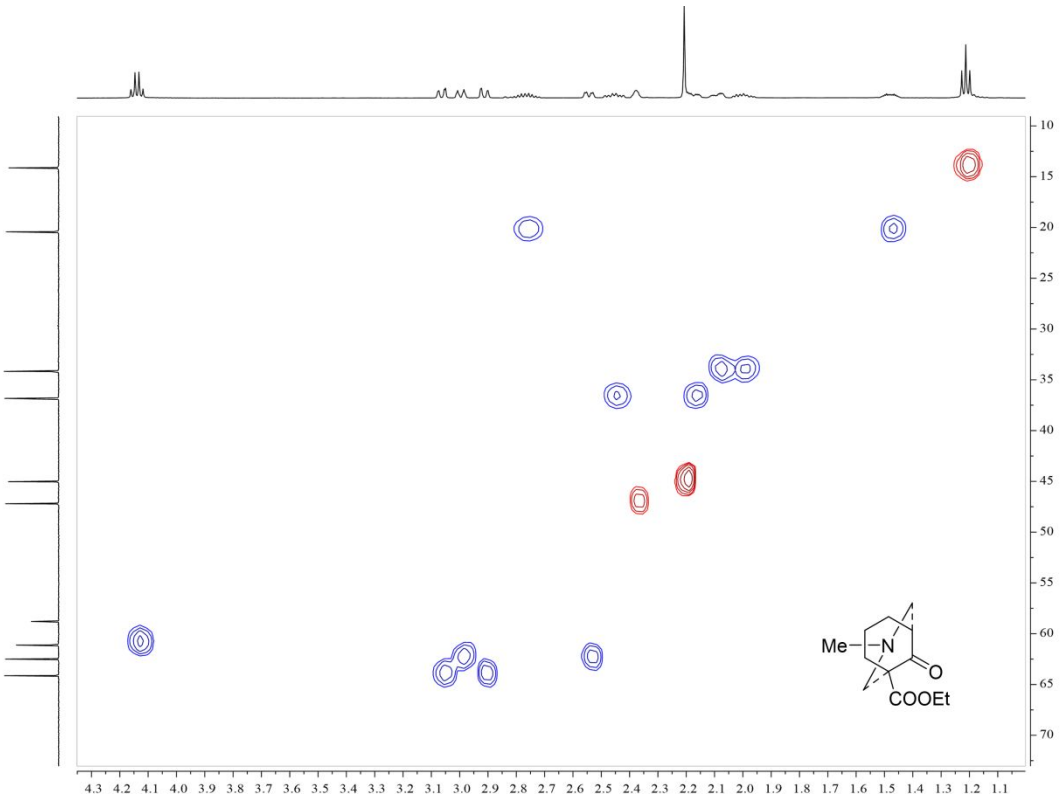

Figure S83. HSQC spectrum of *N*-Me [3.3.1]azabicycle (**6**) in $CDCl_3$

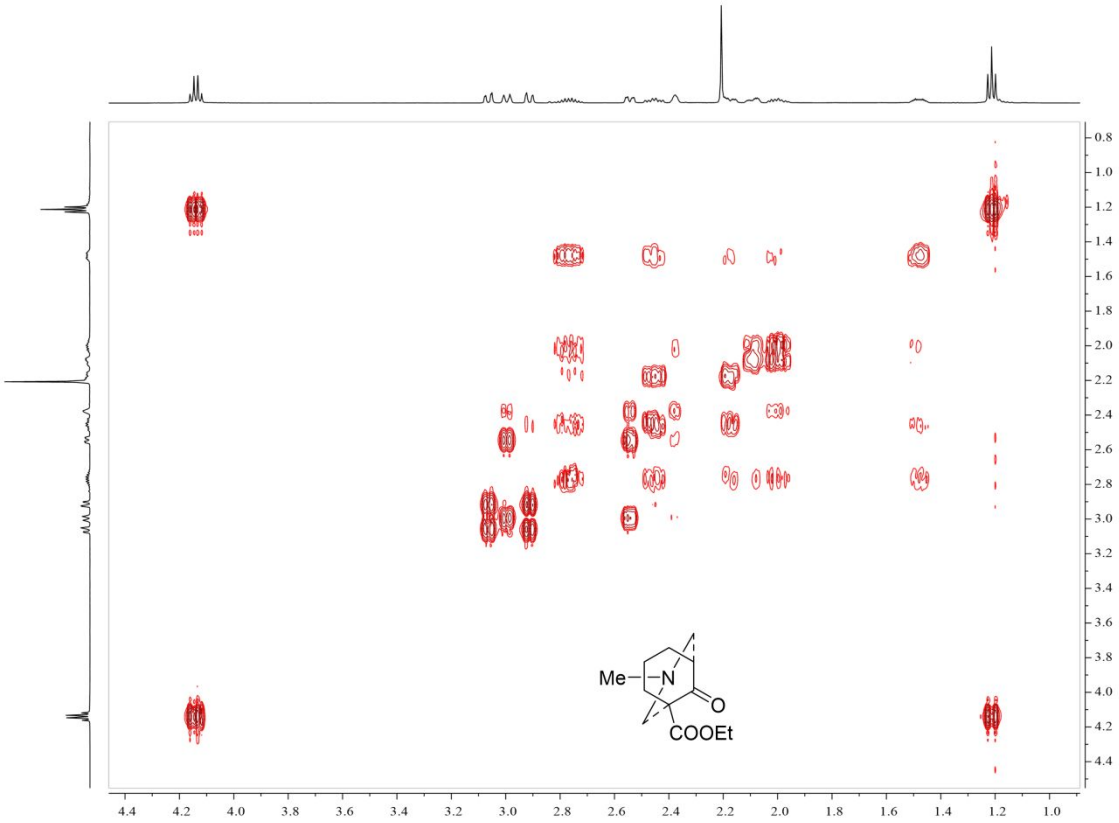

Figure S84. COSY spectrum of *N*-Me [3.3.1]azabicycle (**6**) in $CDCl_3$

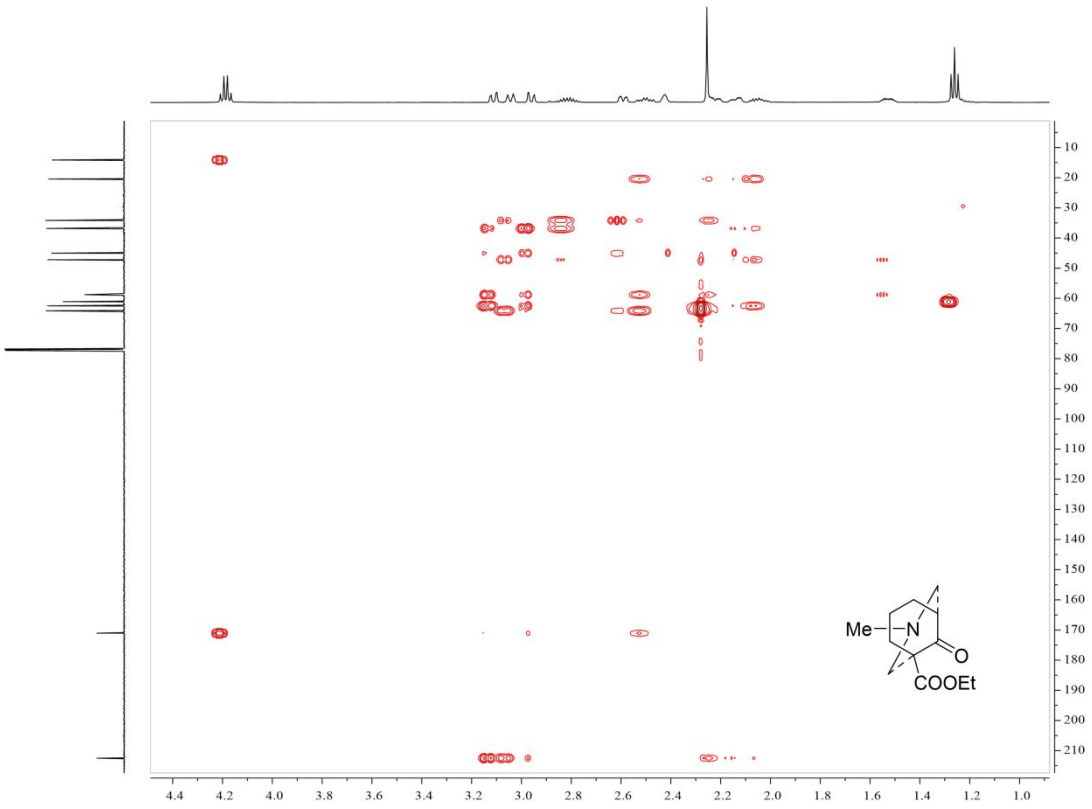

Figure S85. HMBC spectrum of *N*-Me [3.3.1]azabicycle (**6**) in $CDCl_3$

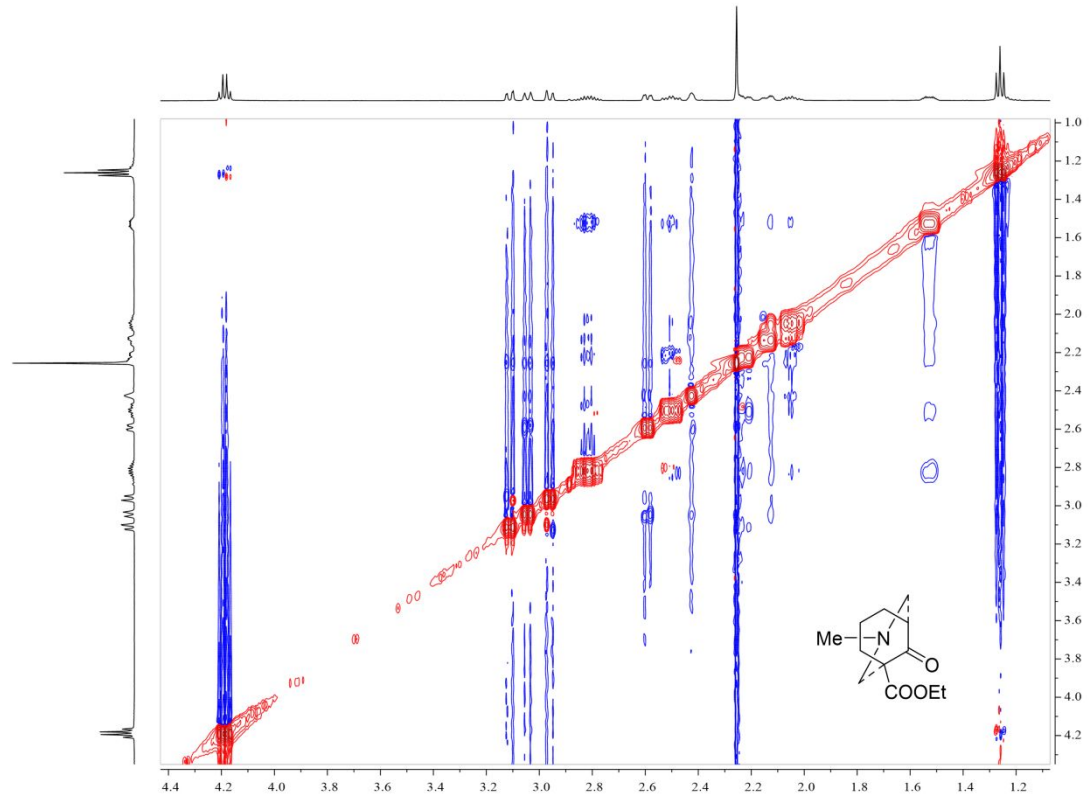

Figure S86. NOESY spectrum of *N*-Me [3.3.1]azabicycle (**6**) in $CDCl_3$

Figure S87. ^{1}H-^{15}N HMBC spectrum of *N*-Me [3.3.1]azabicycle (**6**) in $CDCl_3$

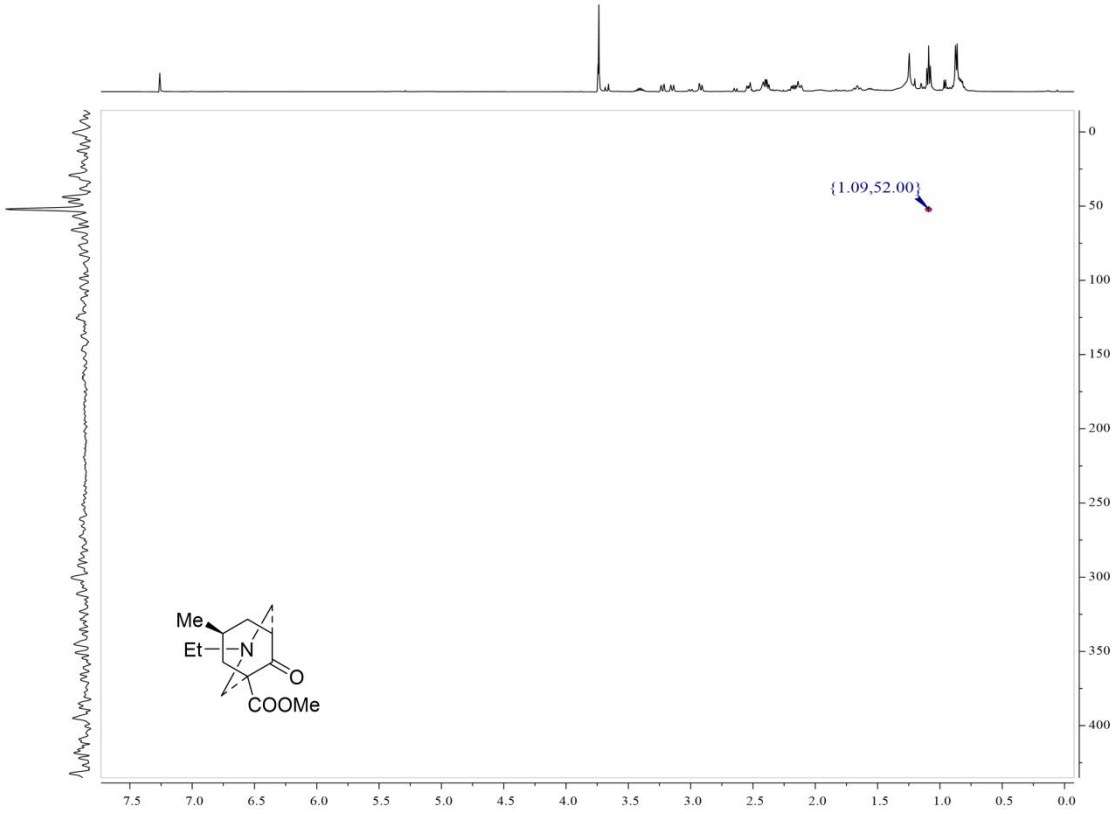

Figure S88. ^{1}H-^{15}N HMBC spectrum of 7-Me [3.3.1]azabicycle (**7**) in $CDCl_3$

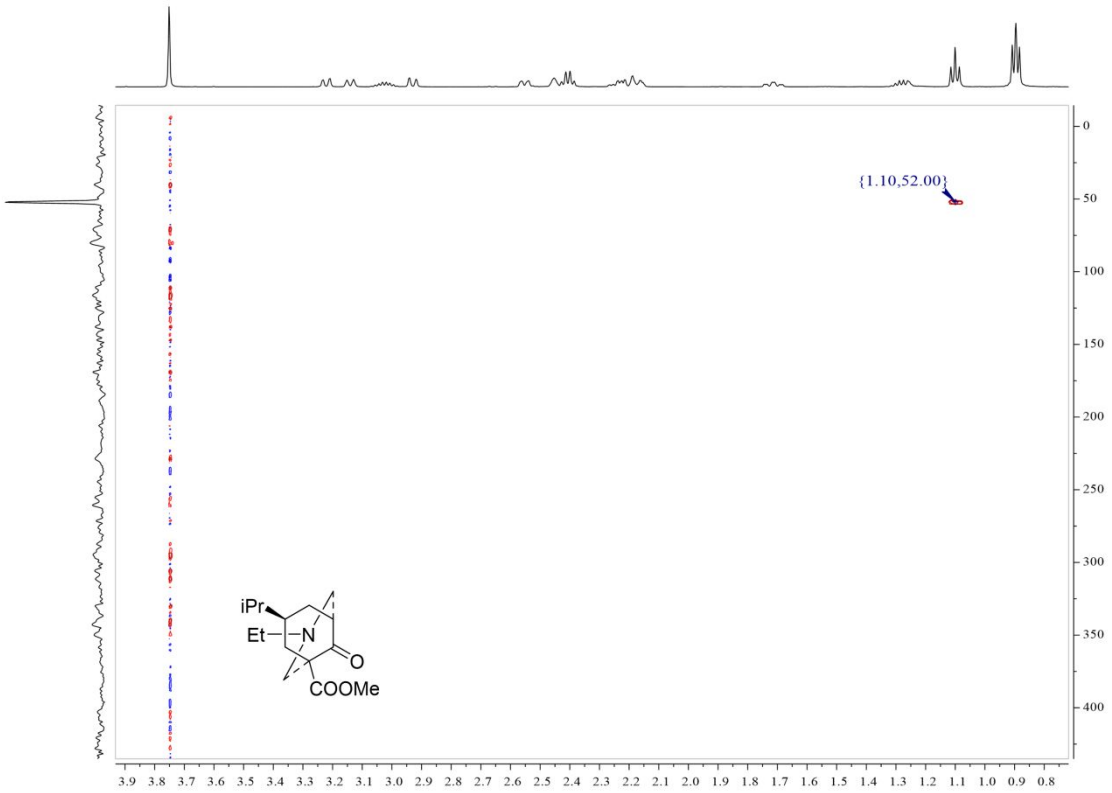

Figure S89. ^{1}H-^{15}N HMBC spectrum of 7-iPr [3.3.1]azabicycle (**8**) in $CDCl_3$

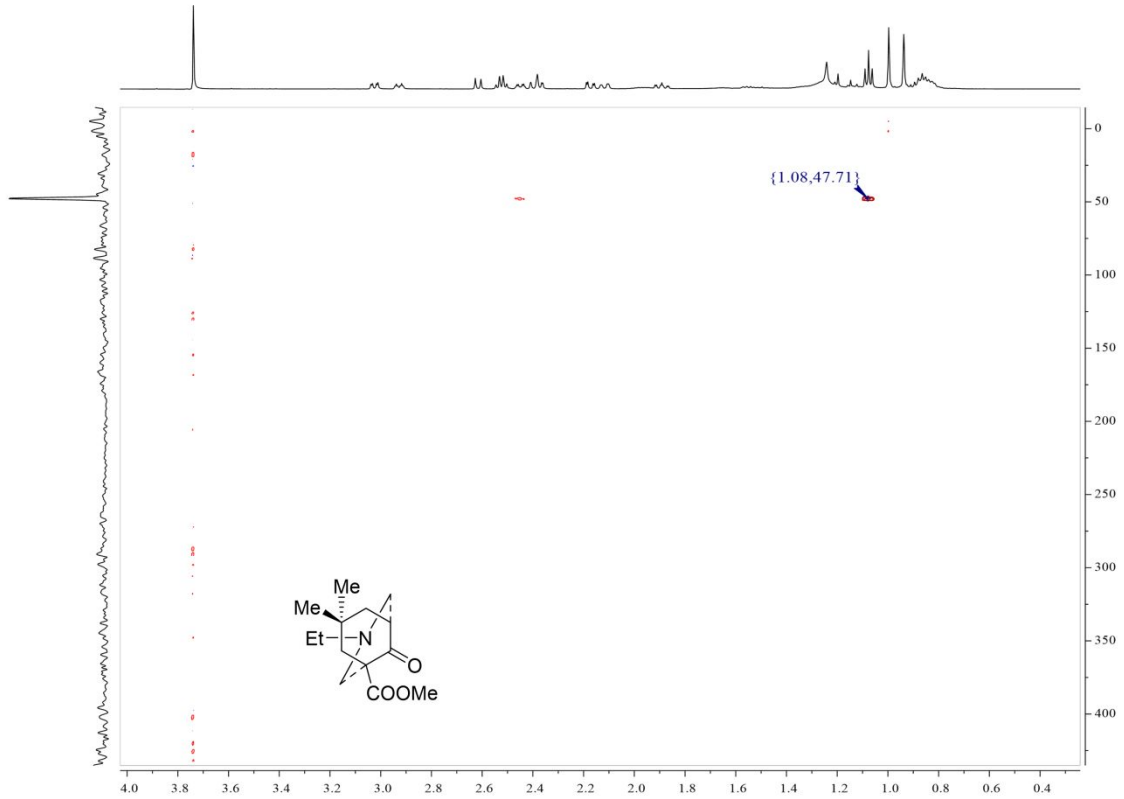

Figure S90. ^{1}H-^{15}N HMBC spectrum of 7,7-diMe [3.3.1]azabicycle (**9**) in $CDCl_3$

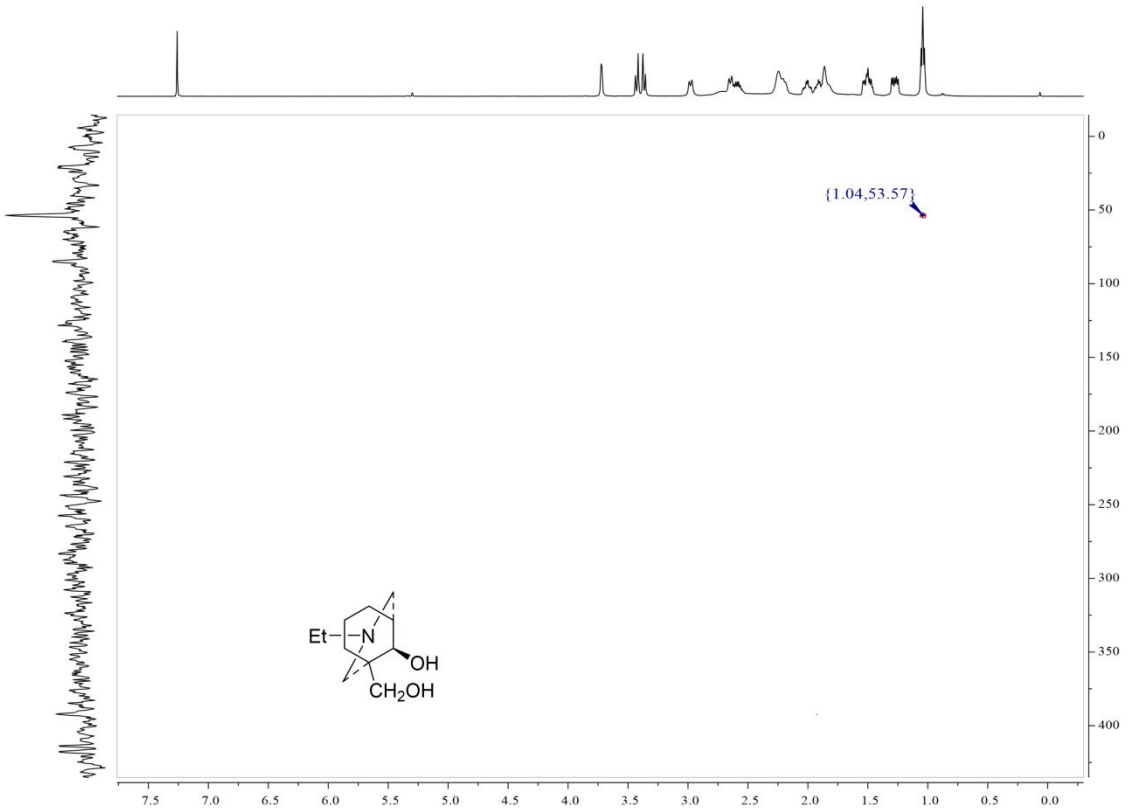

Figure S91. ^{1}H-^{15}N HMBC spectrum of diol (**10**) in $CDCl_3$

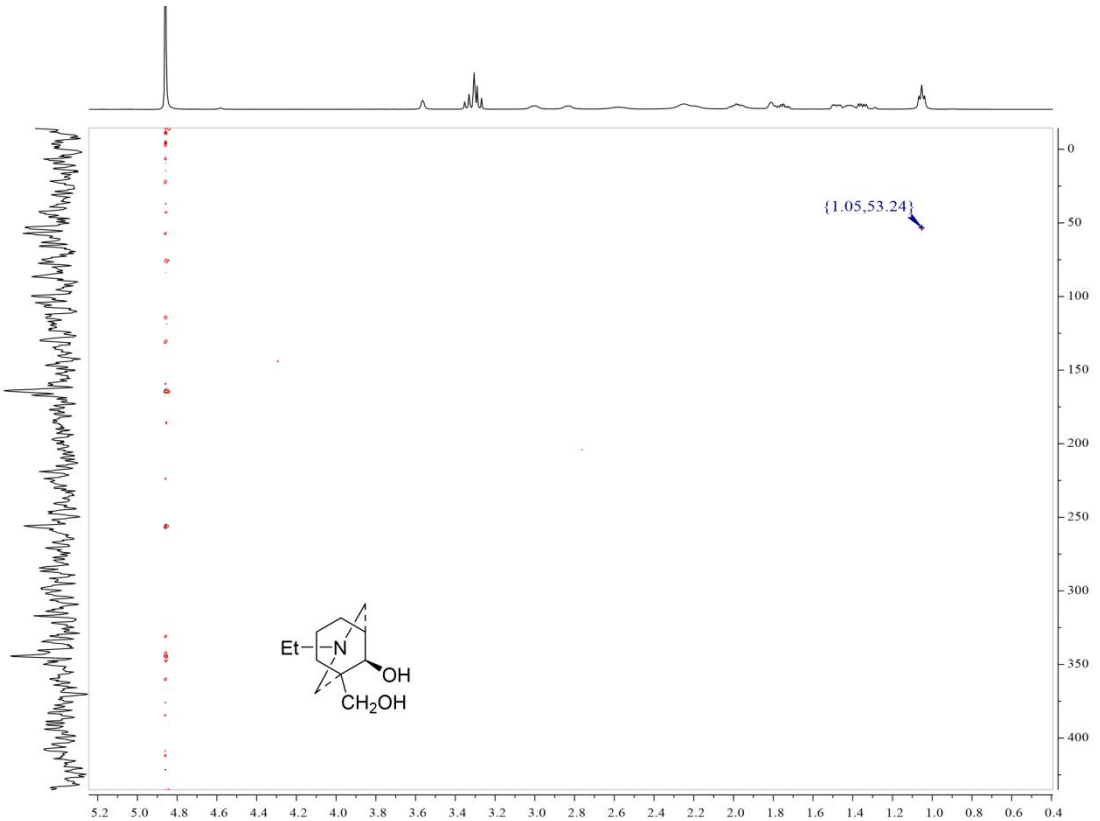

Figure S92. ^{1}H-^{15}N HMBC spectrum of diol (**10**) in CD_3OD

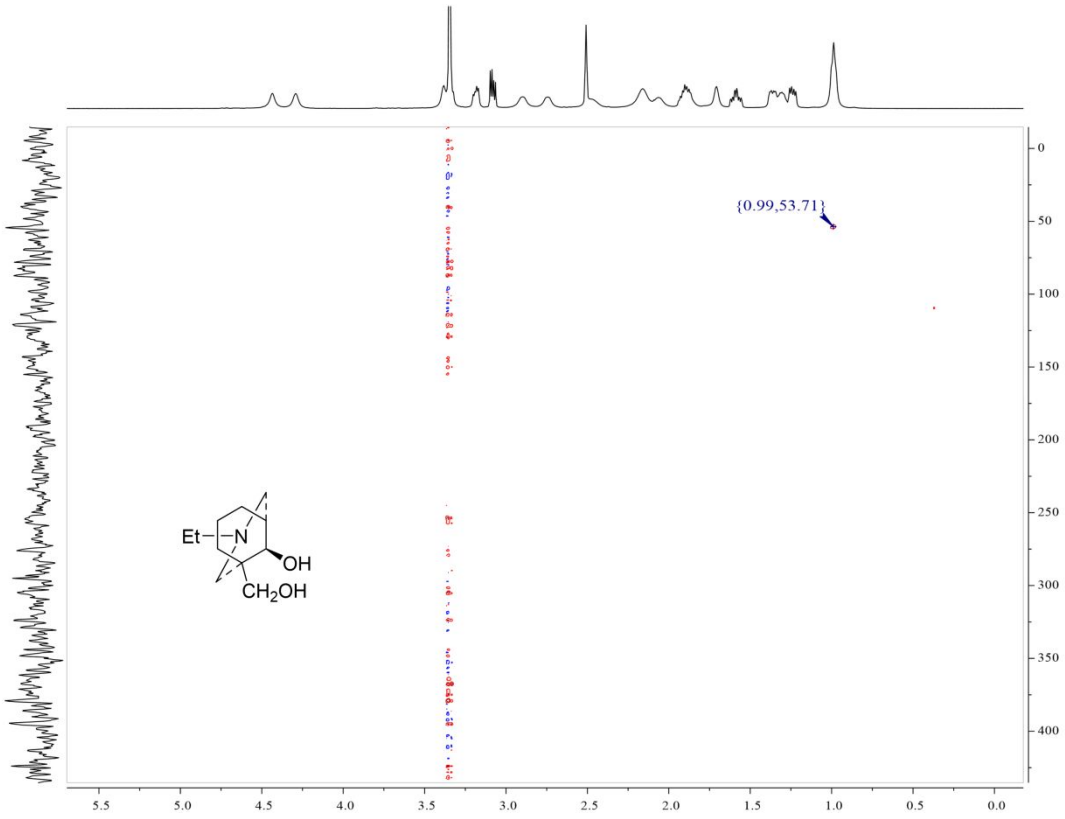

Figure S93. ^{1}H-^{15}N HMBC spectrum of diol (**10**) in d_6-DMSO

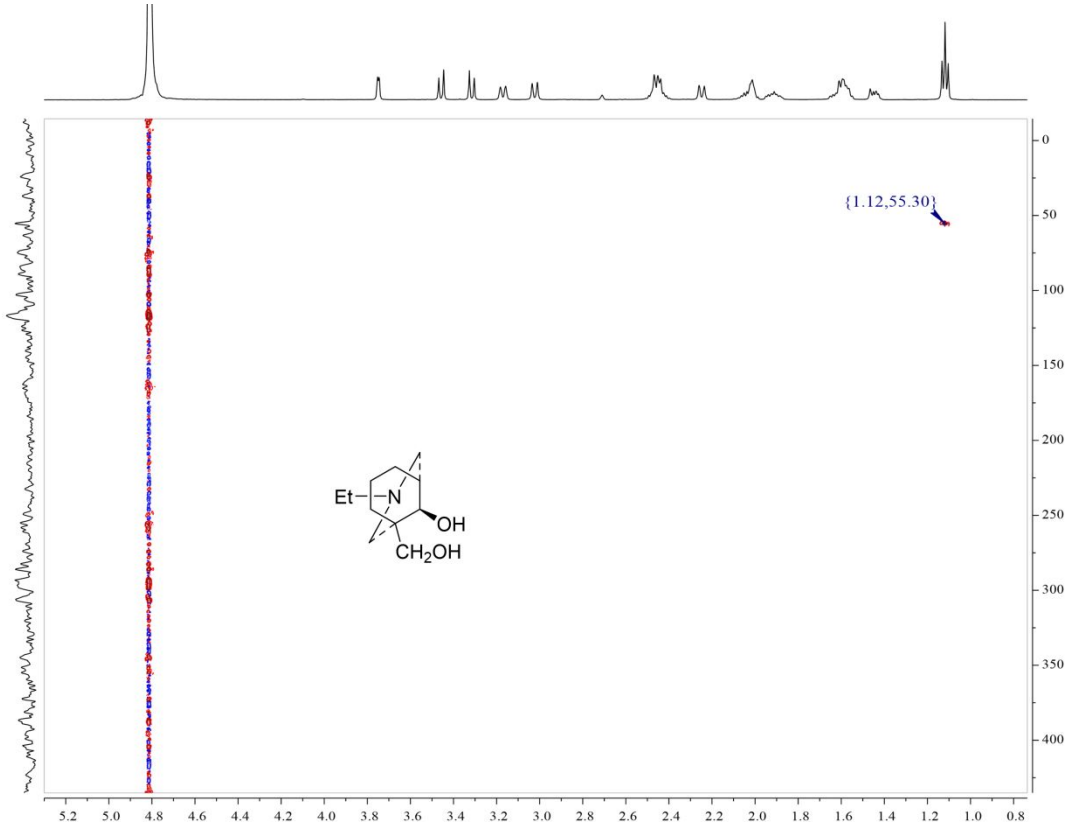

Figure S94. ^{1}H-^{15}N HMBC spectrum of diol (**10**) in D_2O (with additional 2 drops of d_6-DMSO)

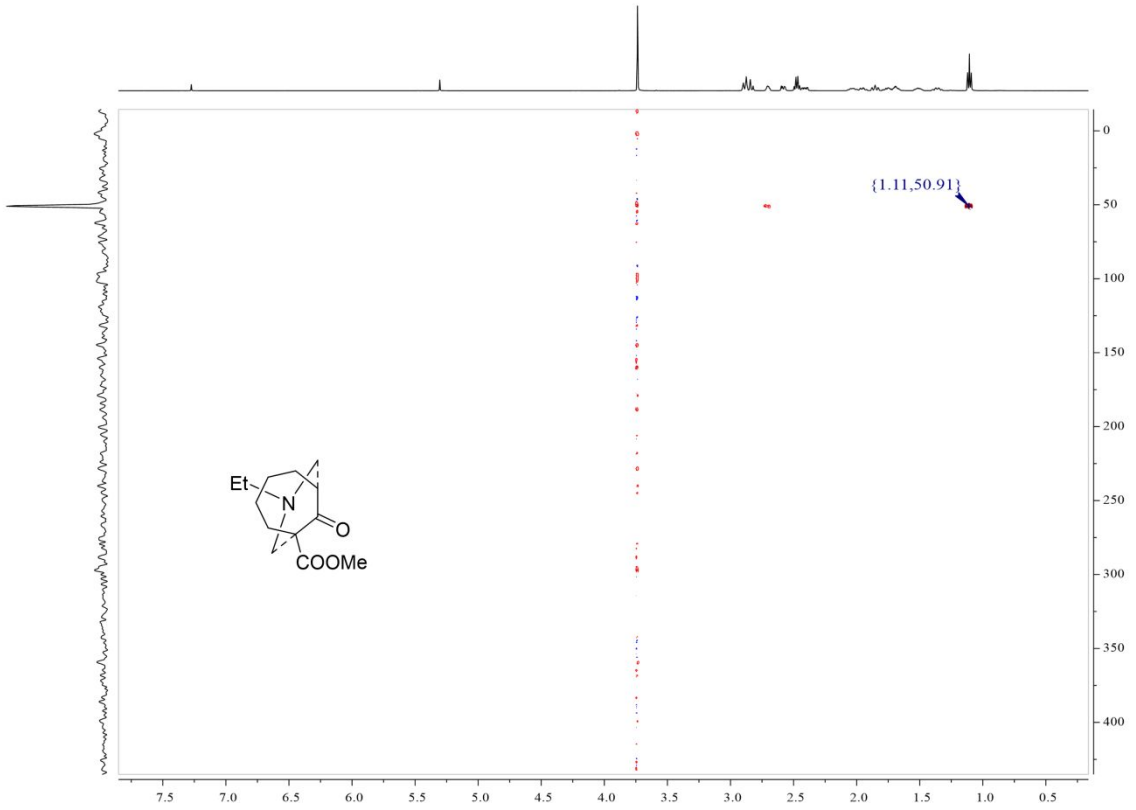

Figure S95. ^{1}H-^{15}N HMBC spectrum of [4.3.1]azabicycle (**11**) in $CDCl_3$

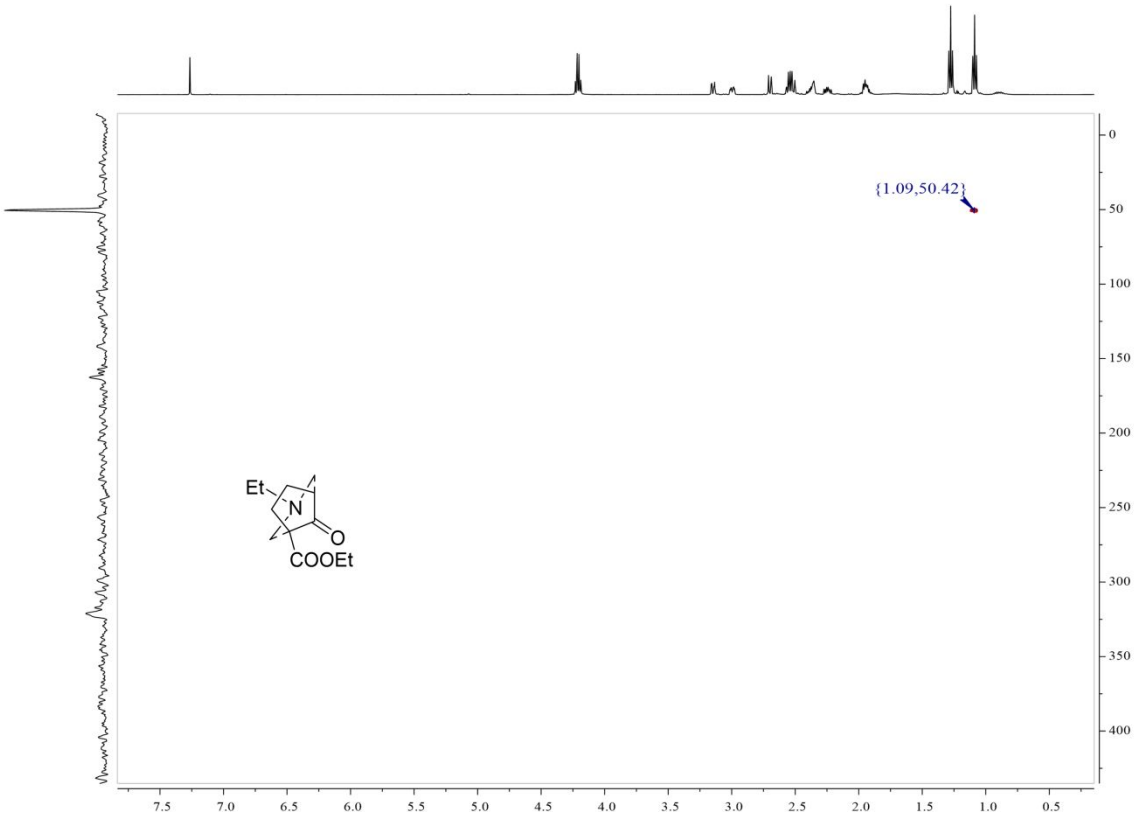

Figure S96. ^{1}H-^{15}N HMBC spectrum of [3.2.1]azabicycle (**12**) in $CDCl_3$

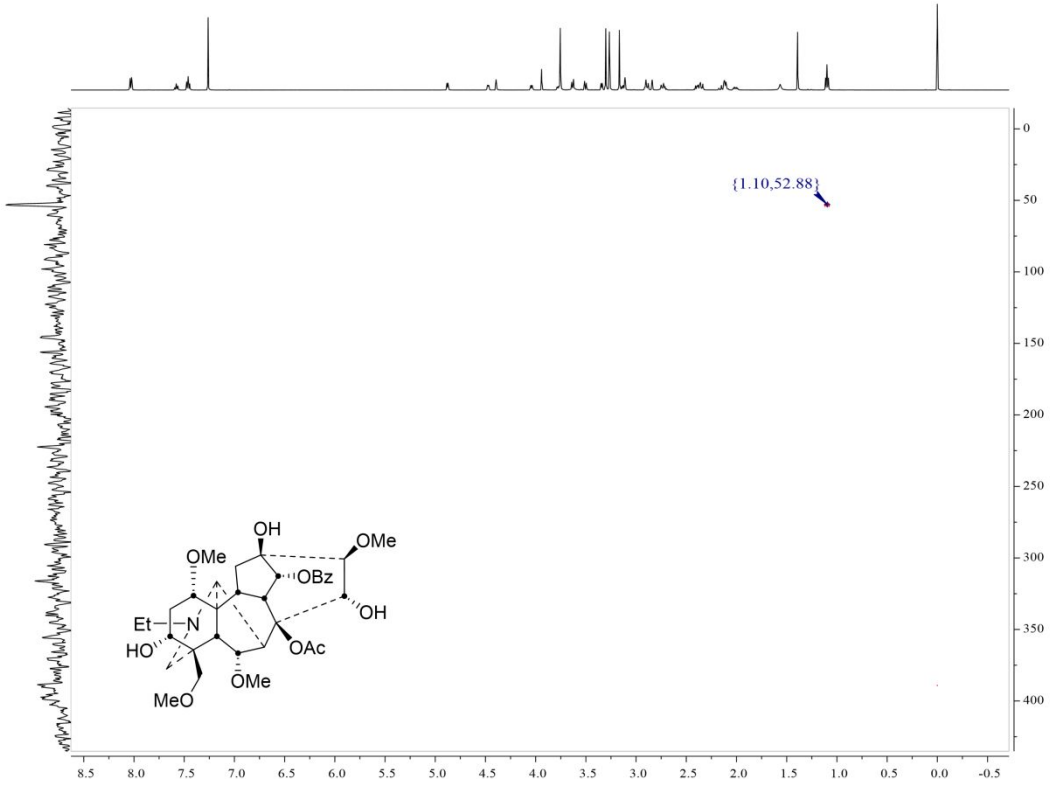

Figure S97. ^{1}H-^{15}N HMBC spectrum of aconitine (**13**) in $CDCl_3$

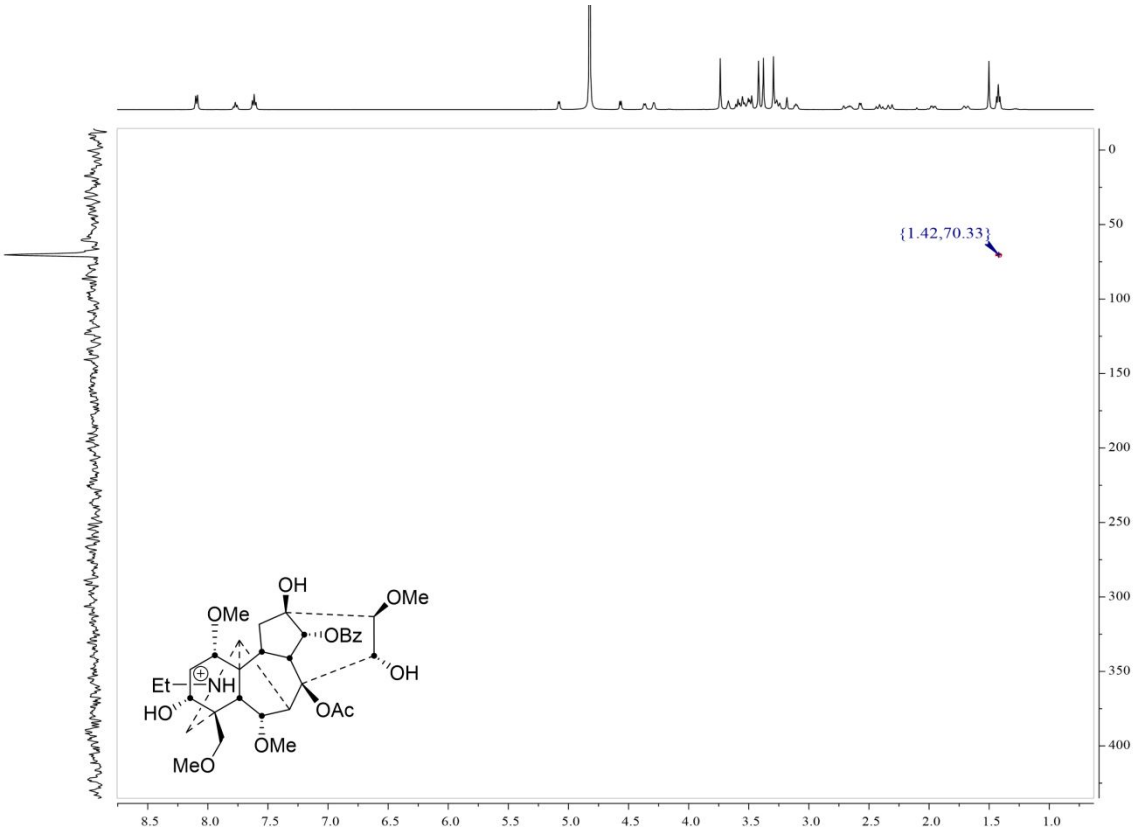

Figure S98. ^{1}H-^{15}N HMBC spectrum of aconitine HCl salt (**13'**) in D_2O (with additional 2 drops of d_6-DMSO)

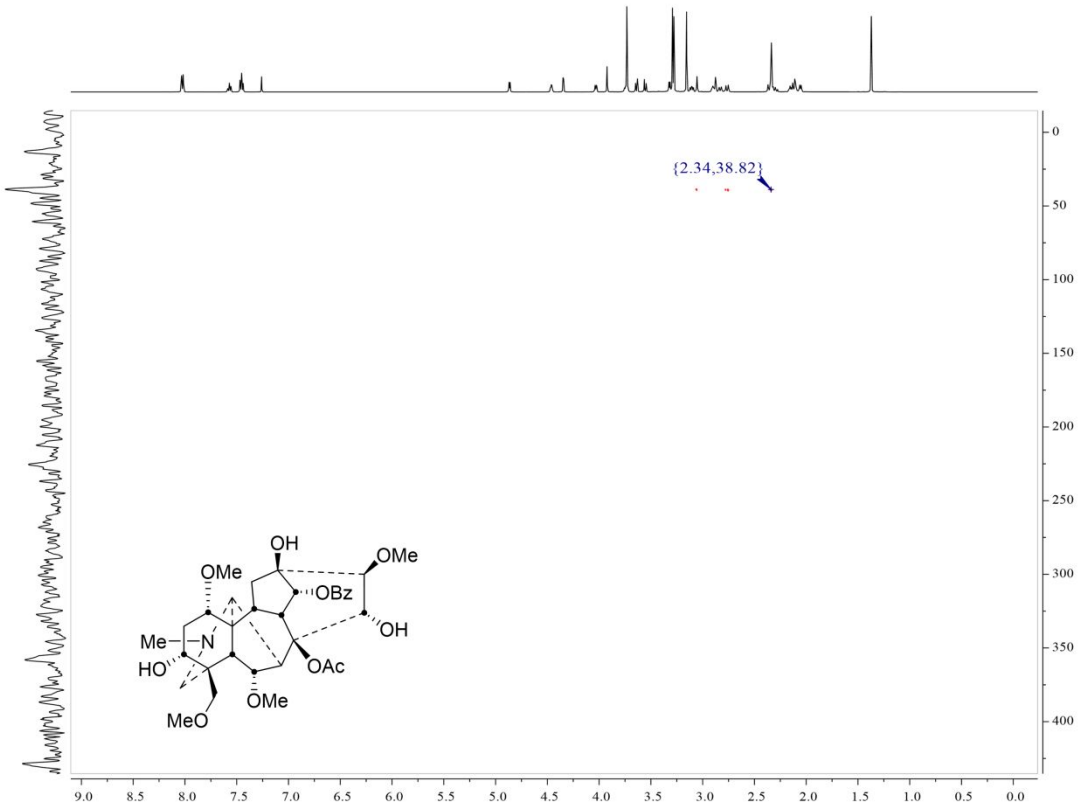

Figure S99. ^{1}H-^{15}N HMBC spectrum of mesaconitine (**14**) in $CDCl_3$

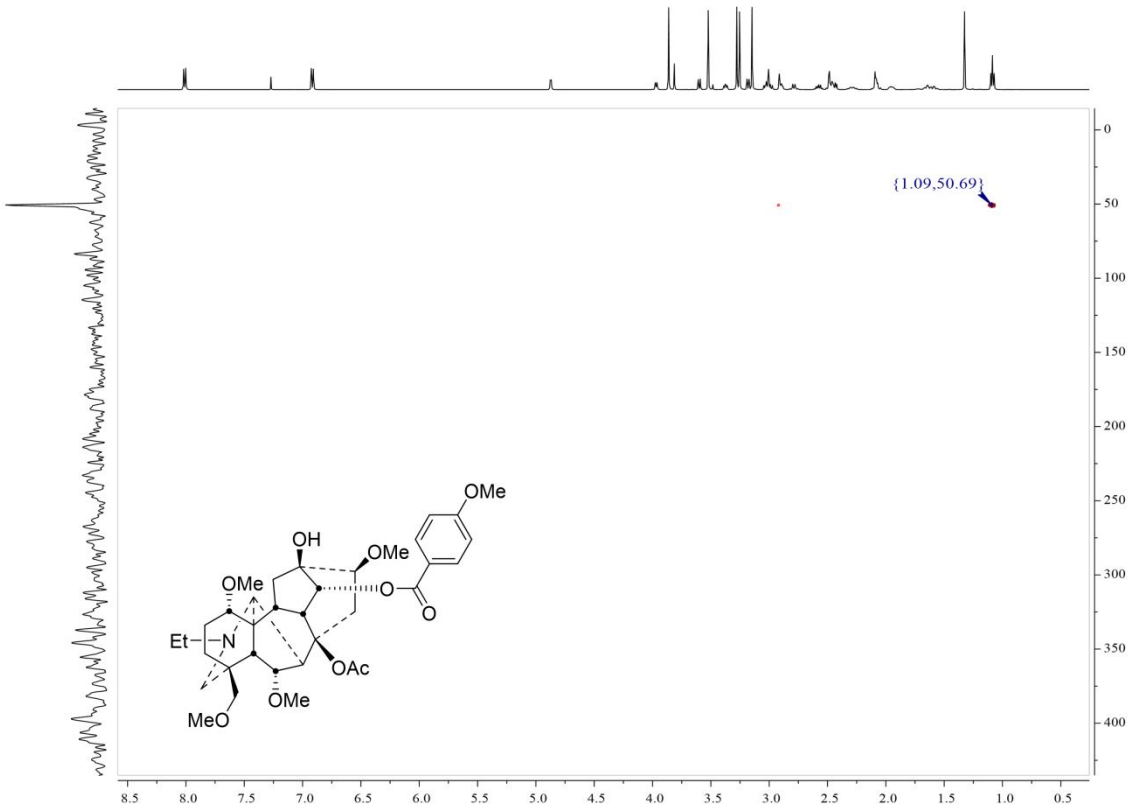

Figure S100. ^{1}H-^{15}N HMBC spectrum of crassicauline A (**15**) in $CDCl_3$

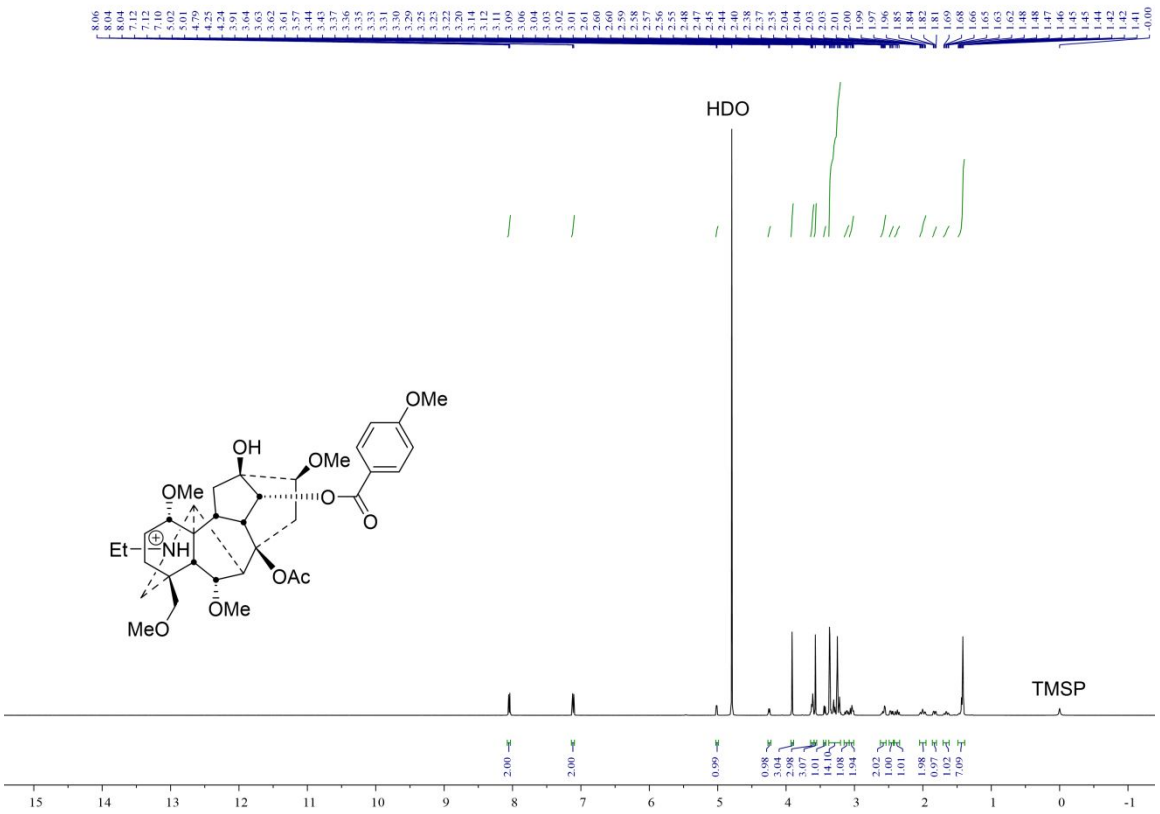

Figure S101. ^{1}H NMR spectrum of crassicauline A HCl salt (**15'**) in D_2O

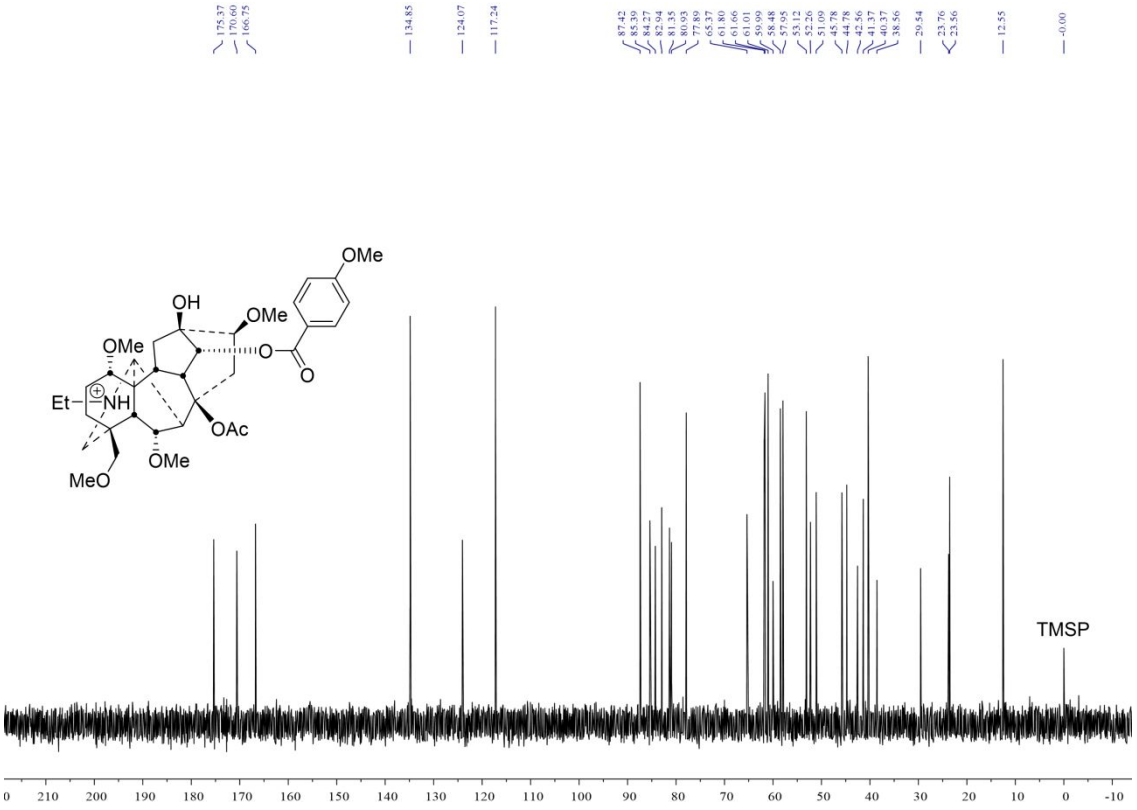

Figure S102. ^{13}C NMR spectrum of crassicauline A HCl salt (**15'**) in D_2O

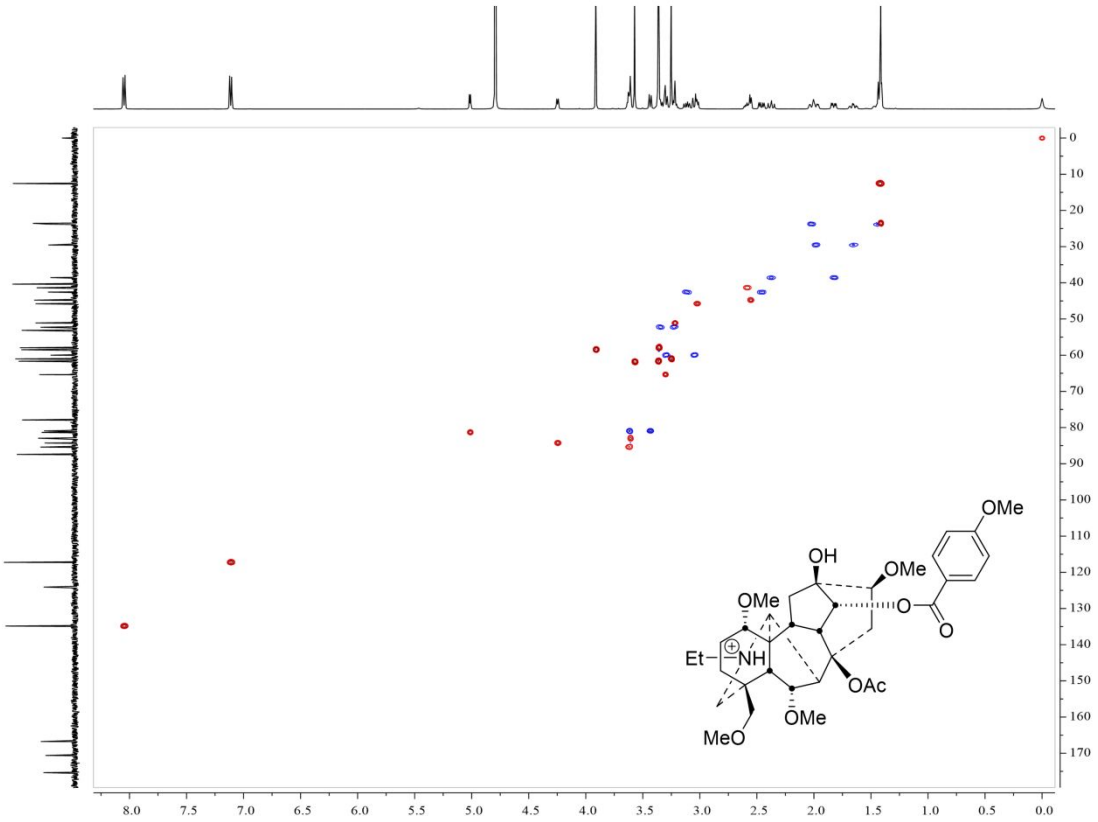

Figure S103. HSQC spectrum of crassicauline A HCl salt (**15'**) in D_2O

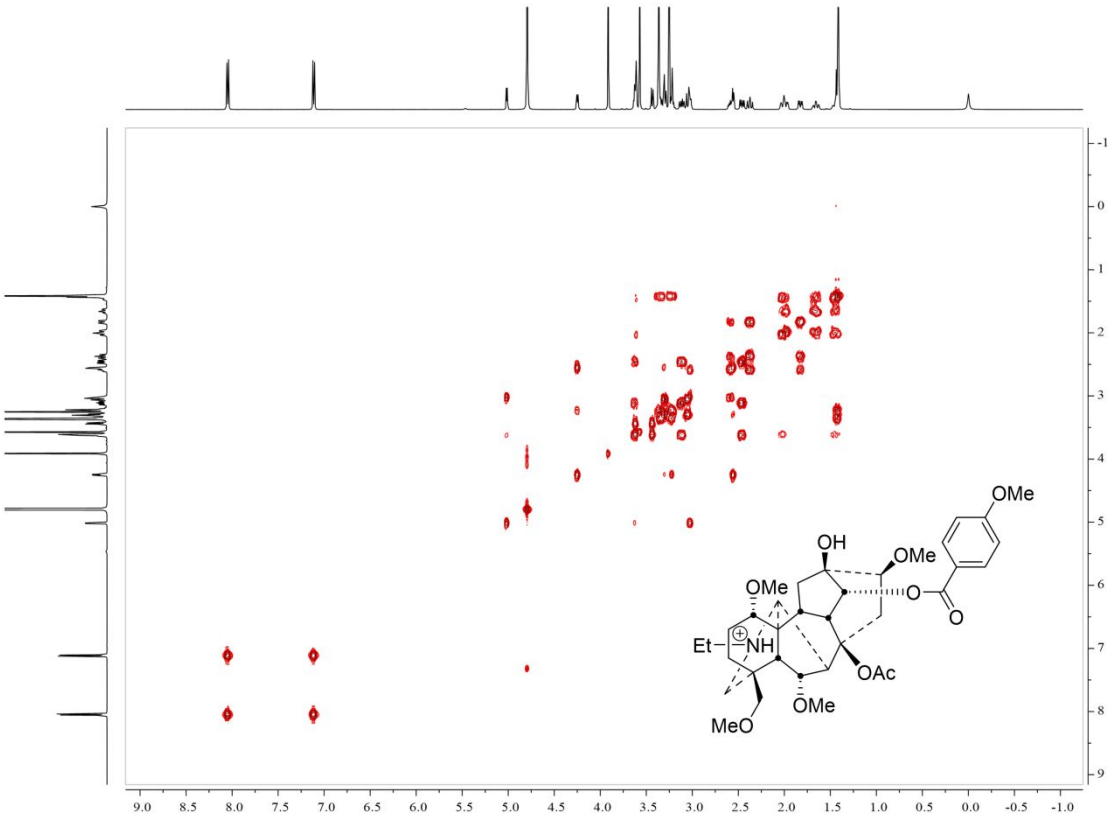

Figure S104. COSY spectrum of crassicauline A HCl salt (**15'**) in D_2O

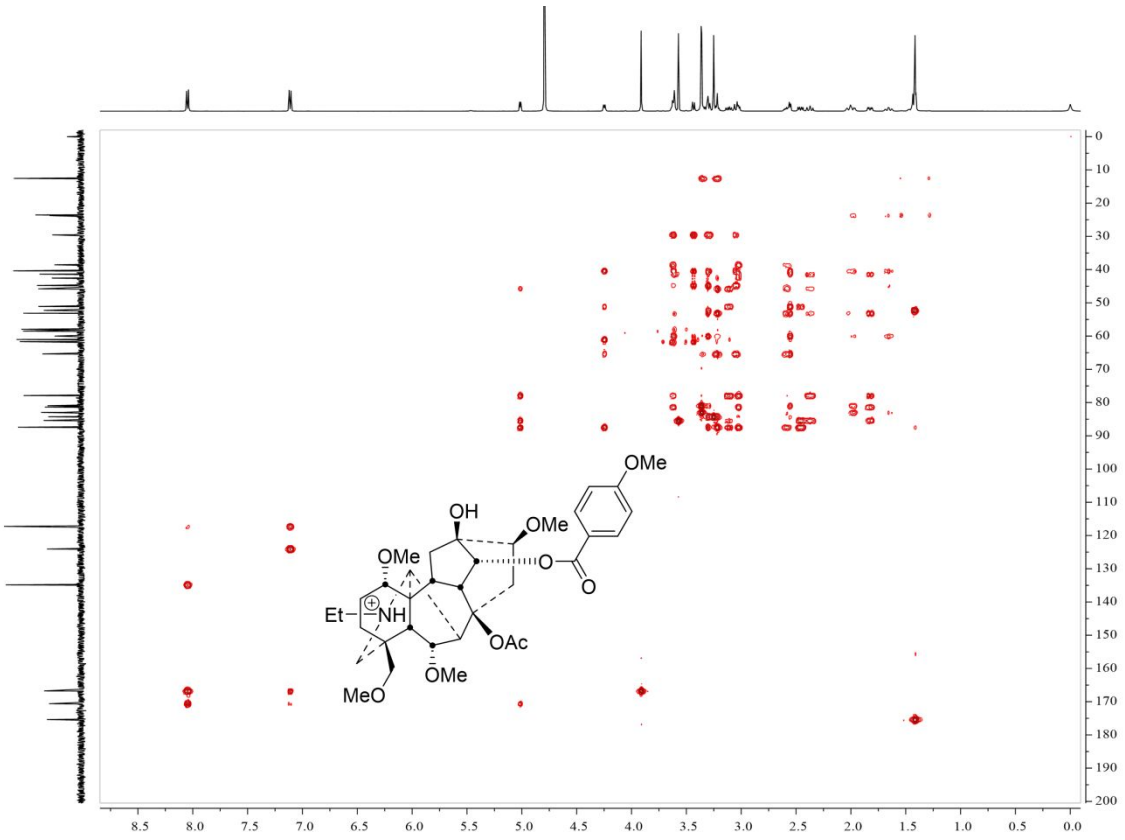

Figure S105. HMBC spectrum of crassicauline A HCl salt (**15'**) in D_2O

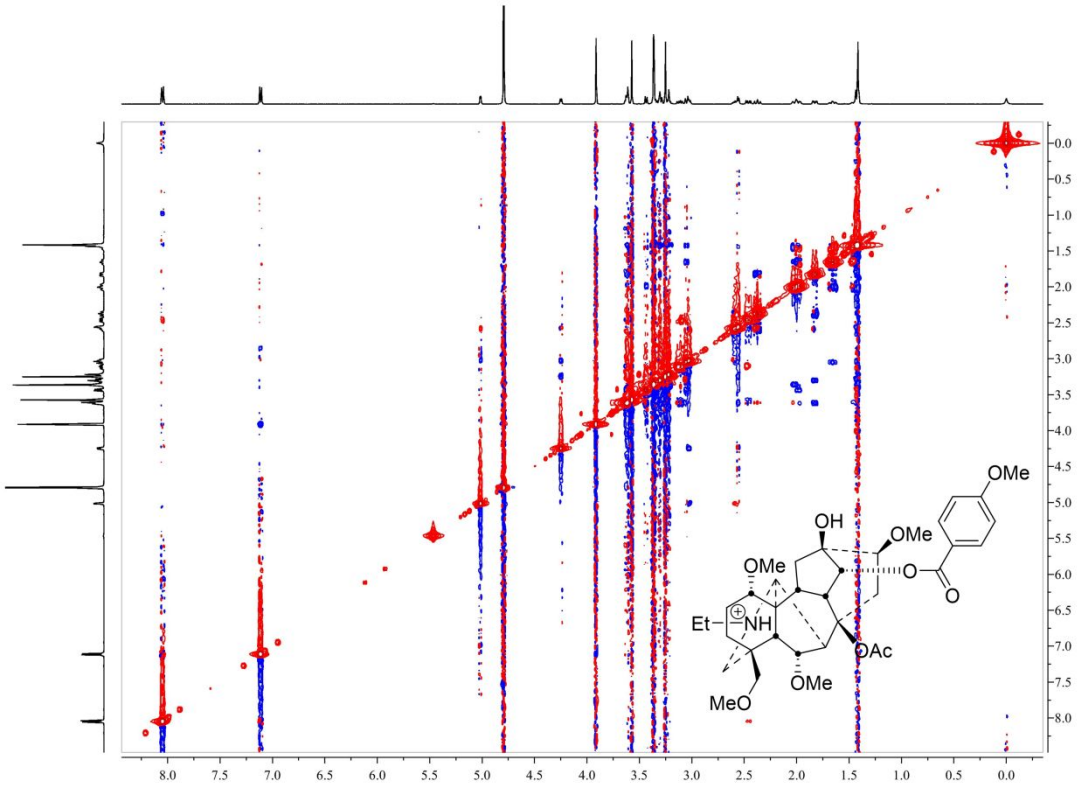

Figure S106. NOESY spectrum of crassicauline A HCl salt (**15'**) in D_2O

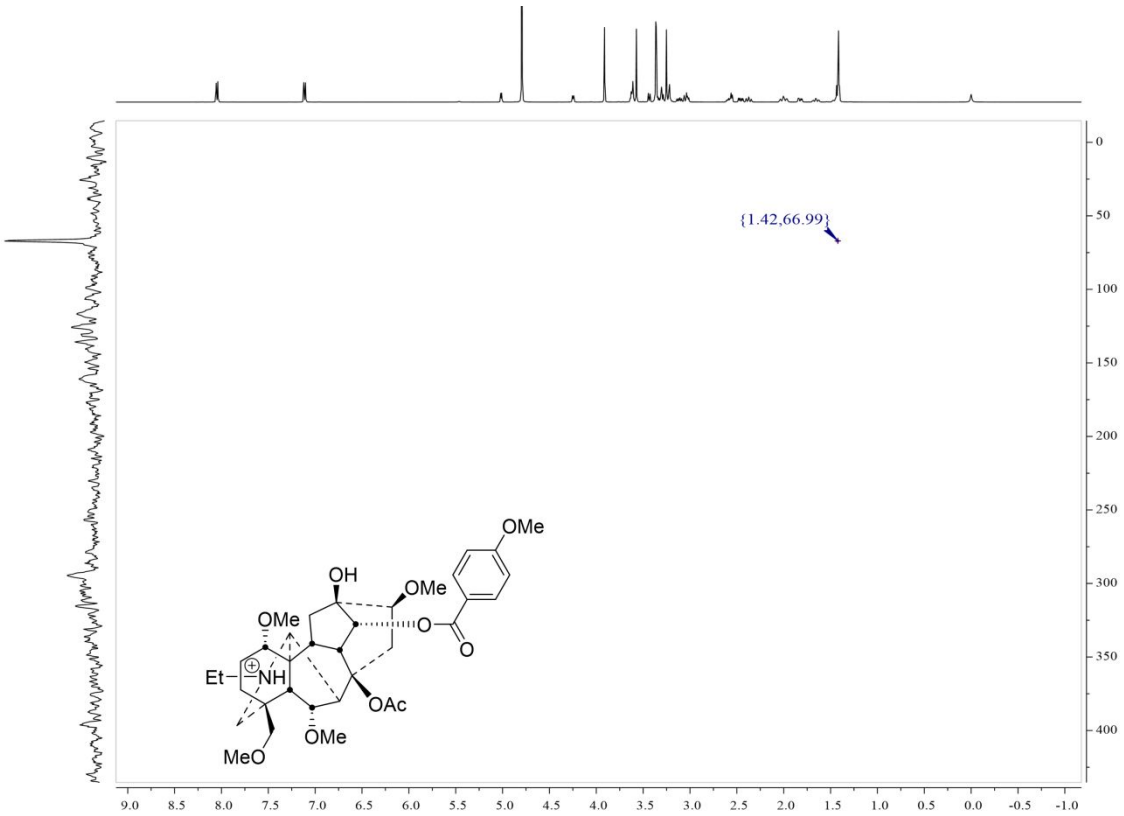

Figure S107. ^{1}H-^{15}N HMBC spectrum of crassicauline A HCl salt (**15'**) in D_2O

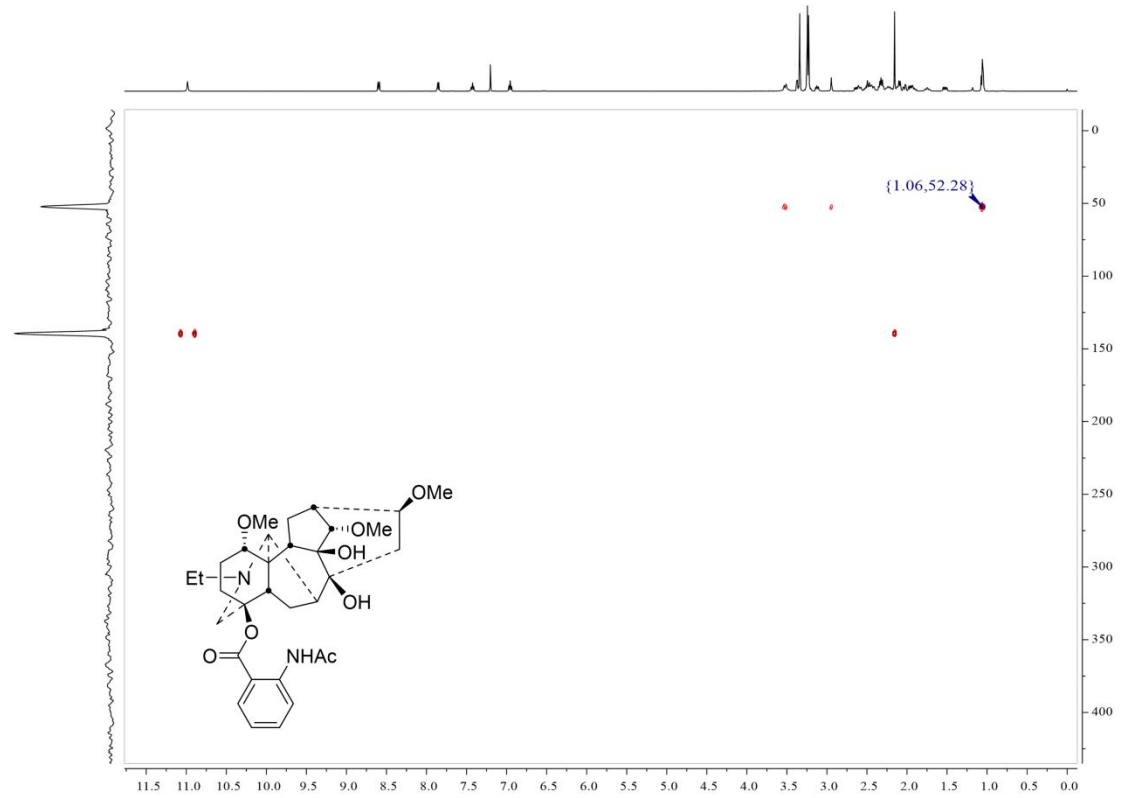

Figure S108. ^{1}H-^{15}N HMBC spectrum of lappaconitine (**16**) in $CDCl_3$

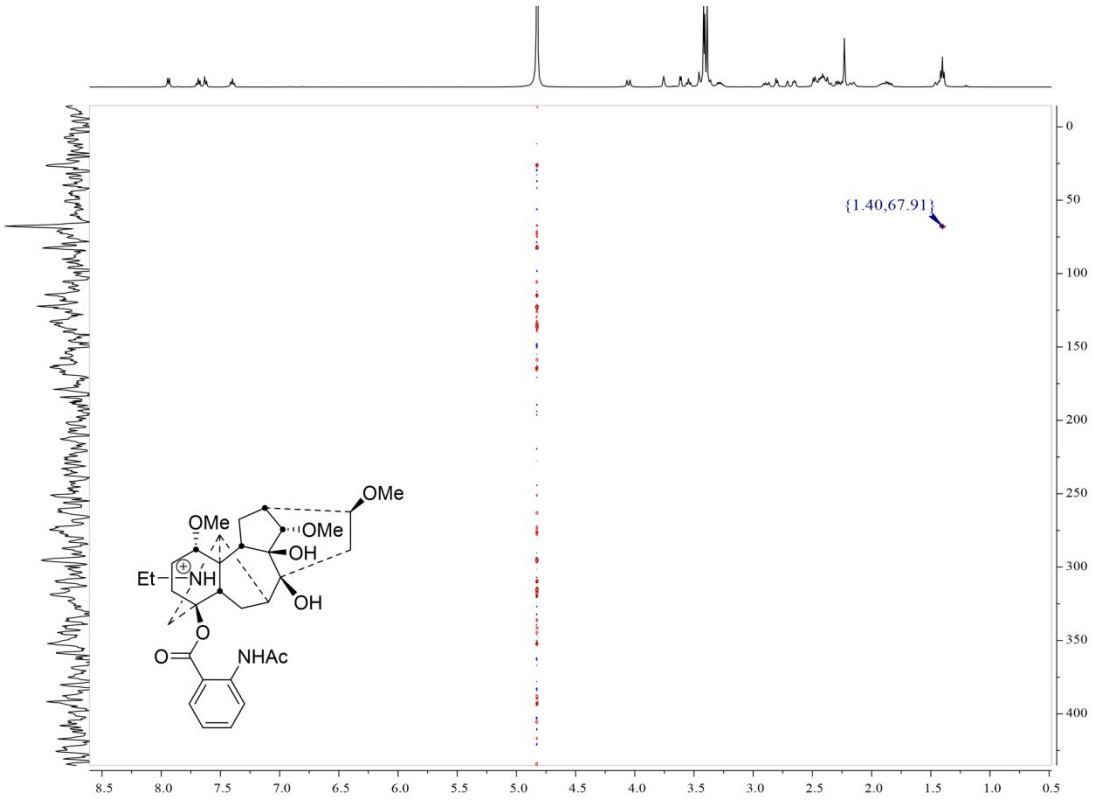

Figure S109. ^{1}H-^{15}N HMBC spectrum of lappaconitine HBr salt (**16'**) in D_2O (with additional 2 drops of d_6-DMSO)

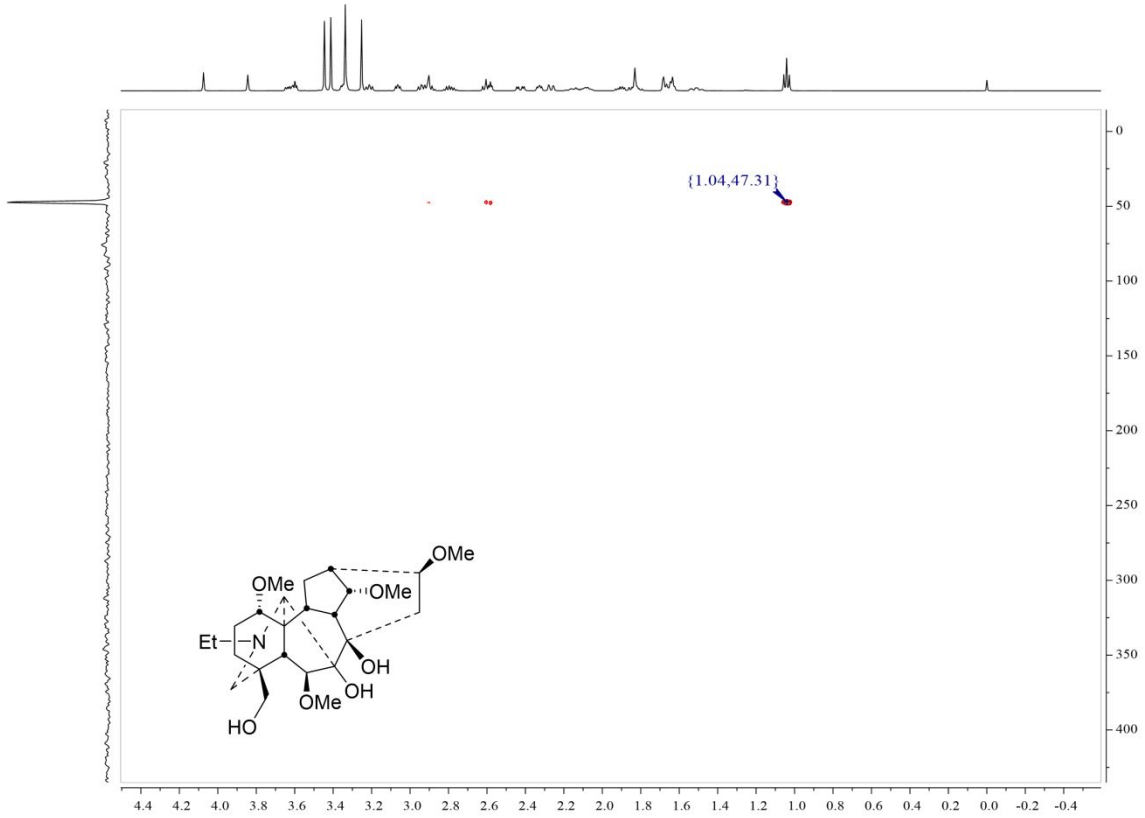

Figure S110. ^{1}H-^{15}N HMBC spectrum of lycoctonine (**17**) in $CDCl_3$

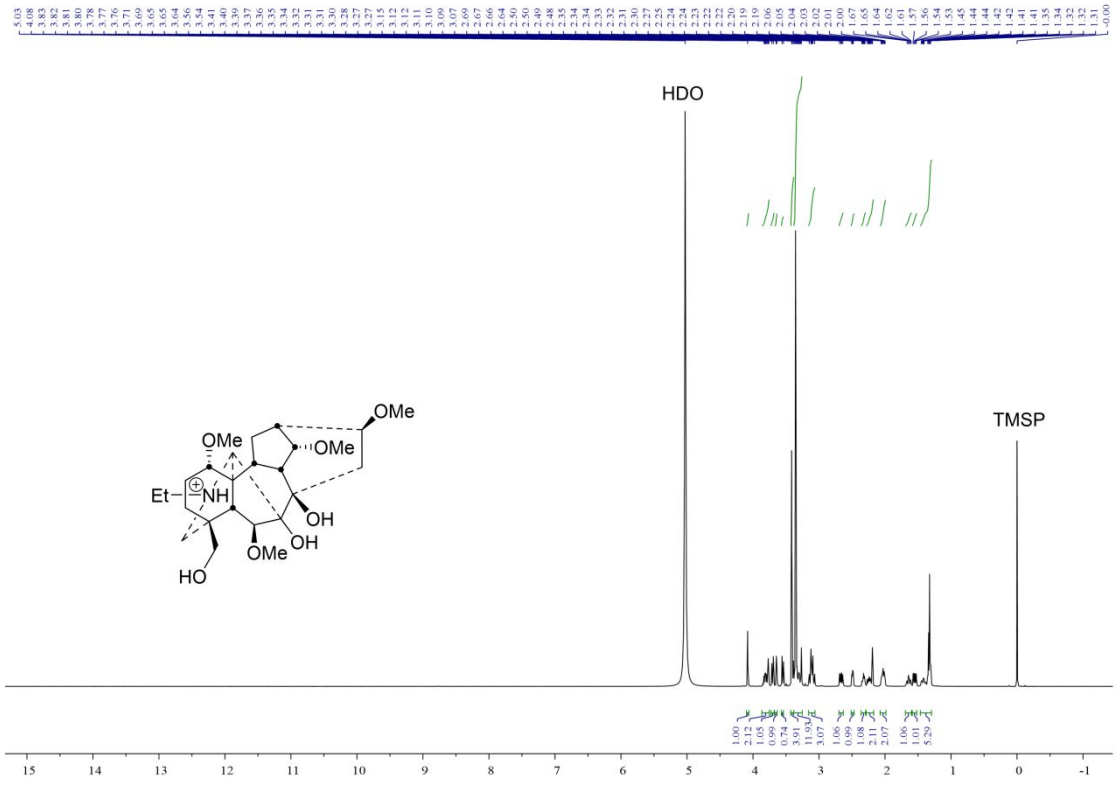

Figure S111. ^{1}H NMR spectrum of lycoctonine HCl salt (**17'**) in D_2O (with additional 2 drops of d_6-DMSO and drops of DCl in 35% in D_2O, pD ~2)

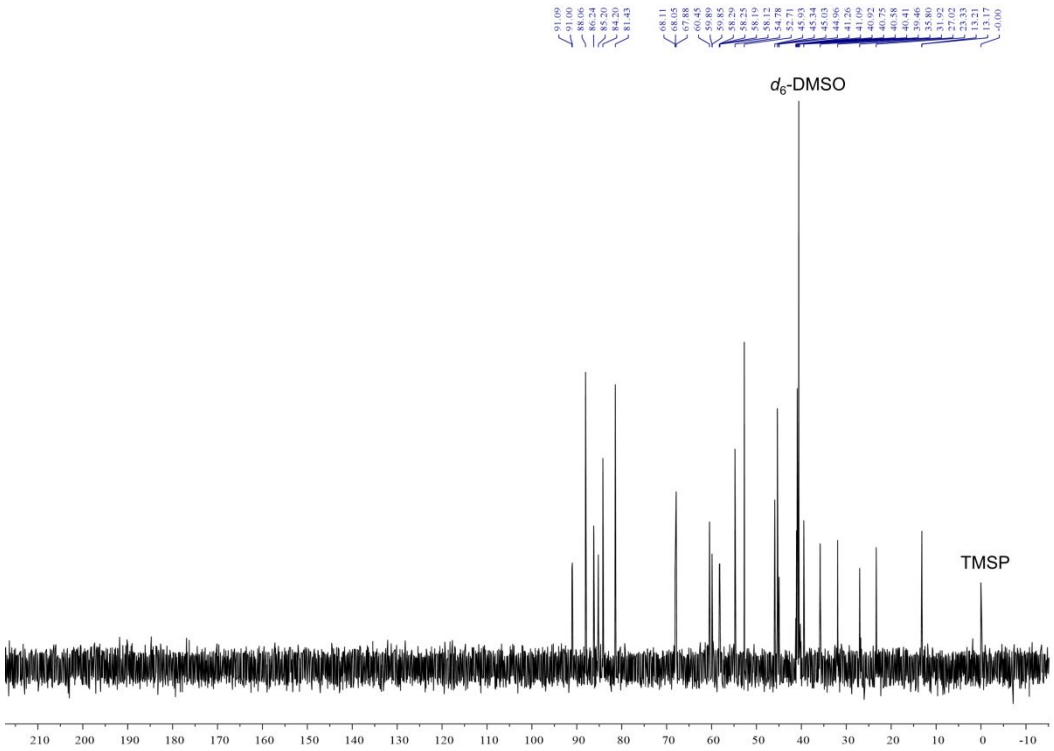

Figure S112. ^{13}C NMR spectrum of lycoctonine HCl salt (**17'**) in D_2O (with additional 2 drops of d_6-DMSO and drops of DCl in 35% in D_2O, pD ~2)

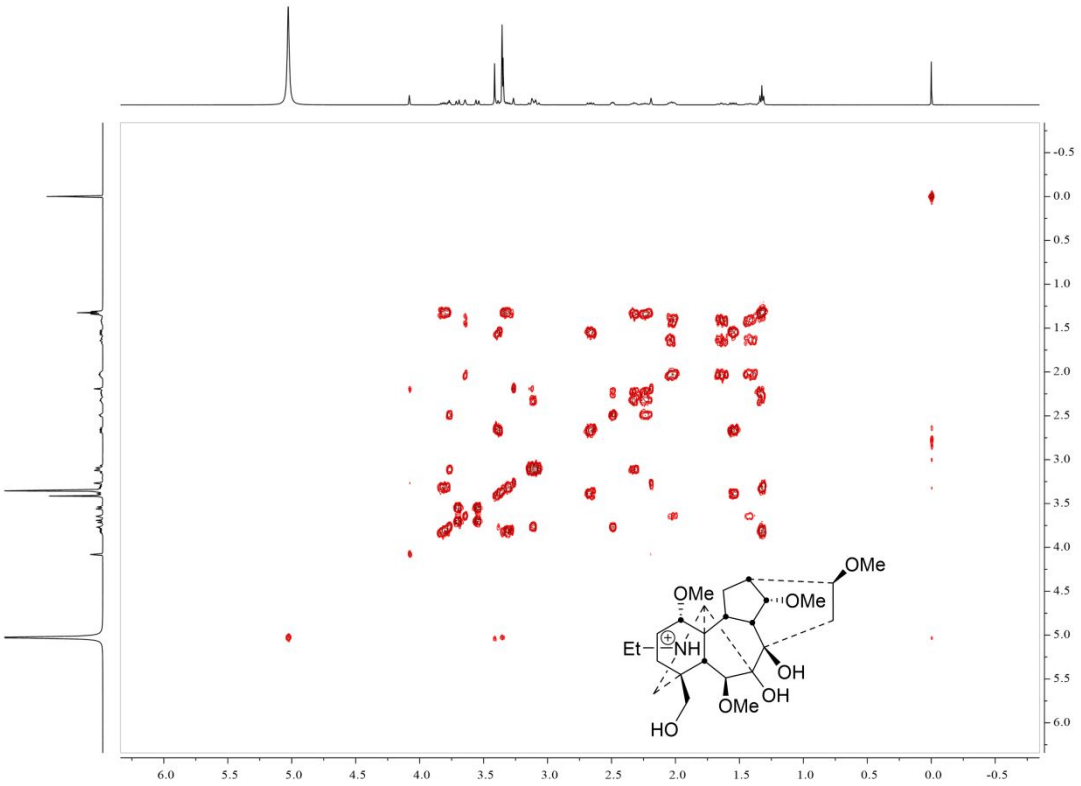

Figure S113. COSY spectrum of lycoctonine HCl salt (**17'**) in D_2O (with additional 2 drops of d_6-DMSO and drops of DCl in 35% in D_2O, pD ~2)

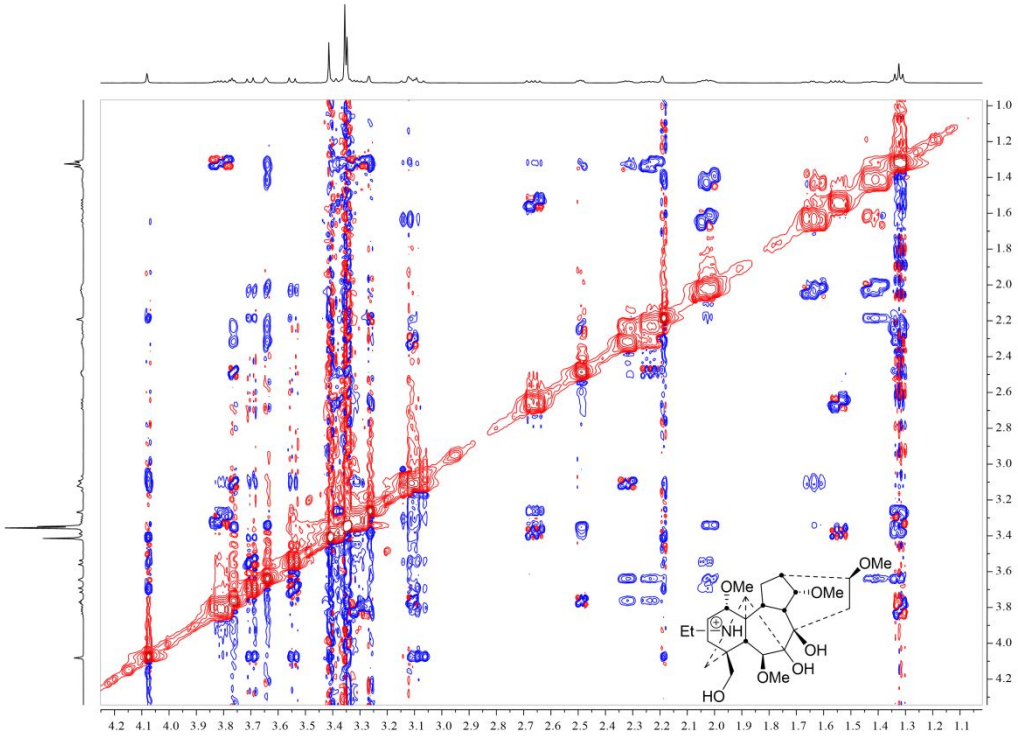

Figure S114. NOESY spectrum of lycoctonine HCl salt (**17'**) in D_2O (with additional 2 drops of d_6-DMSO and drops of DCl in 35% in D_2O, pD ~2)

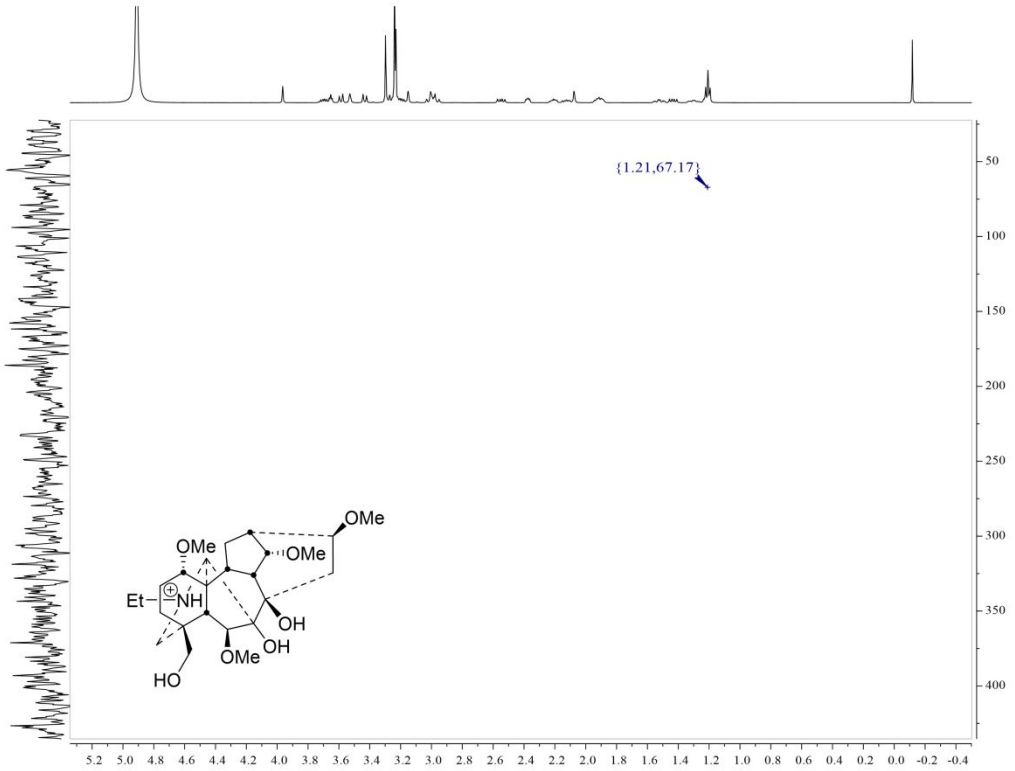

Figure S115. ^{1}H-^{15}N HMBC spectrum of lycoctonine HCl salt (**17'**) in D_2O (with additional 2 drops of d_6-DMSO and drops of DCl in 35% in D_2O, pD ~2)

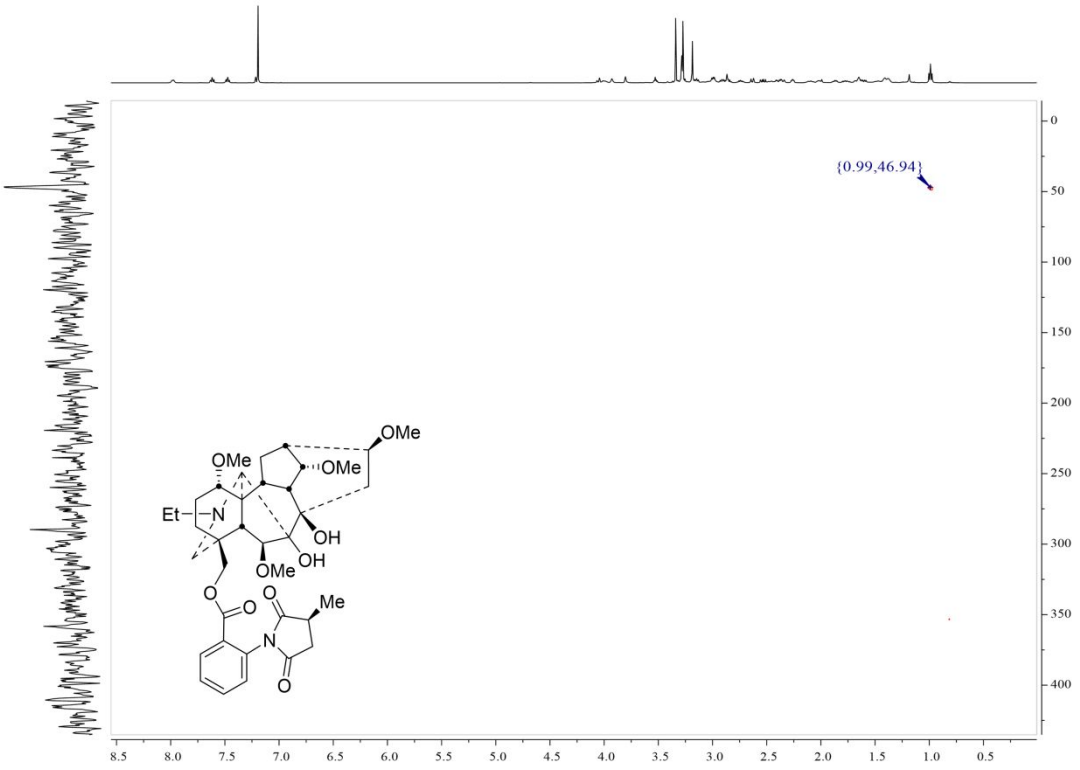

Figure S116. ^{1}H-^{15}N HMBC spectrum of MLA perchlorate (**18**) in $CDCl_3$

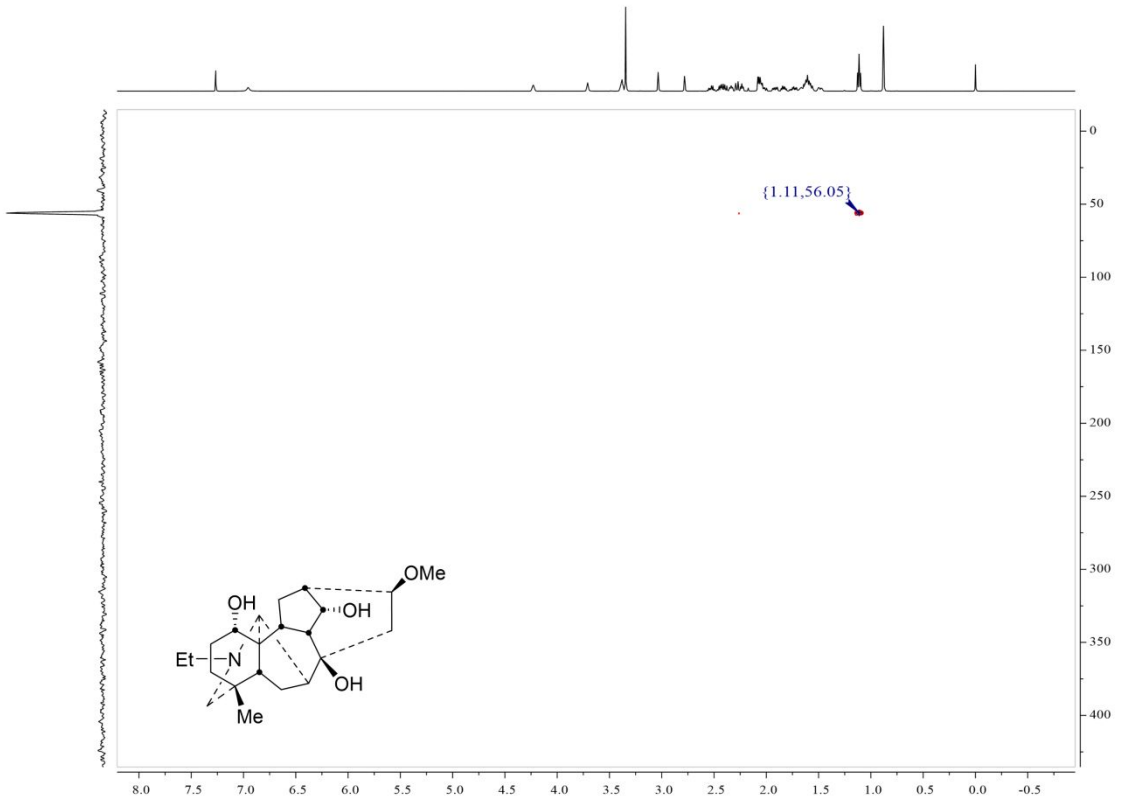

Figure S117. ^{1}H-^{15}N HMBC spectrum of karacoline (**19**) in $CDCl_3$

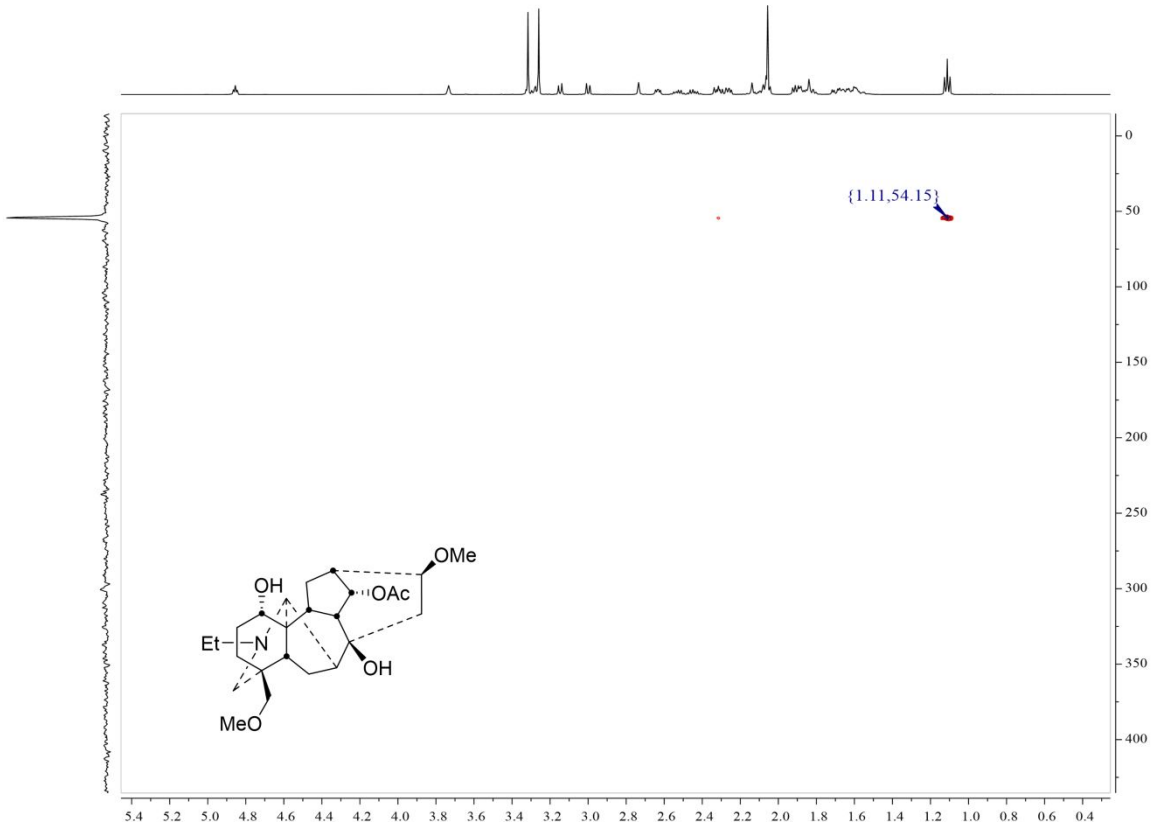

Figure S118. ^{1}H-^{15}N HMBC spectrum of condelphine (**20**) in $CDCl_3$

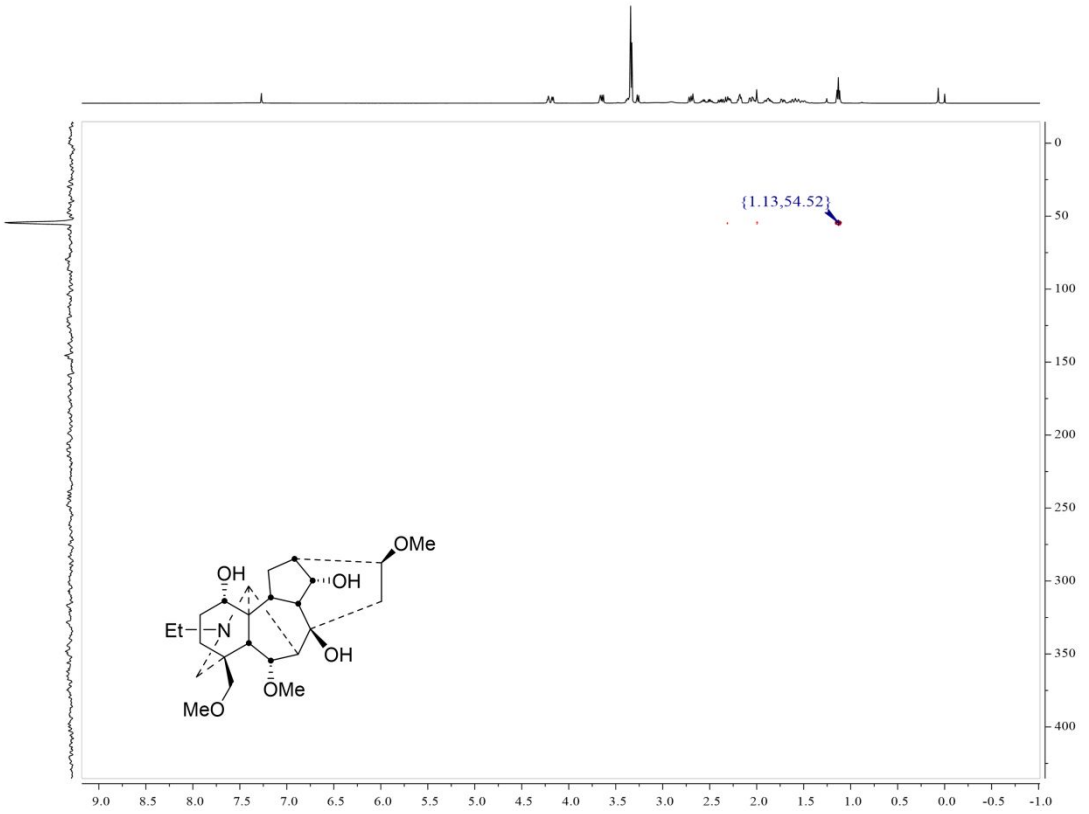

Figure S119. ^{1}H-^{15}N HMBC spectrum of neoline (**21**) in $CDCl_3$

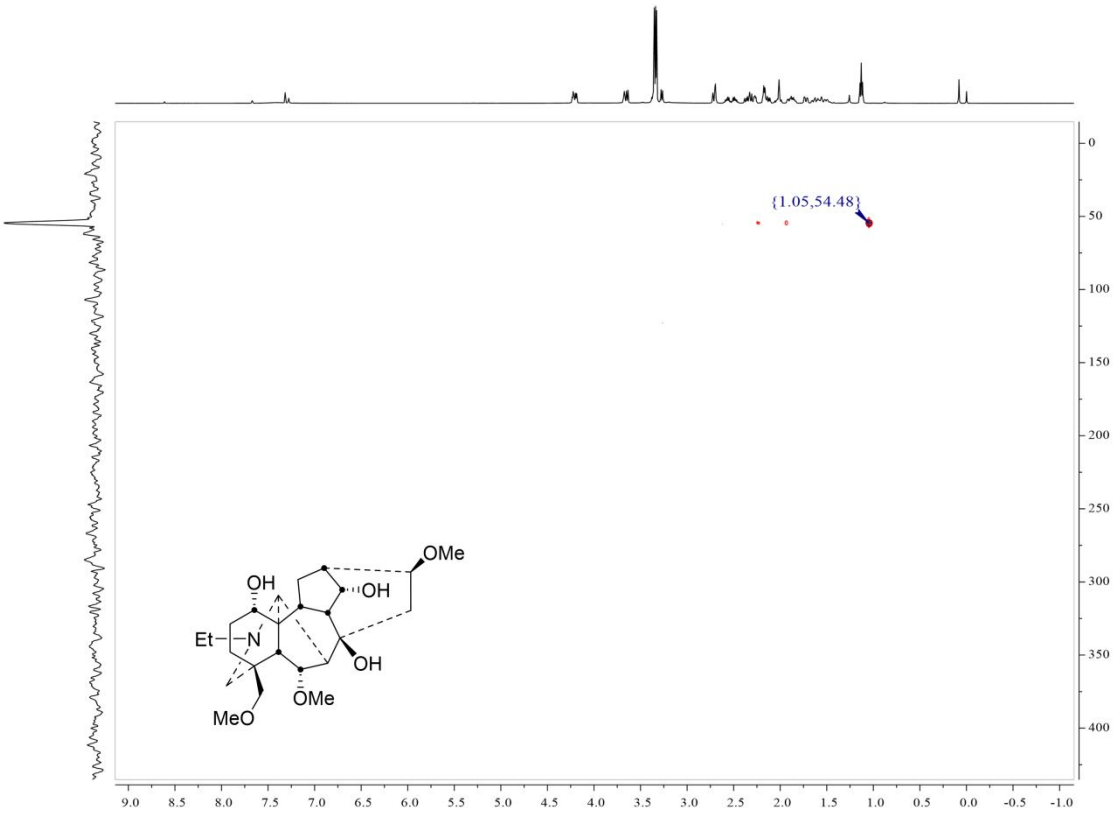

Figure S120. ^{1}H-^{15}N HMBC spectrum of neoline (**21**) in $CDCl_3$ with additional 2 drops of d_5-pyridine

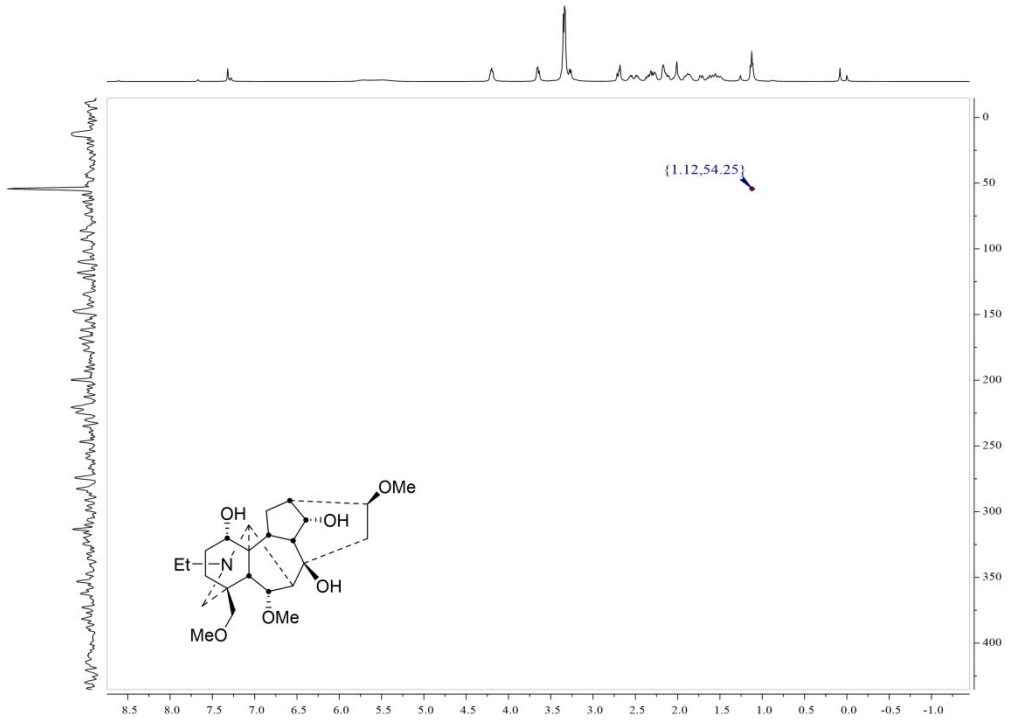

Figure S121. ^{1}H-^{15}N HMBC spectrum of neoline (**21**) in $CDCl_3$ with additional 2 drops of d_5-pyridine and 2 drops of NaOD solution (30% in D_2O, w/w)

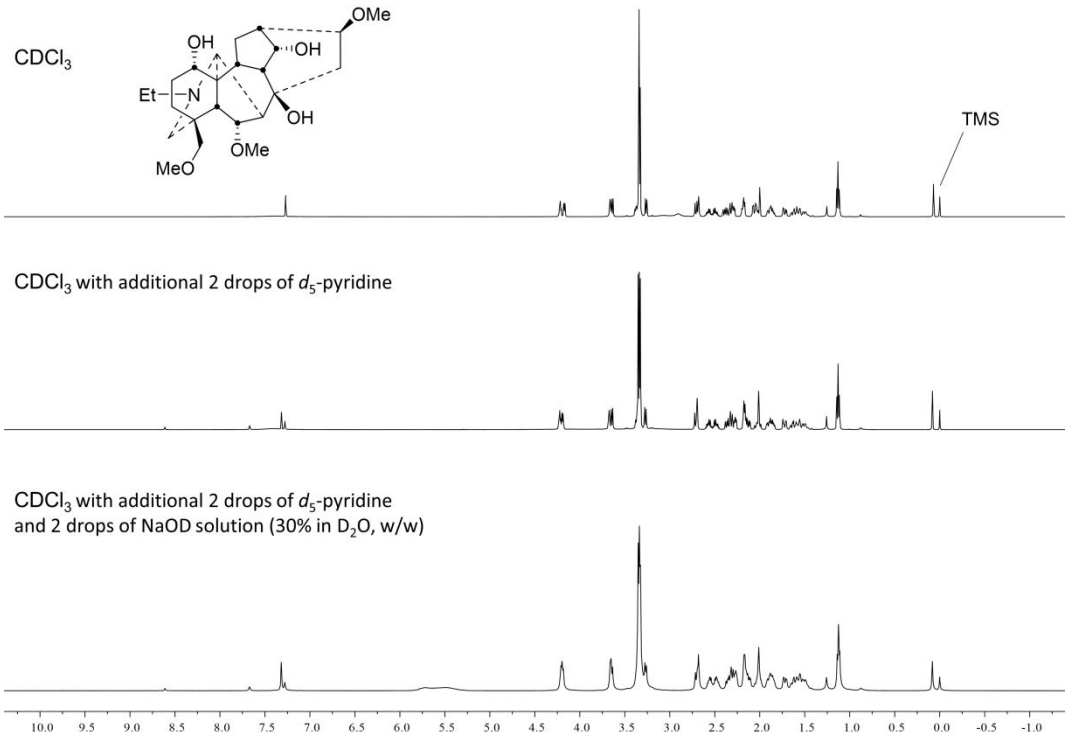

Figure S121. Comparison of ^{1}H NMR spectra between those of neoline (**21**) in $CDCl_3$, in $CDCl_3$ with additional 2 drops of d_5-pyridine, and in $CDCl_3$with additional 2 drops of d_5-pyridine and 2 drops of NaOD solution (30% in D_2O, w/w)