Supplementary Material for:

Patterned Recognitions of Amines and Ammonium Ions by a Pyridine-Based Helical Oligoamide Host

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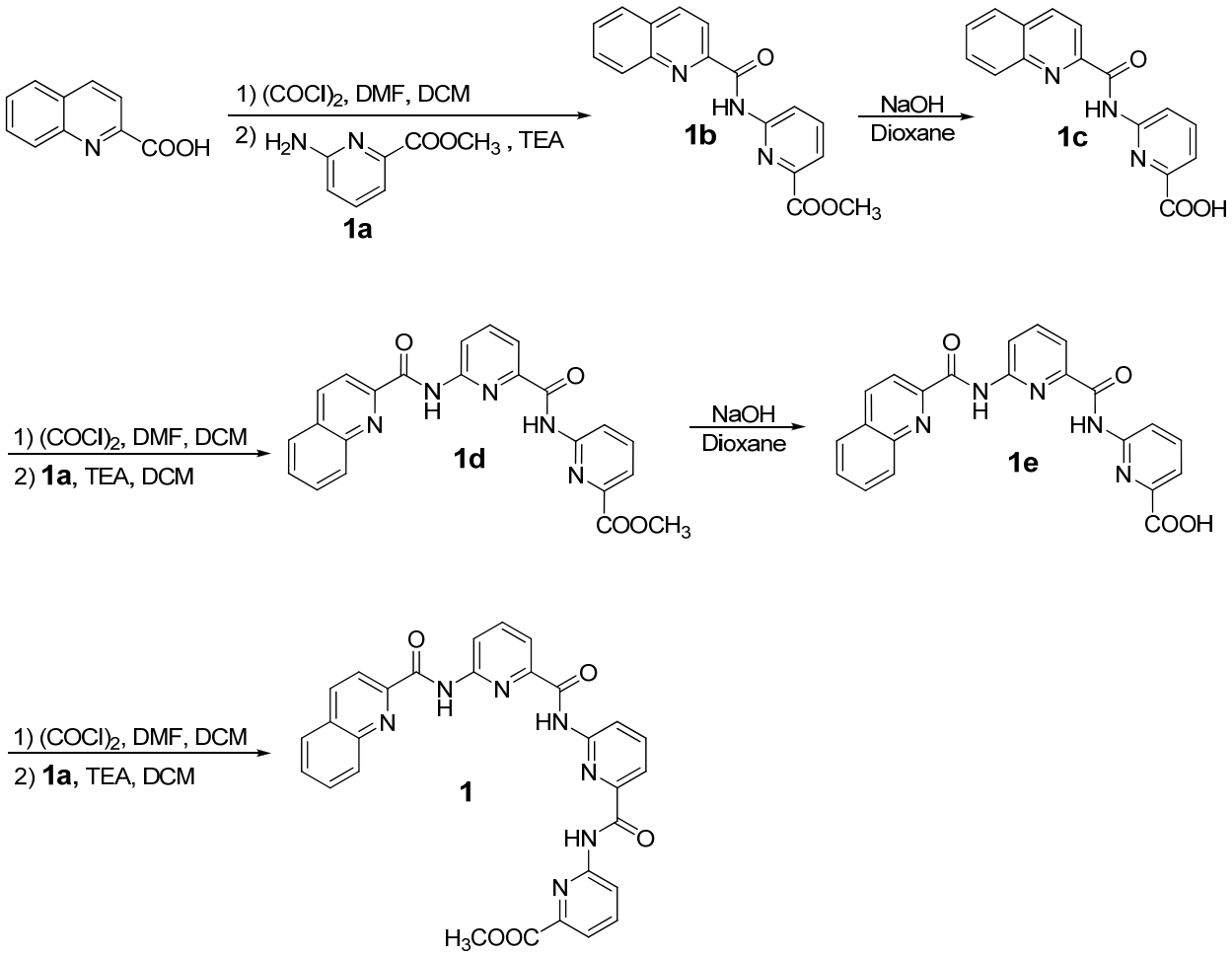
1. General Remarks

All the reagents were obtained from commercial suppliers and used as received unless otherwise stated. Aqueous solutions were prepared from distilled water. The organic solutions from all liquid extractions were dried over anhydrous sodium sulphate for a minimum of 15 minutes before filtration. Reactions were monitored by thin-layer chromatography (TLC) on silica gel pre-coated glass plates (0.25 mm thickness, 60F-254, E., Merck). Chemical yields refer to pure isolated substances. Melting point (mp) of the compounds was measured using Büchi Melting point B540. Mass spectra were obtained using instrumentation which includes Finnigan MAT95XL-T and Micromass VG7035. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AMX500 (500 MHz) spectrometer. In addition, key compounds were characterized by 2D NOESY and X-Ray Diffraction. The solvent signal of $CDCl_3$ and DMSO-d_6 in ^{1}H NMR were referenced at δ = 7.26 ppm and δ = 2.50 ppm respectively. Coupling constants (*J* values) are reported in Hertz (Hz). ^{1}H NMR data are recorded in the order: chemical shift value, multiplicity (s: singlet; d: doublet; t: triplet; q: quartet; m: multiplet; br: broad), coupling constant and number of protons that gave rise to the signal, where applicable. ^{13}C NMR spectra are proton-decoupled and the solvent peaks of $CDCl_3$ and DMSO-d_6 were referenced at δ = 77.0 ppm and 39.5 ppm respectively. 2D NMR experiments were recorded on a Bruker DRX500 (500 MHz) spectrometer, unless otherwise stated. $CDCl_3$ and DMSO-d_6 were purchased from Cambridge Isotope Laboratories, Inc. and used without further purification unless otherwise stated. 'Neutralized' $CDCl_3$ refer to $CDCl_3$ that was passed through a column of basic alumina to remove the DCl in the solvent.

2. Scheme S1. Synthetic Route that Affords Tetramer 1



3. Synthetic Procedures & Characterization

The synthesis of the **amine 1a** had been reported in the following journal article:

(1) Ong, W. Q.; Zhao, H.; Du, Z.; Yeh, J. Z. Y.; Ren, C.; Tan, L. Z. W.; Zhang, K.; Zeng, H. *Chem. Commun.* **2011**, *47*, 6416.

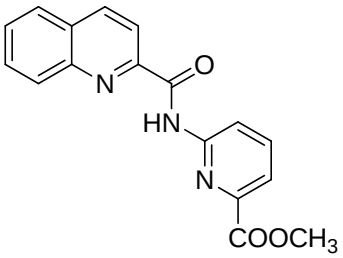
General procedure for coupling using oxalyl chloride:

The acid (1.0 mmol) was dissolved in dry dichloromethane (10ml) in a round bottom flask. DMF (0.1 ml) was added, followed by the dropwise addition of oxalyl chloride (2.0 mmol) into the round bottom flask. The reaction mixture was stirred for 2 hrs and the solvent and excess oxalyl chloride were removed *in vacuo* and dry dichloromethane (10 ml) was added to the acid chloride in nitrogen atmosphere. Minimal amount of dry dichloromethane was added to a mixture containing the amine (1.5 mmol) and triethylamine (2.0 mmol) and the mixture was injected into the acid chloride. The mixture was allowed to stir for 1 hr at room temperature and after the reaction, the product was washed with water (2 x 10ml), 1M HCl (2 x 10ml) and 1M NaOH (2 x 10ml). The solvent was removed *in vacuo* to give the crude product and subjected to either recrystallization or flash column chromatography to afford the pure product.

General procedure for hydrolysis using sodium hydroxide:

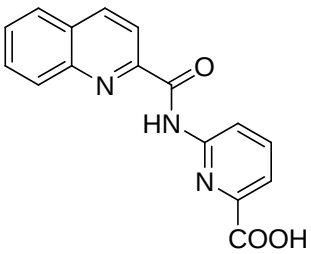
Solid NaOH (3.0 mmol) was dissolved in minimal amount of deionized water and was then added into the round bottom flask containing the ester (1.0 mmol) in dioxane (10 ml). The mixture was stirred at room temperature overnight and the solvent was then removed *in vacuo*.

Water (20 ml), MeOH (20 ml) and solid $KHSO_4$ (0.54 g, 4.0 mmol) was then added. The suspension was then filtered, washed and the residue obtained was dried to give the acid.



Compound 1b:

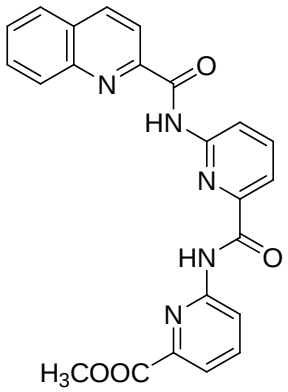
Melting Point: 218.5–219.0 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.90 (s, 1H), 8.74 (dd, 1H, J_d = 6.9 Hz, J_d = 2.7 Hz), 8.37 (s, 2H), 8.27 (d, 1H, *J* = 8.4 Hz), 7.90–7.95 (m, 3H), 7.82 (t, 1H, *J* = 8.0 Hz), 7.66 (t, 1H, *J* = 7.6 Hz), 4.04 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.40, 163.27, 151.46, 148.69, 146.48, 146.38, 139.30, 137.81, 130.48, 129.97, 129.57, 128.48, 127.69, 121.28, 118.63, 117.87, 52.99. HRMS-EI: calculated for $[M]^+$ ($C_{17}H_{13}N_3O_3$): *m/z* 307.0957, found: *m/z* 307.0958.



Compound 1c:

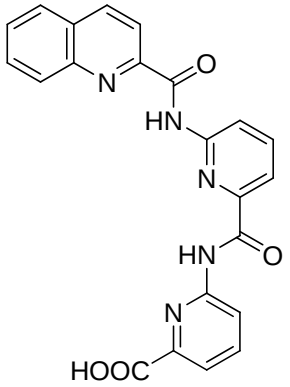
^{1}H NMR (500 MHz, DMSO-d_6): δ 13.33 (s, 1H), 10.68 (s, 1H), 8.66 (d, 1H, *J* = 8.9 Hz), 8.51 (d, 1H, *J* = 8.2 Hz), 8.29 (d, 2H, *J* = 8.9 Hz), 8.08–8.13 (m, 2H), 7.91 (t, 1H, *J* = 7.3 Hz), 7.86 (d,

1H, *J* = 7.6 Hz), 7.77 (t, 1H, *J* = 7.4 Hz). ^{13}C NMR (125 MHz, DMSO-d_6): δ 165.55, 162.33, 150.34, 148.40, 147.05, 145.75, 140.03, 138.67, 130.94, 129.28, 129.26, 128.72, 128.11, 120.86, 118.35, 116.57. HRMS-ESI: calculated for $[M+Na]^+$ ($C_{16}H_{11}N_3O_3{}^{23}Na$): *m/z* 316.0693, found: *m/z* 316.0696.



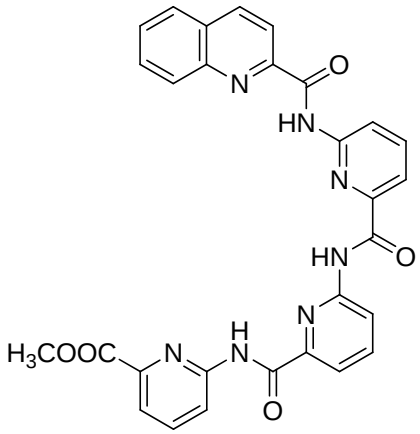
Compound 1d:

Melting Point: 244.5–245.0 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.80 (s, 1H), 10.46 (s, 1H), 8.71–8.76 (m, 2H), 8.49 (d, 1H, *J* = 8.3 Hz), 8.39 (s, 2H), 8.09 (d, 1H, *J* = 6.2 Hz), 8.00 (t, 1H, *J* = 7.9 Hz), 7.91–7.94 (m, 3H), 7.82–7.85 (m, 1H), 7.66–7.70 (m, 1H), 4.07 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.39, 163.26, 162.76, 151.48, 150.23, 148.65, 147.47, 146.58, 146.23, 140.00, 139.43, 137.97, 130.40, 130.33, 129.67, 128.58, 127.70, 121.48, 118.88, 118.70, 118.22, 117.63, 53.13. HRMS-EI: calculated for $[M]^+$ ($C_{23}H_{17}N_5O_4$): *m/z* 427.1281, found: *m/z* 427.1295.



Compound 1e:

^{1}H NMR (500 MHz, DMSO-d_6): δ 13.37 (br, 1H), 11.21 (s, 1H), 10.72 (s, 1H), 8.67 (d, 1H, *J* = 8.4 Hz), 8.58 (d, 1H, *J* = 8.3 Hz), 8.49 (d, 1H, *J* = 8.4 Hz), 8.29–8.34 (m, 2H), 8.19 (t, 1H, *J* = 7.8 Hz), 8.14 (d, 1H, *J* = 8.0 Hz), 8.09 (t, 1H, *J* = 8.0 Hz), 7.99 (d, 1H, *J* = 7.7 Hz), 7.95 (t, 1H, *J* = 7.5 Hz), 7.87 (d, 1H, *J* = 7.0 Hz), 7.78 (t, 1H, *J* = 7.3 Hz). ^{13}C NMR (125 MHz, DMSO-d_6): δ 165.67, 163.24, 162.34, 150.64, 149.98, 149.01, 147.40, 147.23, 145.88, 140.56, 139.79, 138.46, 130.86, 129.37, 129.18, 128.65, 128.16, 120.90, 118.73, 118.35, 117.40, 117.12. HRMS-EI: calculated for $[M]^+$ ($C_{22}H_{15}N_5O_4$): *m/z* 413.1124, found: *m/z* 413.1133.



Compound 1:

Melting Point: 266.4–267.0 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.92 (s, 1H), 10.48 (s, 1H), 10.42 (s, 1H), 8.78 (d, 1H, J = 8.6 Hz), 8.73 (dd, 1H, J_d = 6.8 Hz, J_d = 2.8 Hz), 8.69 (d, 1H, J = 8.2 Hz), 8.39 (s, 2H), 8.36 (d, 1H, J = 8.3 Hz), 7.90–8.13 (m, 7H), 7.63–7.72 (m, 2H), 3.63 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.22, 163.20, 162.72, 151.44, 150.27, 150.10, 148.68, 147.56, 147.45, 146.47, 146.30, 140.06, 140.00, 139.37, 137.91, 130.31, 129.61, 128.48, 127.64, 121.43, 118.93, 118.87, 118.71, 118.15, 117.86, 117.73, 52.76. HRMS-EI: calculated for $[M]^+$ ($C_{29}H_{21}N_7O_5$): *m/z* 547.1604, found: *m/z* 547.1611.

4. (a) 2D NOESY Spectra of Tetramer 1

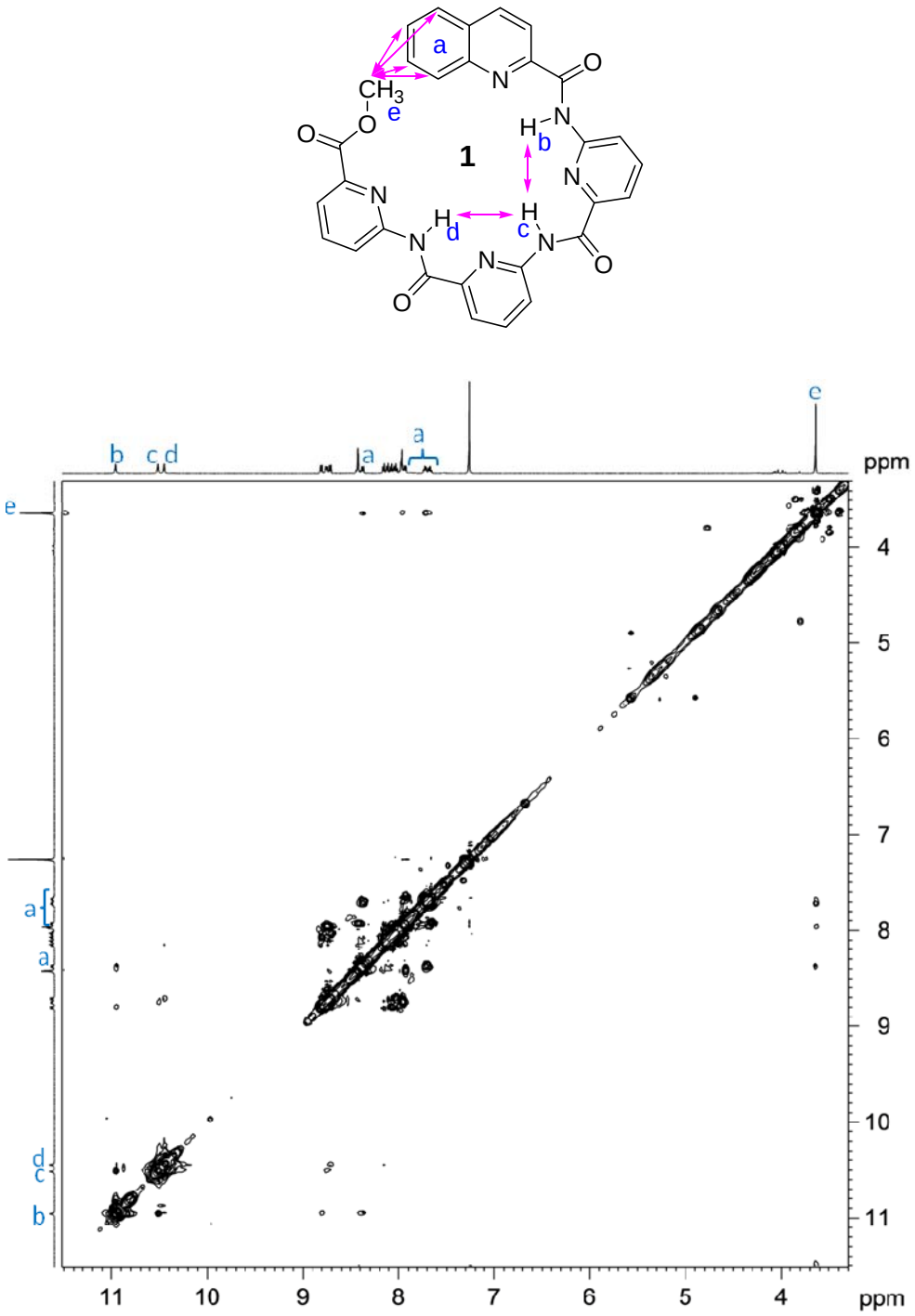


Figure S1. 2D NOESY spectrum containing NOE contacts seen in **1** as revealed by 2D NOESY study (5 mM, 300 K, $CDCl_3$, AMX 500 MHz, mixing time = 500 ms).

(b) 2D NOESY Spectra of Tetramer 1 + Octylamine

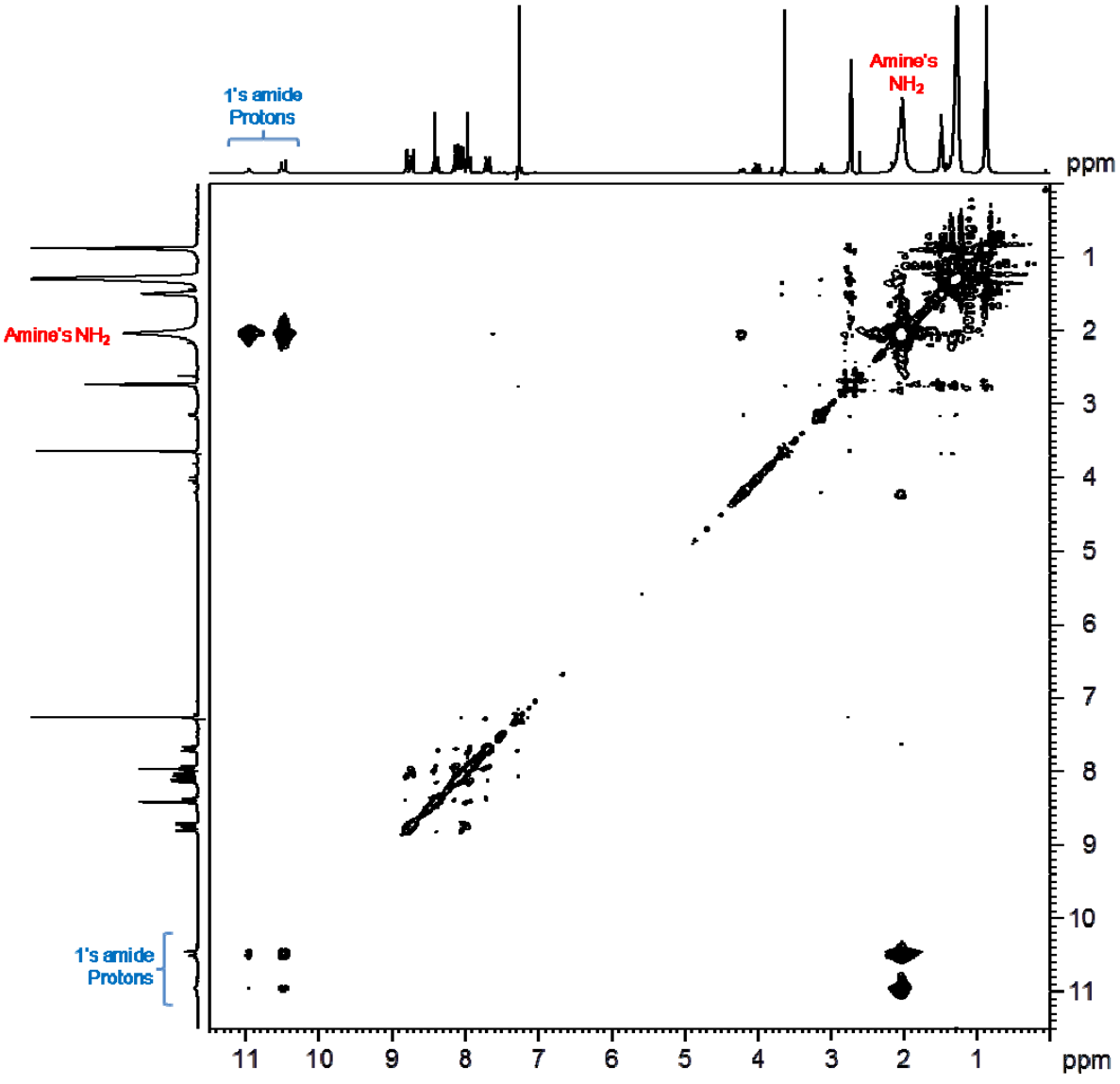


Figure S2. 2D NOESY spectrum containing NOE contacts seen in host **1** even in the presence of octylamine guest as revealed by 2D NOESY study (5 mM, 300 K, $CDCl_3$, AMX 500 MHz, mixing time = 500 ms). The large cross peaks observed between amine's NH_2 protons and amide protons highly likely should arise from the chemical exchange. The persistence of the folded structure by **1** can be seen from the NOEs among the amide protons and their large chemical shift values.

(c) 2D NOESY Spectra of Tetramer 1 + Piperidine

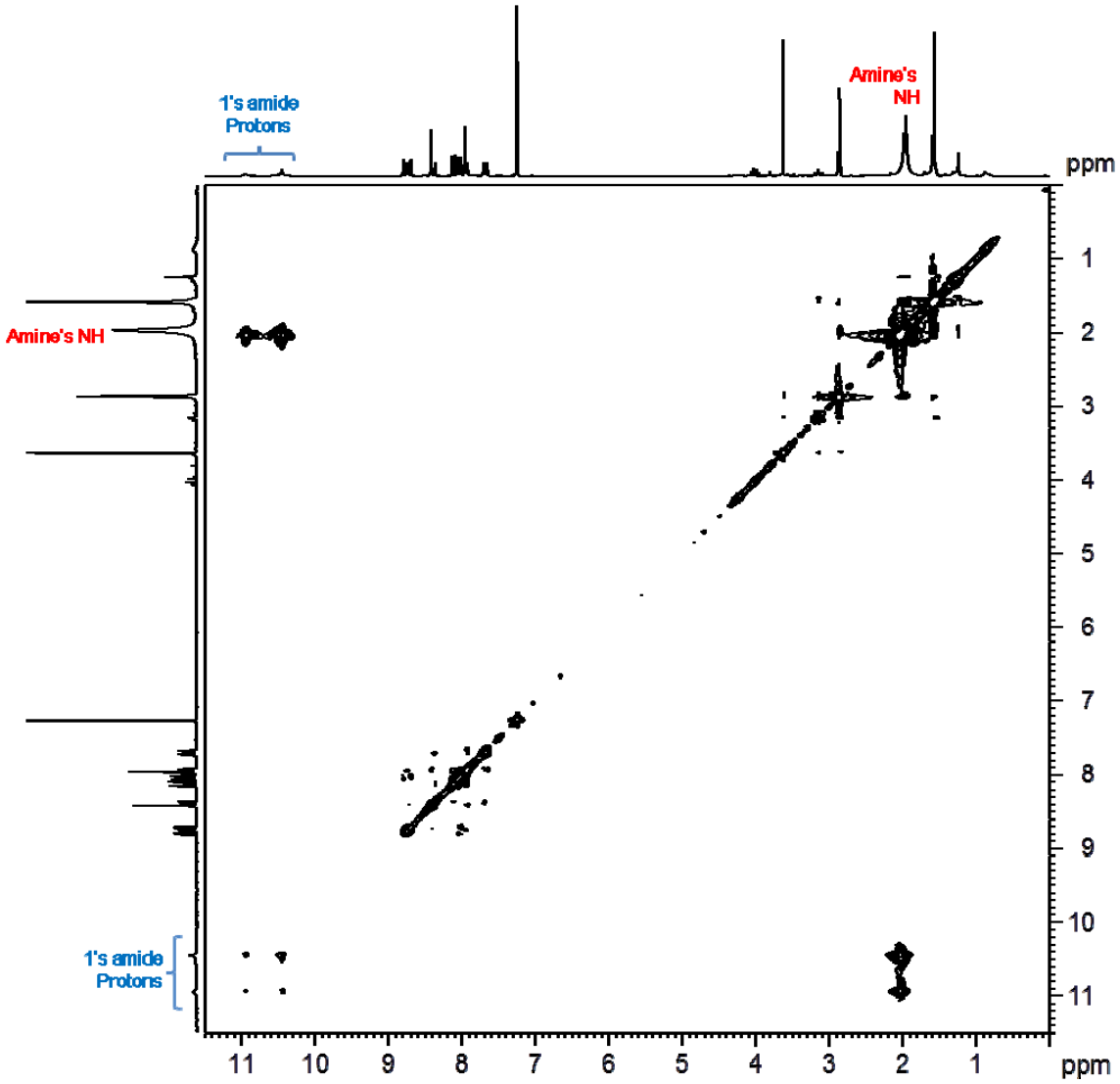


Figure S3. 2D NOESY spectrum containing NOE contacts seen in host **1** even in the presence of piperidine guest as revealed by 2D NOESY study (5 mM, 300 K, $CDCl_3$, AMX 500 MHz, mixing time = 500 ms). The large cross peaks observed between amine's NH_2 protons and amide protons highly likely should arise from the chemical exchange. The persistence of the folded structure by **1** can be seen from the NOEs among the amide protons and their large chemical shift values.

5. Titration ^{1}H NMR Spectra of Oligoamide 1 with Various Guests

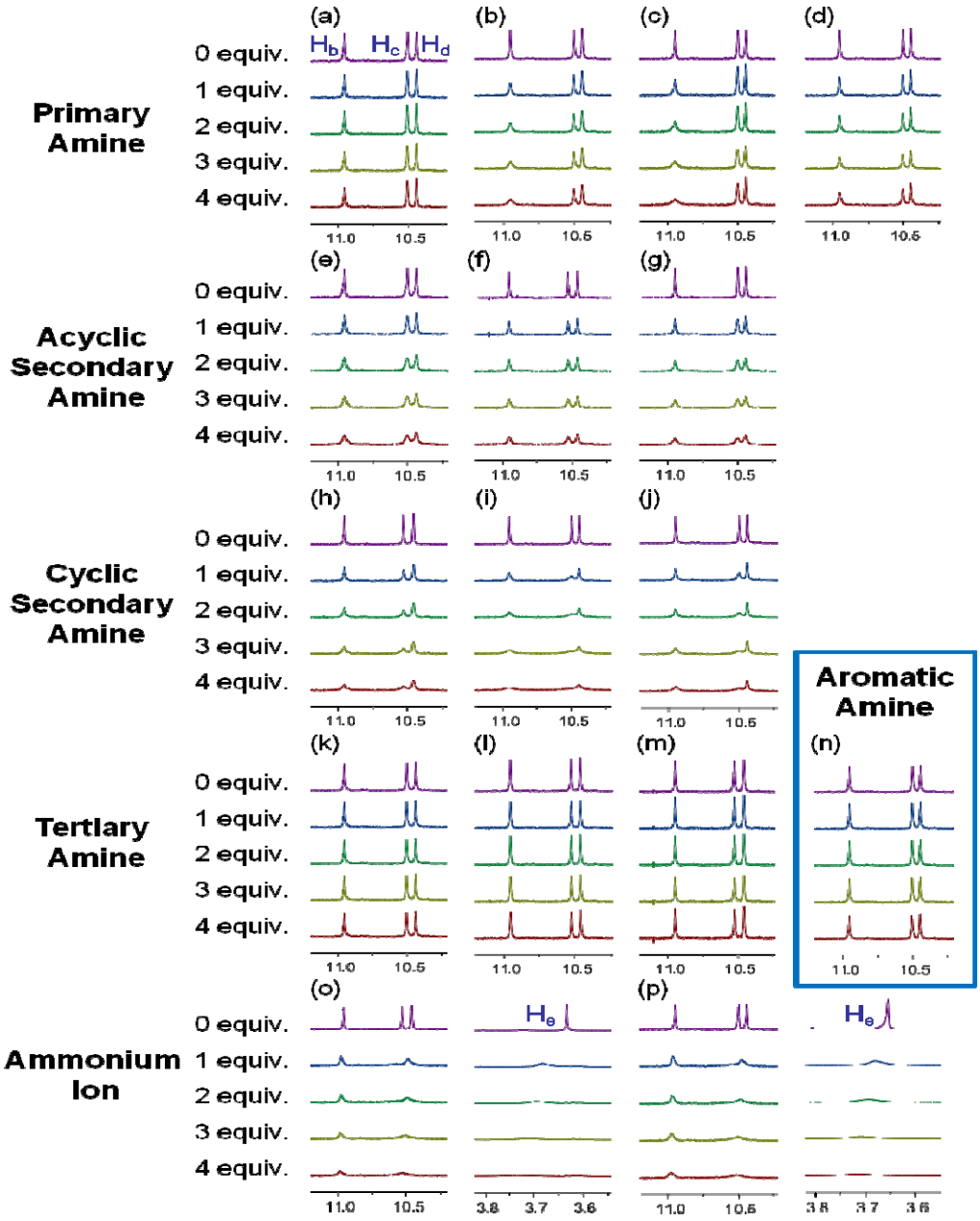


Figure S4. Overview of the expanded ^{1}H NMR (2 mM, "normal" $CDCl_3$) fingerprint regions for amide protons *b*-*d* and ester methyl protons *e* of **1** in the presence of up to four equivalents of (a) isopropylamine, (b) 1-aminooctane, (c) 1,8-diaminooctane, (d) 2,2'-(ethylenedioxy)-bis(ethylamine), (e) di-*n*-propylamine, (f) di-*n*-hexylamine, (g) di-*n*-octylamine, (h) azetidine, (i) pyrrolidine, (j) piperidine, (k) triethylamine, (l) diisopropylethylamine, (m) 1-methylpiperidine, (n) aniline, (o) 1-octylammonium perchlorate and (p) di-*n*-octylammonium perchlorate.

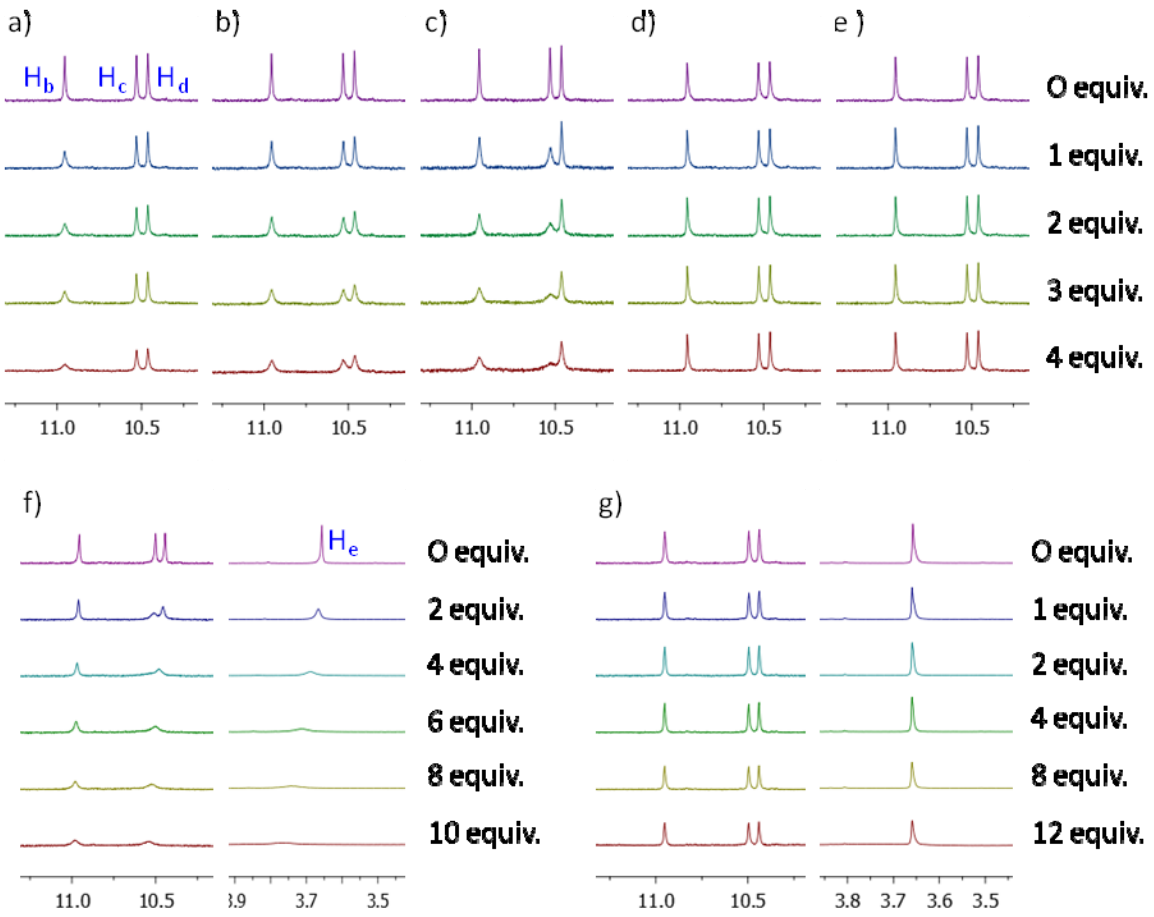


Figure S5. Representative ^{1}H NMR (2 mM, 'neutralized' $CDCl_3$ treated with basic alumina) fingerprint regions for amide protons *b*-*d* and ester methyl protons *e* of **1** in the presence of up to four equivalents of a) 1-octylamine, b) di-*n*-octylamine, c) piperidine, d) triethylamine, e) aniline or up to ten and twelve equivalents of f) 1-octylammonium perchlorate and g) di-*n*-octylammonium perchlorate respectively.

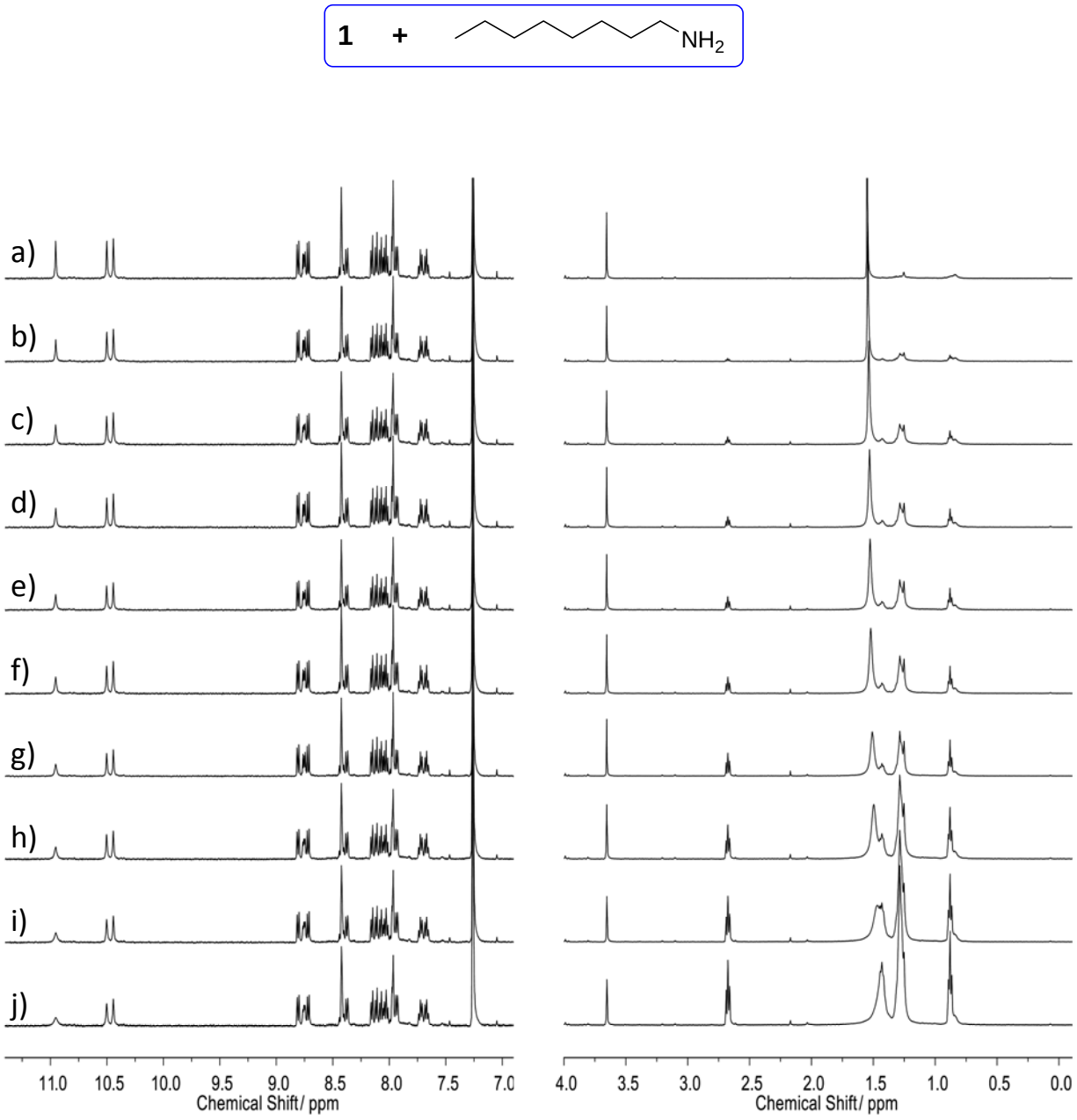


Figure S6. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of 1-octylamine.

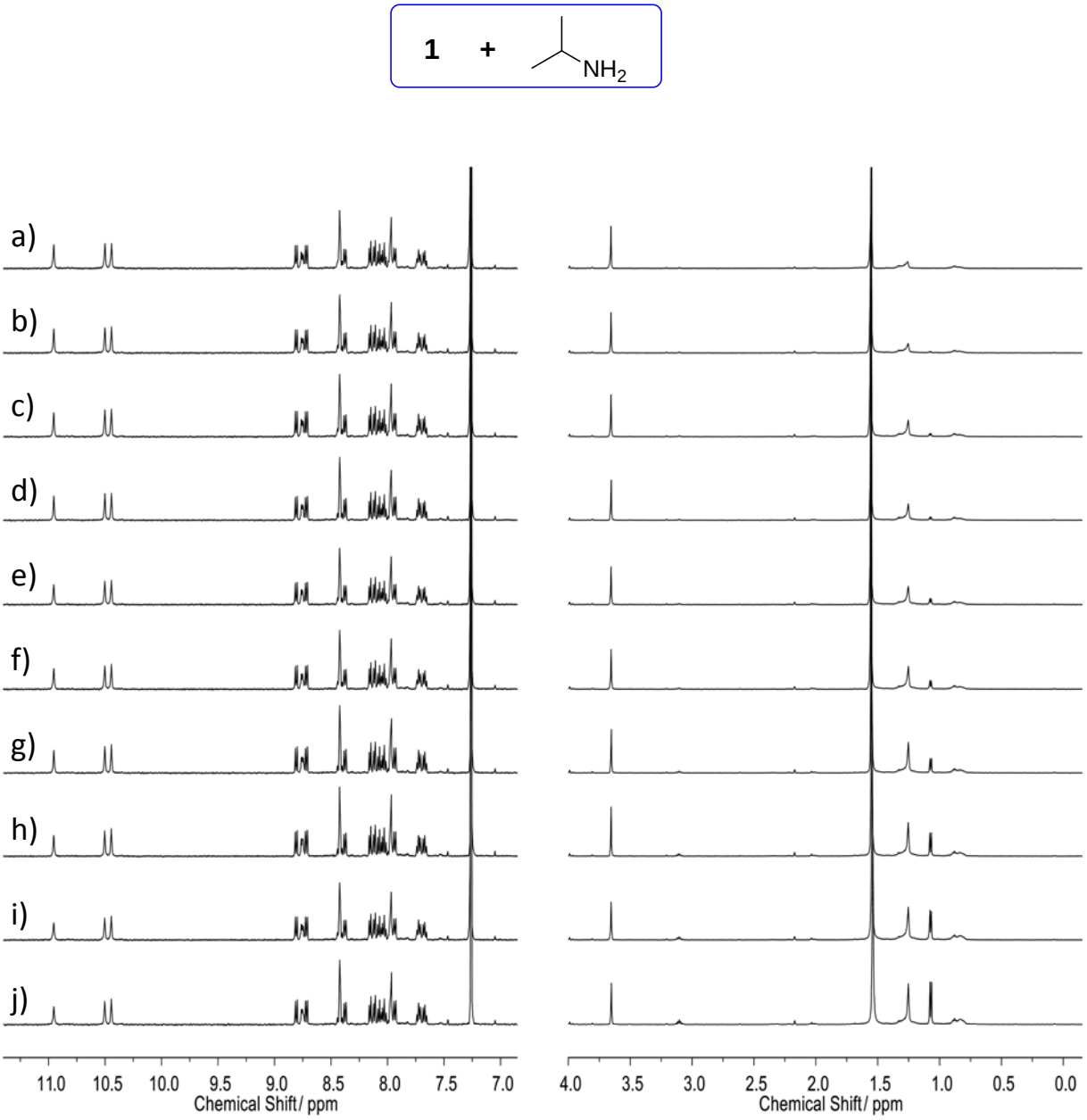


Figure S7. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of isopropylamine.

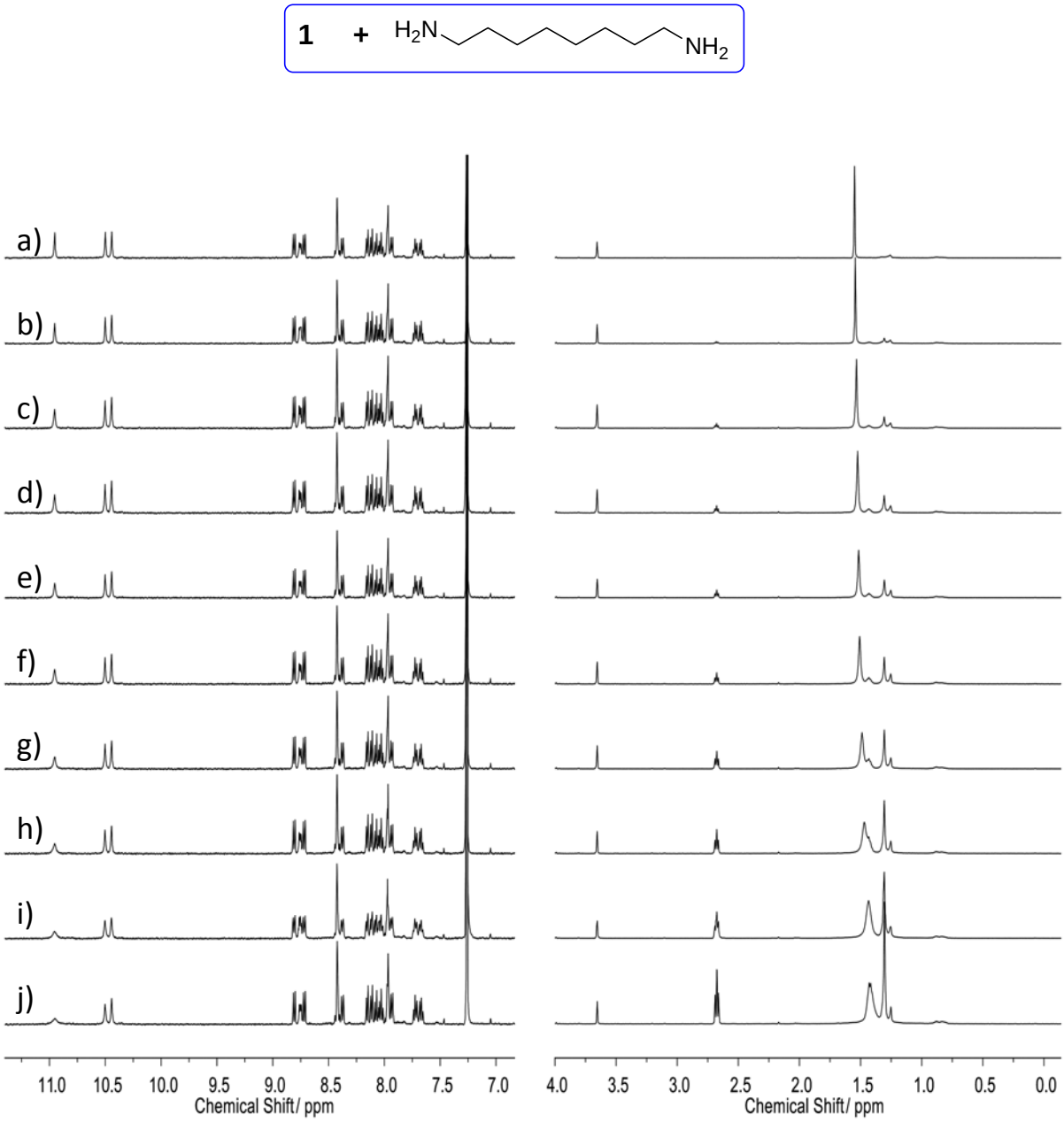
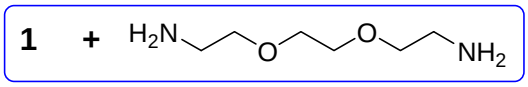


Figure S8. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of 1,8-diaminooctane.



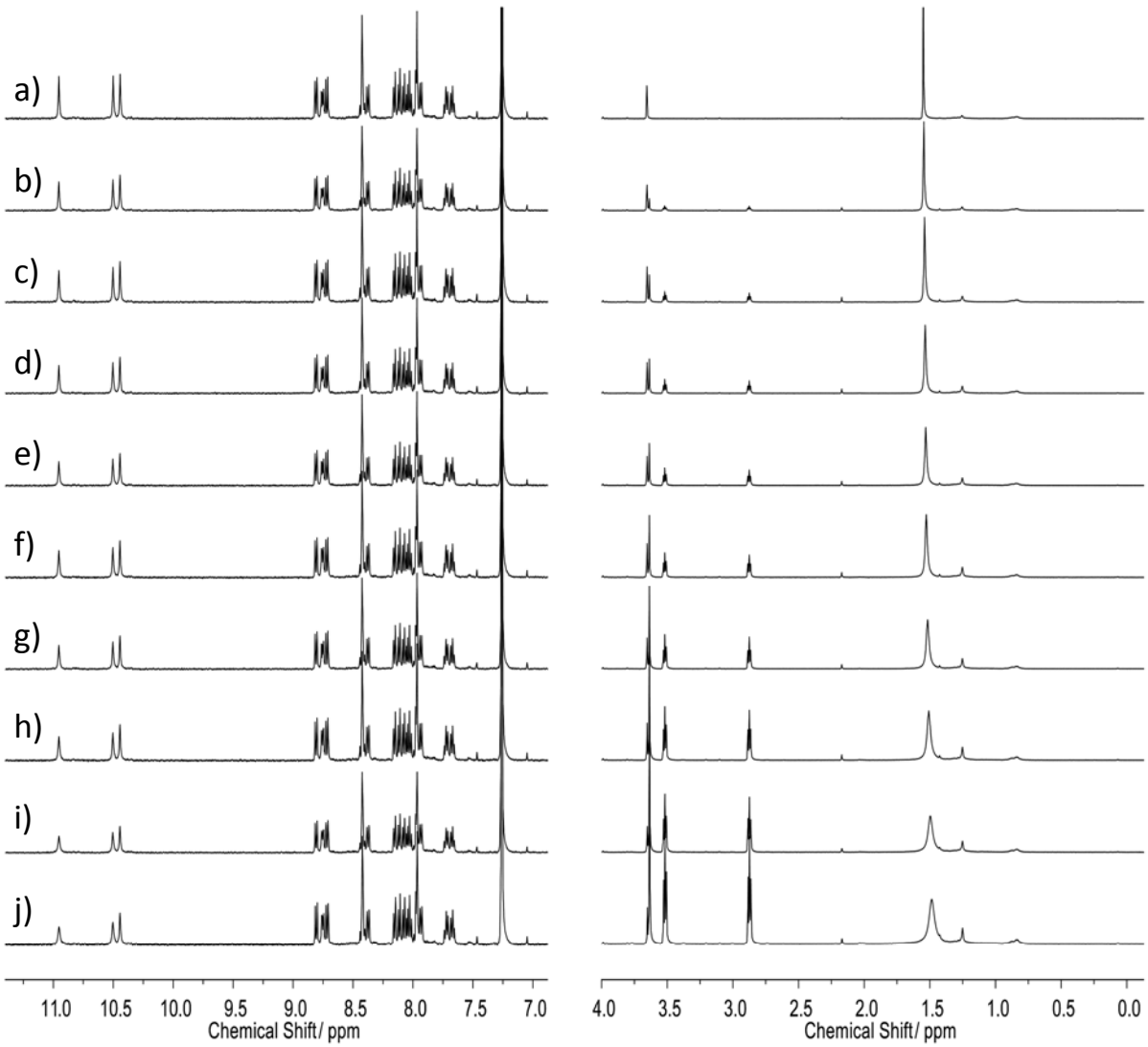


Figure S9. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of 2,2'-(ethylenedioxy)bis(ethylamine).

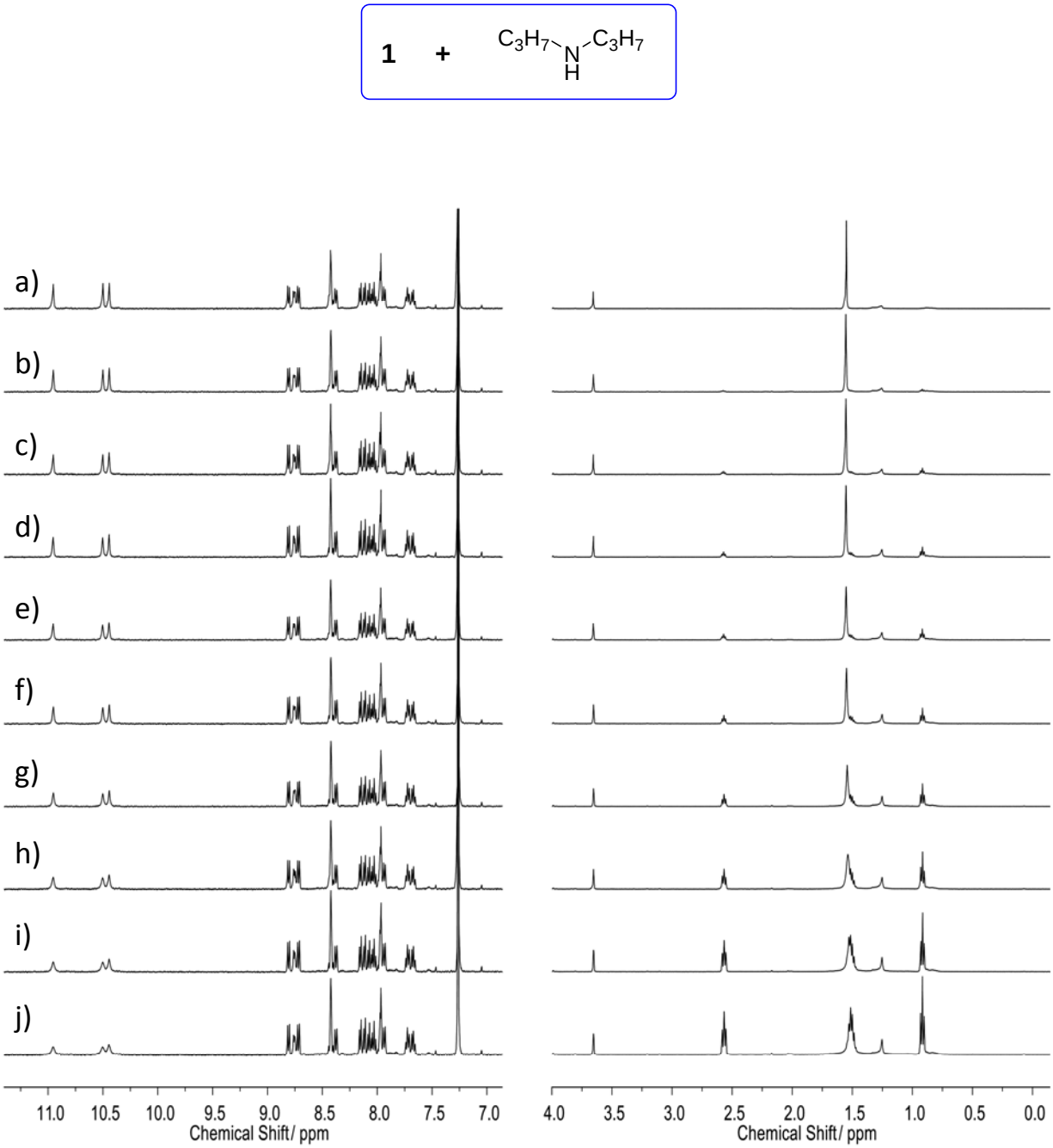


Figure S10. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of di-*n*-propylamine.

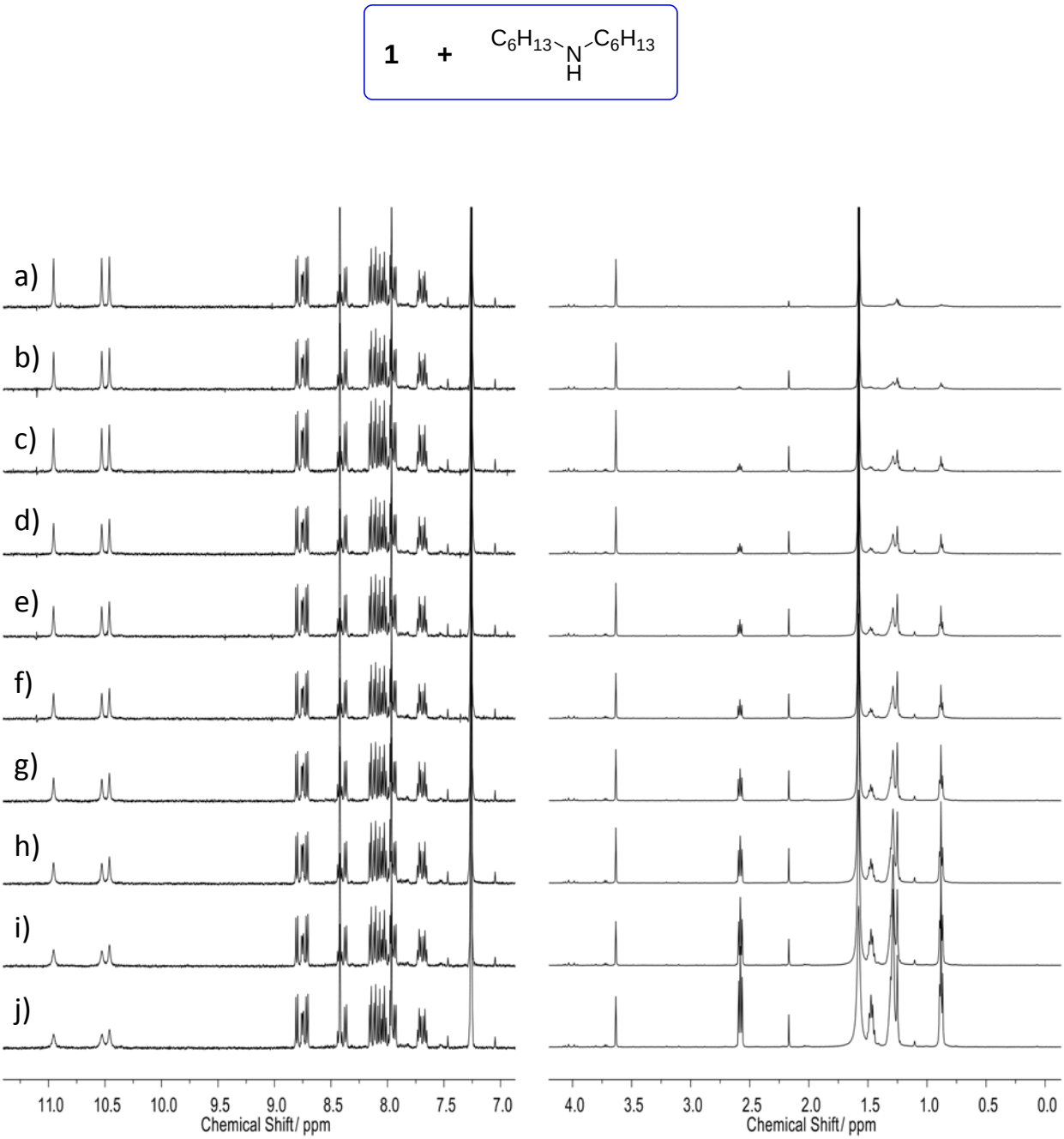
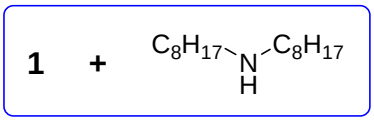


Figure S11. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of di-*n*-hexylamine.



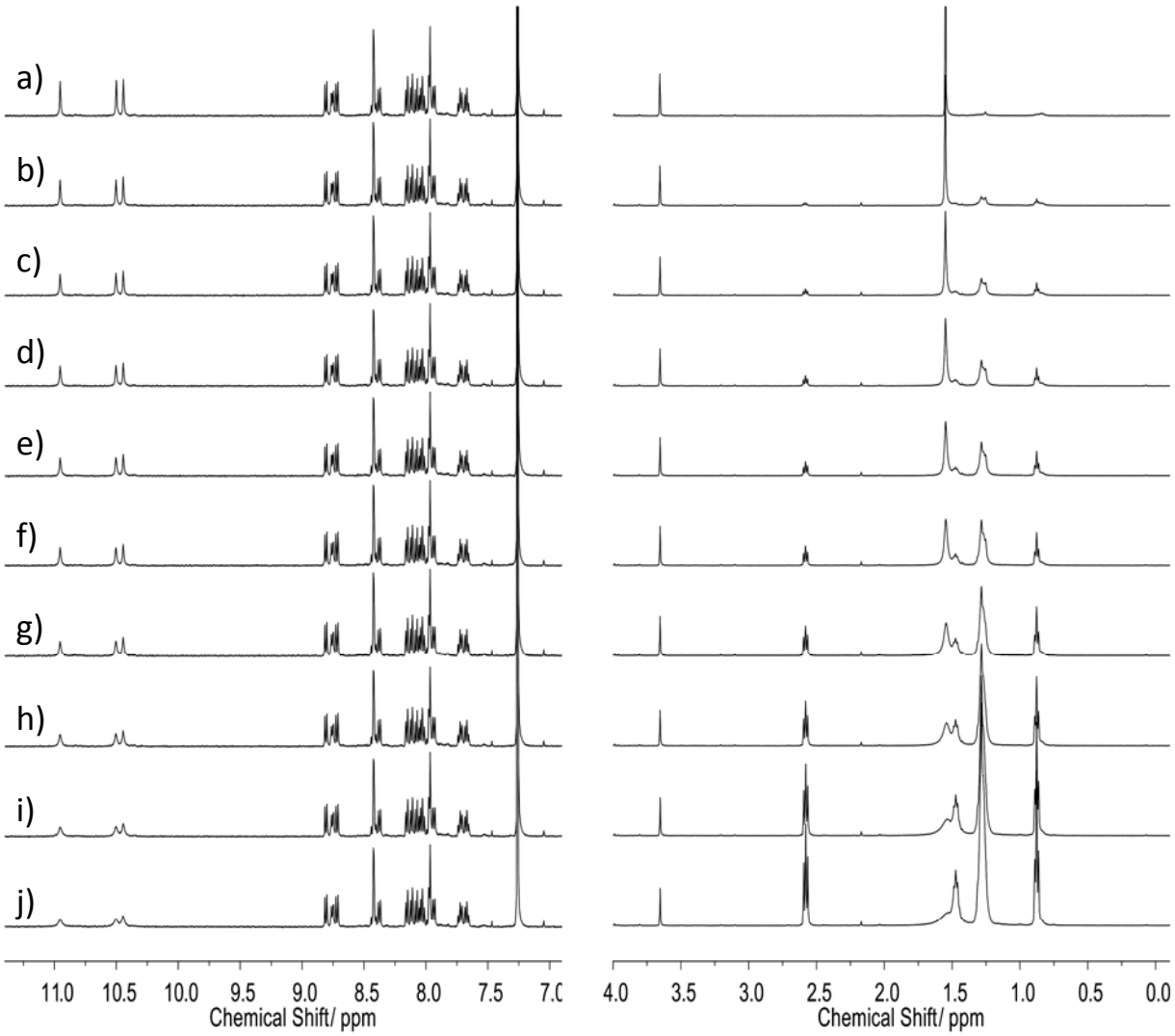


Figure S12. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of di-*n*-octylamine.

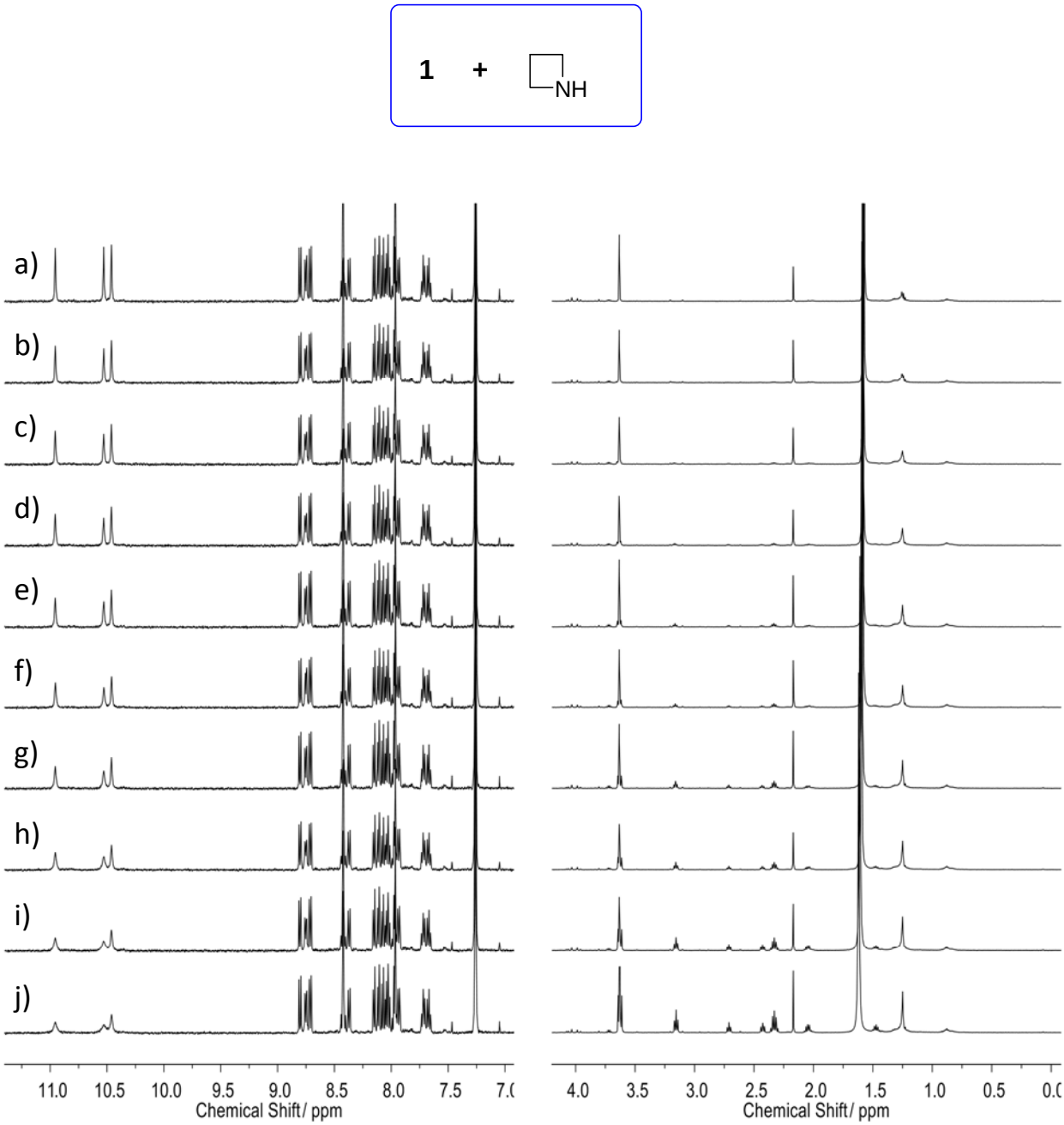


Figure S13. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of azetidine.

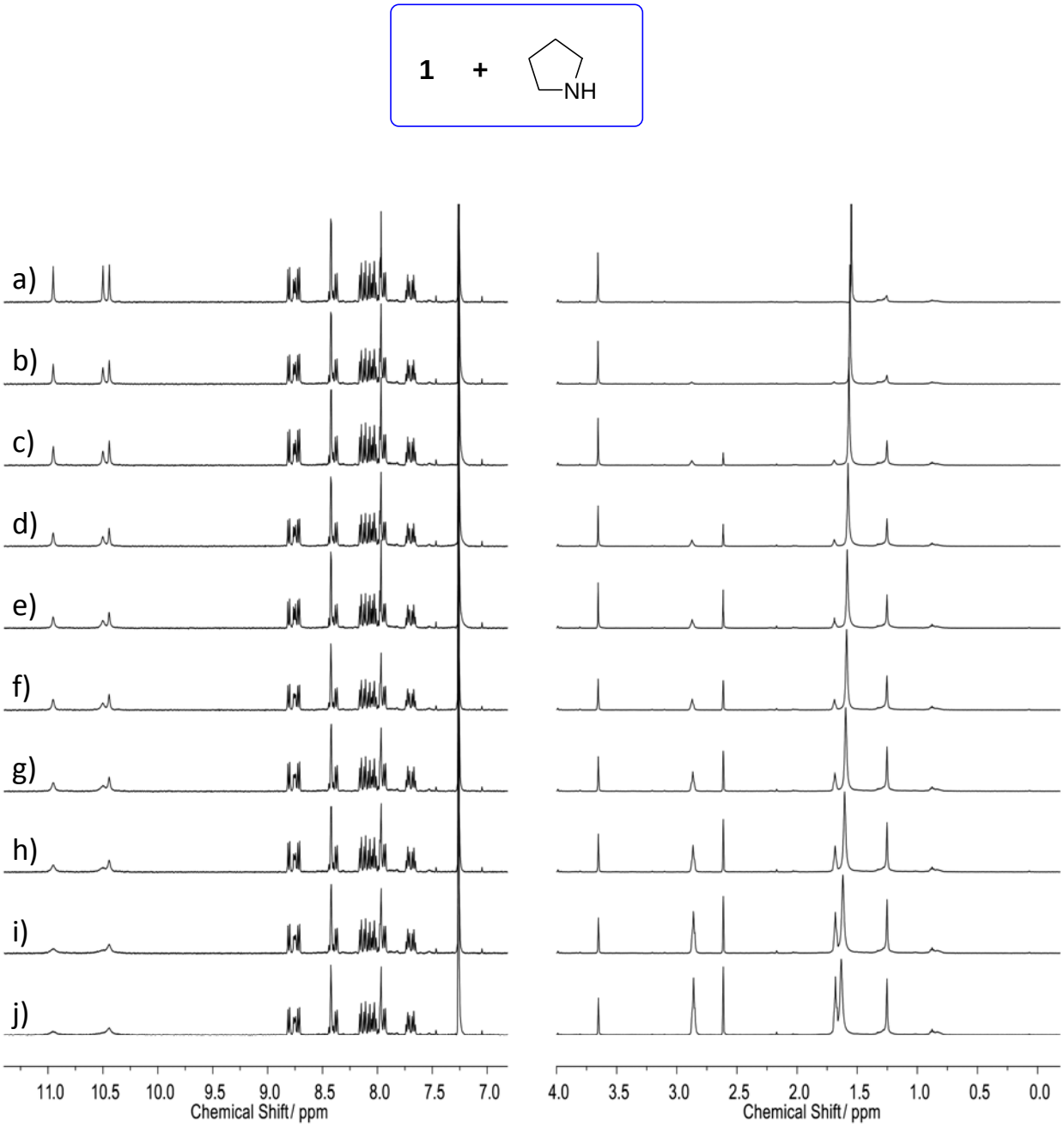


Figure S14. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of pyrrolidine.

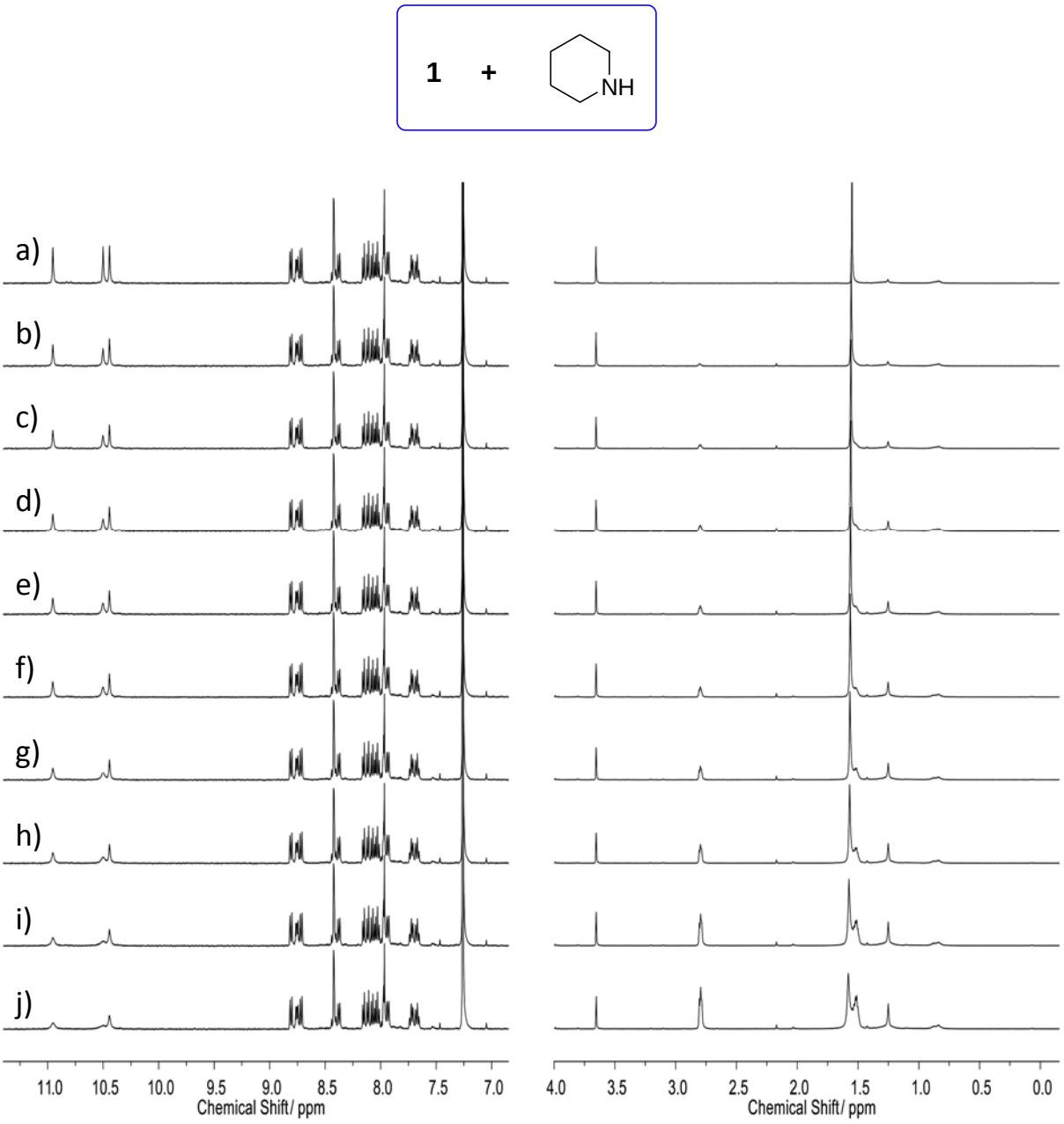


Figure S15. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of piperidine.

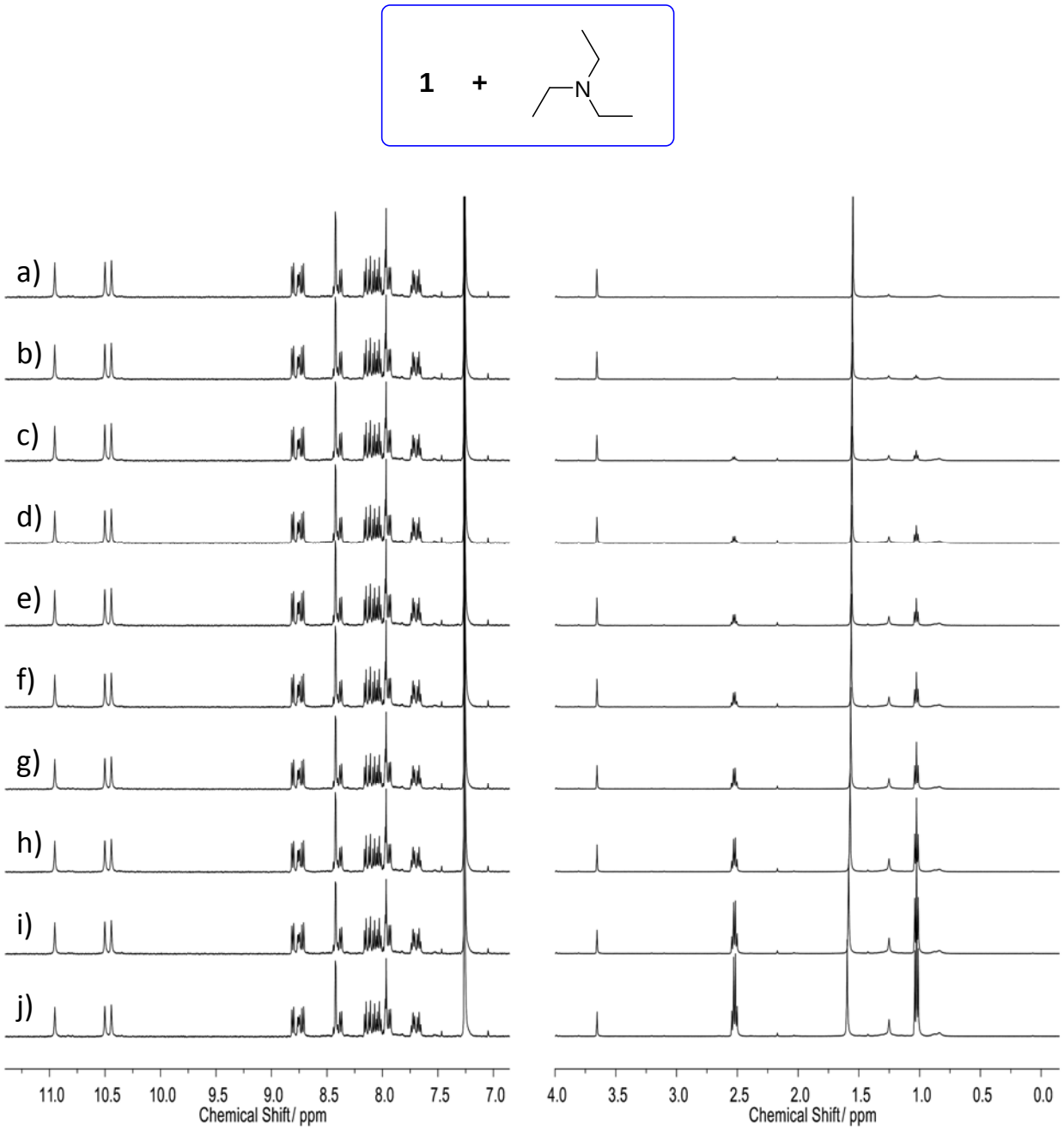


Figure S16. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of triethylamine.

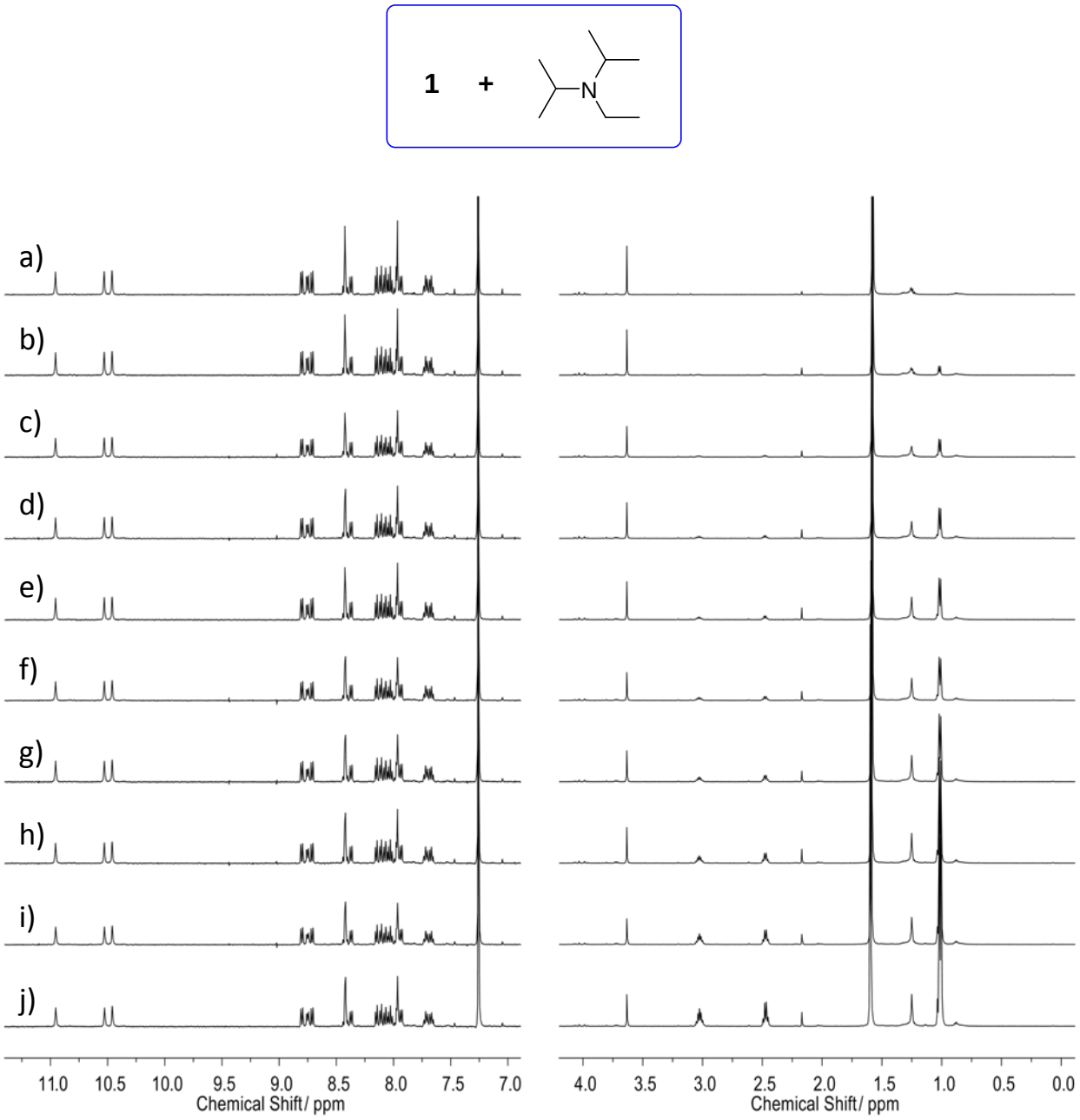


Figure S17. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of diisopropylethylamine.

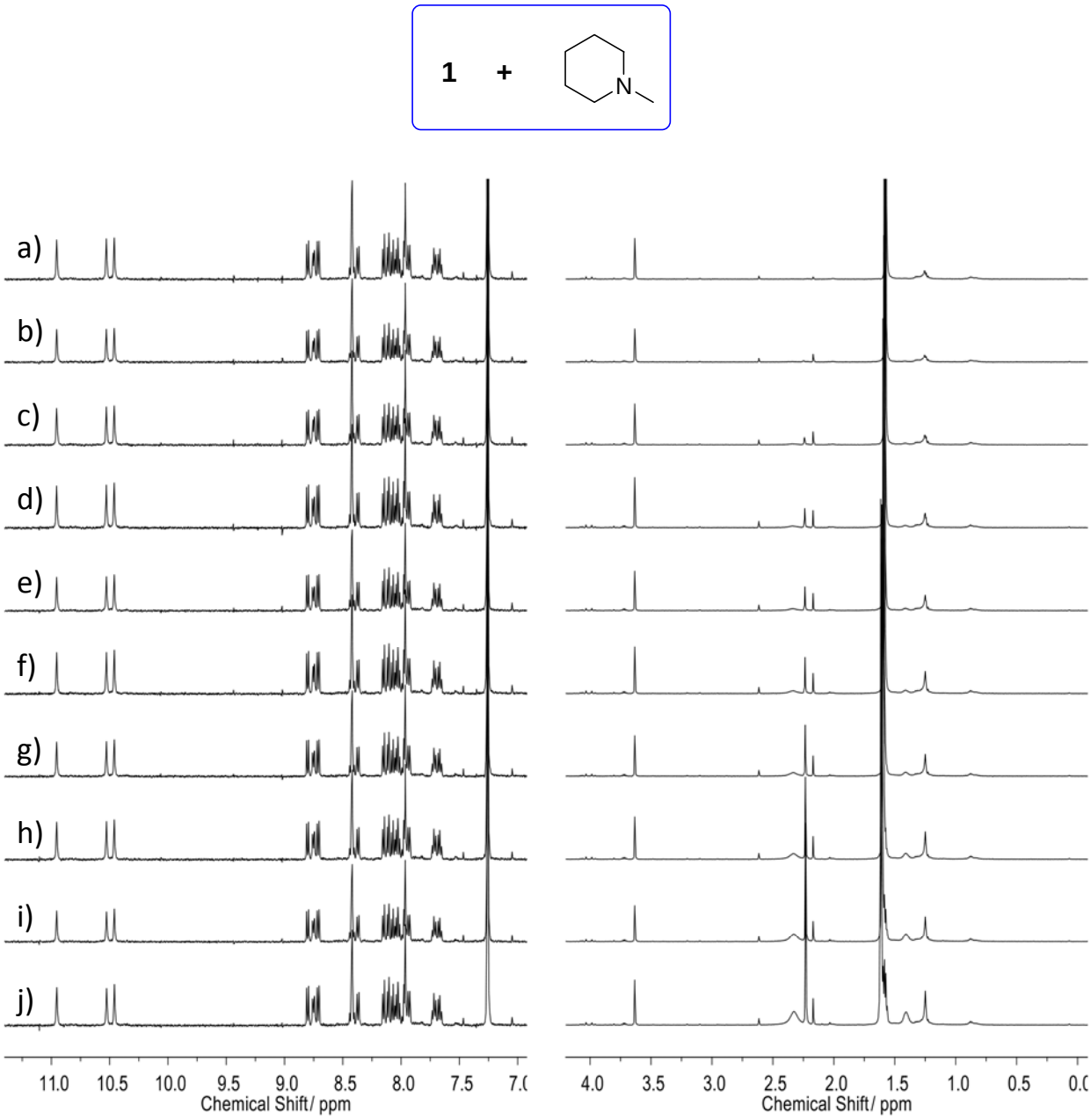


Figure S18. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of 1-methylpiperidine.

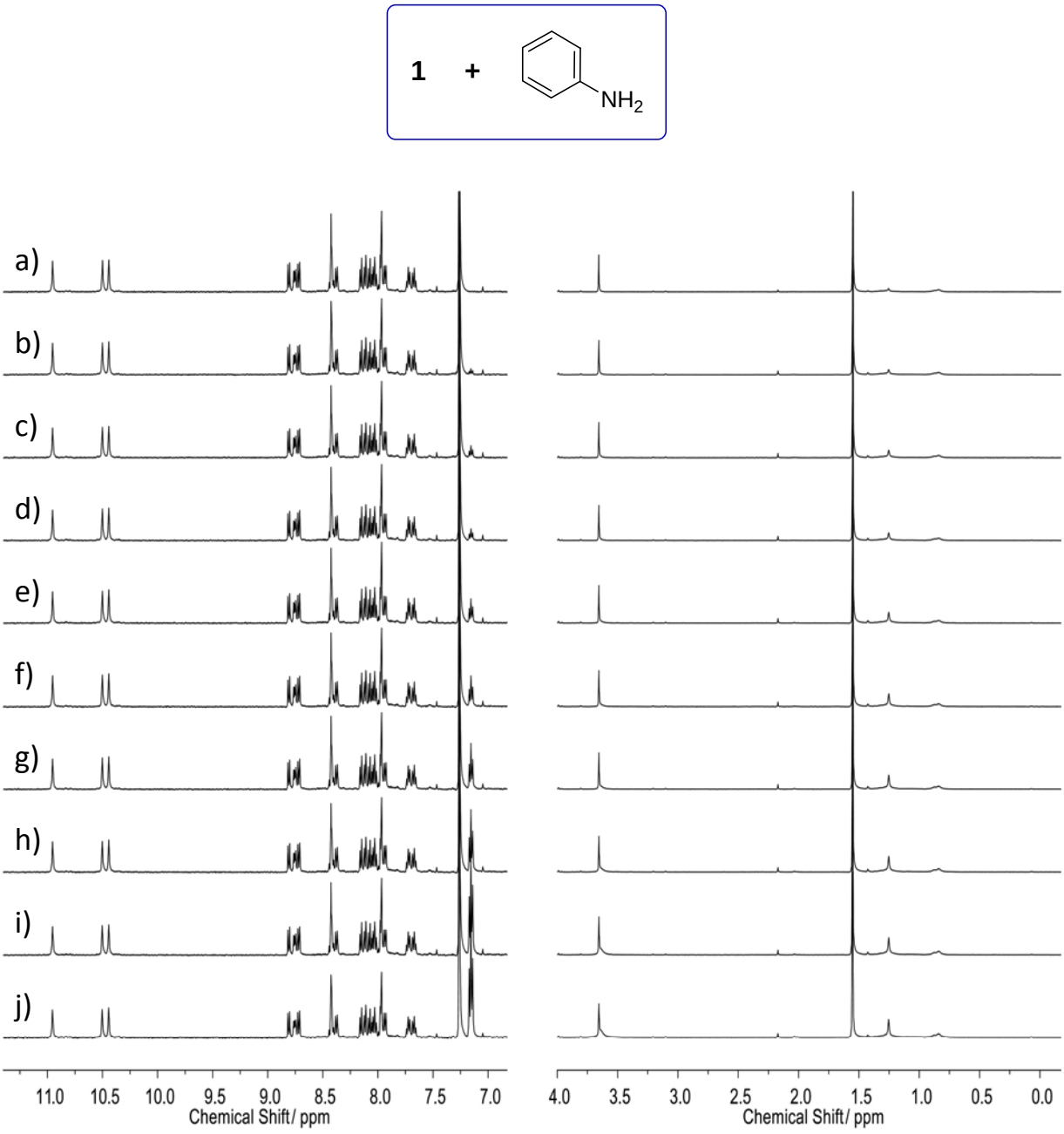
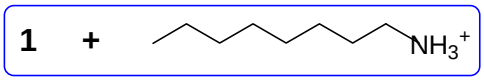


Figure S19. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of aniline.



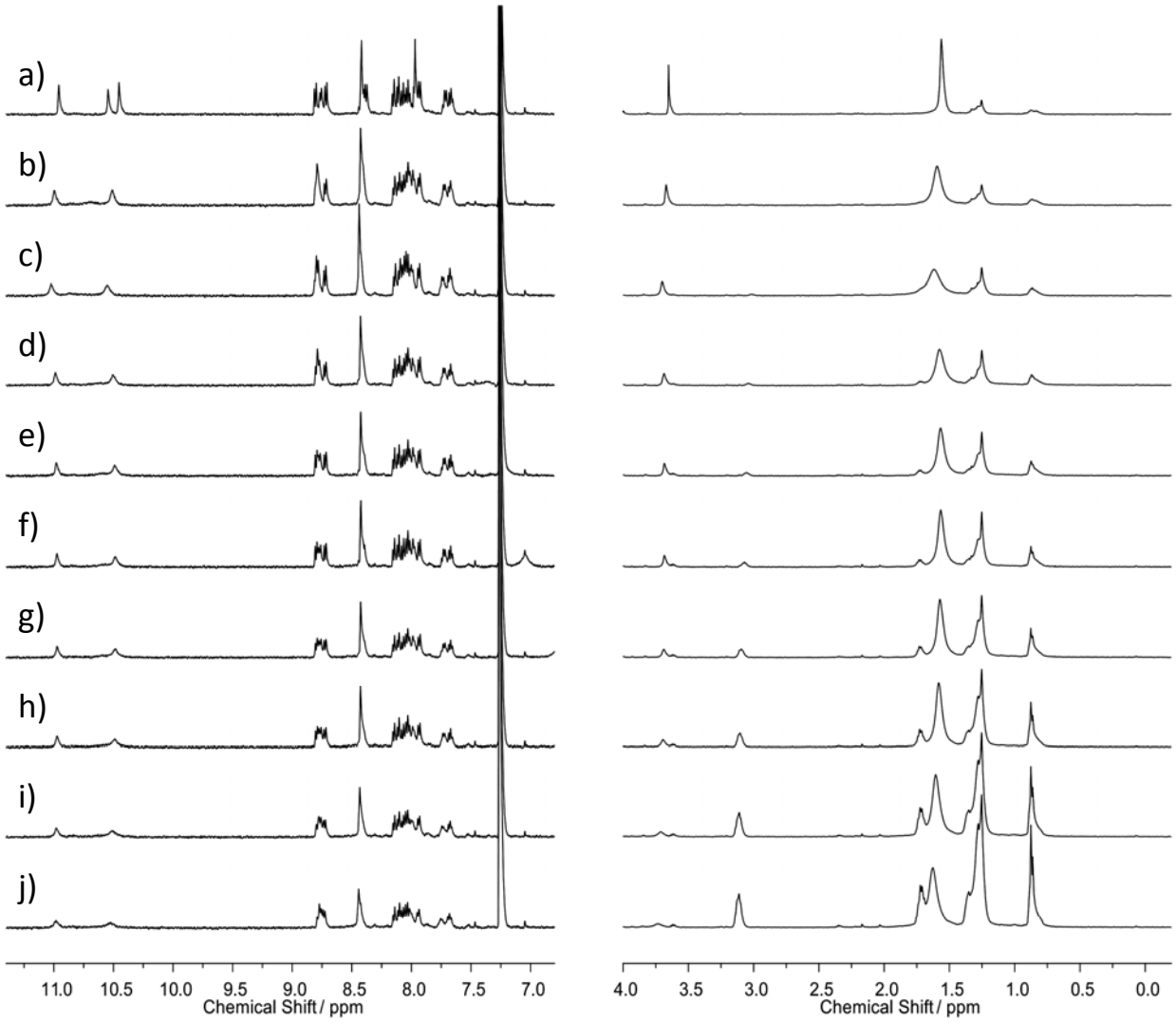
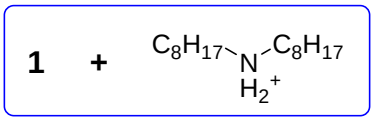


Figure S20. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of 1-octylammonium perchlorate.



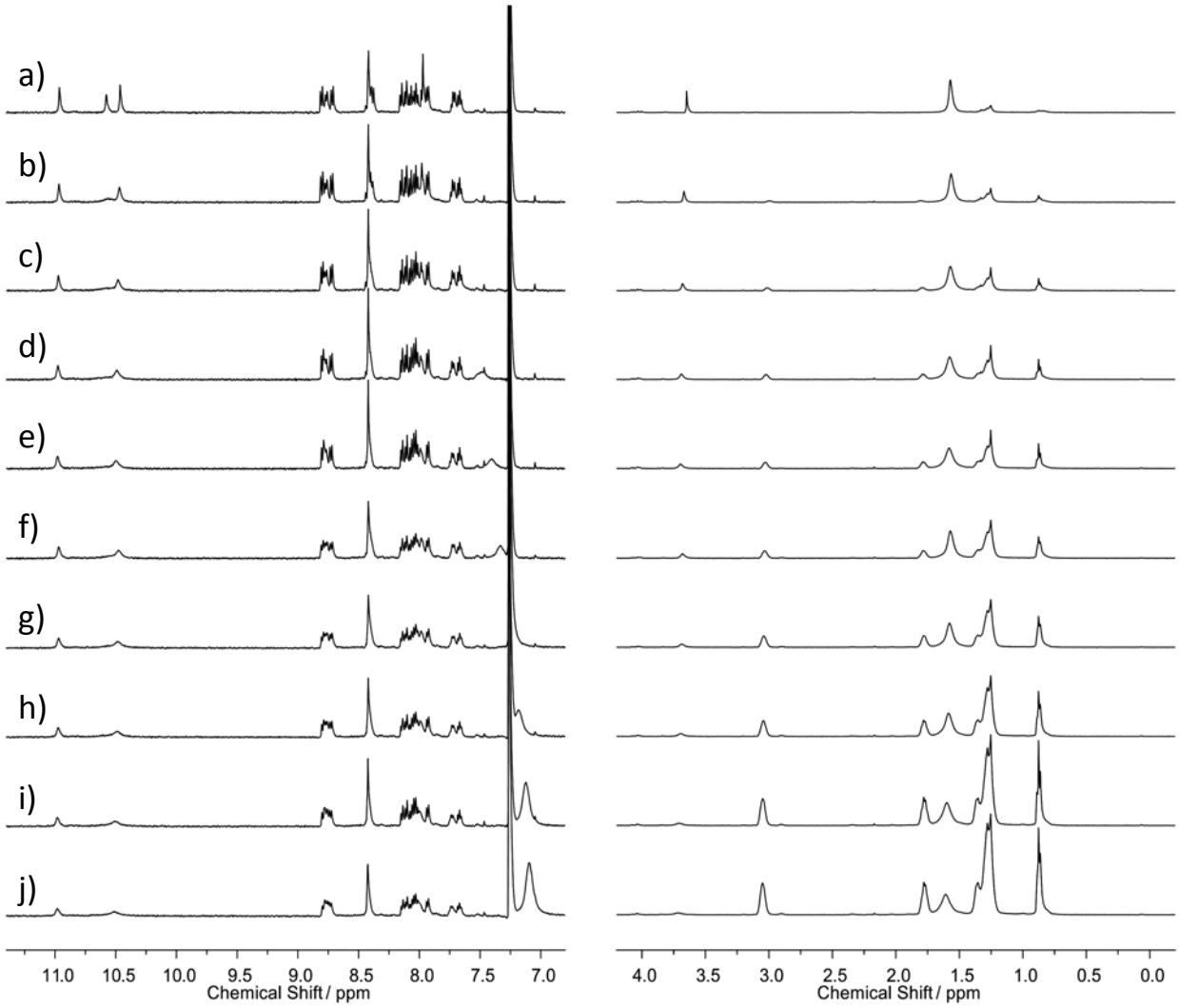


Figure S21. Expanded ^{1}H NMR (500 MHz) (i) from 11.4 ppm to 7 ppm and (ii) 4 ppm to 0 ppm of **1** (2 mM in "normal" $CDCl_3$) with (a) 0.0 equiv., (b) 0.2 equiv., (c) 0.4 equiv., (d) 0.6 equiv., (e) 0.8 equiv., (f) 1.0 equiv., (g) 1.5 equiv., (h) 2.0 equiv., (i) 3.0 equiv., (j) 4.0 equiv. of di-*n*-octylammonium perchlorate.

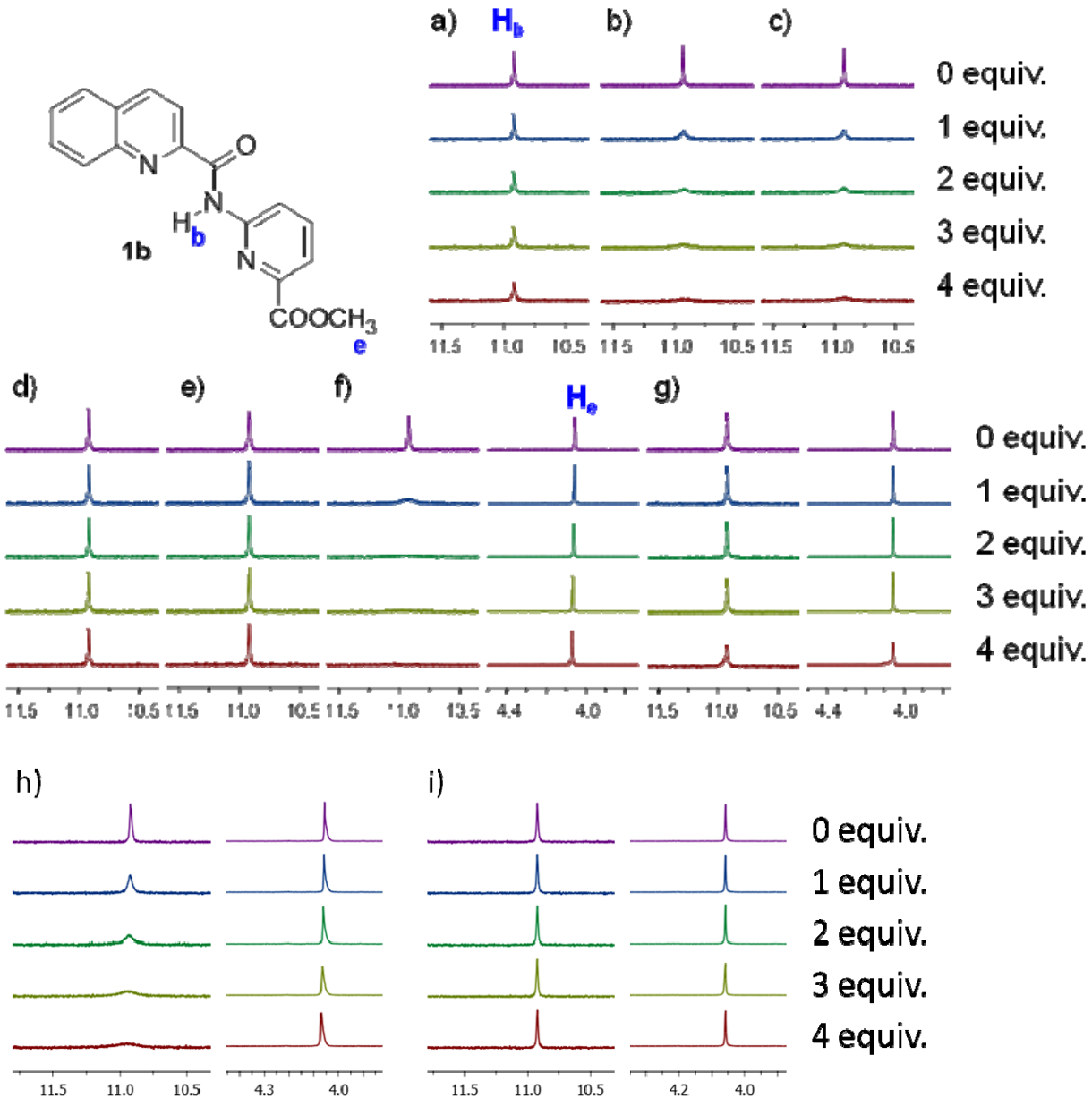


Figure S22. Representative ^{1}H NMR (2 mM) fingerprint regions for amide protons *b* and ester methyl protons *e* of dimer **1b** in the presence of up to four equivalents of a) 1-octylamine, b) di-*n*-octylamine, c) piperidine, d) triethylamine, e) aniline, f) 1-octylammonium perchlorate and g) di-*n*-octylammonium perchlorate in "normal" $CDCl_3$ and h) 1-octylammonium perchlorate and i) di-*n*-octylammonium perchlorate in 'neutralized' $CDCl_3$.

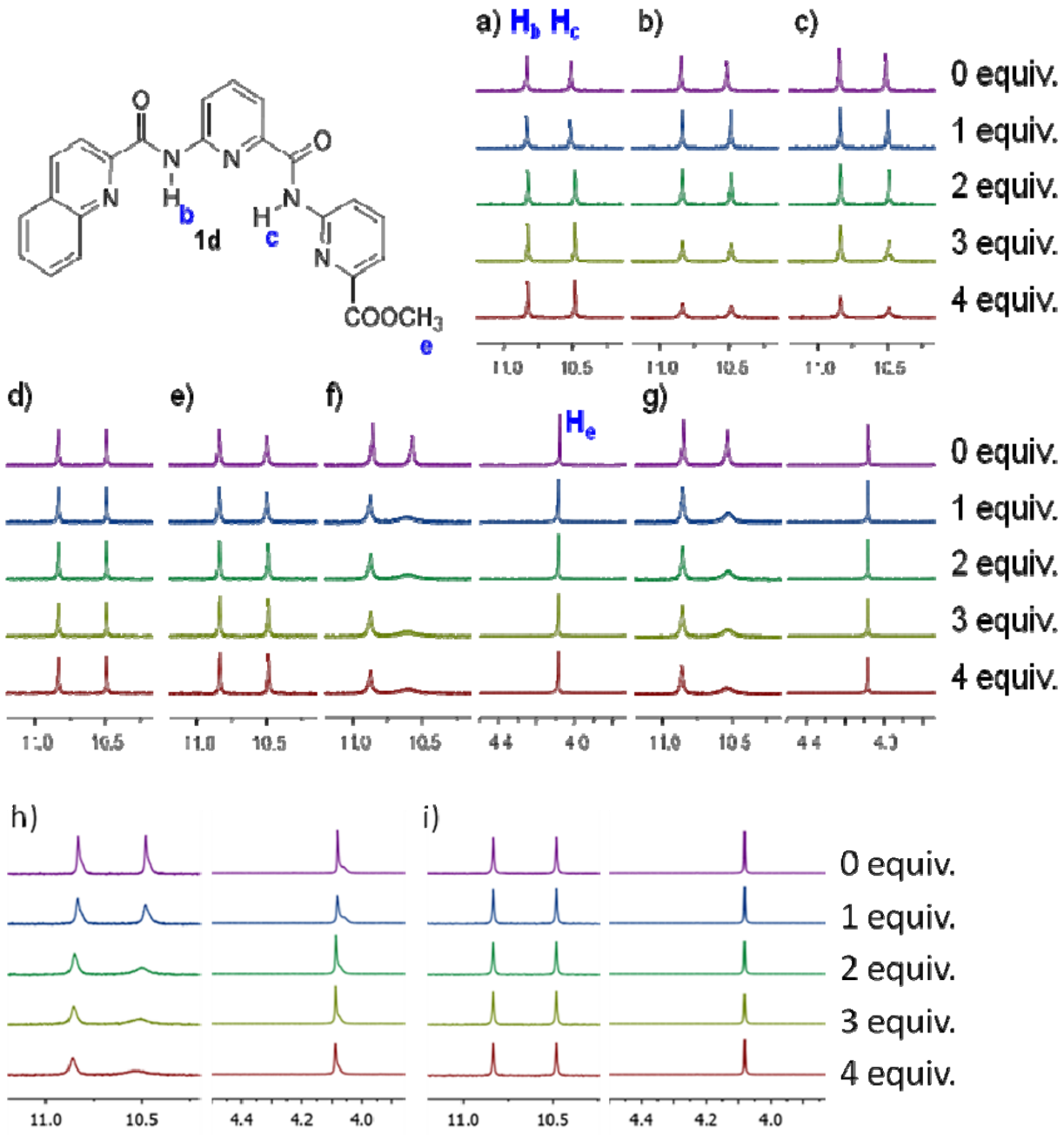


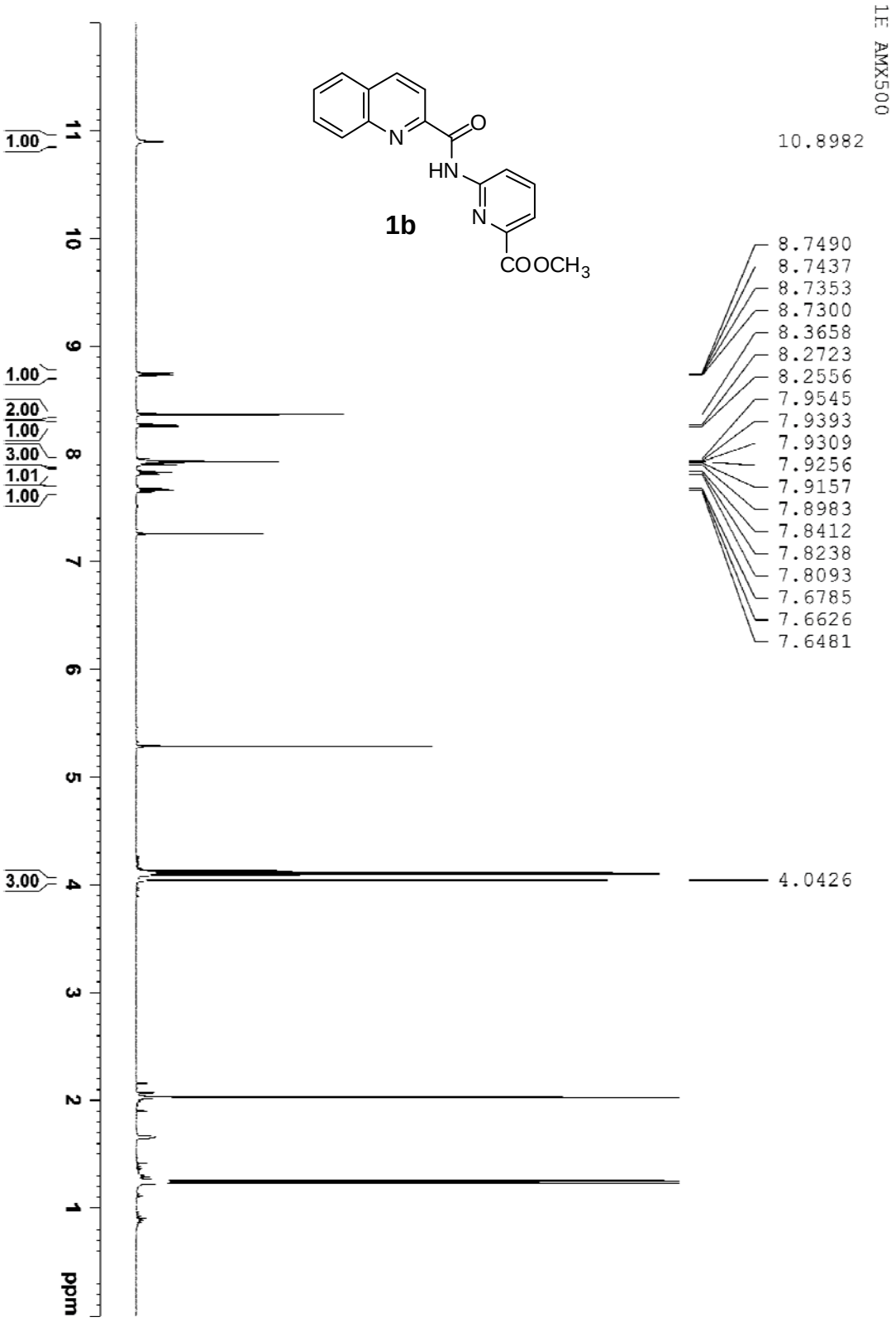
Figure S23. Representative ^{1}H NMR (2 mM) fingerprint regions for amide protons *b*–*c* and ester methyl protons *e* of trimer **1d** in the presence of up to four equivalents of a) 1-octylamine, b) di-*n*-octylamine, c) piperidine, d) triethylamine, e) aniline, f) 1-octylammonium perchlorate and g) di-*n*-octylammonium perchlorate in "normal" $CDCl_3$ and h) 1-octylammonium perchlorate and i) di-*n*-octylammonium perchlorate in 'neutralized' $CDCl_3$.

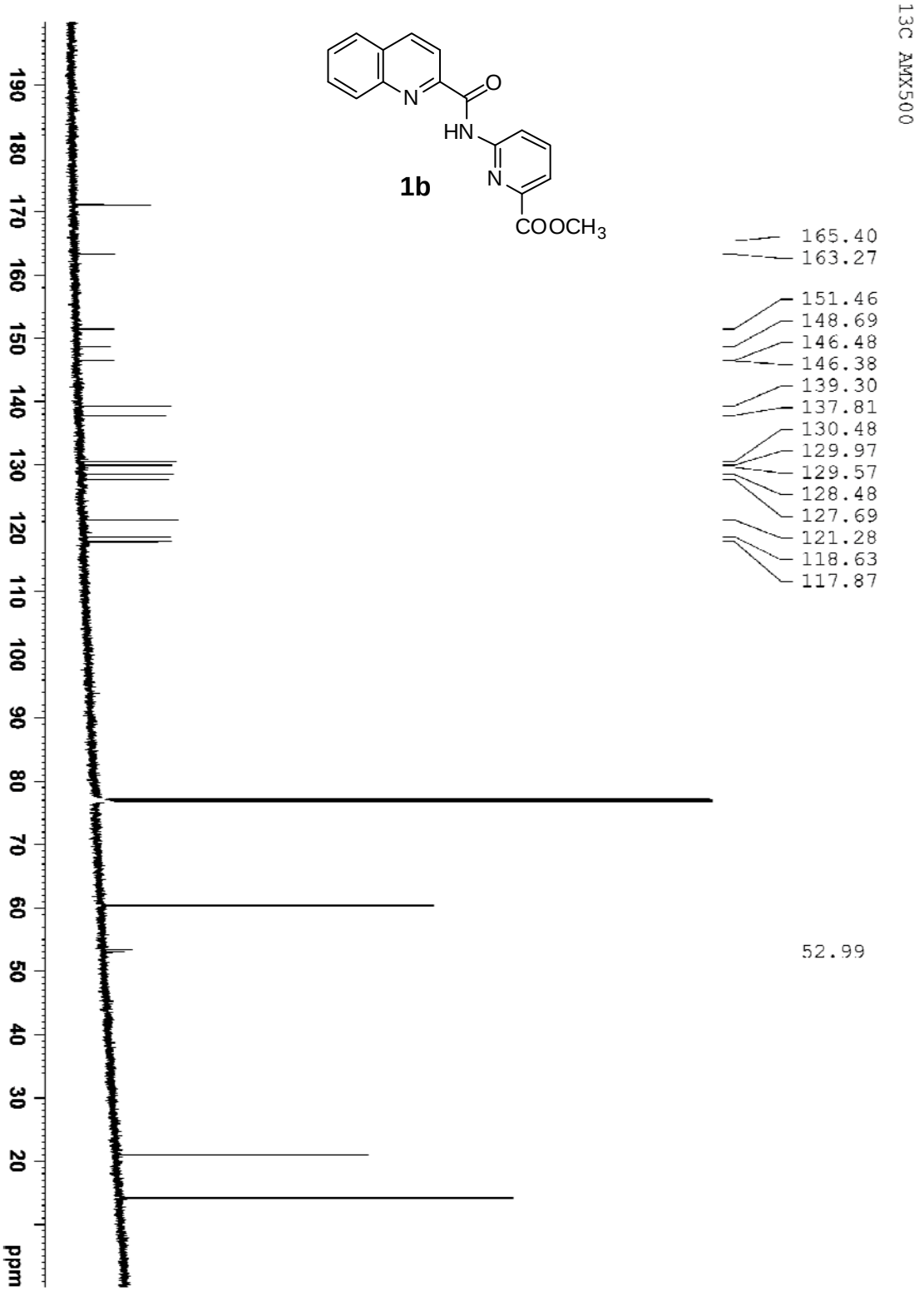
6. *Ab Initio* Molecular Modeling

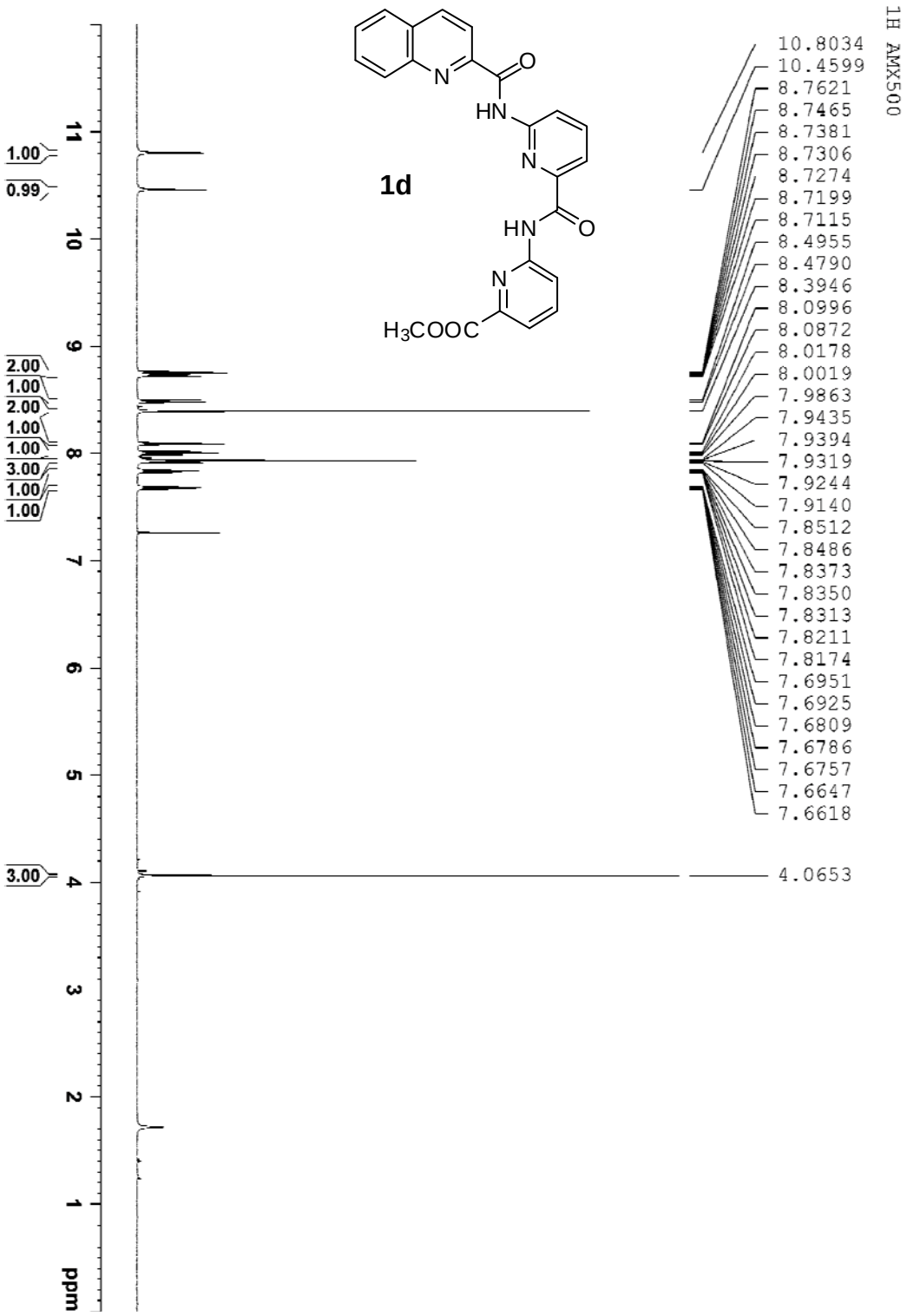
All the calculations were carried out by utilizing the Gaussian 09[1] program package. The geometry optimizations were performed at the density functional theory (DFT) level, and the Becke's three parameter hybrid functional with the Lee-Yang-Parr correlation functional (B3LYP)[2] method was employed to do the calculations. The 6-31G*[3] basic from the Gaussian basis set library has been used in all the calculations. The harmonic vibrational frequencies and zero-point energy corrections were calculated at the same level of theory. Single point energy were obtained at the B3LYP level in conjuction with the 6-311+G (2d, p) basis set with the use of the above optimized geometries, i.e., B3LYP/6-311+G(2d,p)//B3LYP/6-31G.

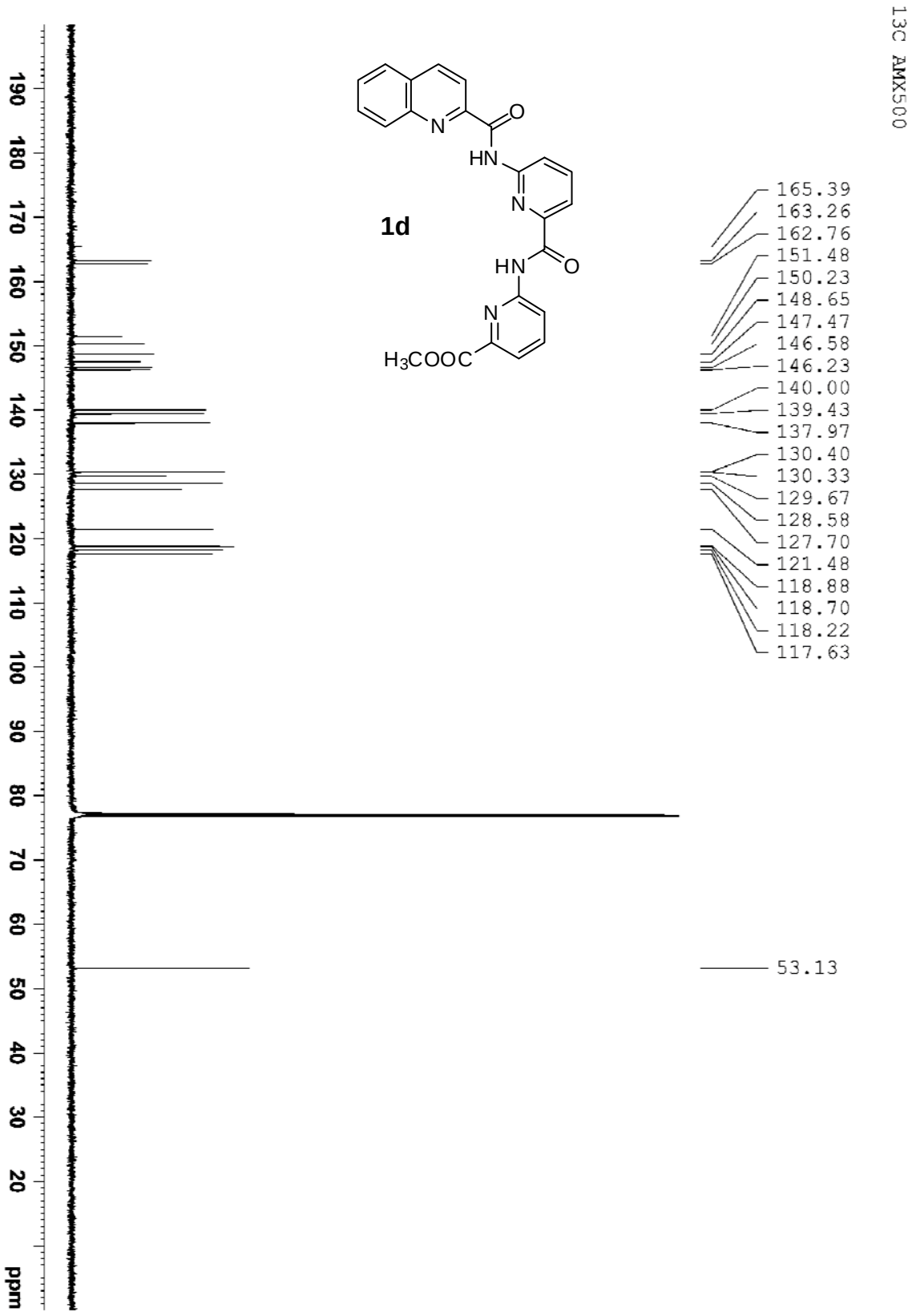
[1] Frisch, M. J.; et al. *Gaussian 09*; Gaussian , Inc.: Wallingford CT, 2009.
[2] Becke, A. D. *J. Chem. Phys.* **1993**, 98, 5648.
[3] Petersson, G. A.; Al-Laham, M. A. *J. Chem. Phys.* **1991**, 94, 6081; Petersson, G. A.; Bennett, A.; Tensfeldt, T. G.; Al-Laham, M. A.; Shirley, W. A.; Mantzaris, J. *J. Chem. Phys.* **1988**, 89, 2193.

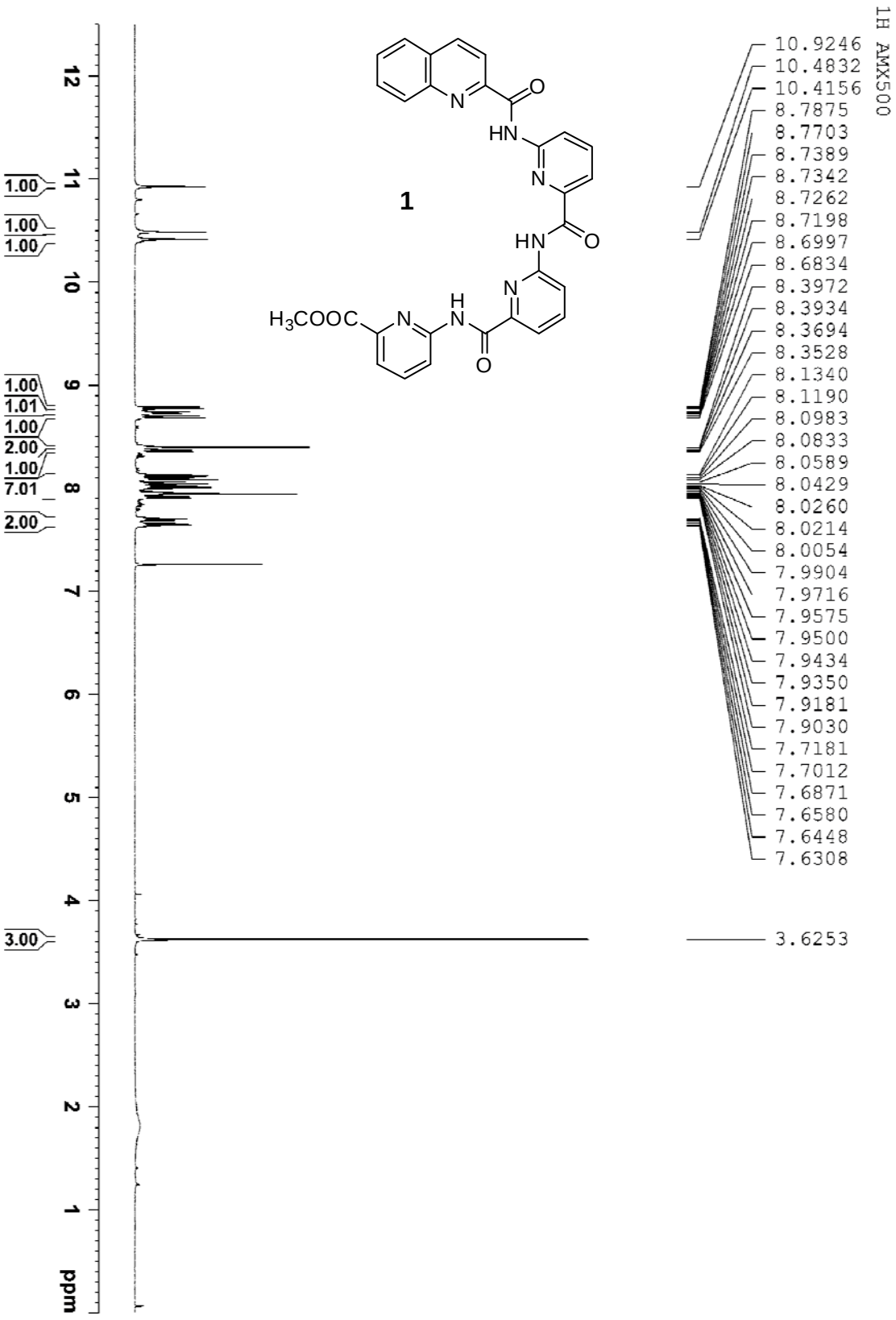
7. ^{1}H and ^{13}C NMR spectra

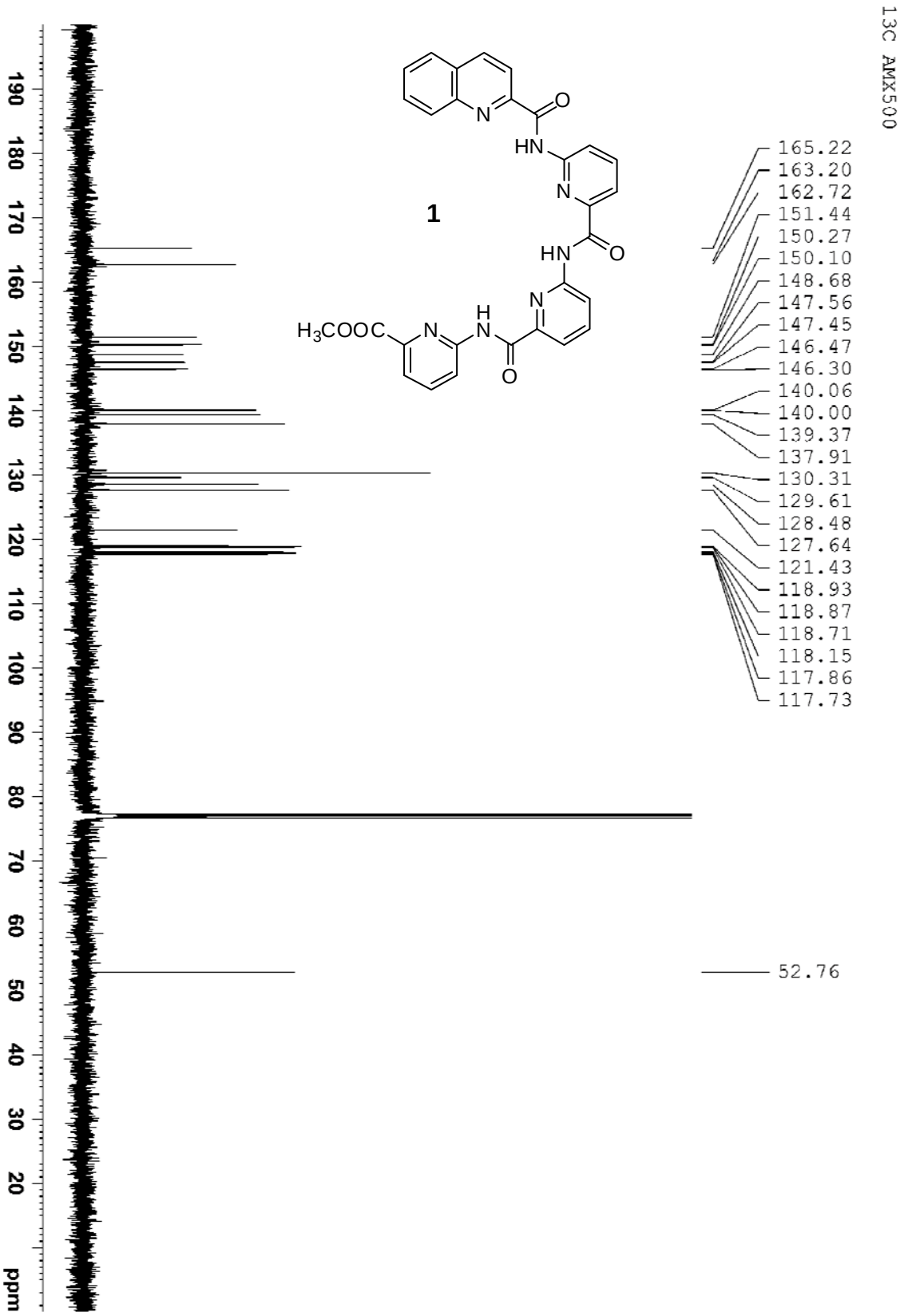



13C AMX500
1b
N
O
HN
N
COOCH3
165.40
163.27
151.46
148.69
146.48
146.38
139.30
137.81
130.48
129.97
129.57
128.48
127.69
121.28
118.63
117.87
52.99
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

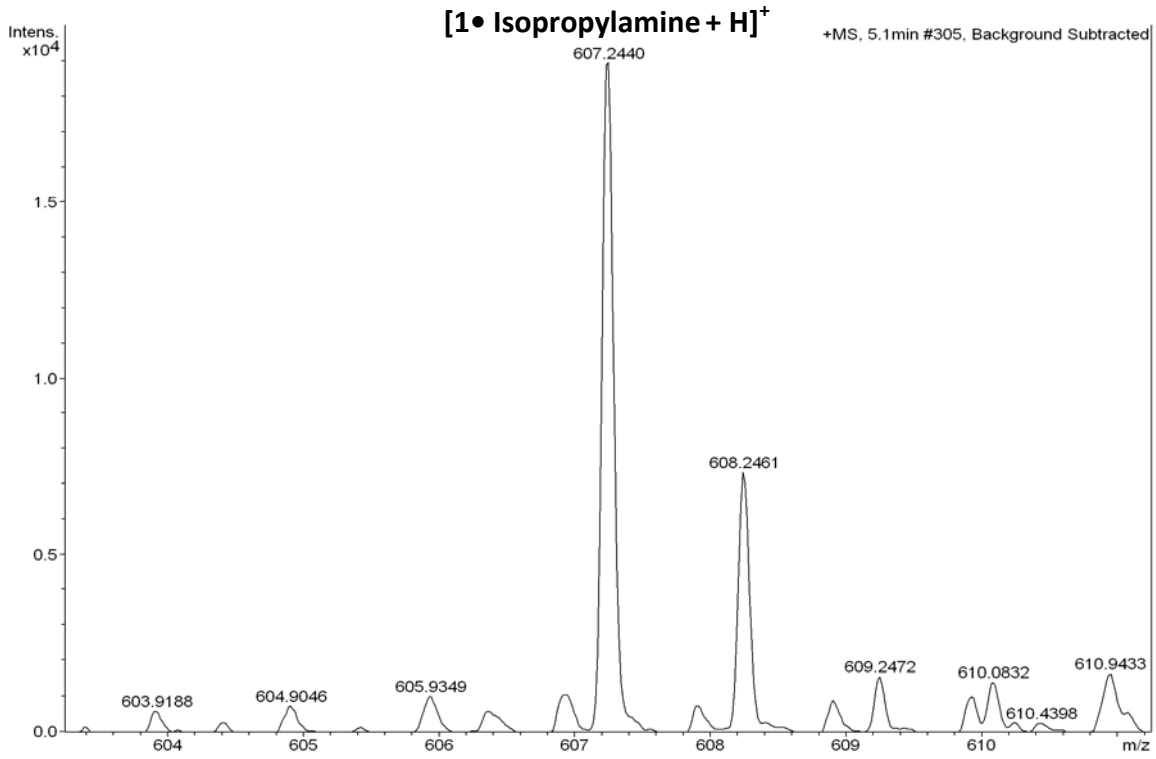


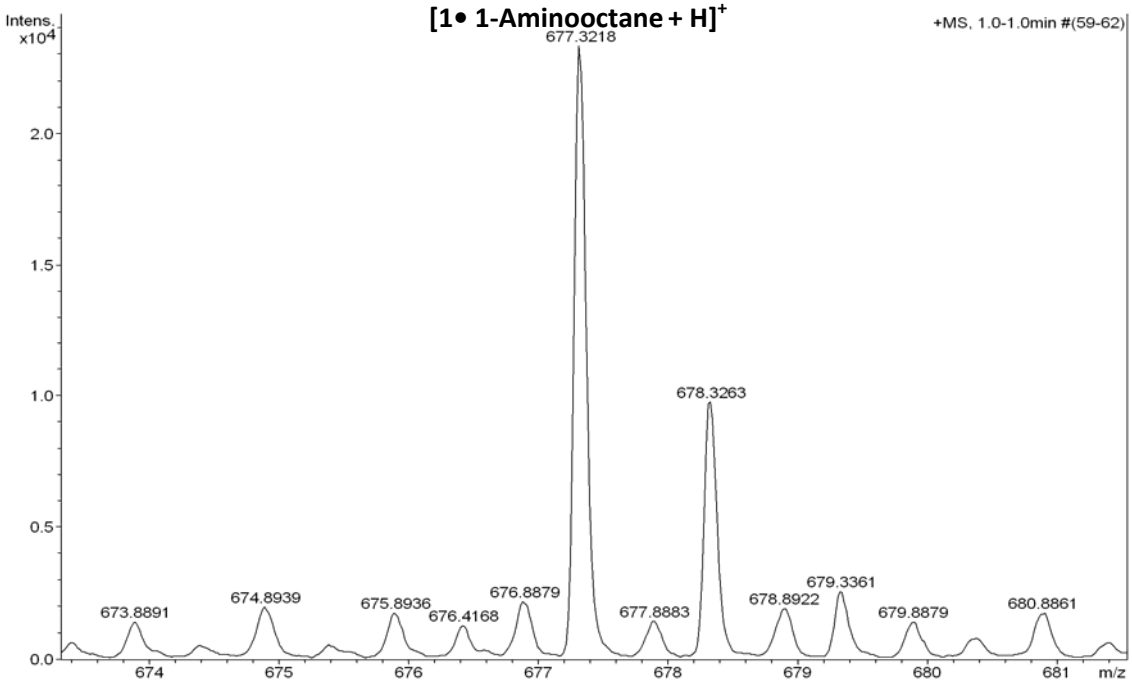


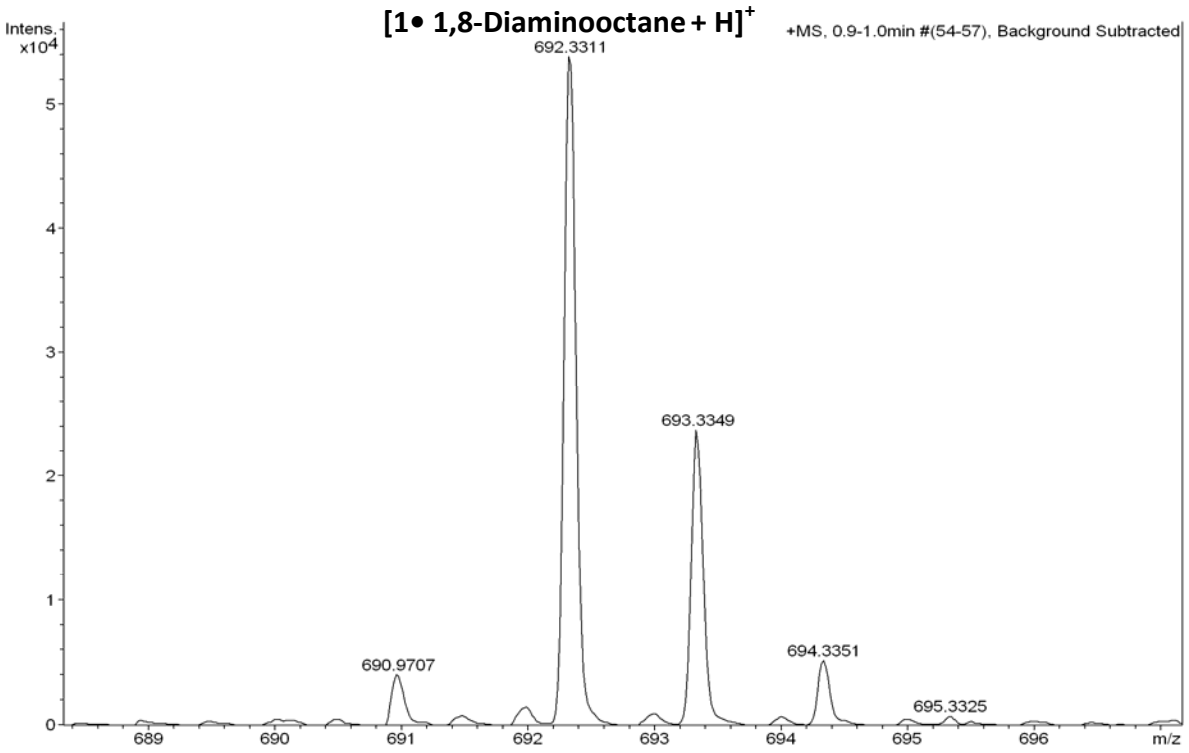

1H AMX500
10.9246
10.4832
10.4156
8.7875
8.7703
8.7389
8.7342
8.7262
8.7198
8.6997
8.6834
8.3972
8.3934
8.3694
8.3528
8.1340
8.1190
8.0983
8.0833
8.0589
8.0429
8.0260
8.0214
8.0054
7.9904
7.9716
7.9575
7.9500
7.9434
7.9350
7.9181
7.9030
7.7181
7.7012
7.6871
7.6580
7.6448
7.6308
3.6253
1.00
1.00
1.00
1.00
1.01
1.00
2.00
1.00
7.01
2.00
3.00
ppm
1
H3COOC
HN
HN
HN
O
O
O
N
N
N
N
H

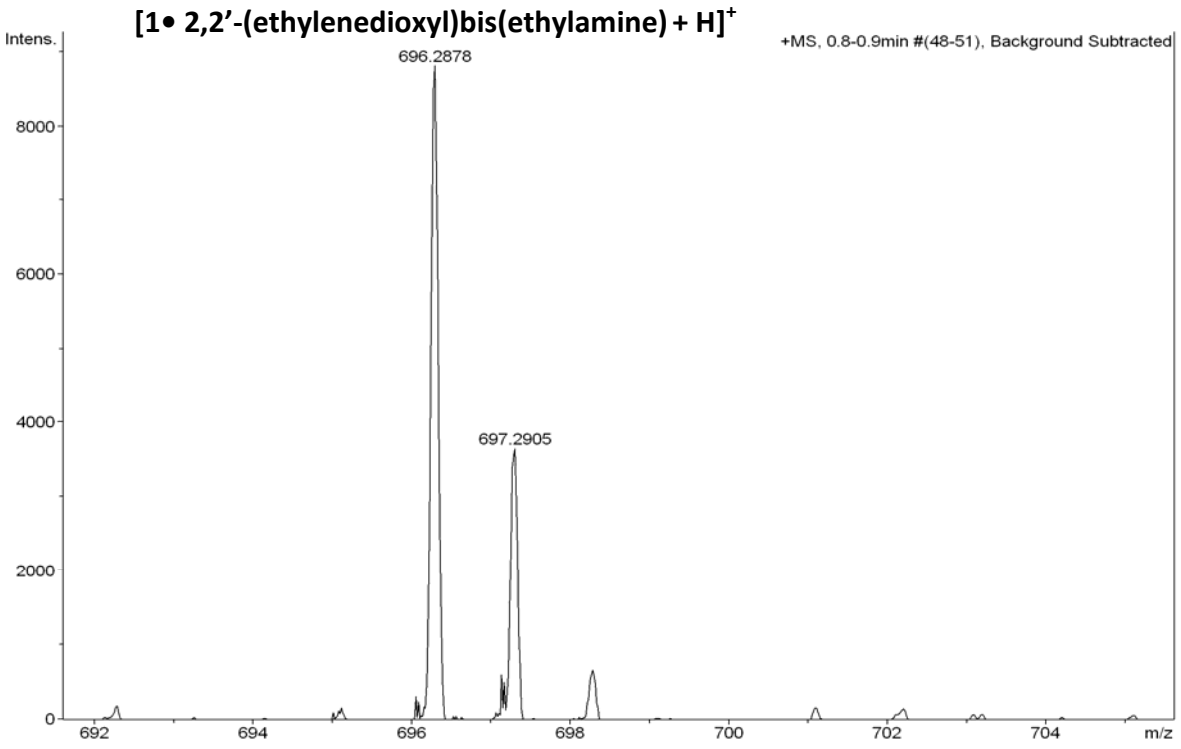


8. HRMS Spectra of [1•Guest] Complexes

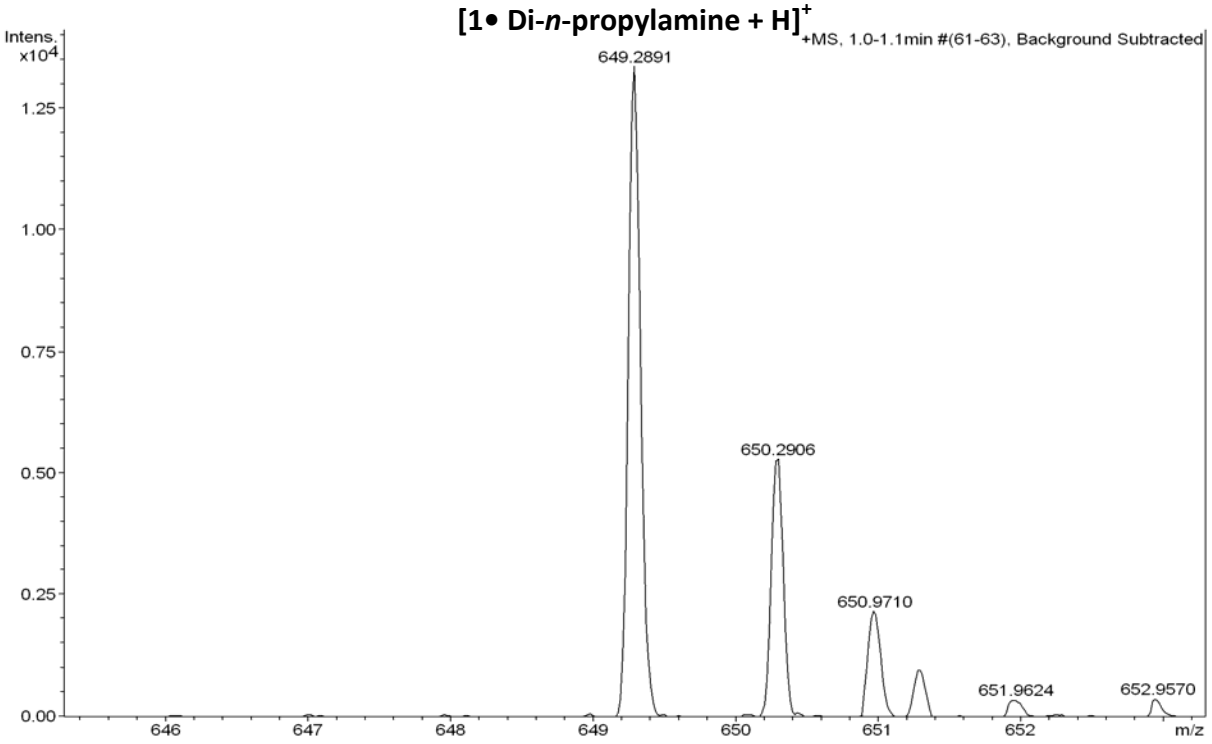




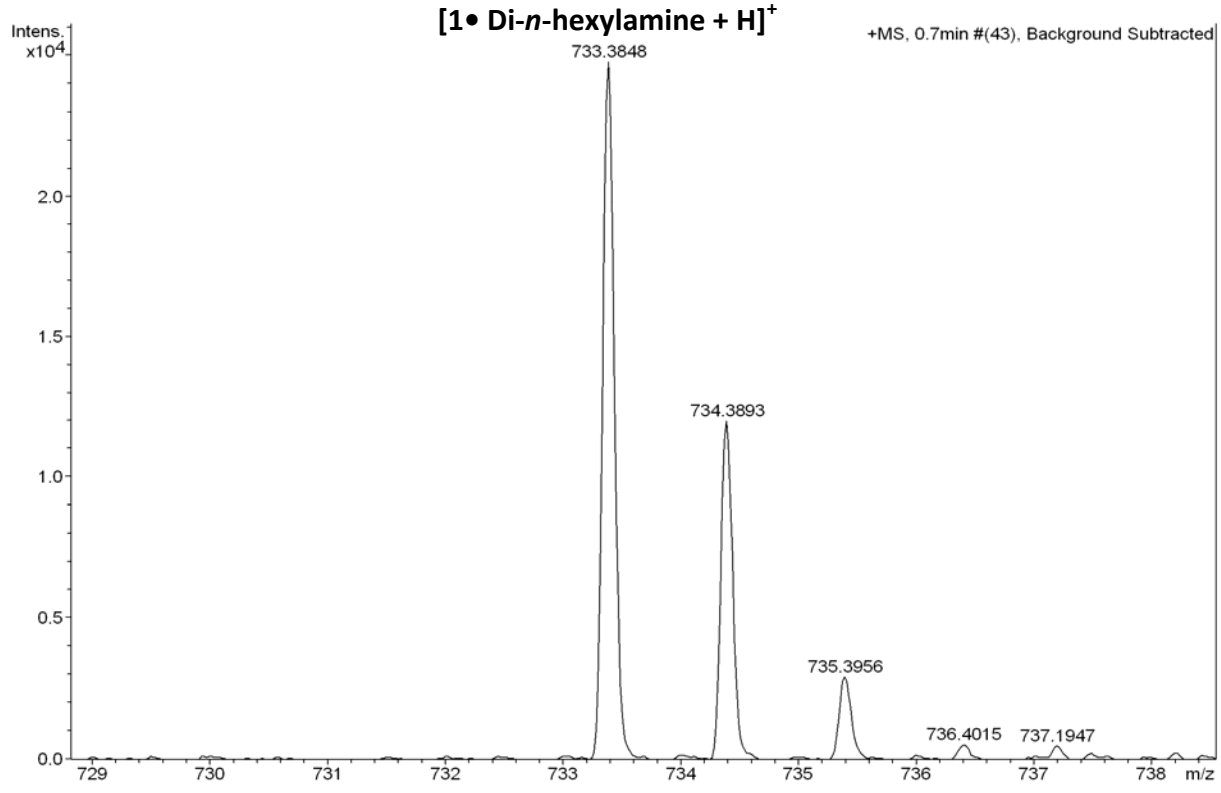

[1• 1,8-Diaminooctane + H]+
+MS, 0.9-1.0min #(54-57), Background Subtracted
Intens.
x10^4
692.3311
693.3349
690.9707
694.3351
695.3325
m/z


[1• 2,2'-(ethylenedioxyl)bis(ethylamine) + H]+
+MS, 0.8-0.9min #(48-51), Background Subtracted
Intens.
696.2878
697.2905
m/z

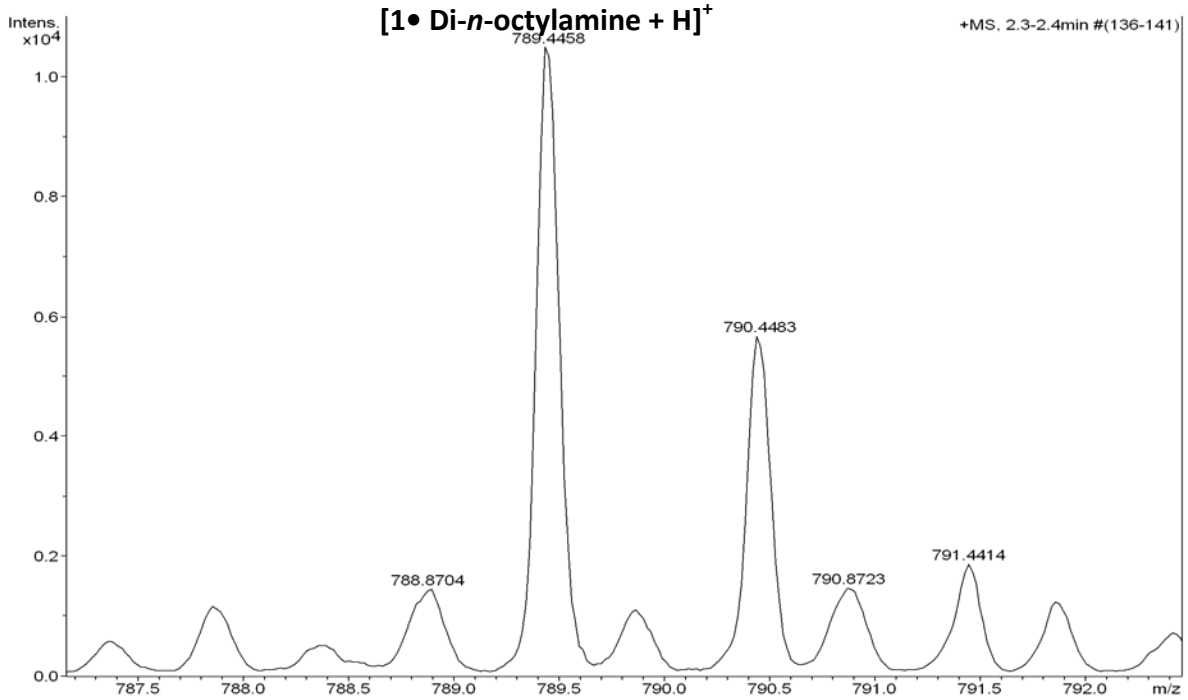
[1• Di-*n*-propylamine + H]$^+$



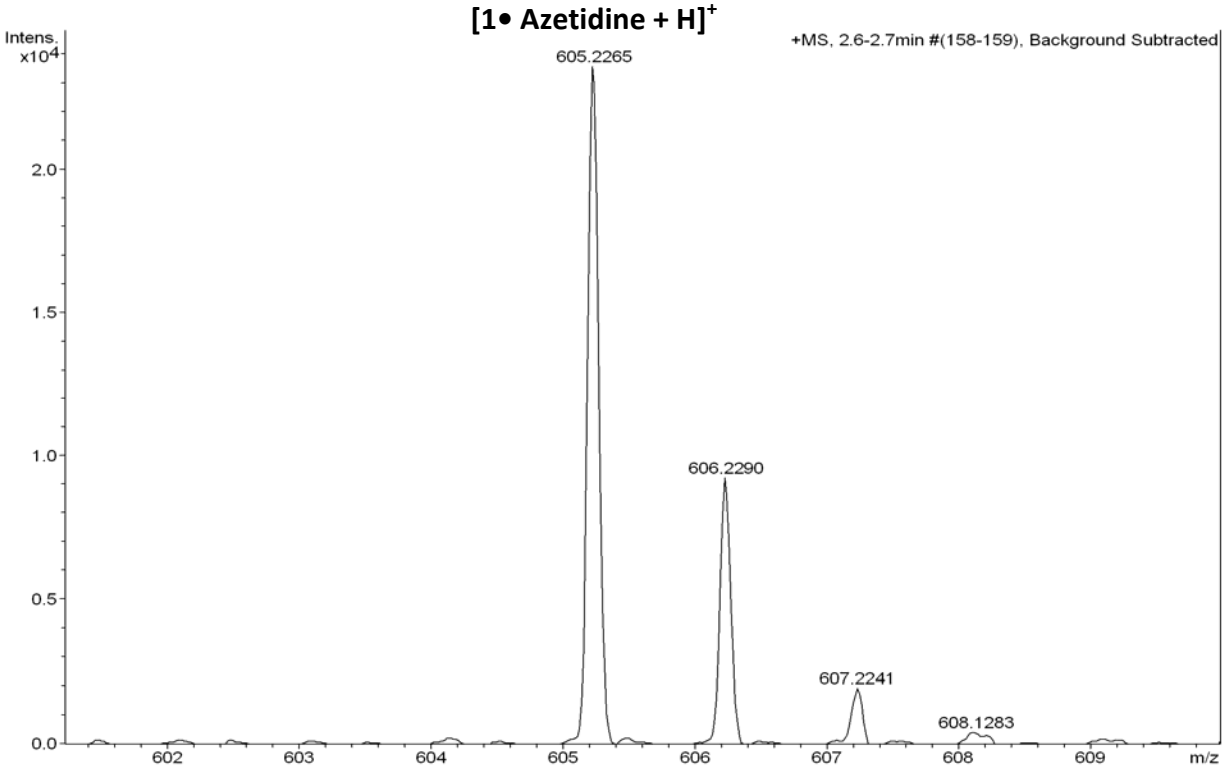
[1• Di-*n*-hexylamine + H]$^+$

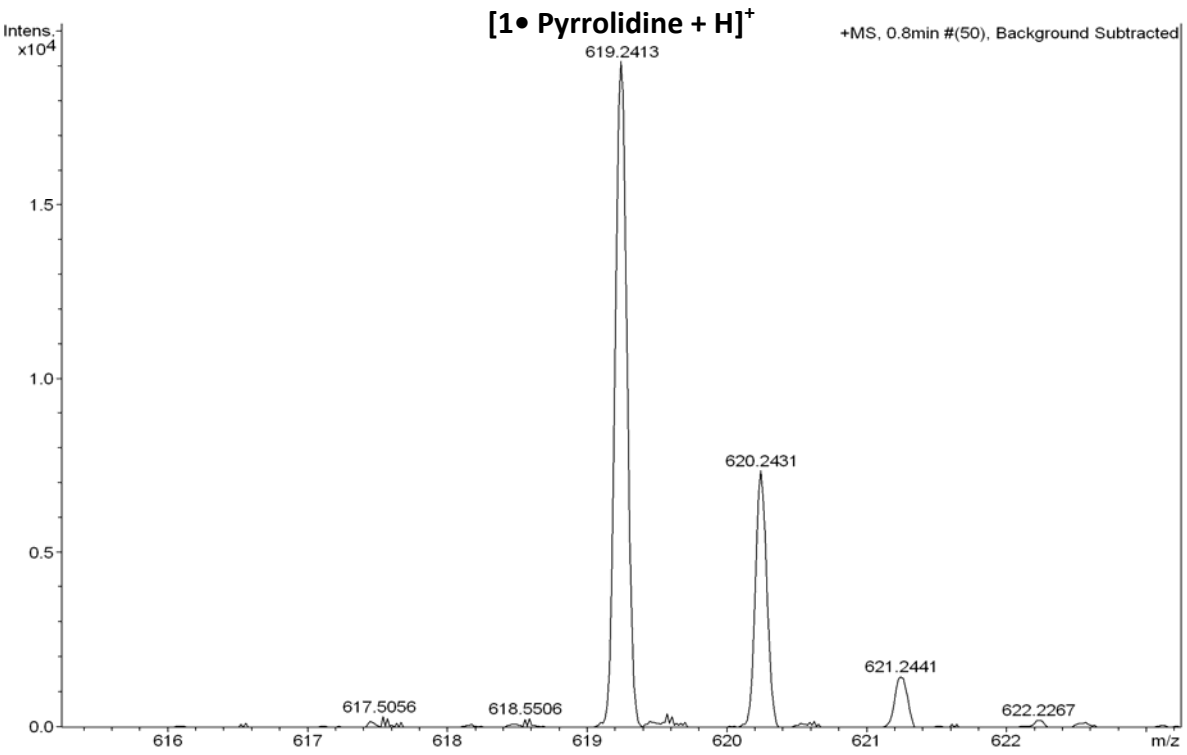


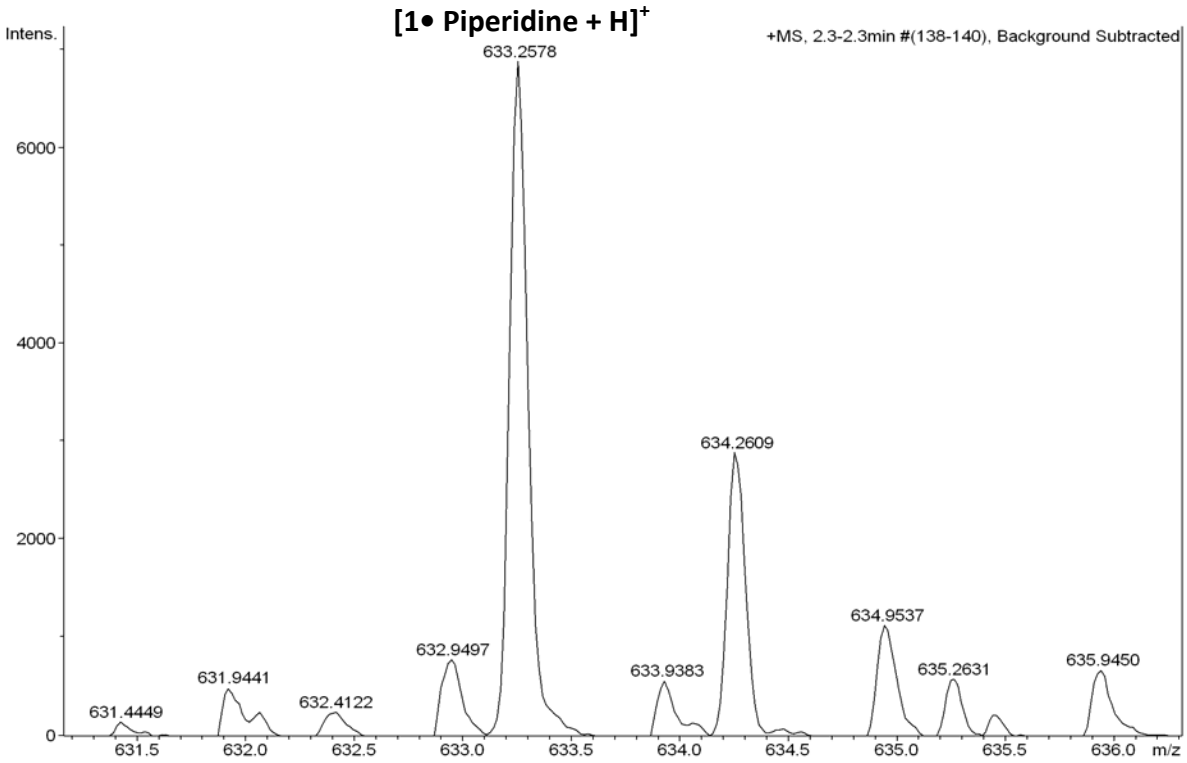
[1• Di-*n*-octylamine + H]$^+$



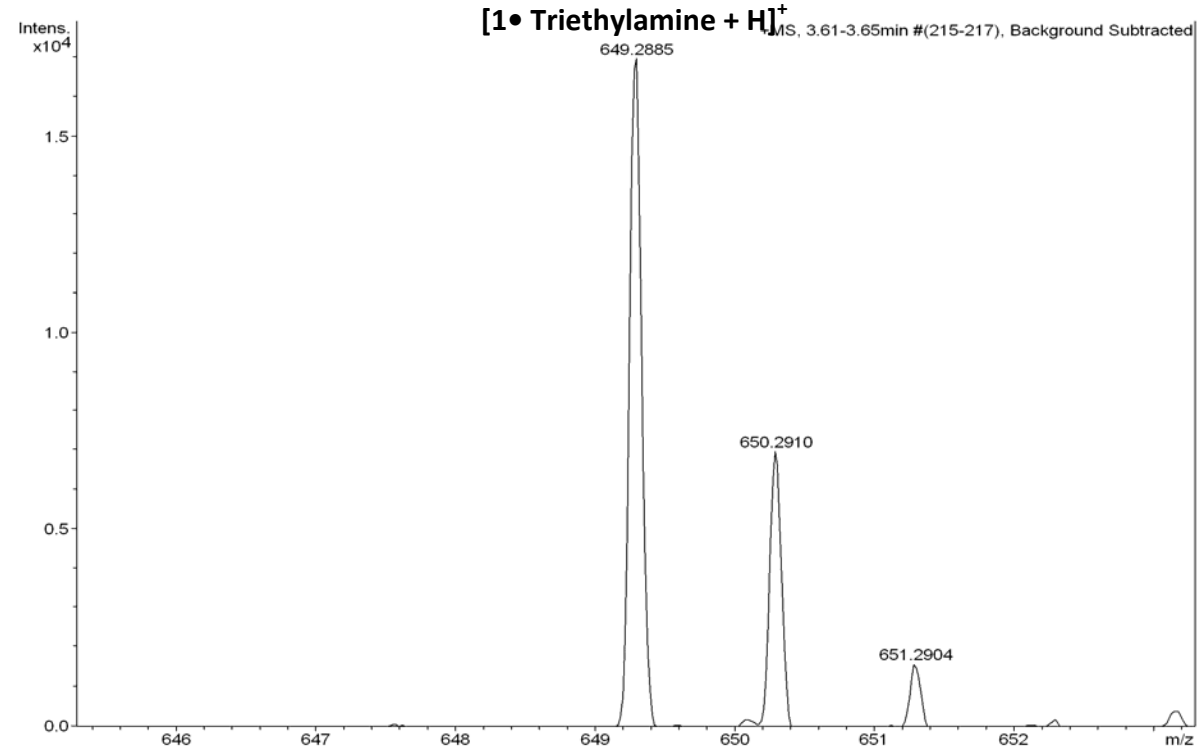
[1• Azetidine + H]$^+$



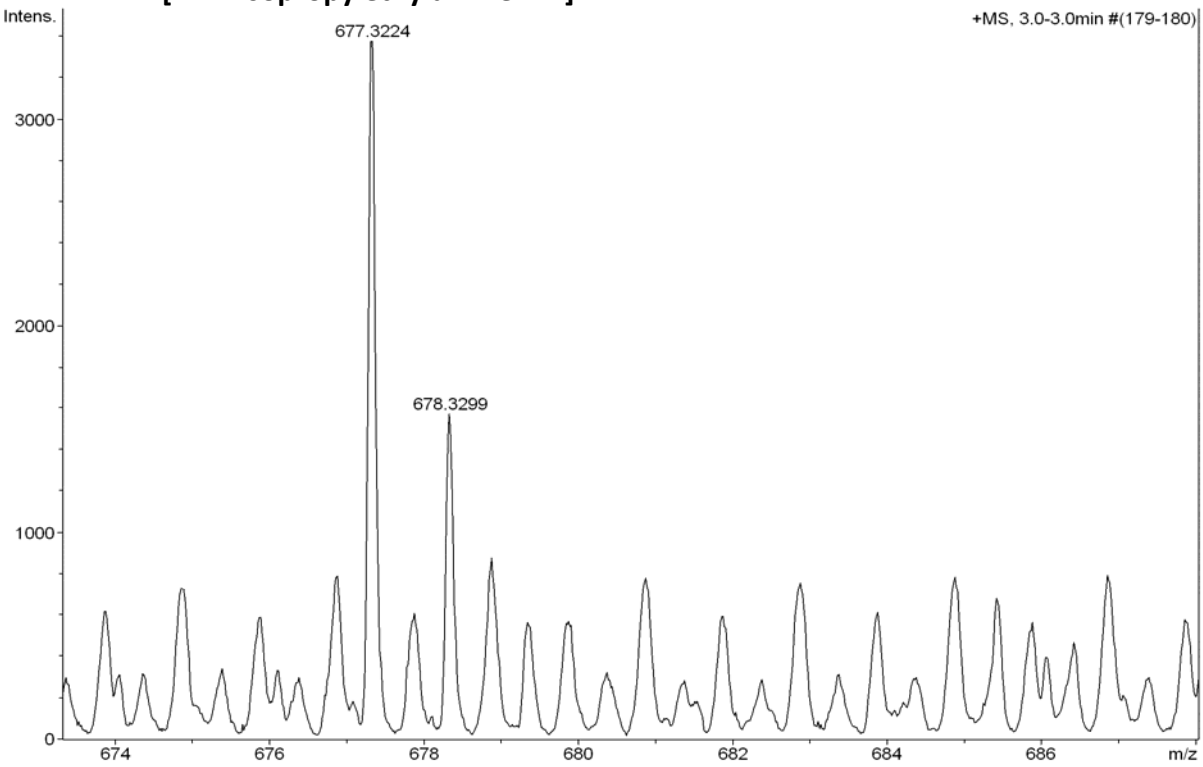

[1• Pyrrolidine + H]+
+MS, 0.8min #(50), Background Subtracted
Intens.
x10^4
619.2413
620.2431
621.2441
617.5056
618.5506
622.2267
m/z


[1• Piperidine + H]+
+MS, 2.3-2.3min #(138-140), Background Subtracted
Intens.
633.2578
634.2609
634.9537
632.9497
631.9441
633.9383
635.2631
635.9450
632.4122
631.4449
m/z

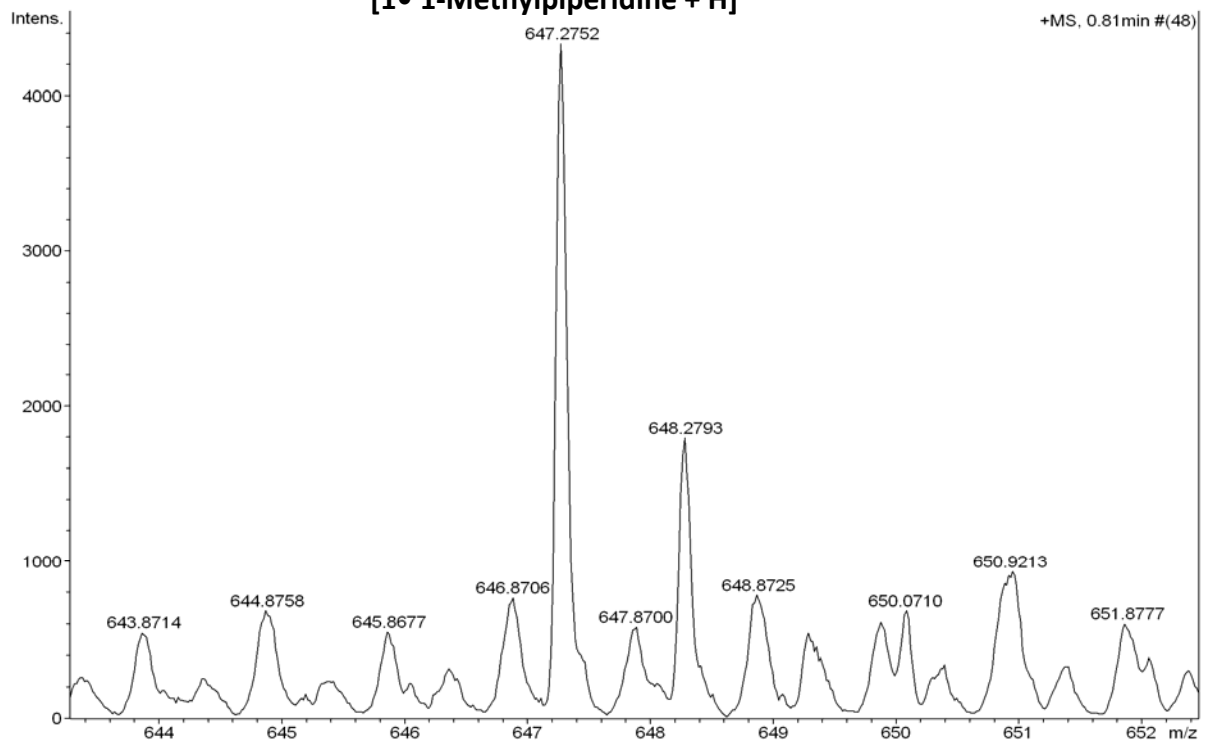
[1• Triethylamine + H]$^+$



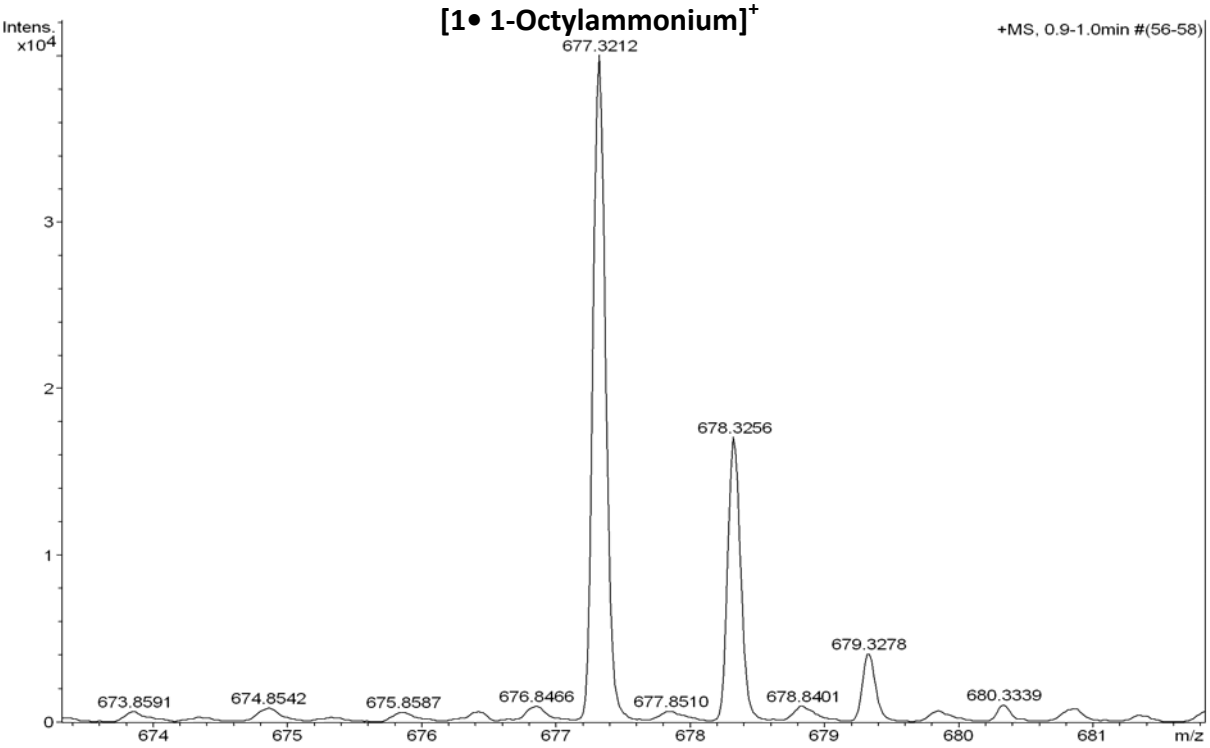
[1• Diisopropylethylamine + H]$^+$

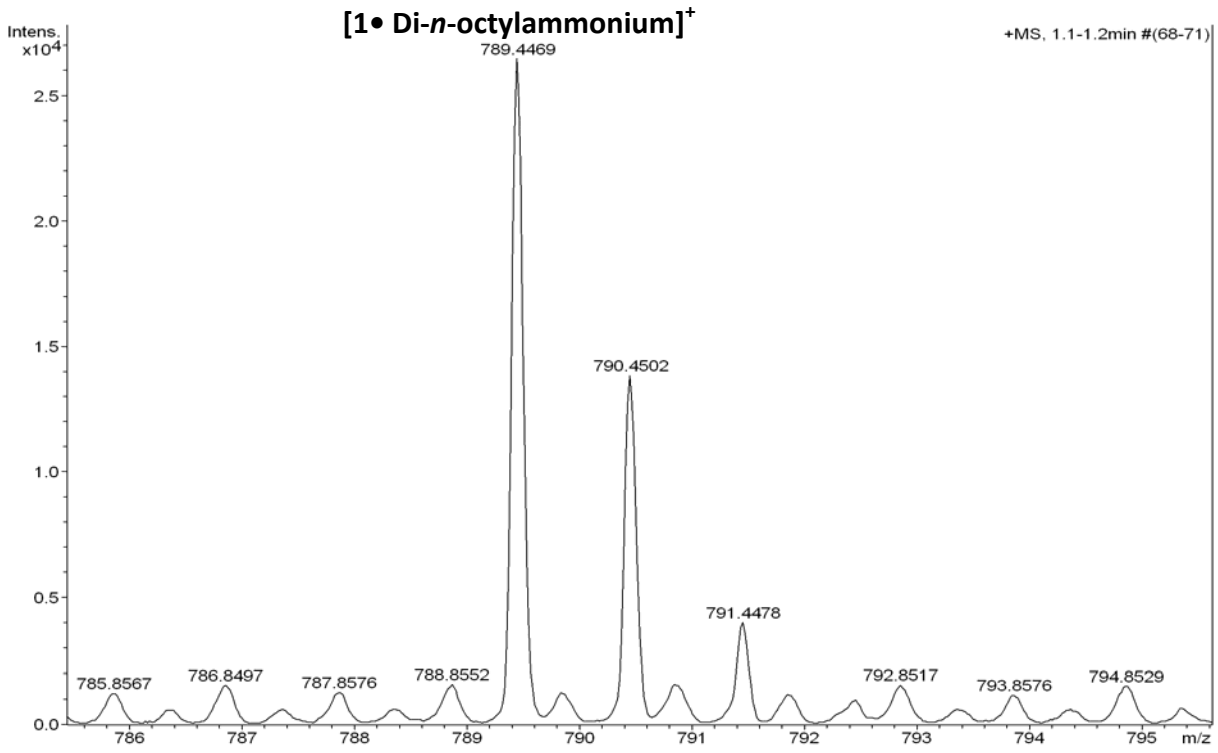


[1• 1-Methylpiperidine + H]$^+$



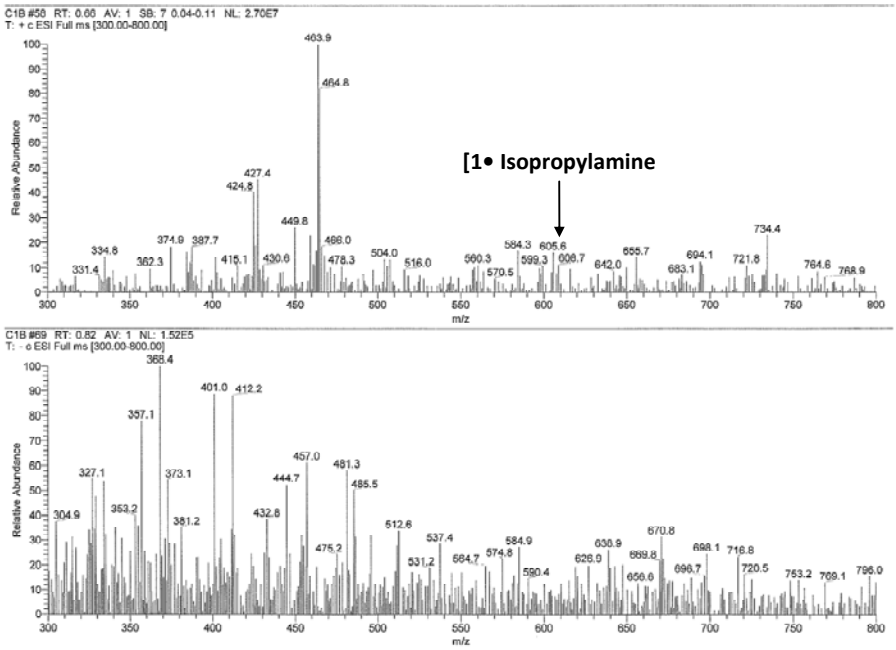
[1• 1-Octylammonium]$^+$



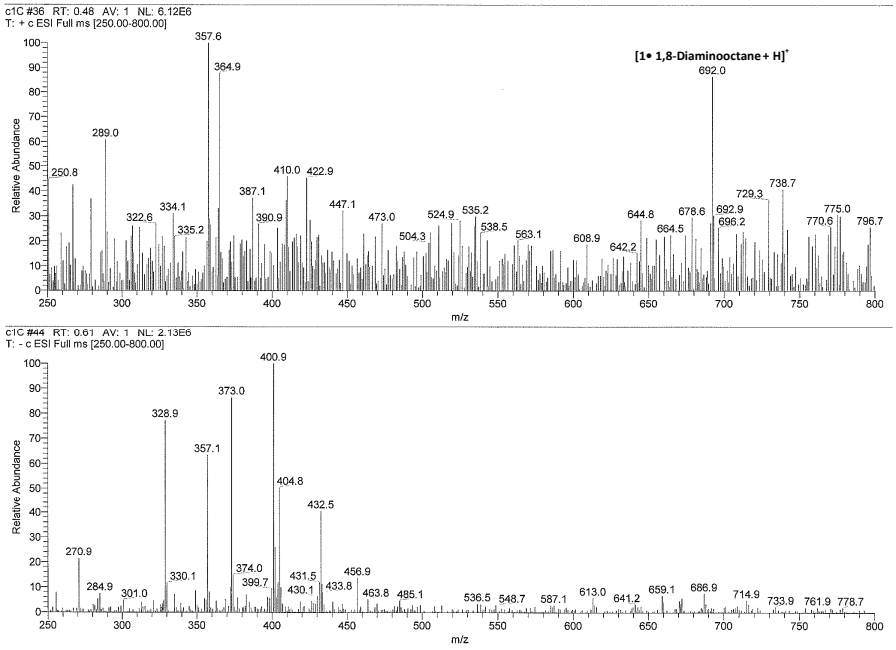

[1• Di-n-octylammonium]+
Intens.
x10^4
+MS, 1.1-1.2min #(68-71)
789.4469
790.4502
791.4478
785.8567
786.8497
787.8576
788.8552
792.8517
793.8576
794.8529
2.5
2.0
1.5
1.0
0.5
0.0
786
787
788
789
790
791
792
793
794
795
m/z

9. LRMS Spectra of [1•Guest] Complexes

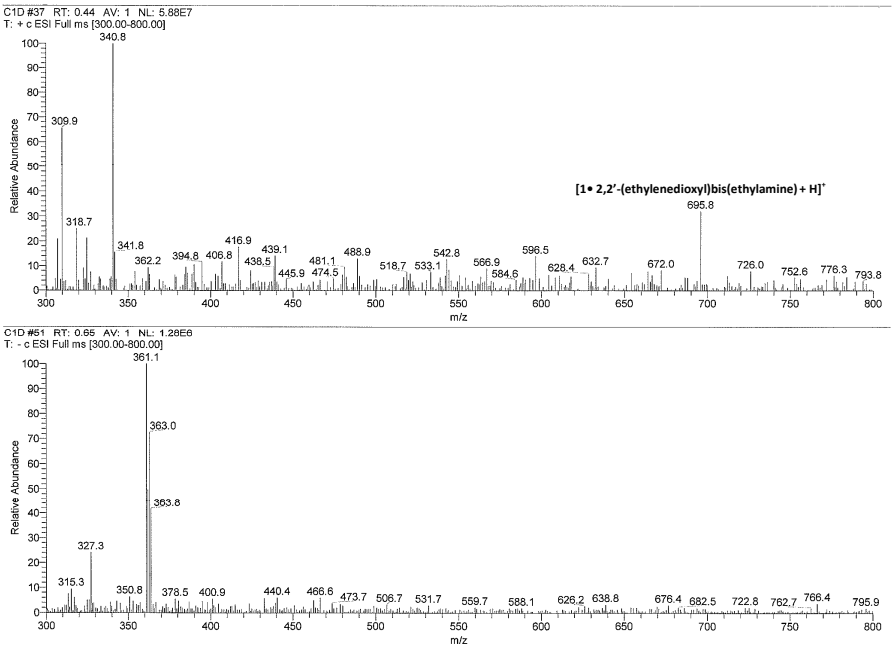
1• Isopropylamine (*m/z* = 607.2440)



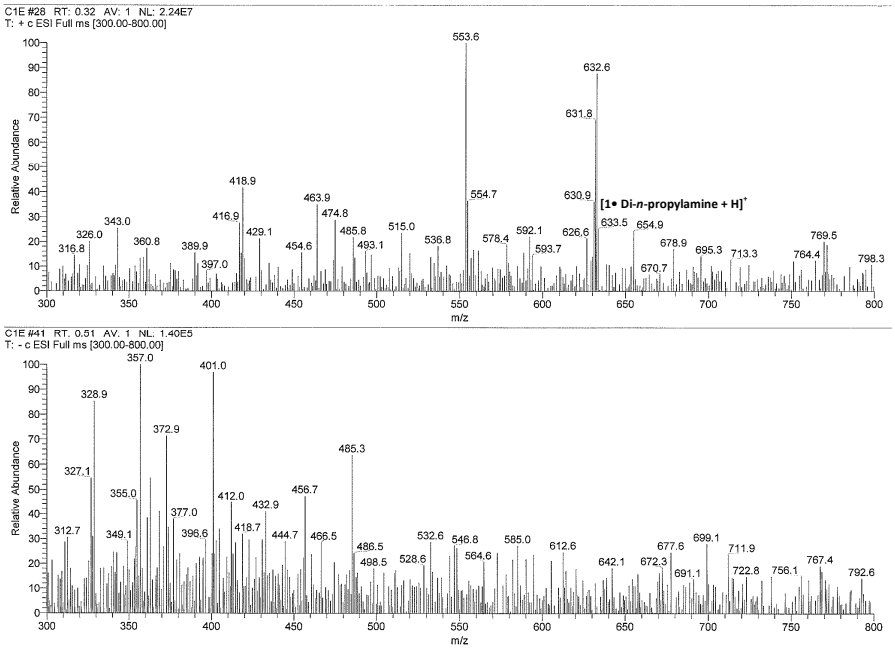
1• 1,8-Diaminooctane (*m/z* =692.3311)



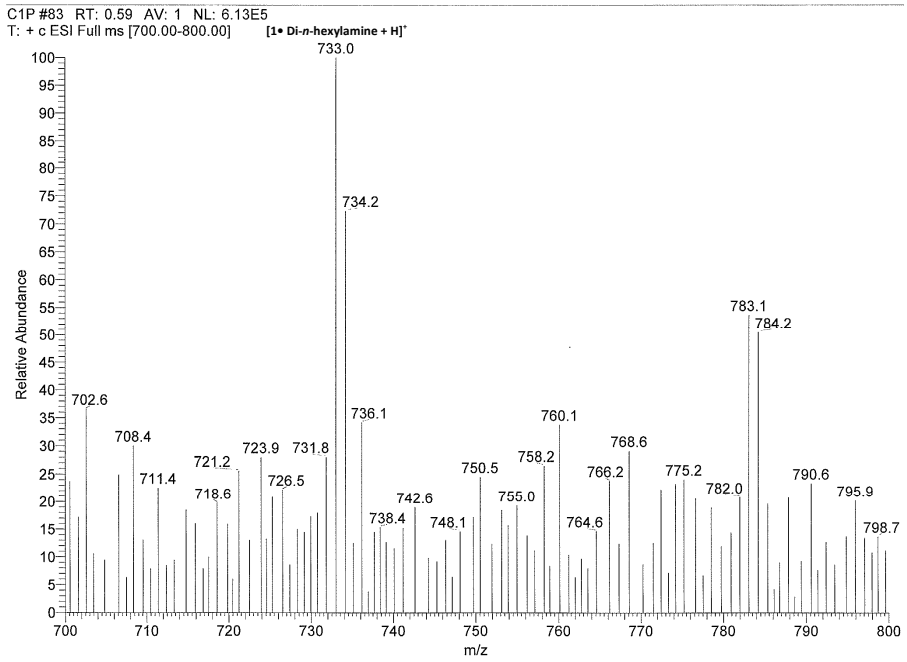
1• 2,2'-(ethylenedioxyl)bis(ethylamine) (*m/z* =696.2878)



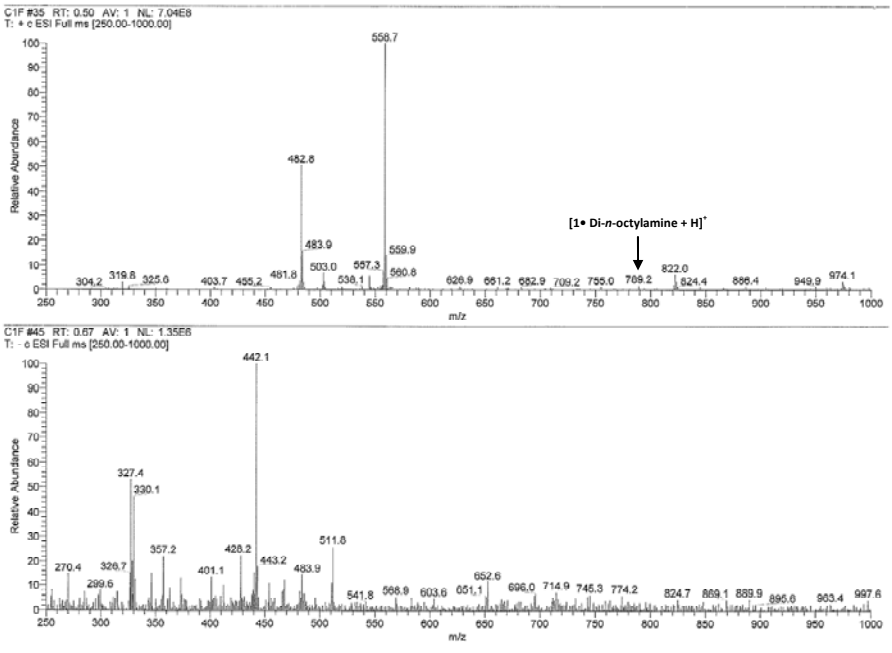
1• Di-*n*-propylamine (*m/z* =649.2891)



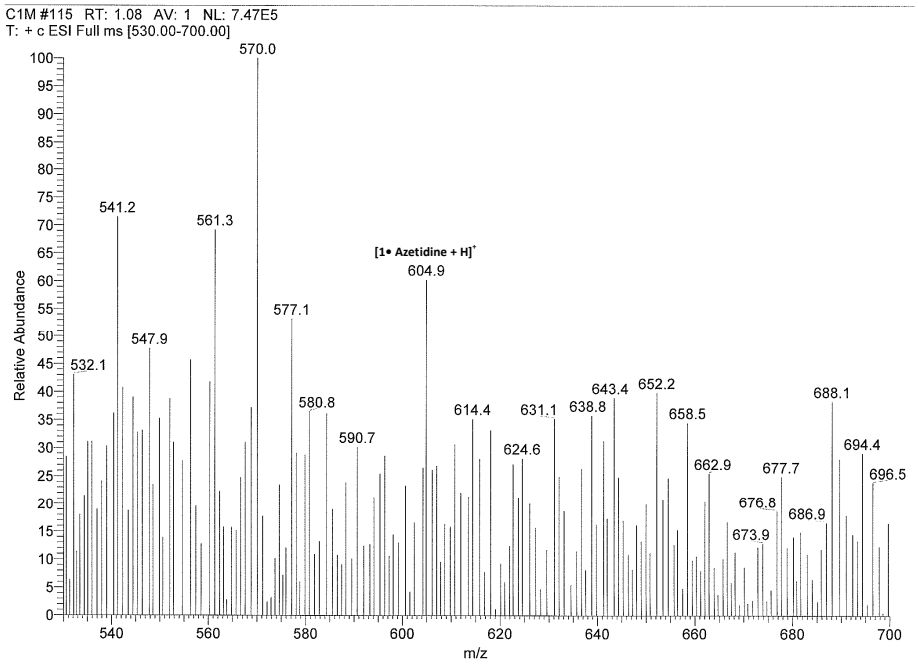
1• Di-*n*-hexylamine (*m/z* =733.3848)



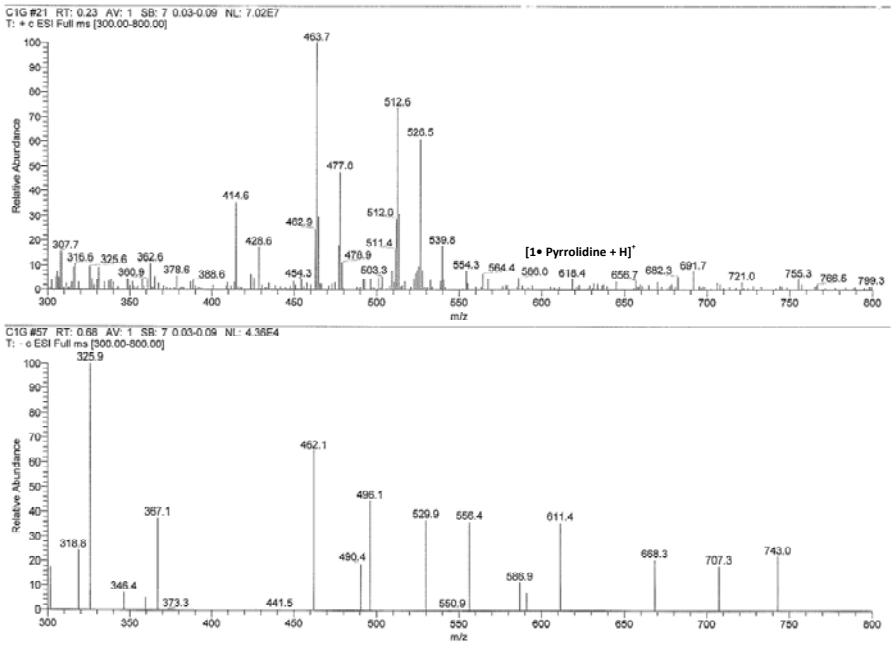
1• Di-*n*-octylamine (*m/z* =789.4458)



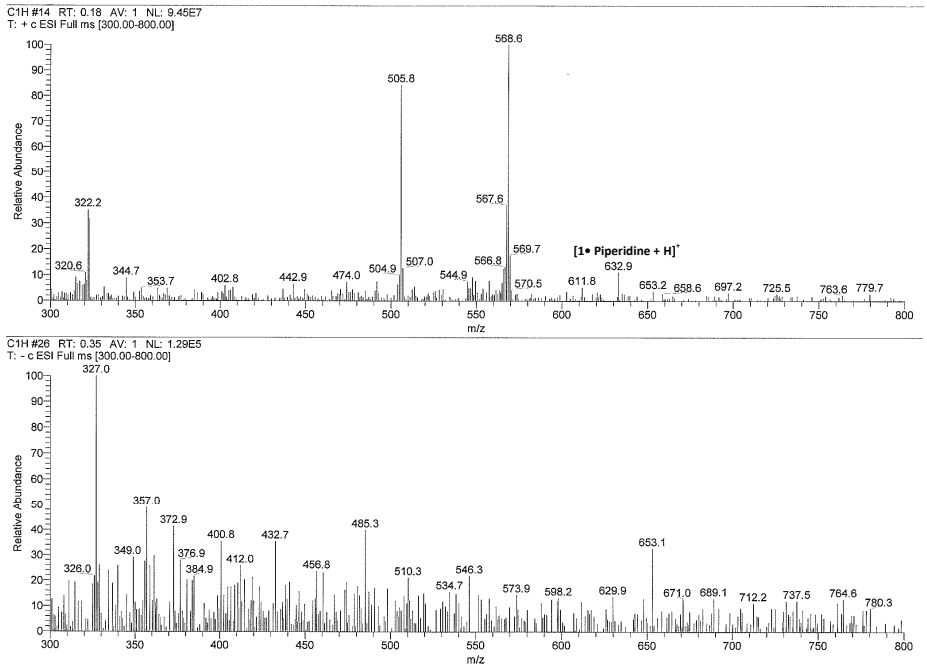
1• Azetidine (*m/z* =605.2265)



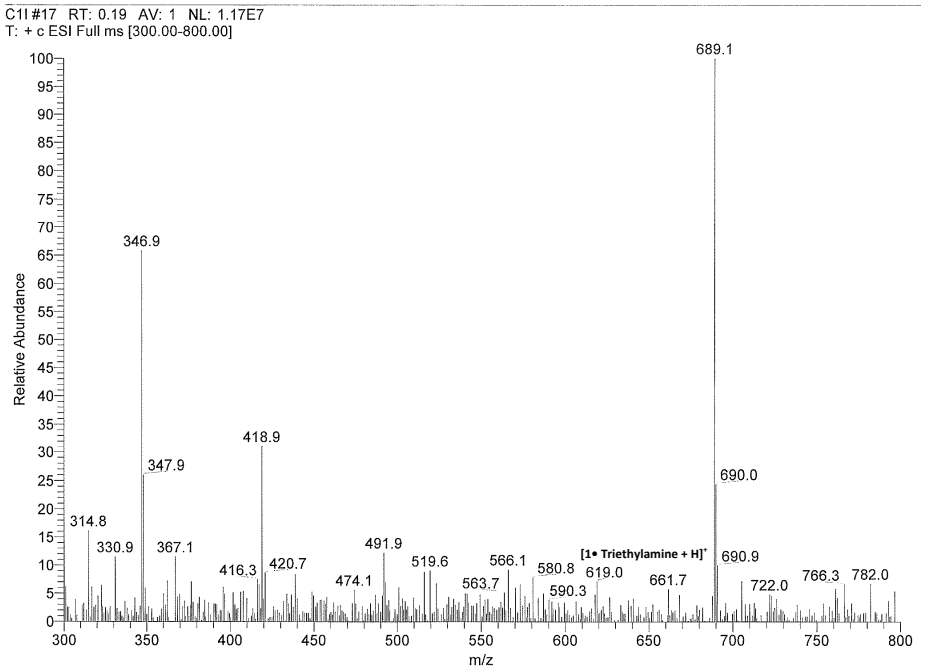
1• Pyrrolidine (*m/z* =619.2413)



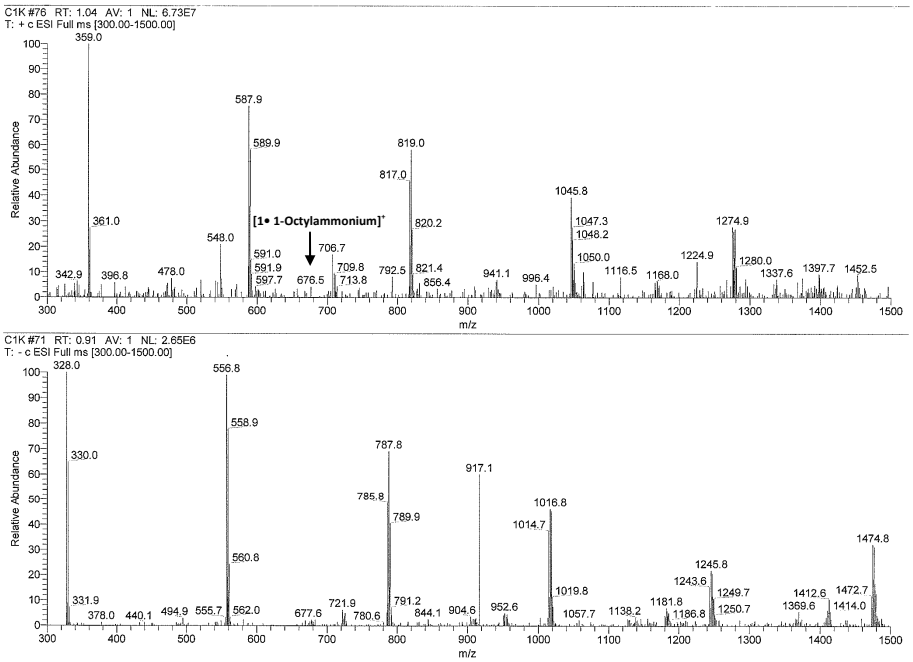
1• Piperidine (*m/z* =633.2578)



1• Triethylamine (*m/z* =649.2885)



1• 1-Octylammonium ion (*m/z* =677.3212)



1• Di-*n*-octylammonium ion (*m/z* =789.4469)