Supplementary Materials

N-benzylethanolammonium ionic liquids and molten salts in the synthesis of ^{68}Ga- and Al^{18}F-labelled radiopharmaceuticals

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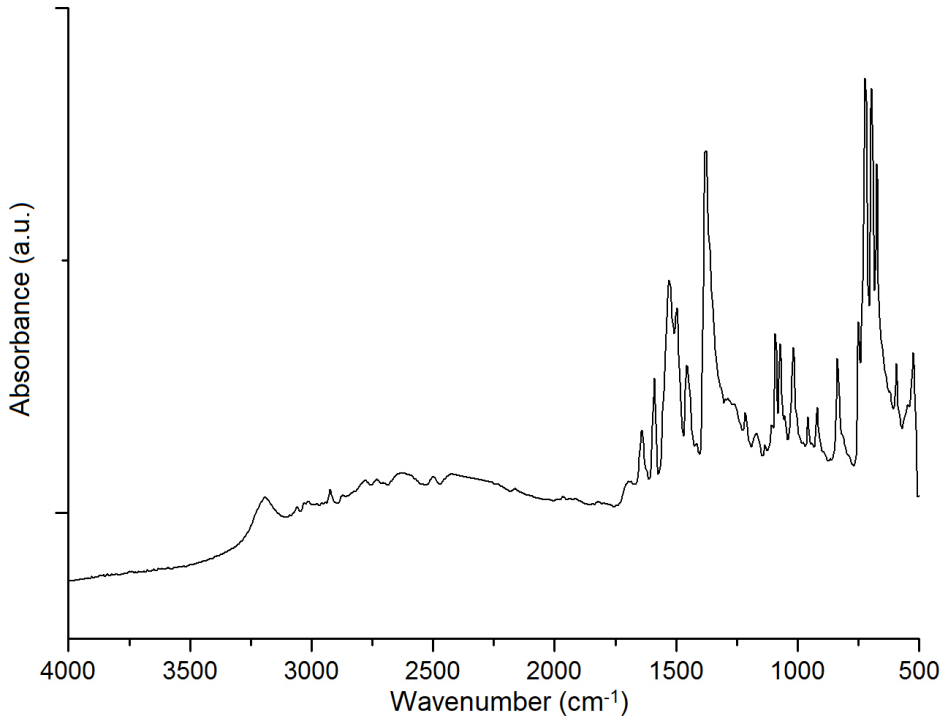

Figure S1. ATR-FTIR spectrum of BEA salt **1**

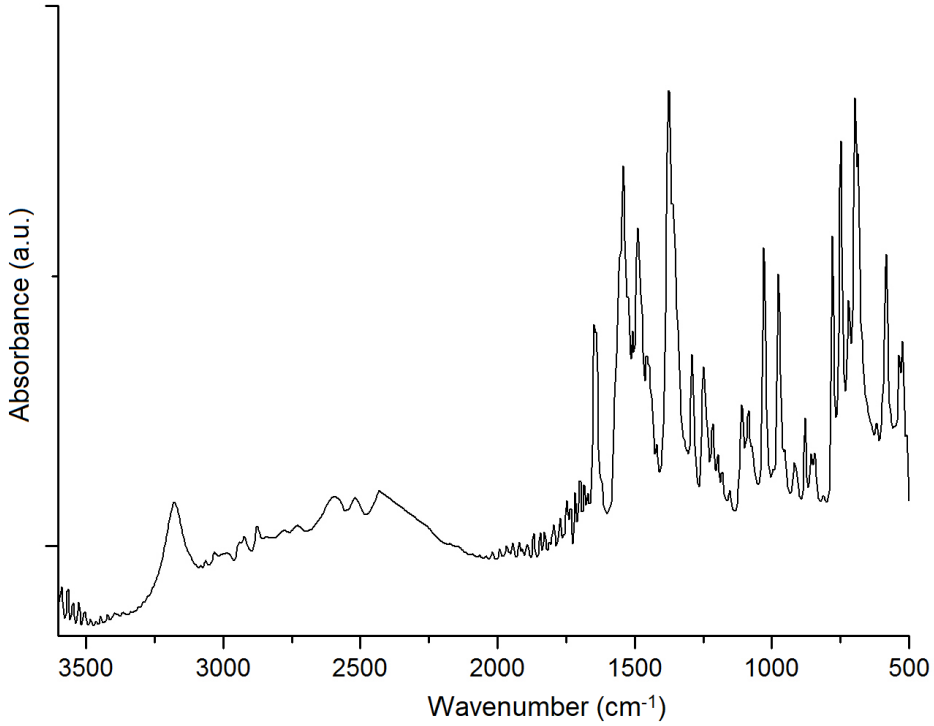

Figure S2. ATR-FTIR spectrum of BEA salt **2**

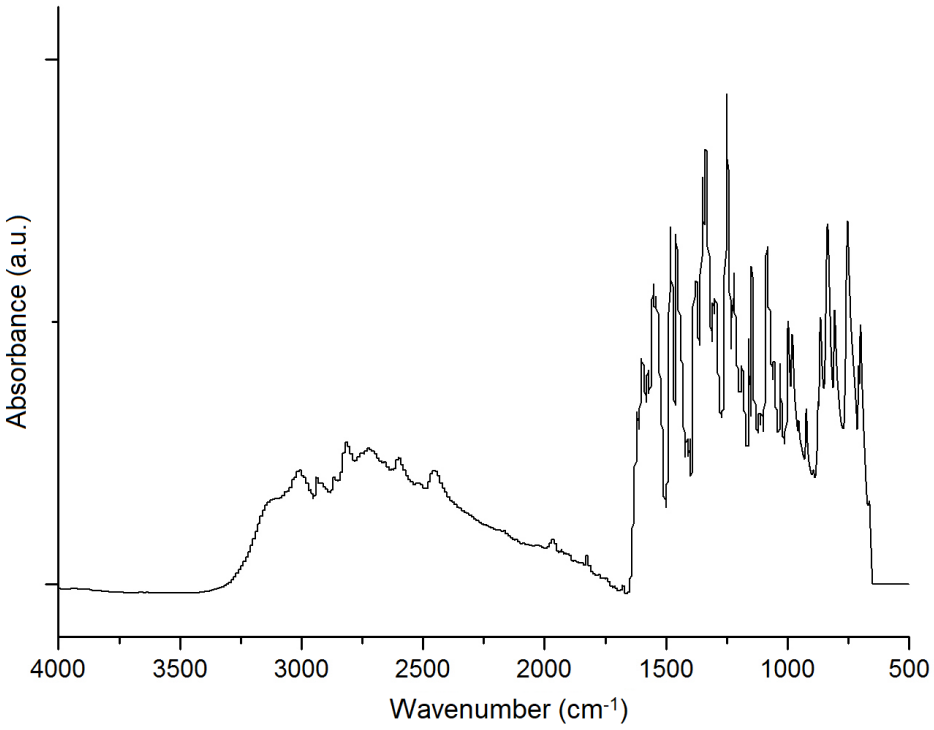

Figure S3. ATR-FTIR spectrum of BEA salt **3**

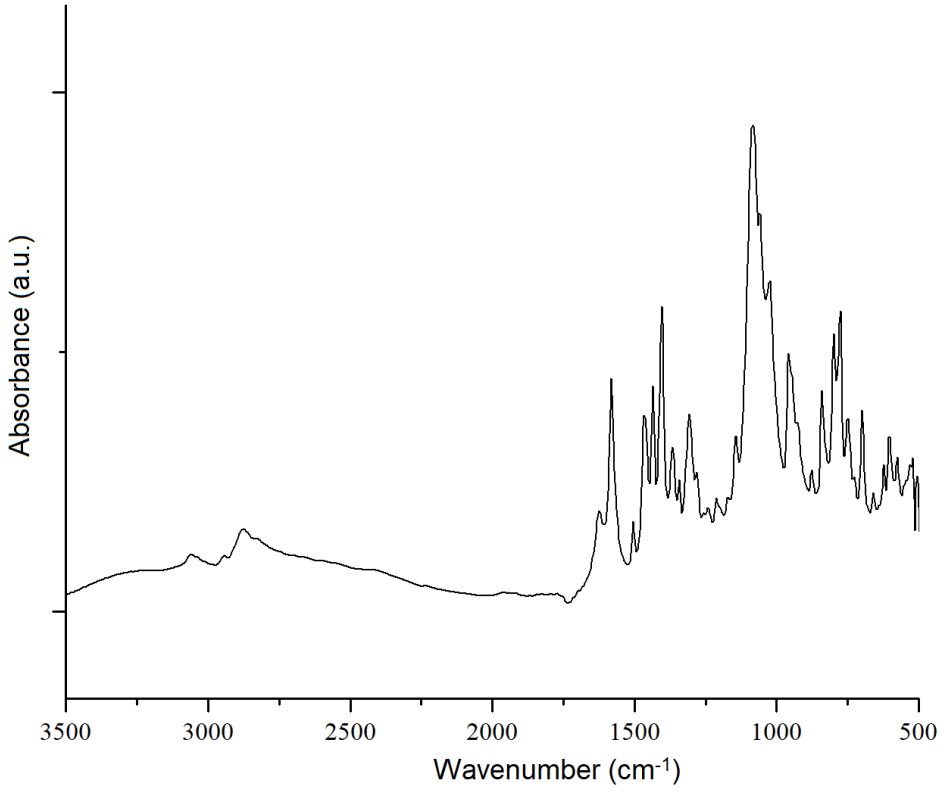

Figure S4. ATR-FTIR spectrum of BEA salt **4**

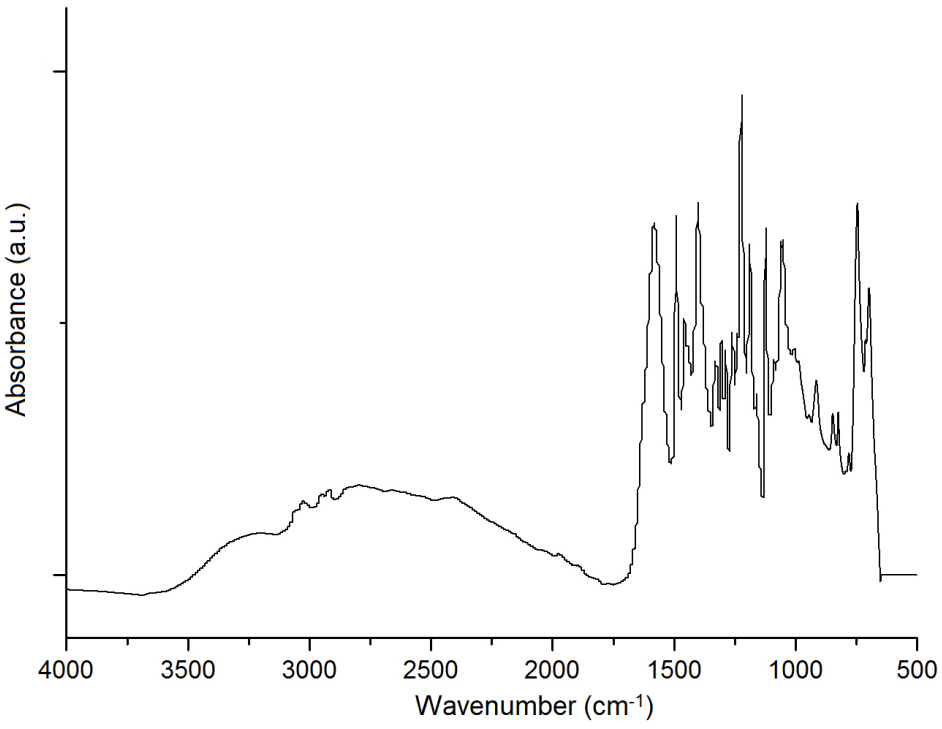

Figure S5. ATR-FTIR spectrum of BEA salt **5**

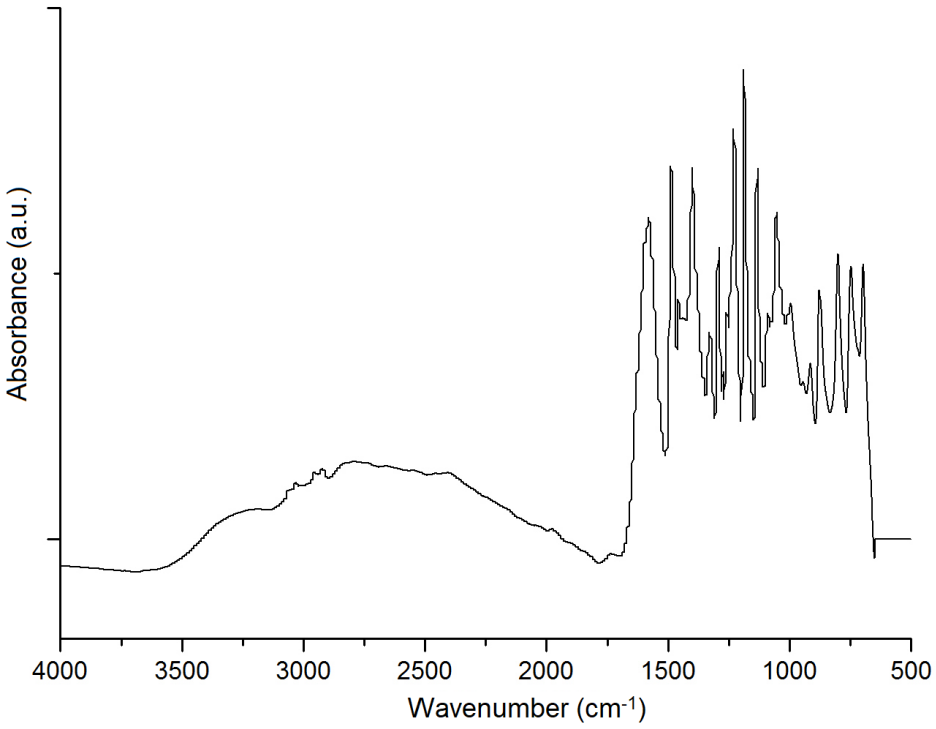

Figure S6. ATR-FTIR spectrum of BEA salt **6**

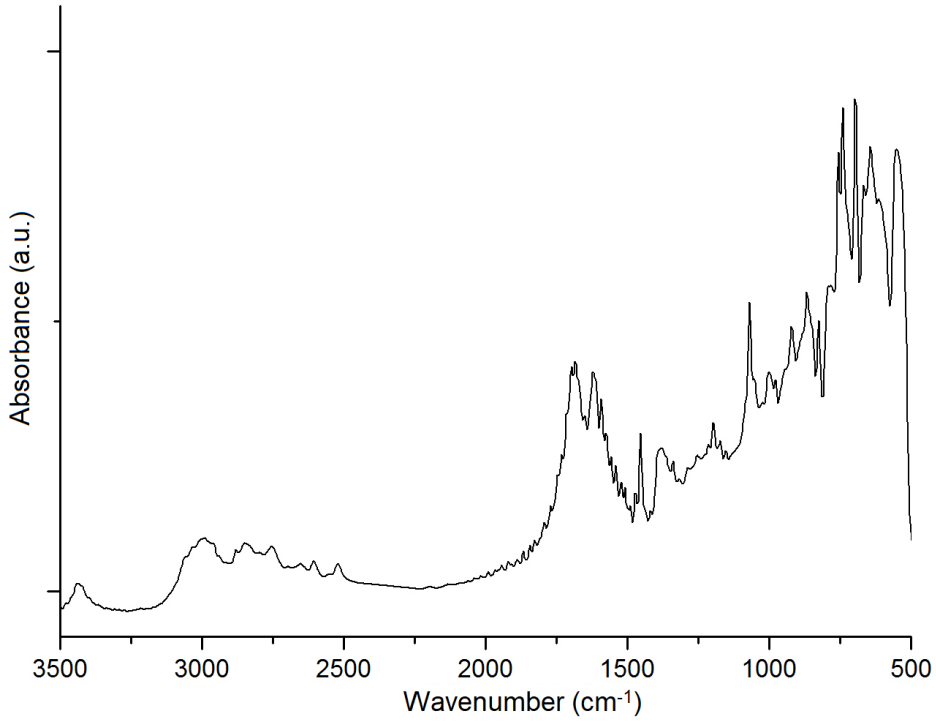

Figure S7. ATR-FTIR spectrum of BEA salt **7**

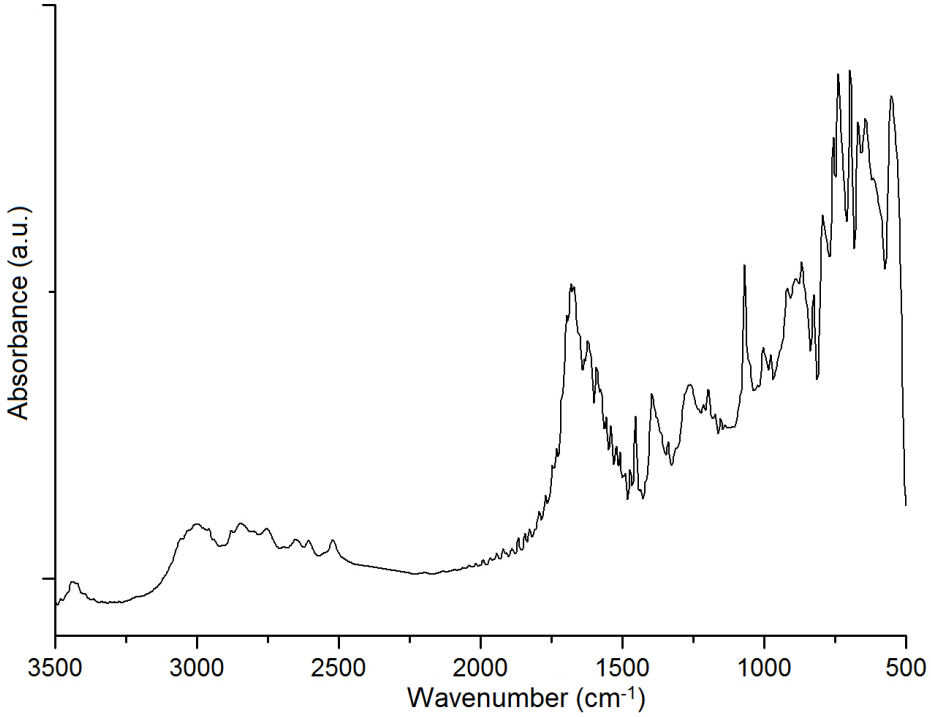

Figure S8. ATR-FTIR spectrum of BEA salt **8**

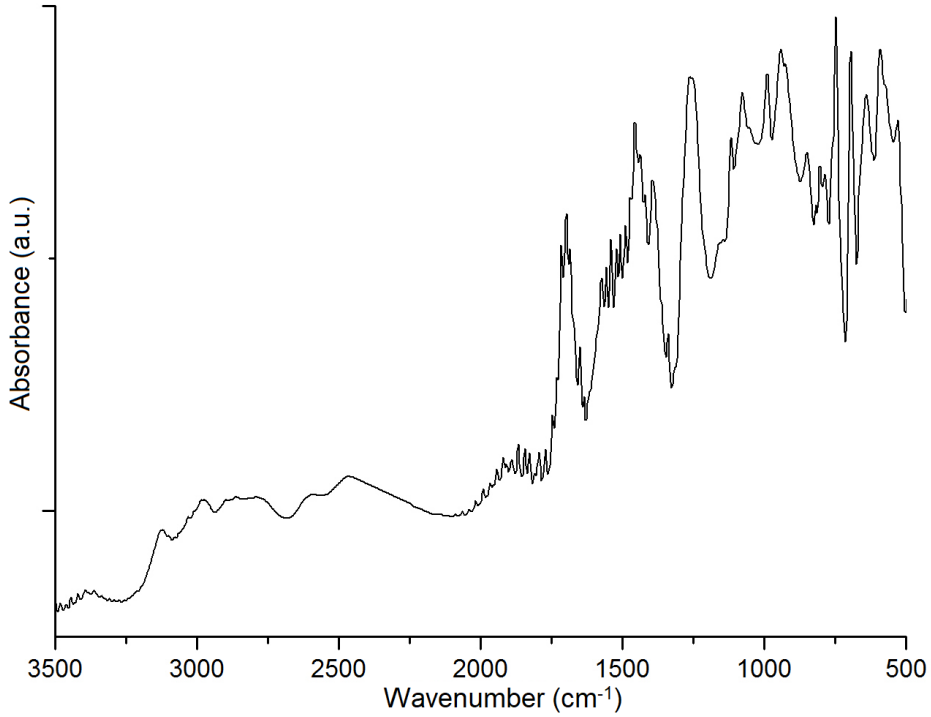

Figure S9. ATR-FTIR spectrum of BEA salt **9**

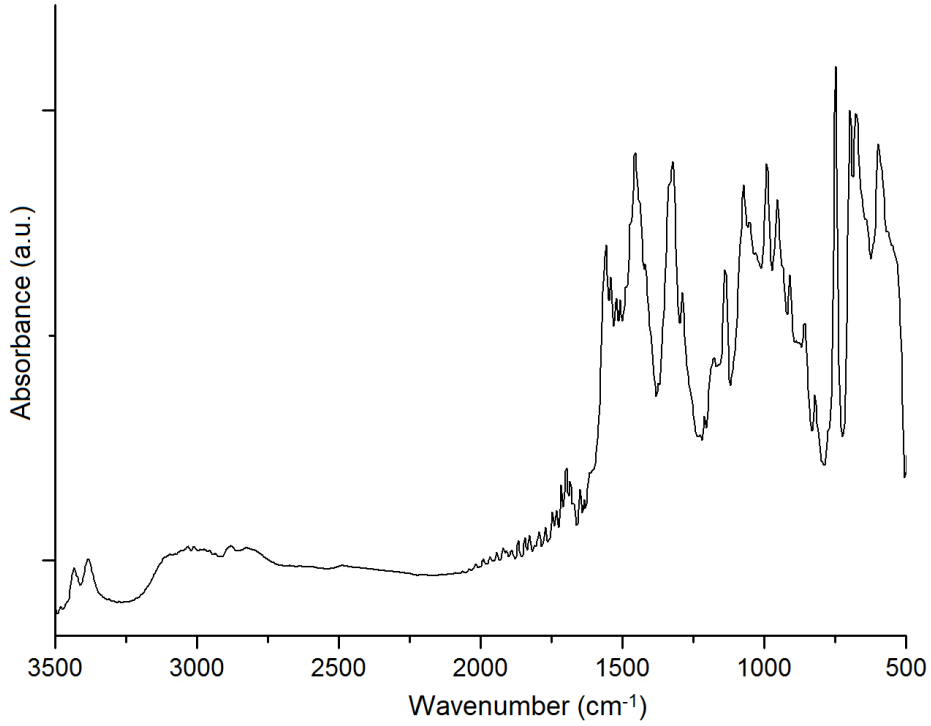

Figure S10. ATR-FTIR spectrum of BEA salt **10**

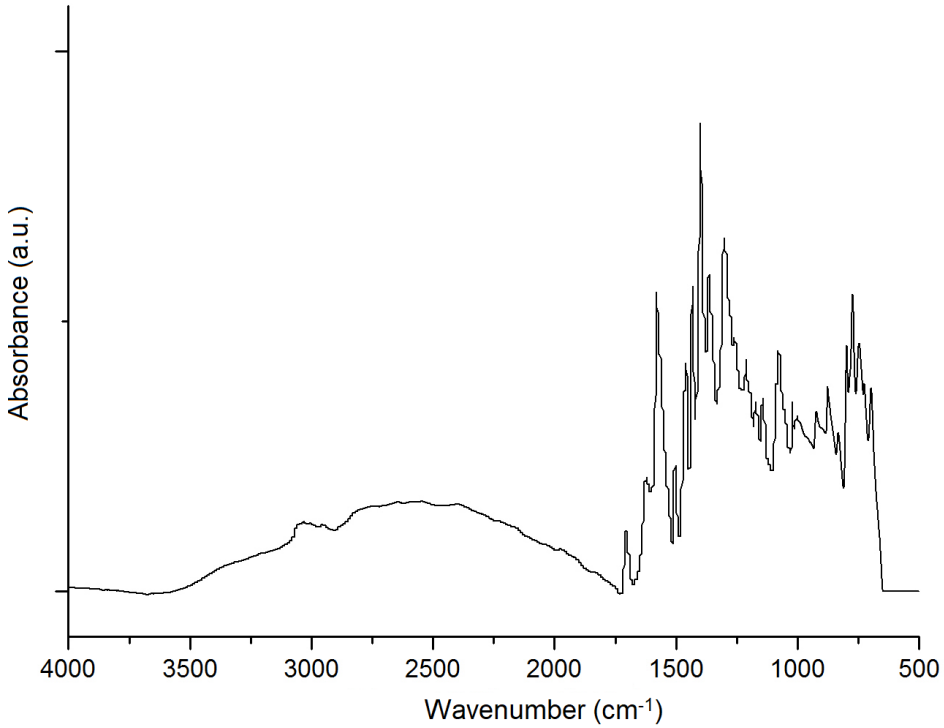

Figure S11. ATR-FTIR spectrum of BEA salt **11**

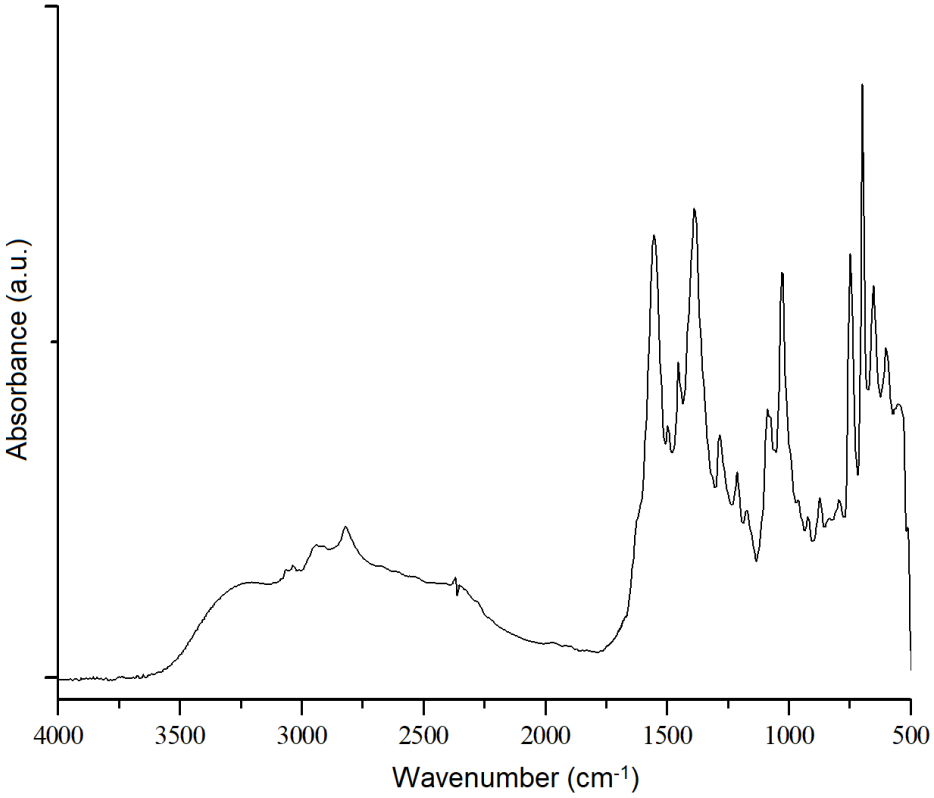

Figure S12. ATR-FTIR spectrum of BEA salt **12**

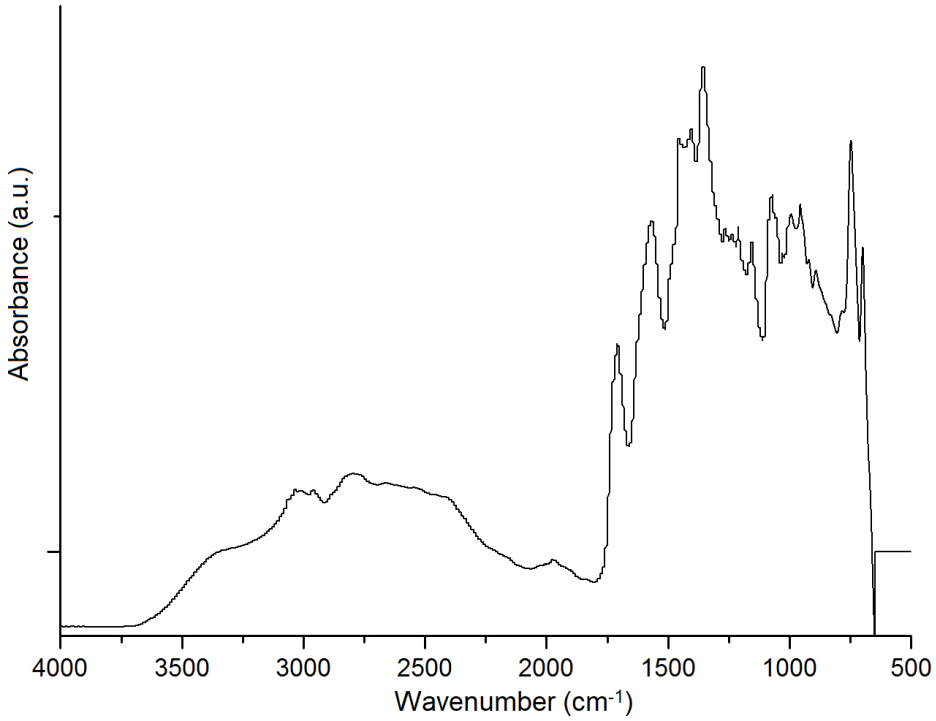

Figure S13. ATR-FTIR spectrum of BEA salt **13**

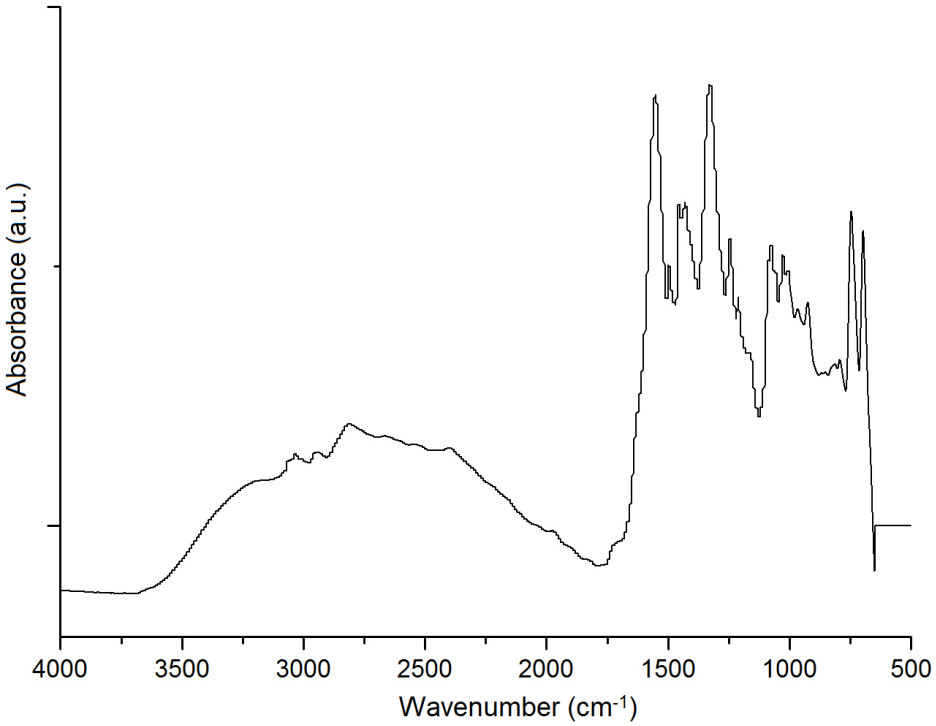

Figure S14. ATR-FTIR spectrum of BEA salt **14**

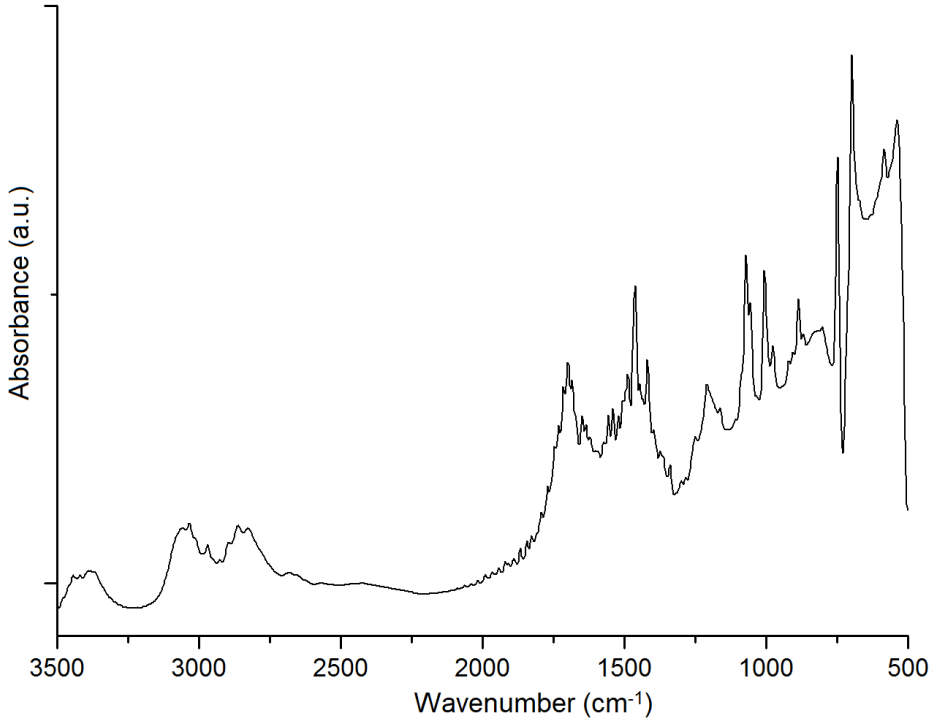

Figure S15. ATR-FTIR spectrum of BEA salt **15**

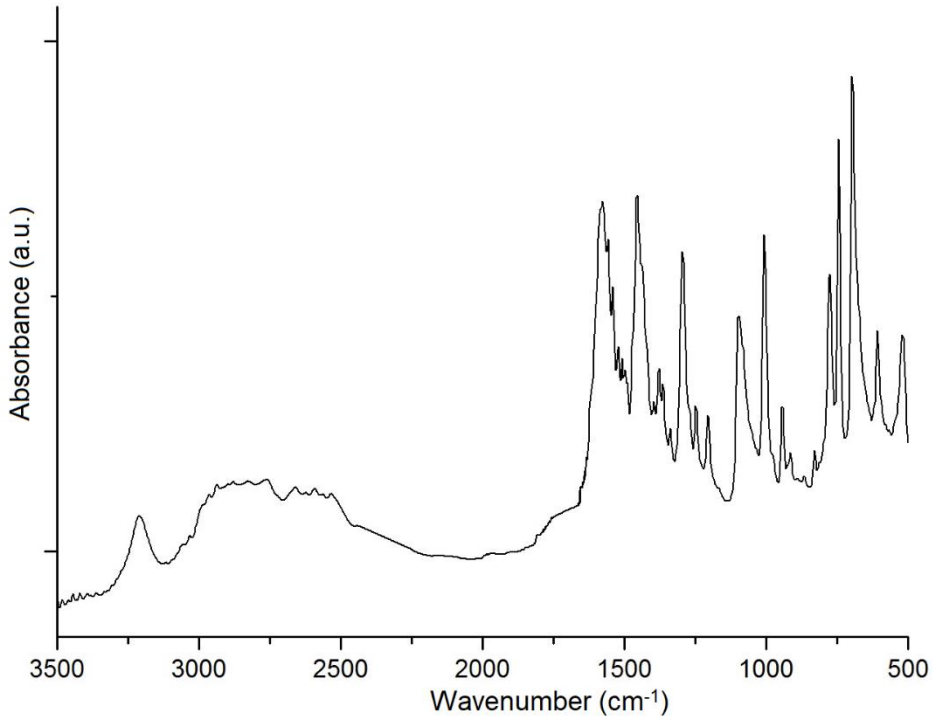

Figure S16. ATR-FTIR spectrum of BEA salt **16**

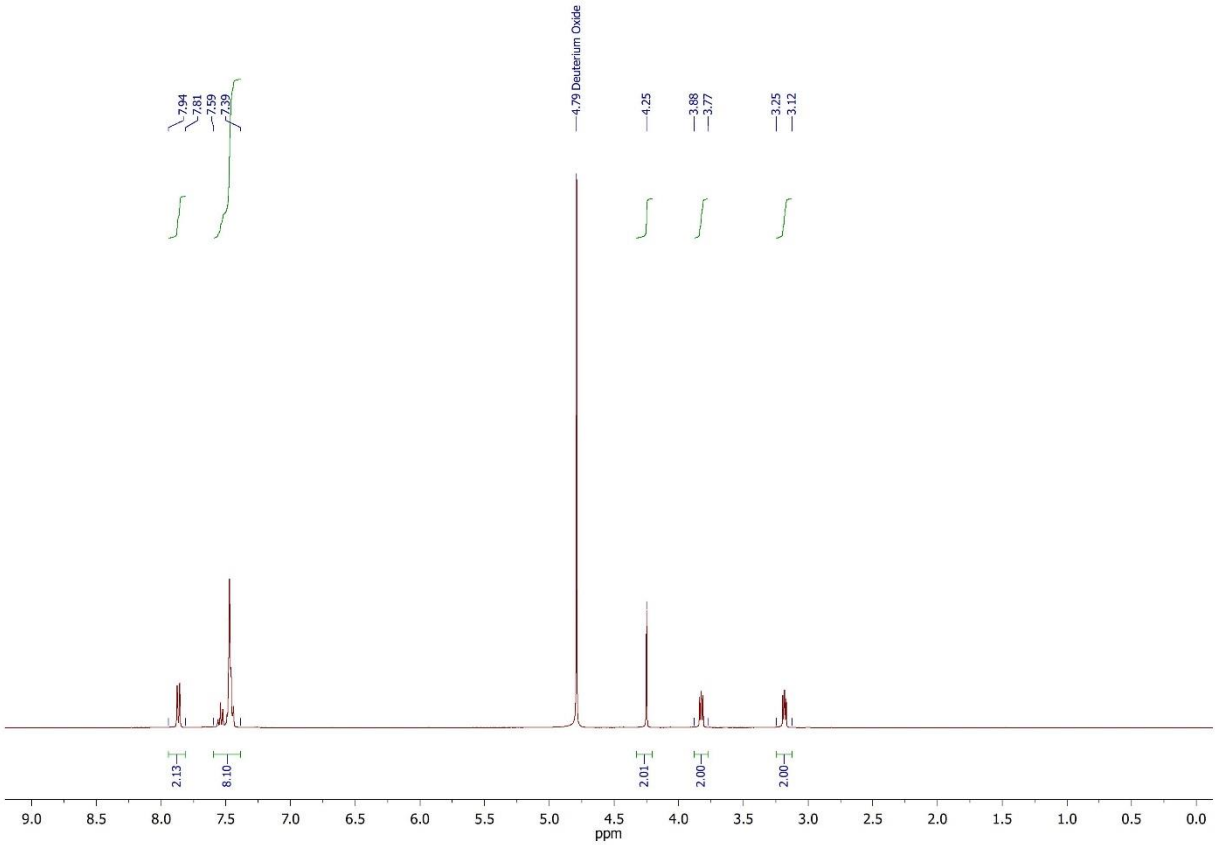

Figure S17 (a). ^{1}H NMR Spectrum of **1** (D_2O, δ, ppm, *J*, Hz)

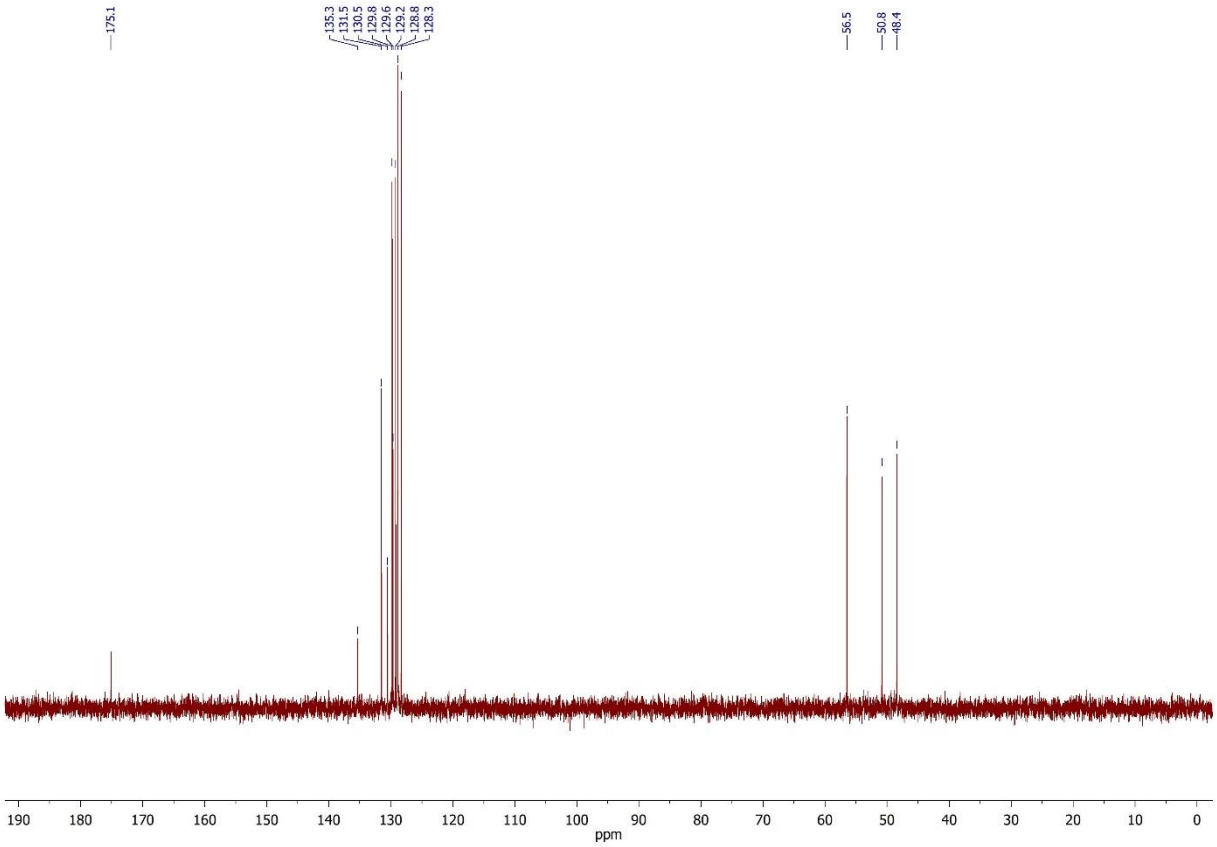

Figure S17 (b). ^{13}C NMR Spectrum of **1** (D_2O, δ, ppm)

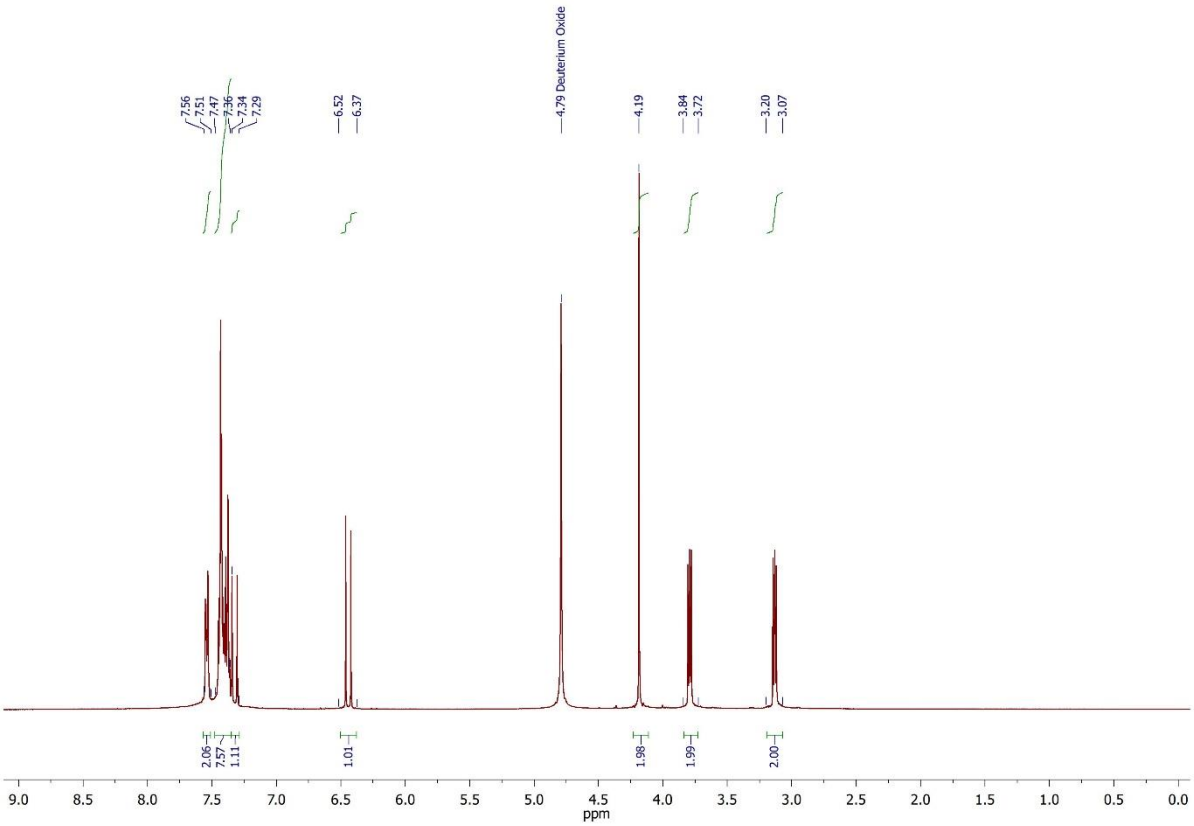

Figure S18 (a). ^{1}H NMR Spectrum of **2** (D_2O, δ, ppm, *J*, Hz)

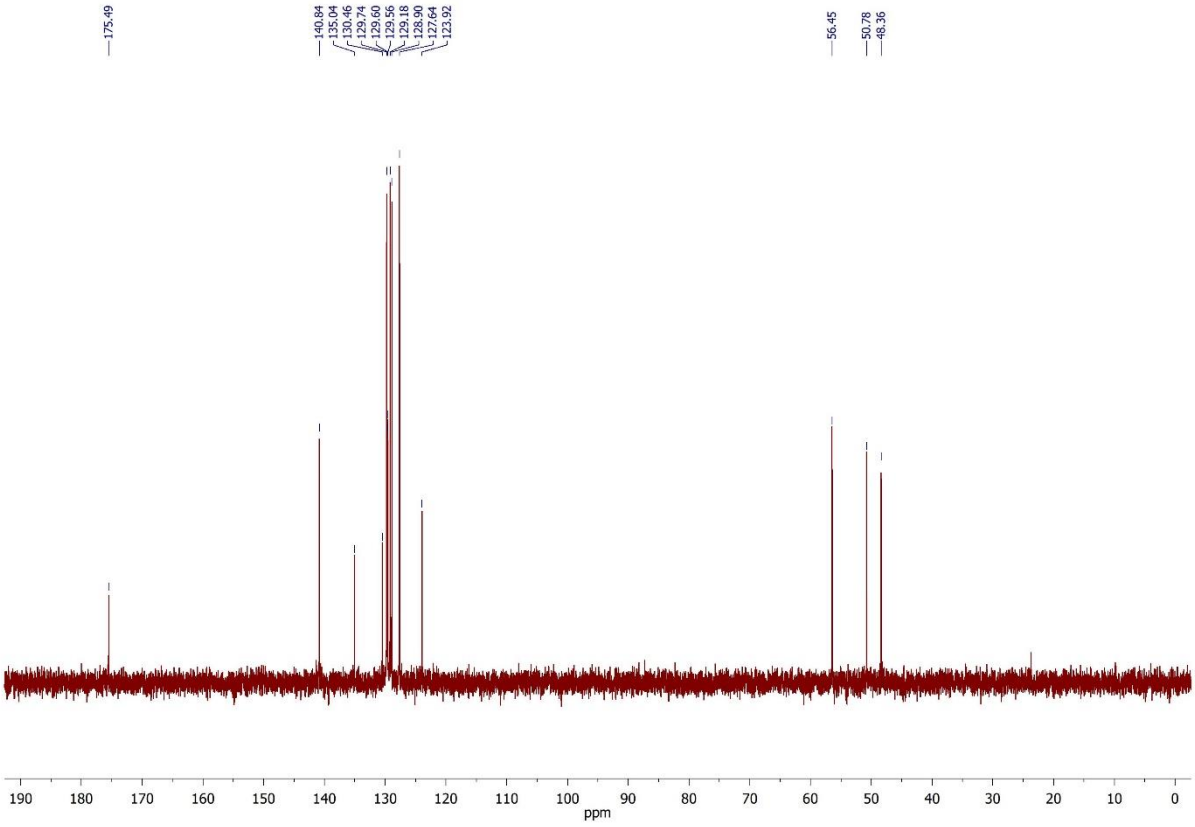

Figure S18 (b). ^{13}C NMR Spectrum of **2** (D_2O, δ, ppm)

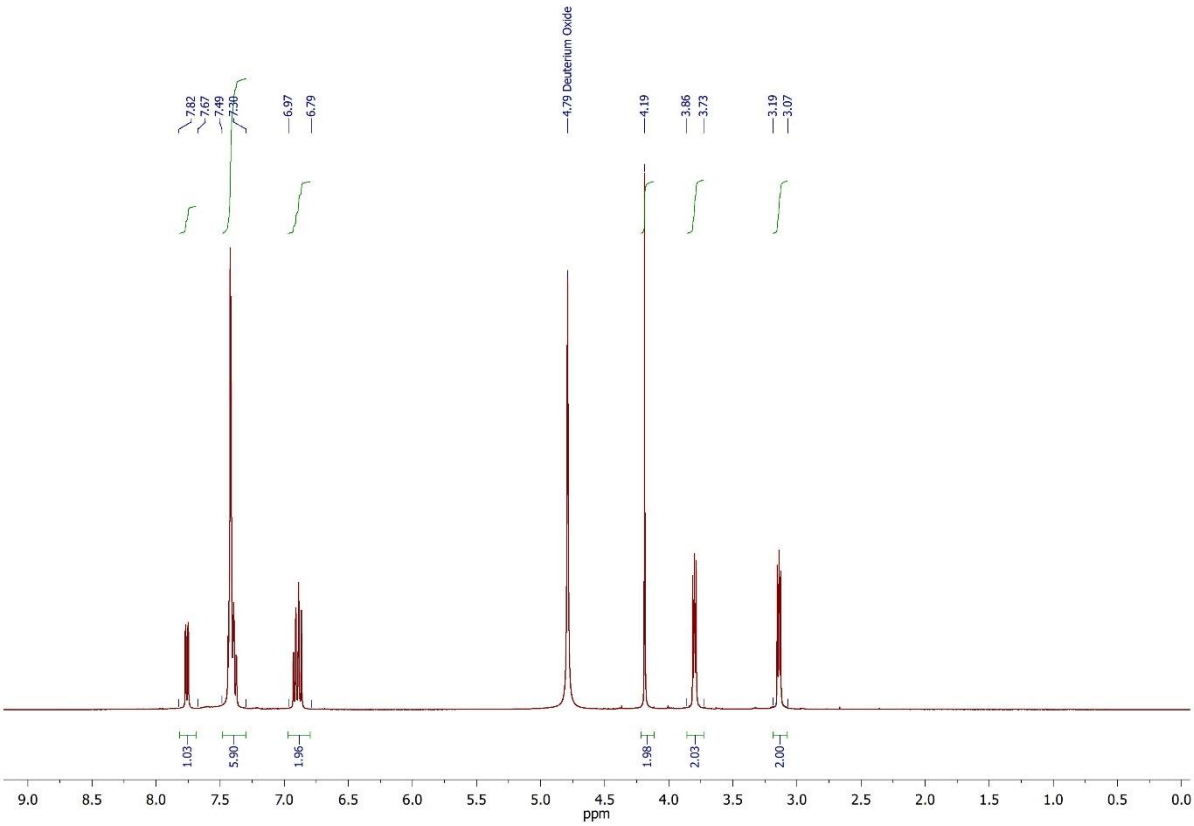

Figure S19 (a). ^{1}H NMR Spectrum of **3** (D_2O, δ, ppm, *J*, Hz)

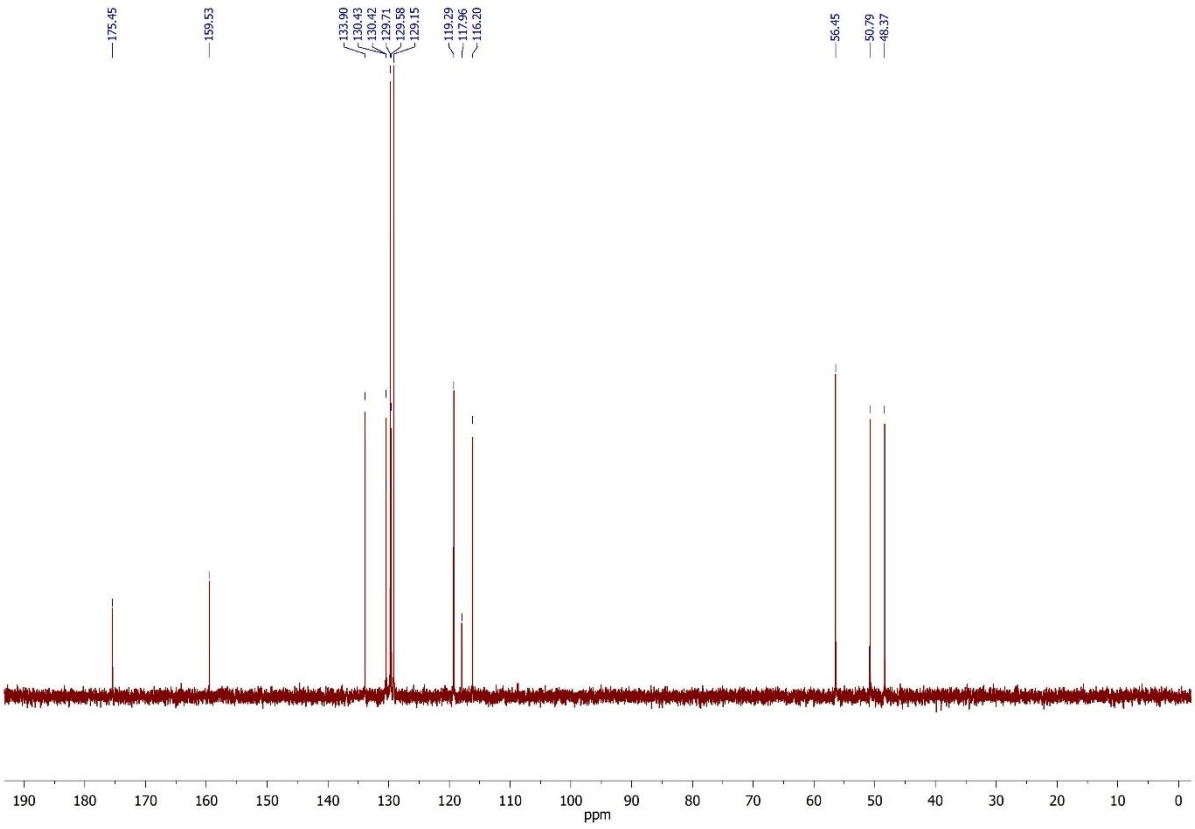

Figure S19 (b). ^{13}C NMR Spectrum of **3** (D_2O, δ, ppm)

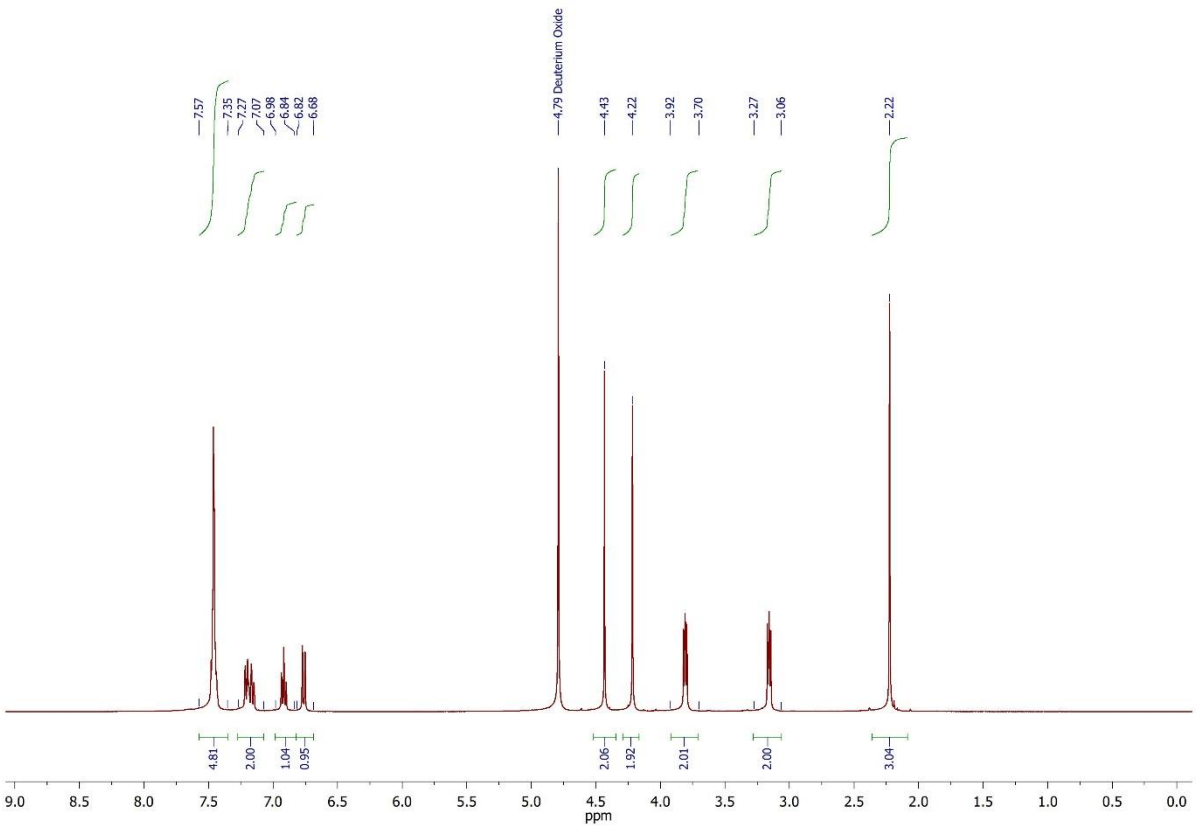

Figure S20 (a). ^{1}H NMR Spectrum of **5** (D_2O, δ, ppm, *J*, Hz)

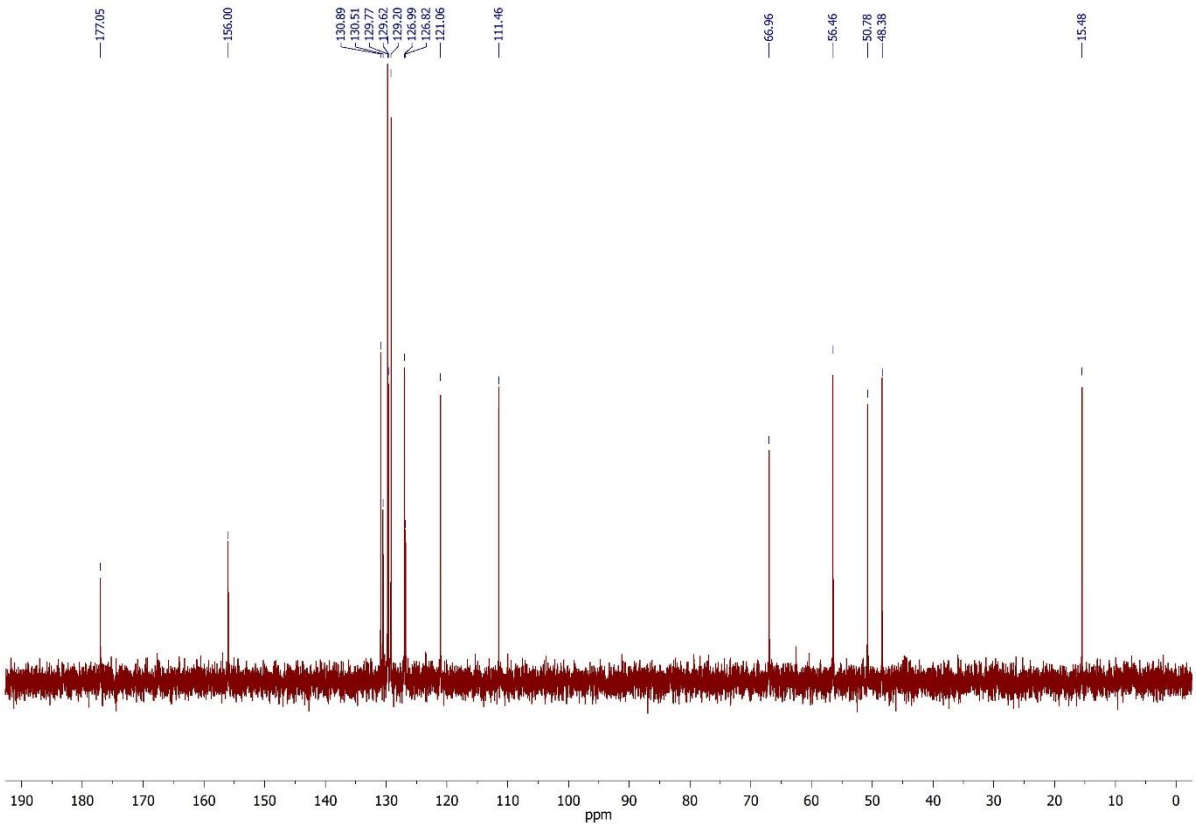

Figure S20 (b). ^{13}C NMR Spectrum of **5** (D_2O, δ, ppm)

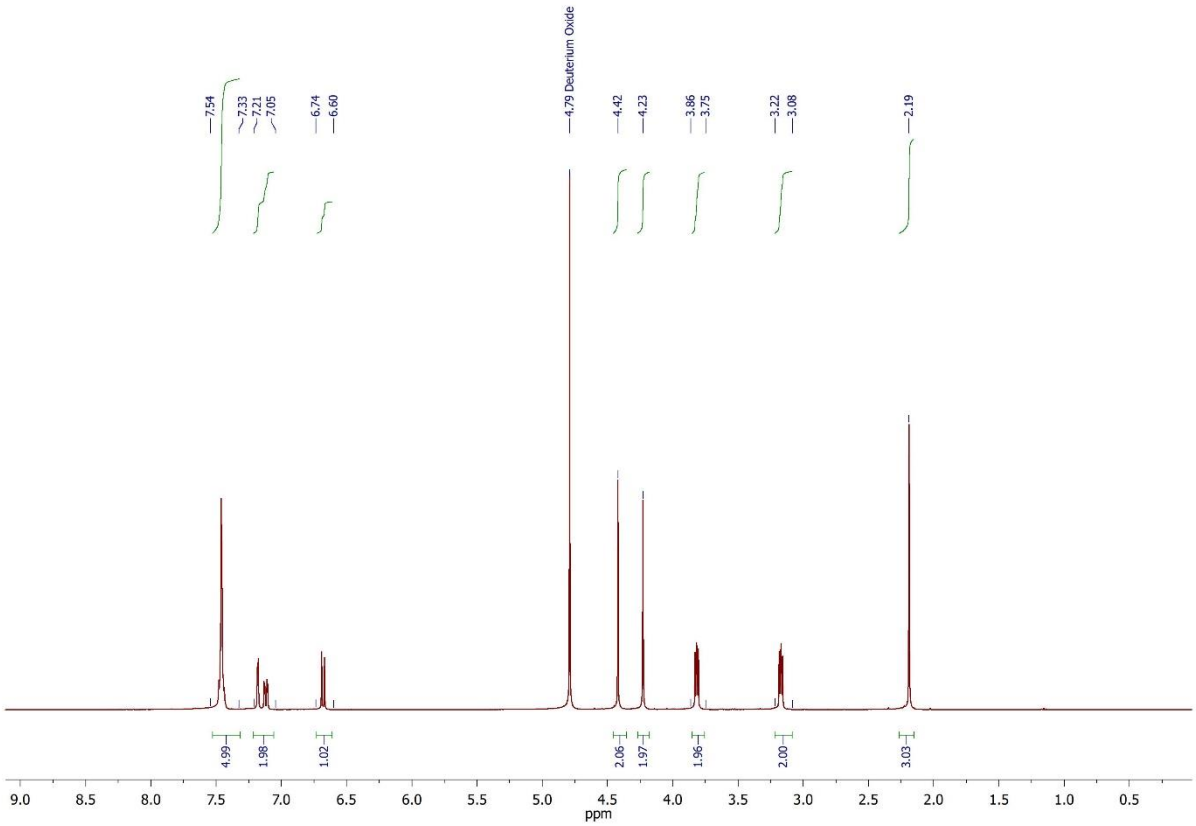

Figure S21 (a).[1]H NMR Spectrum of **6** (D_2O, δ, ppm, *J*, Hz)

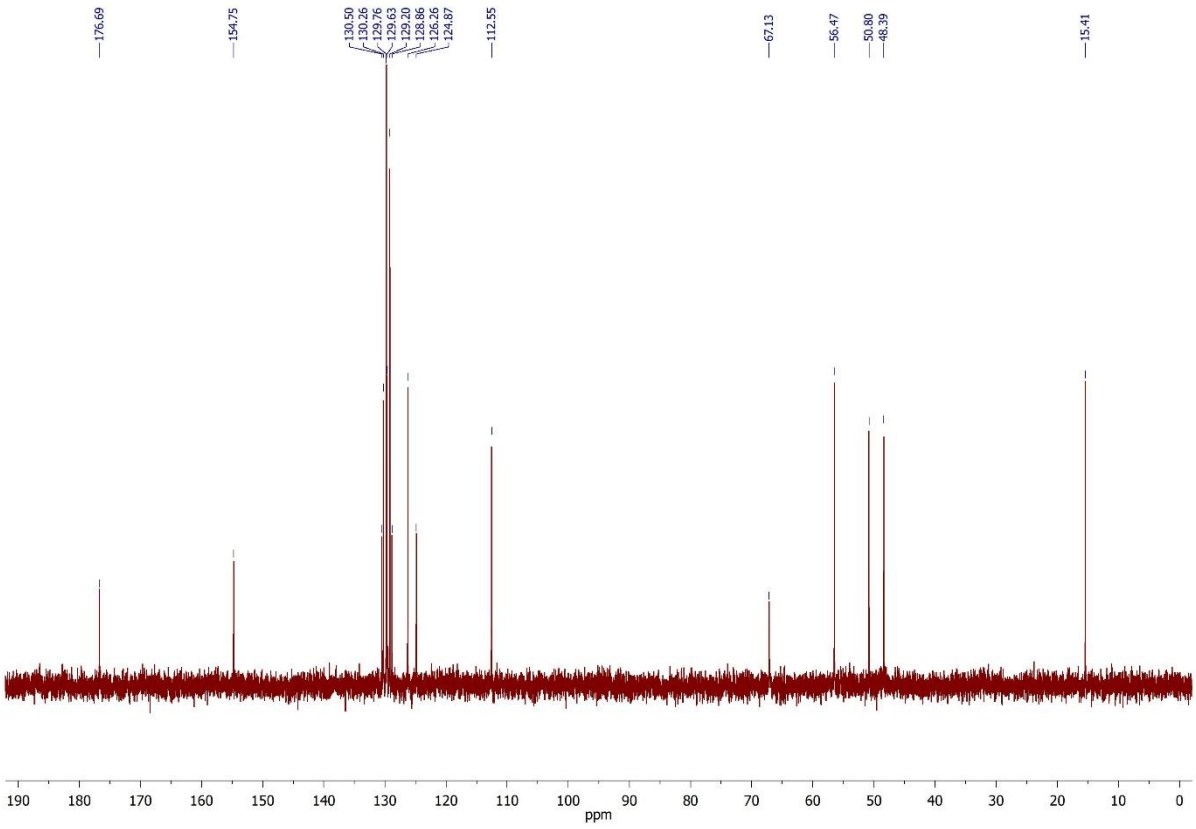

Figure S21 (b). [13]C NMR Spectrum of **6** (D_2O, δ, ppm)

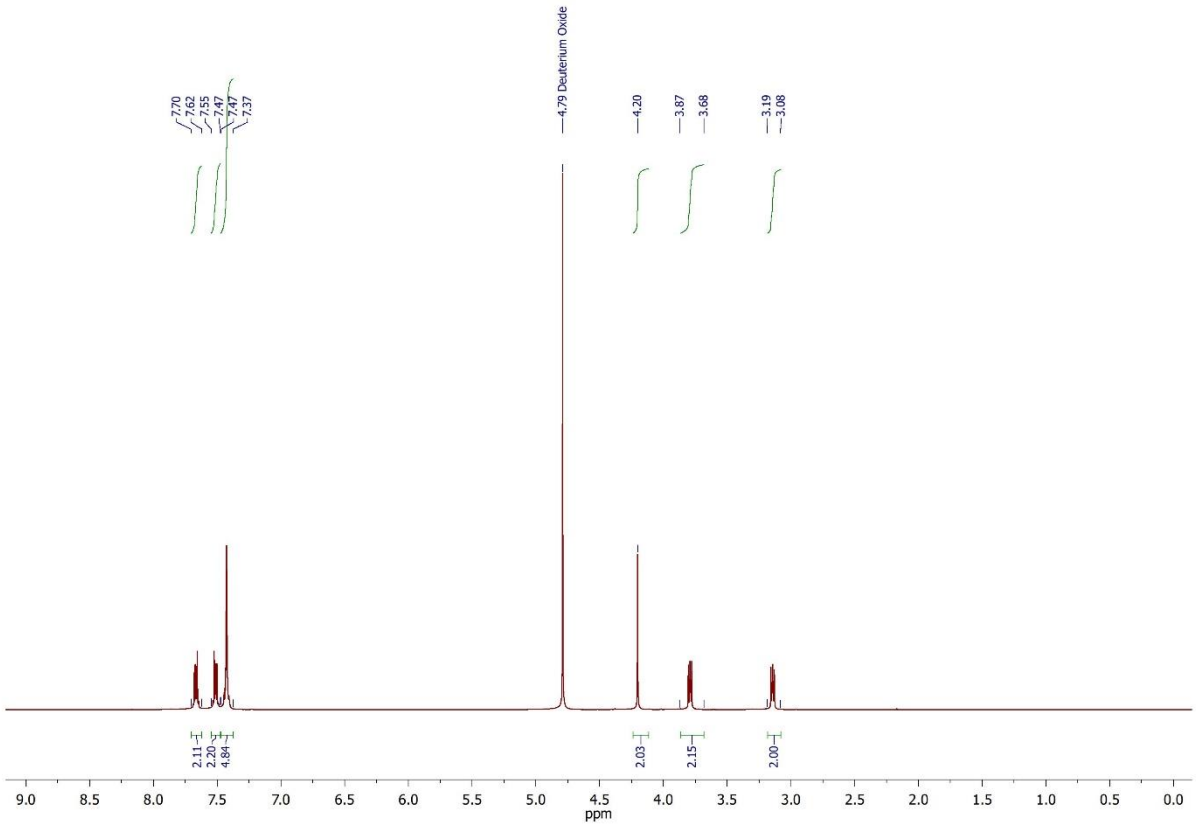

Figure S22 (a). ^{1}H NMR Spectrum of **7** (D_2O, δ, ppm, *J*, Hz)

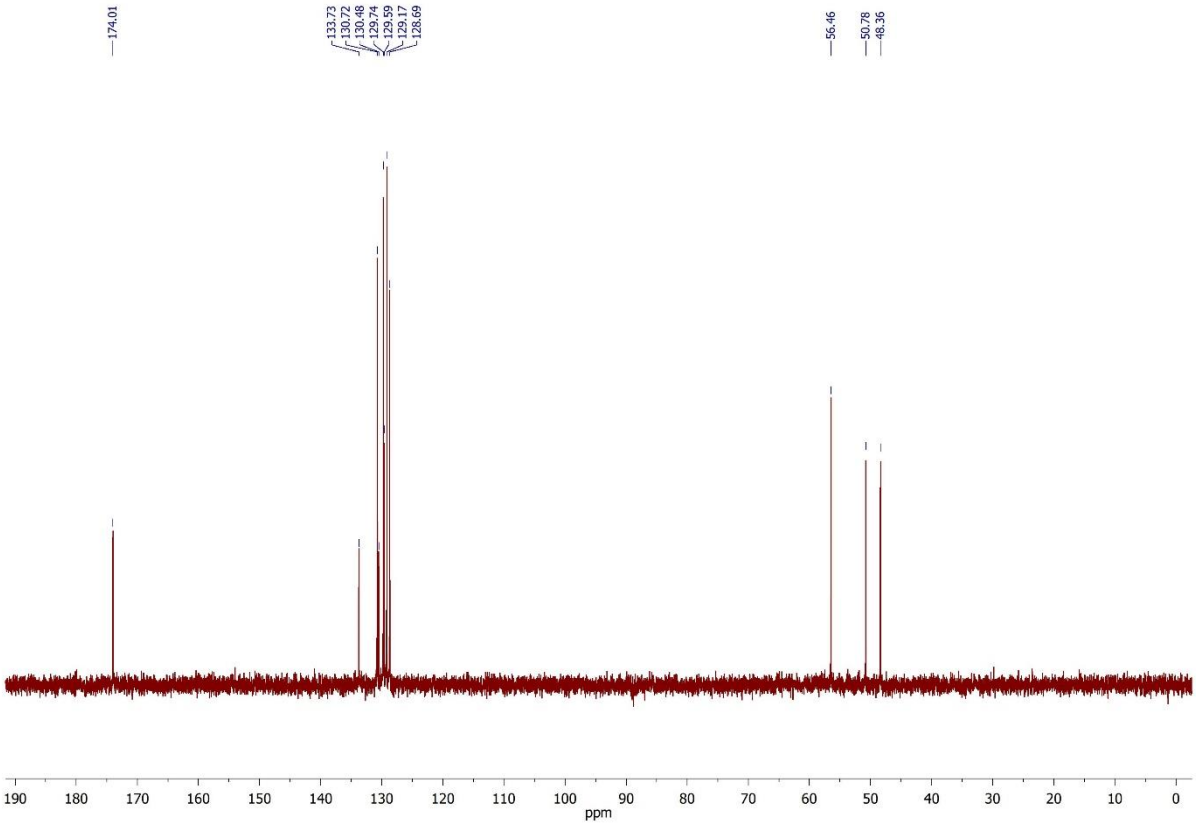

Figure S22 (b). ^{13}C NMR Spectrum of **7** (D_2O, δ, ppm)

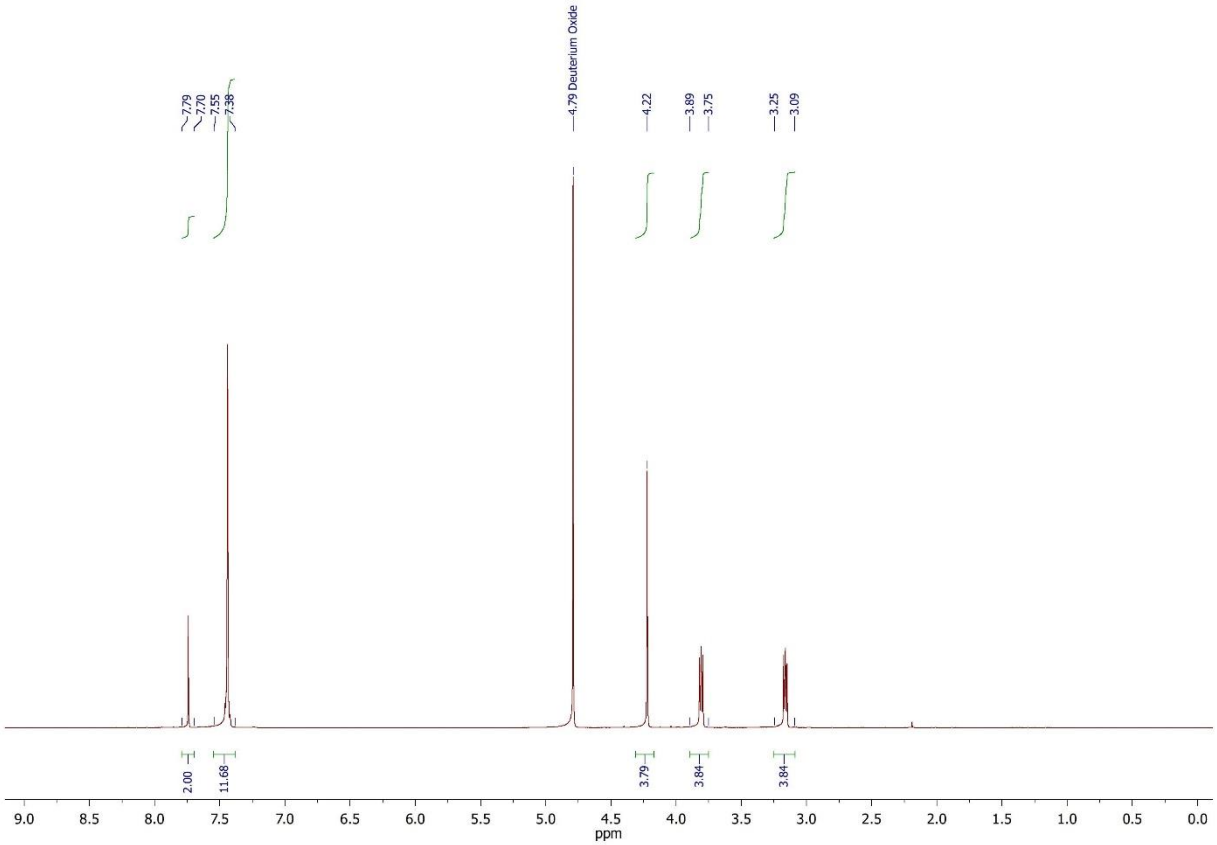

Figure S23 (a). ^{1}H NMR Spectrum of **8** (D_2O, δ, ppm, *J*, Hz)

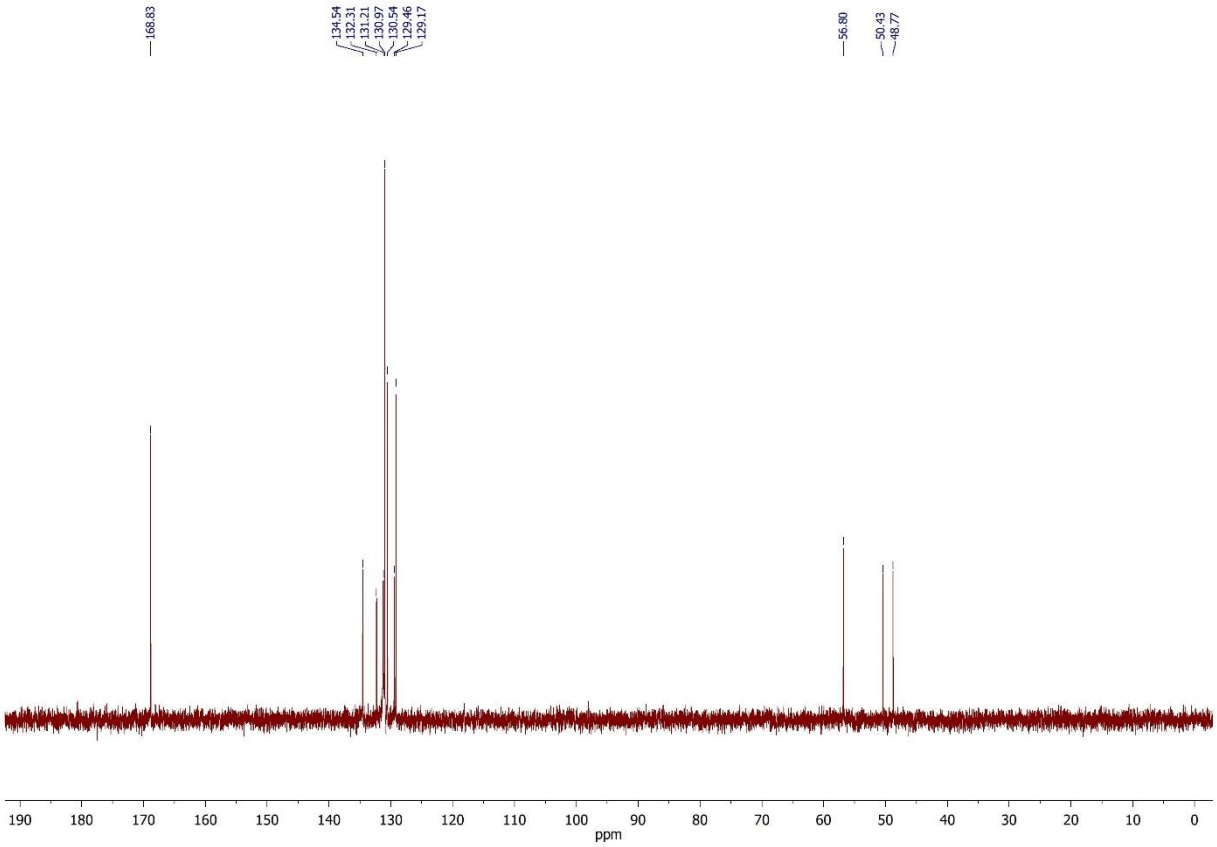

Figure S23 (b). ^{13}C NMR Spectrum of **8** (D_2O, δ, ppm)

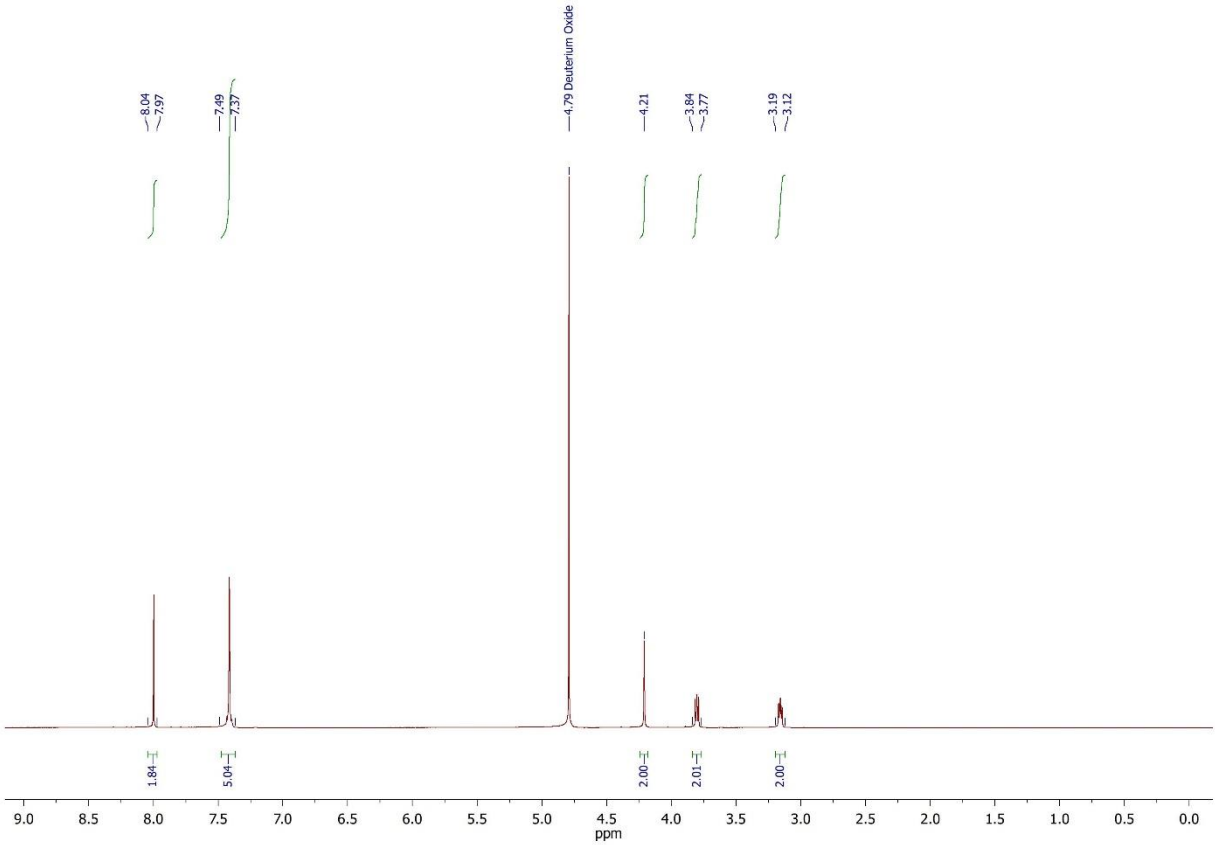

Figure S24 (a). ^{1}H NMR Spectrum of **9** (D_2O, δ, ppm, *J*, Hz)

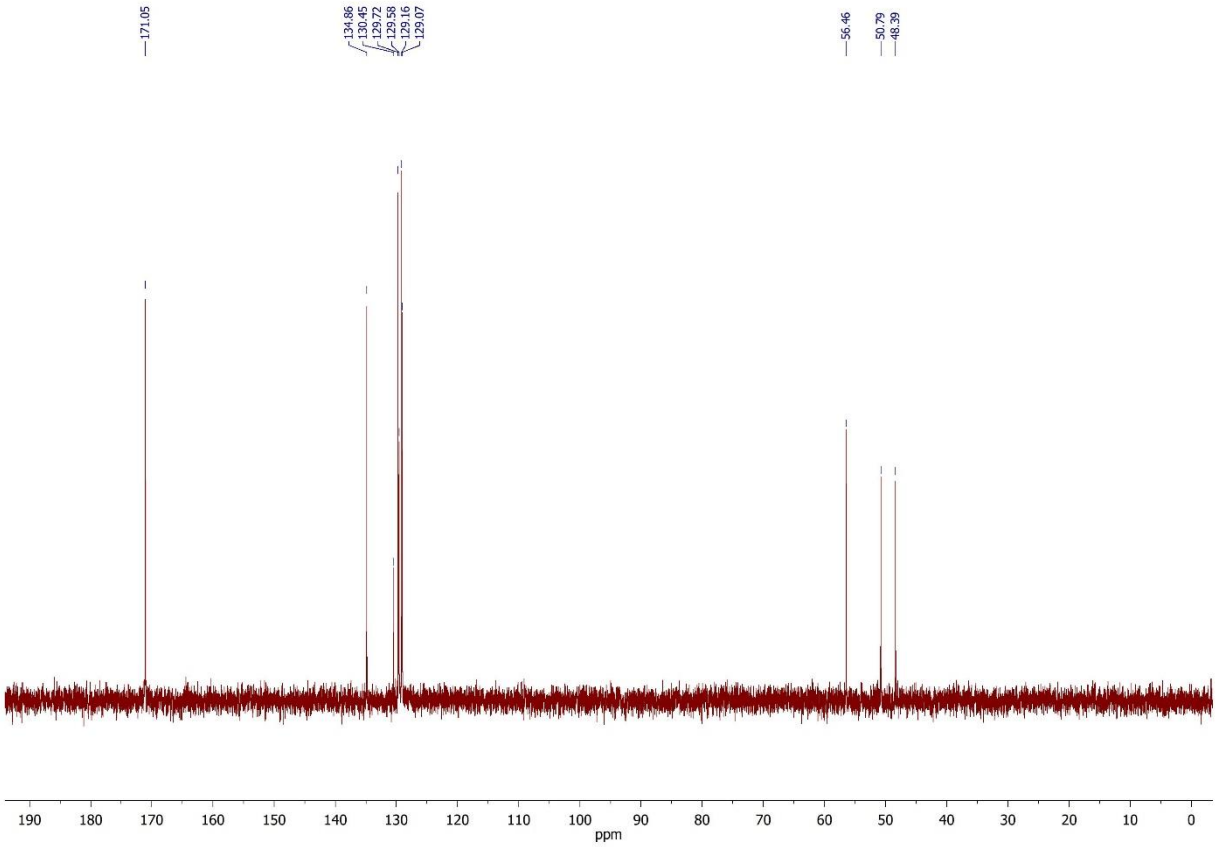

Figure S24 (b). ^{13}C NMR Spectrum of **9** (D_2O, δ, ppm)

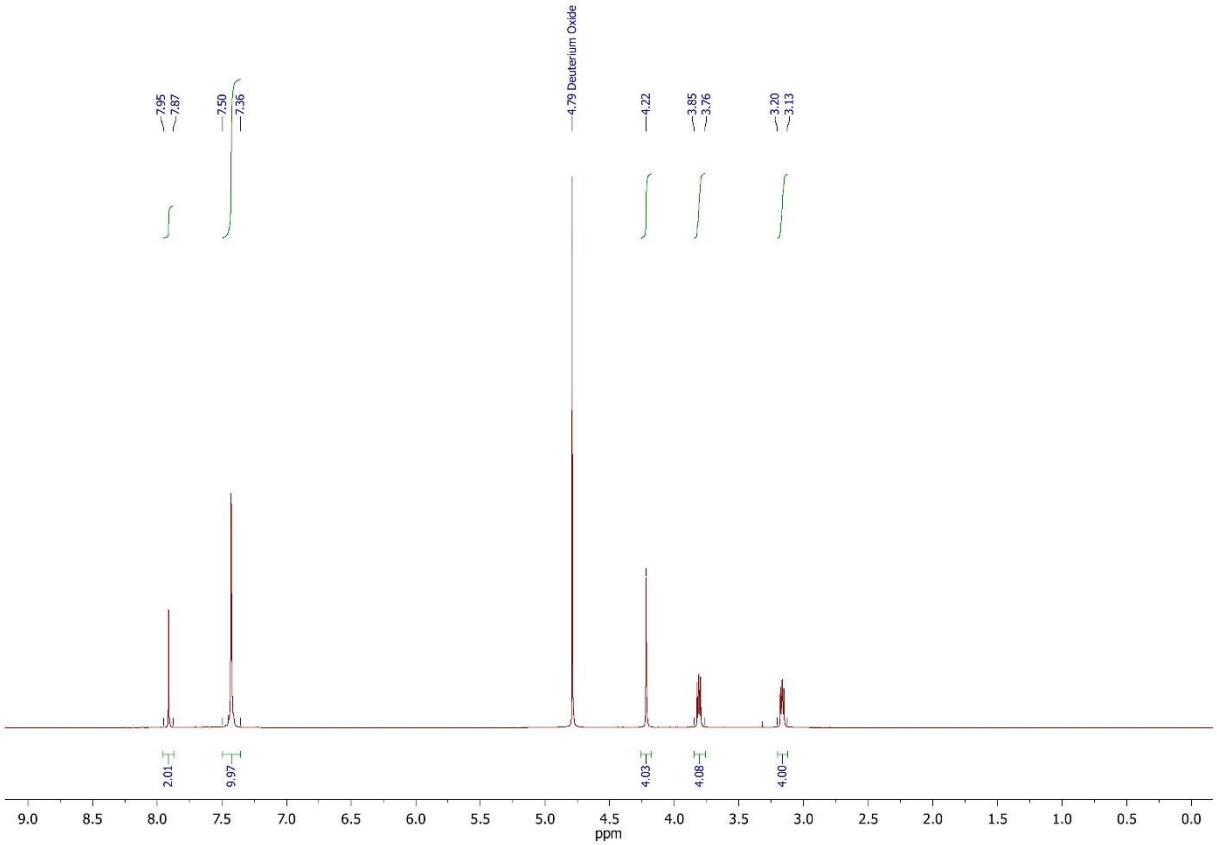

Figure S25 (a). ^{1}H NMR Spectrum of **10** (D_2O, δ, ppm, *J*, Hz)

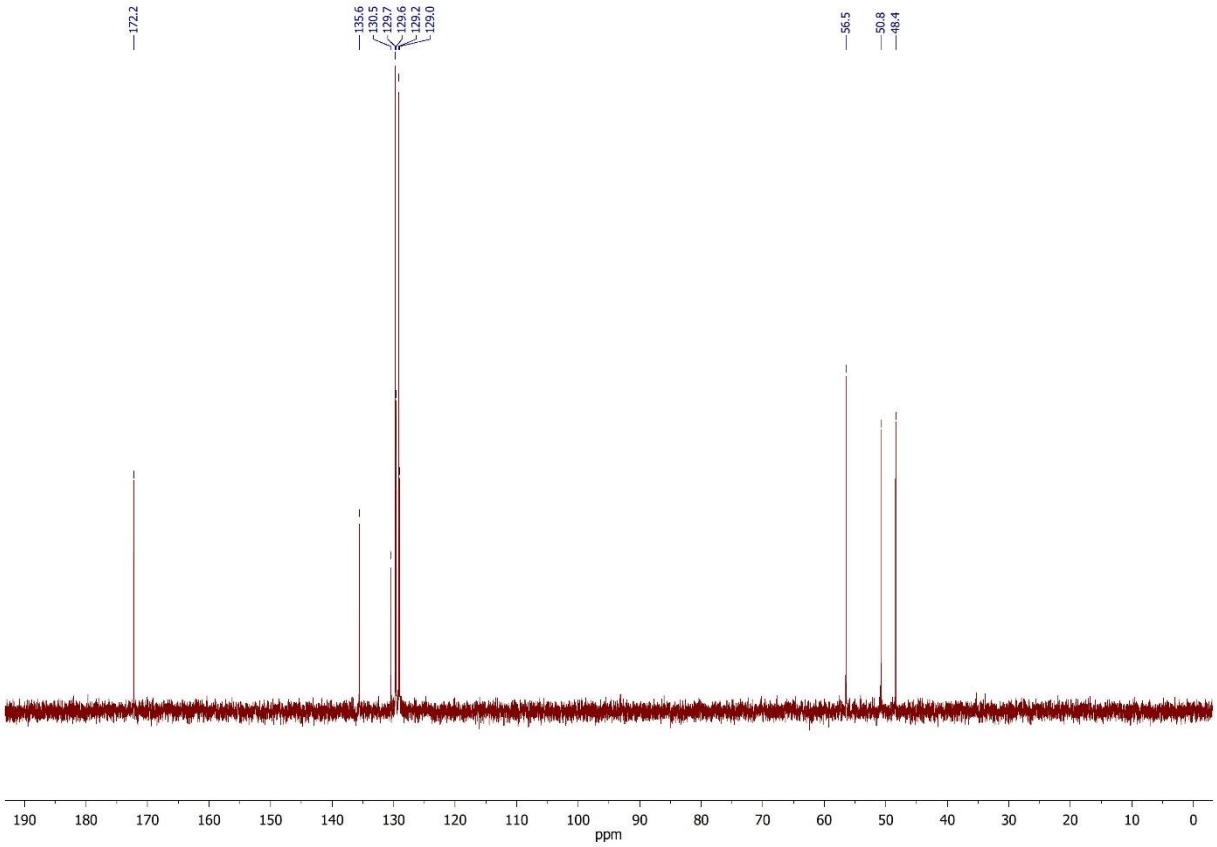

Figure S25 (b). ^{13}C NMR Spectrum of **10** (D_2O, δ, ppm)

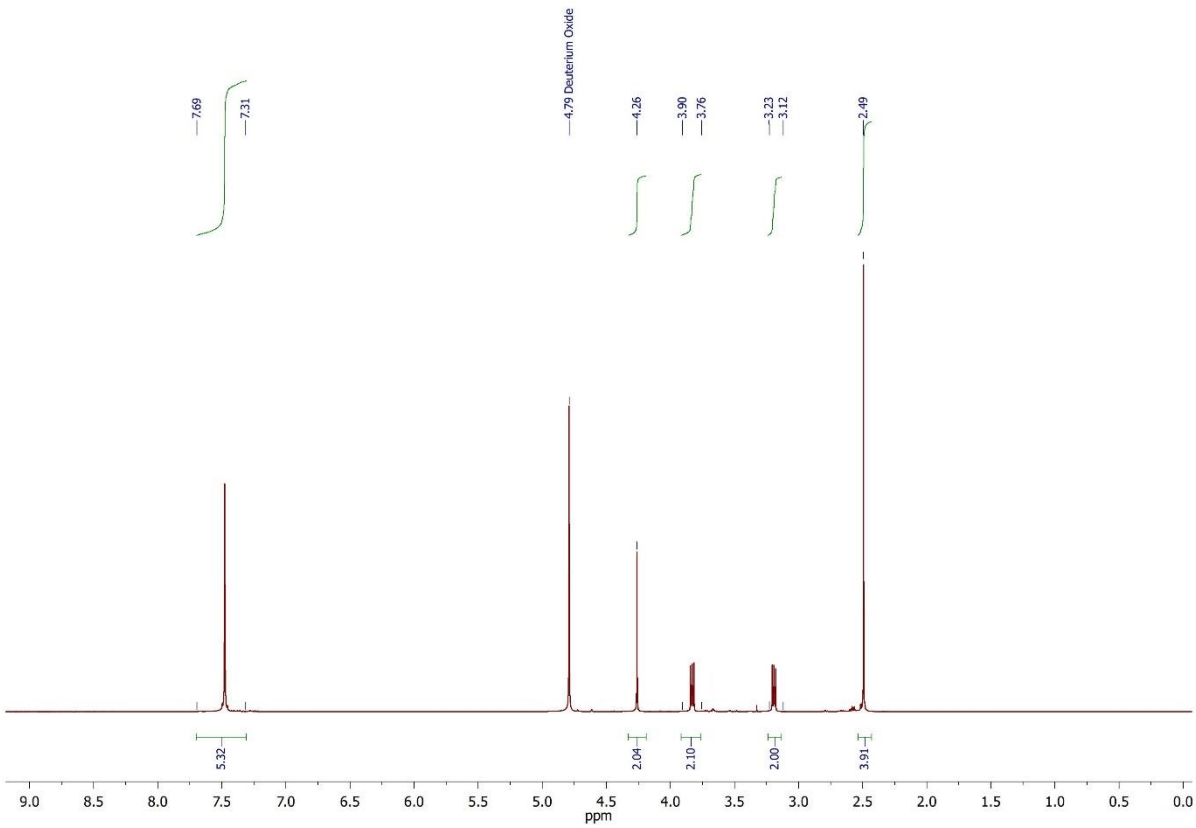

Figure S26 (a). ^{1}H NMR Spectrum of **11** (D_2O, δ, ppm, *J*, Hz)

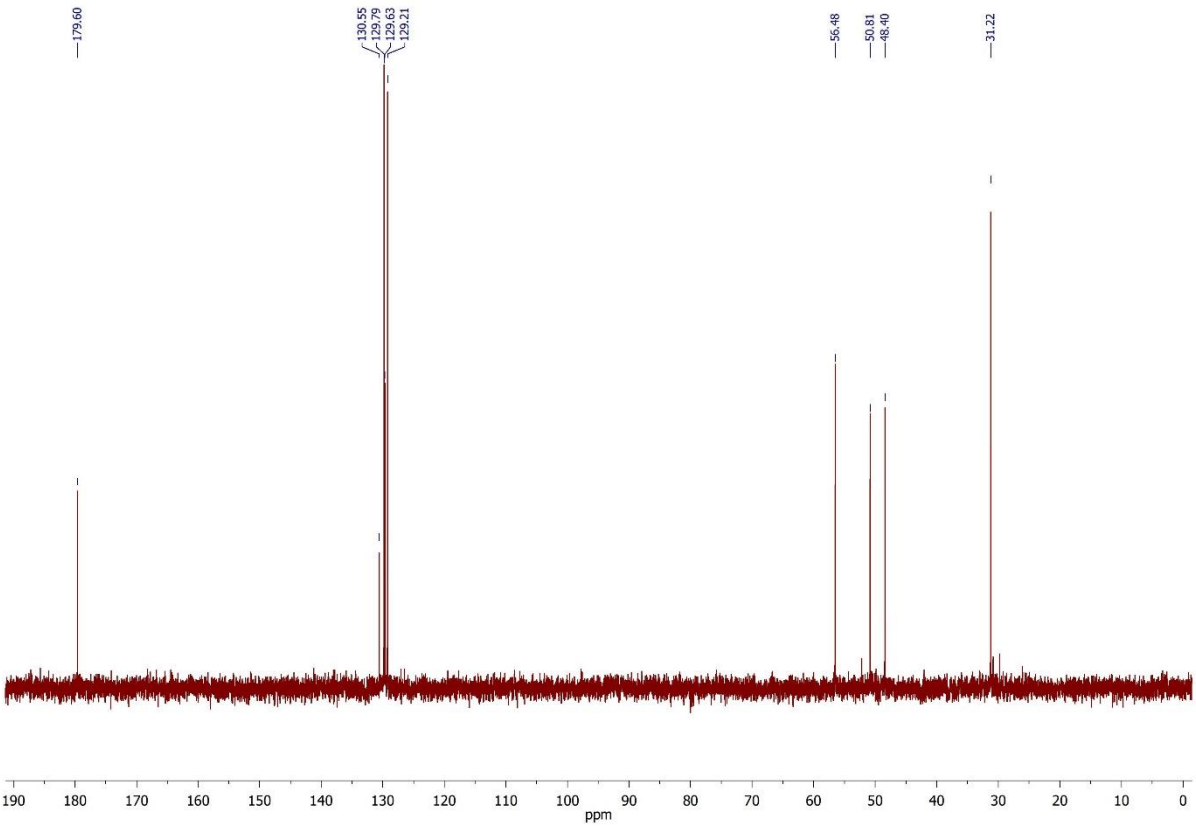

Figure S26 (b). ^{13}C NMR Spectrum of **11** (D_2O, δ, ppm)

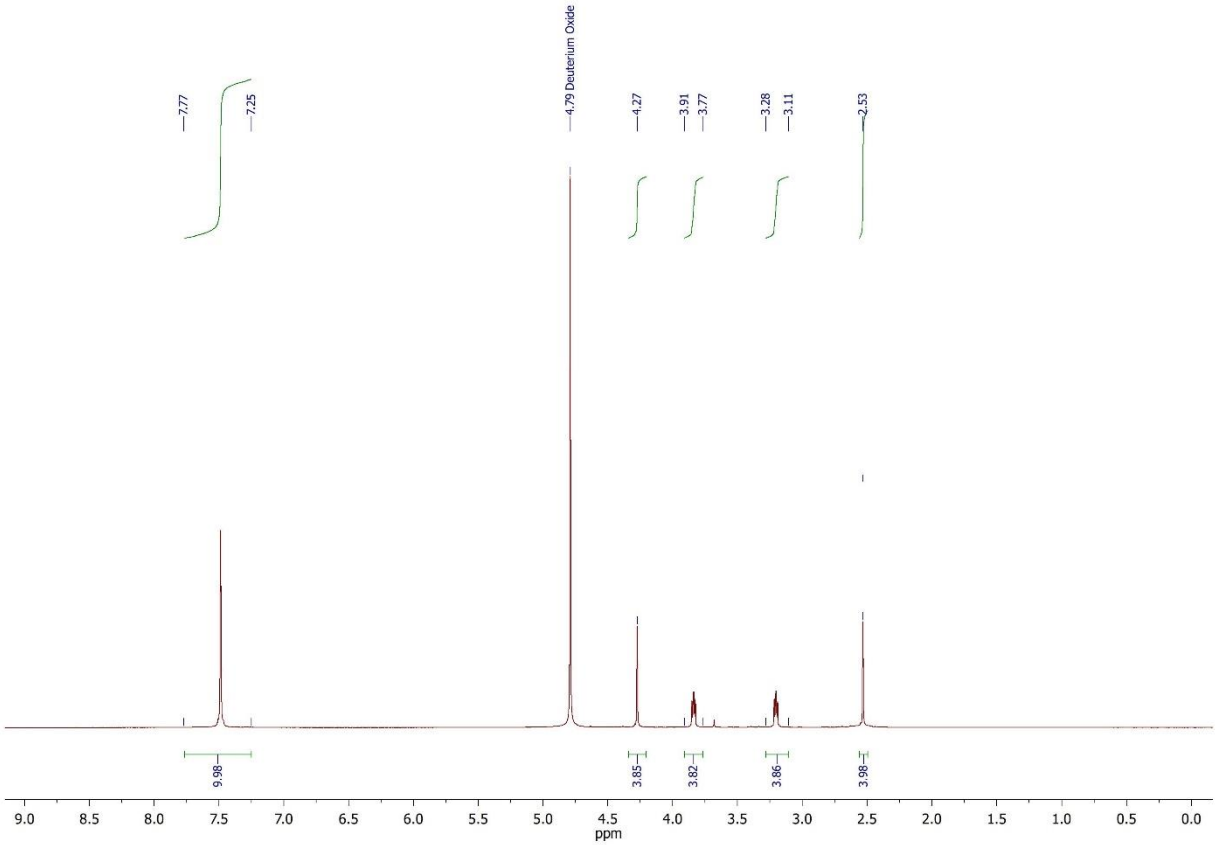

Figure S27 (a). ^{1}H NMR Spectrum of **12** (D_2O, δ, ppm, *J*, Hz)

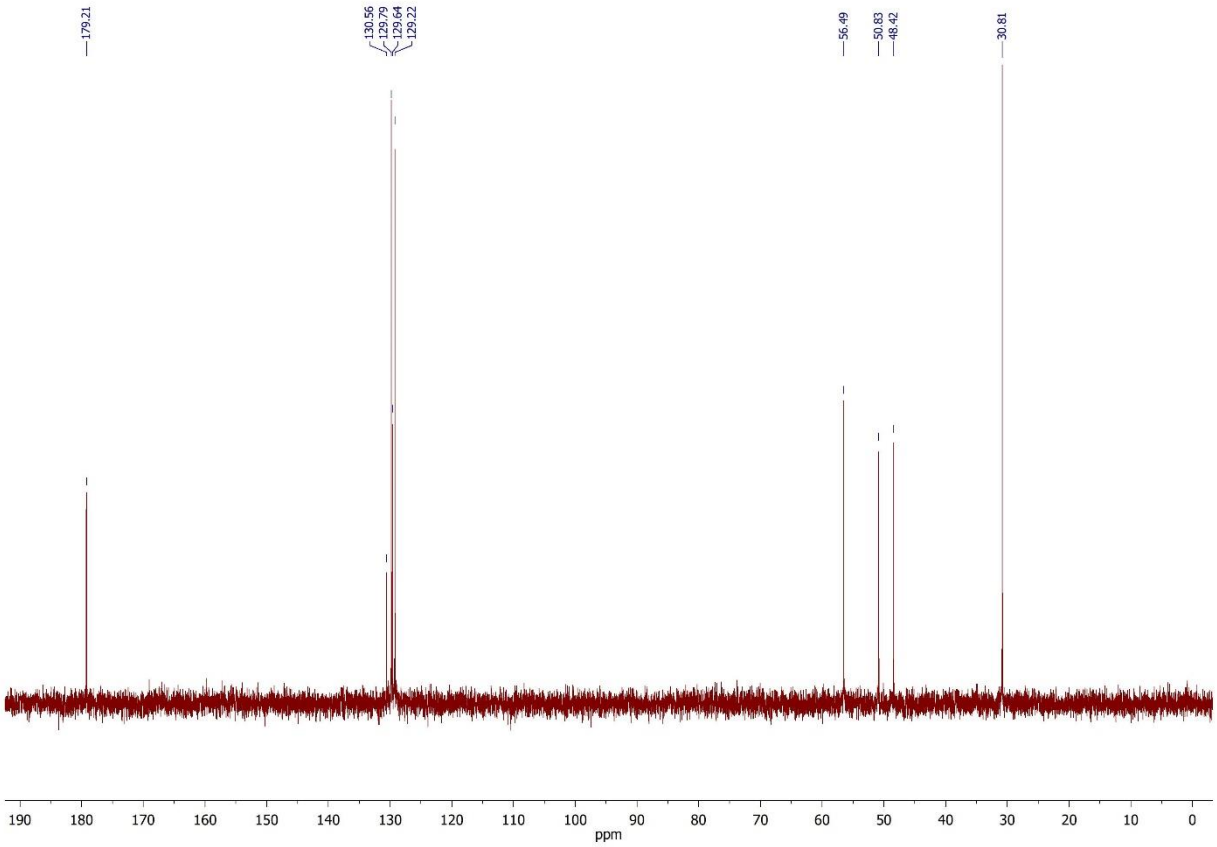

Figure S27 (b). ^{13}C NMR Spectrum of **12** (D_2O, δ, ppm)

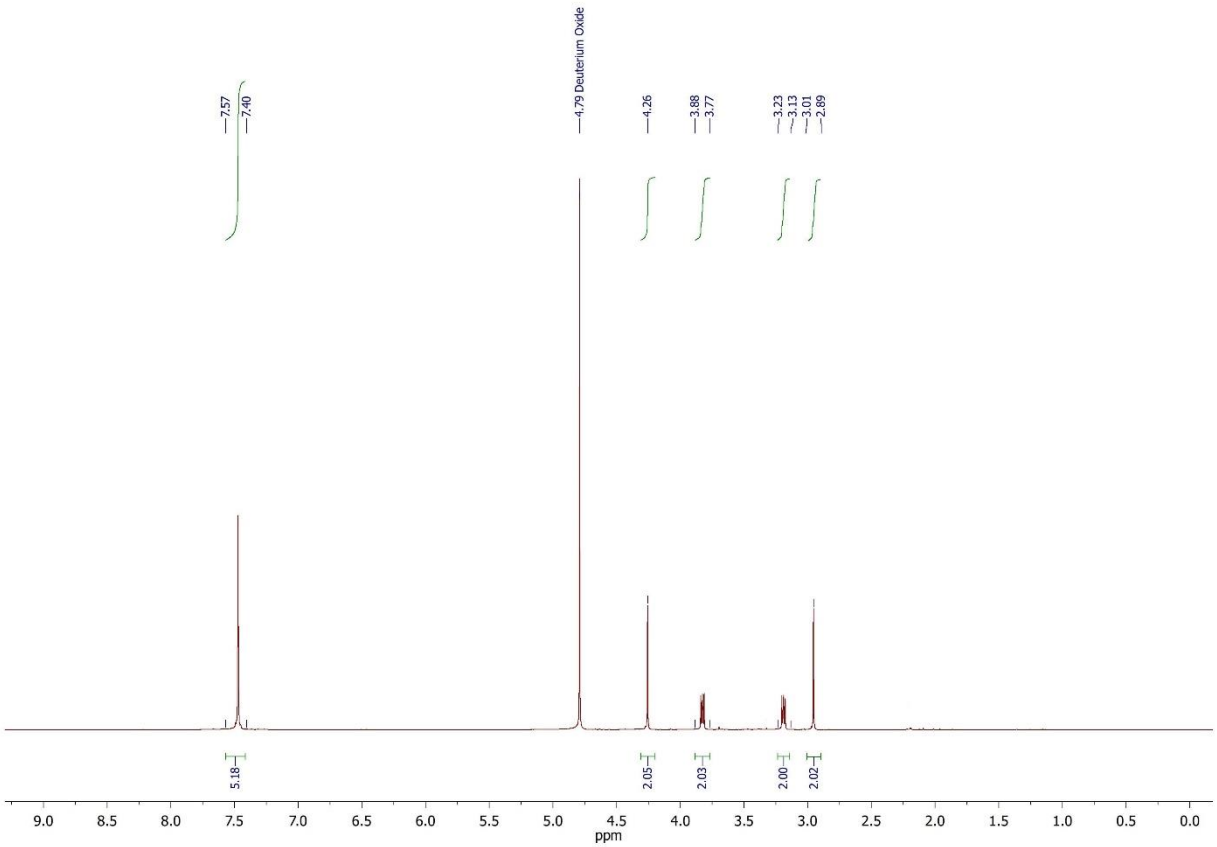

Figure S28 (a). ^{1}H NMR Spectrum of **13** (D_2O, δ, ppm, *J*, Hz)

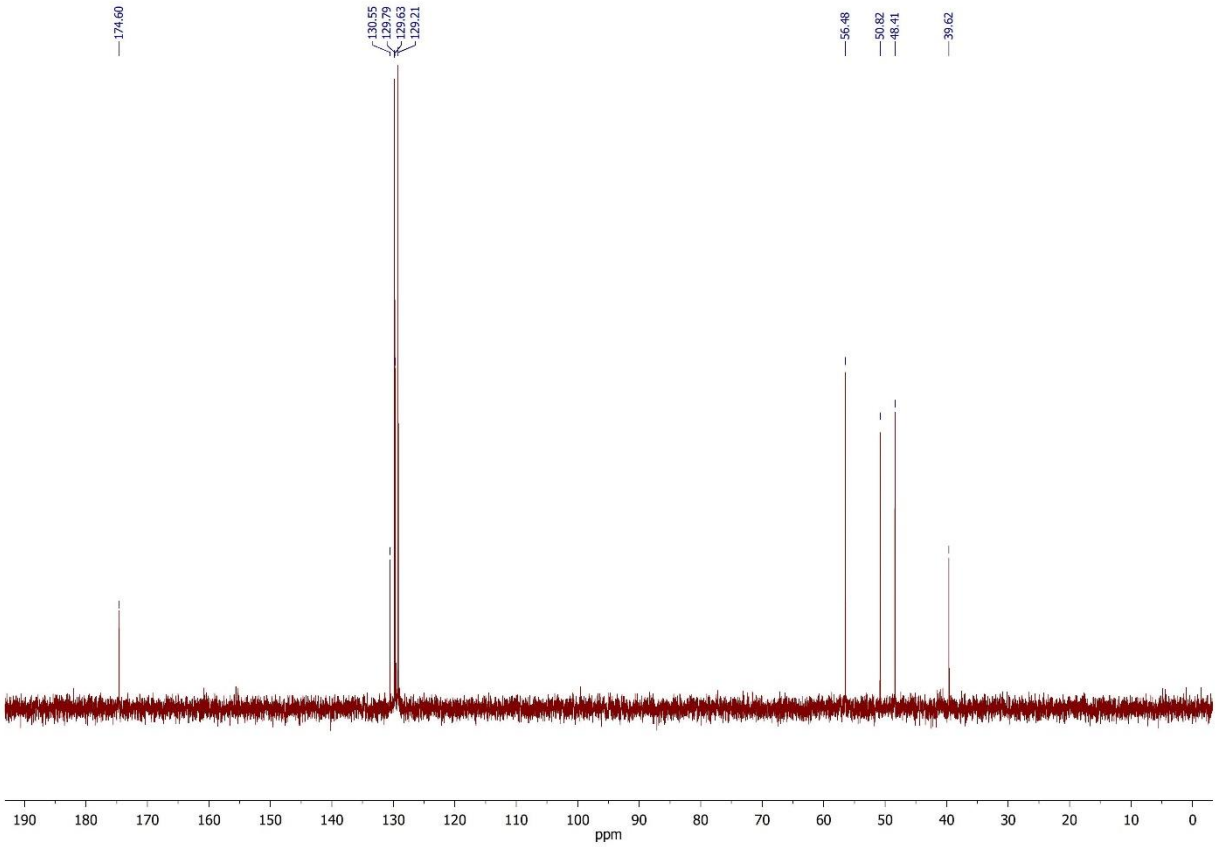

Figure S28 (b). ^{13}C NMR Spectrum of **13** (D_2O, δ, ppm)

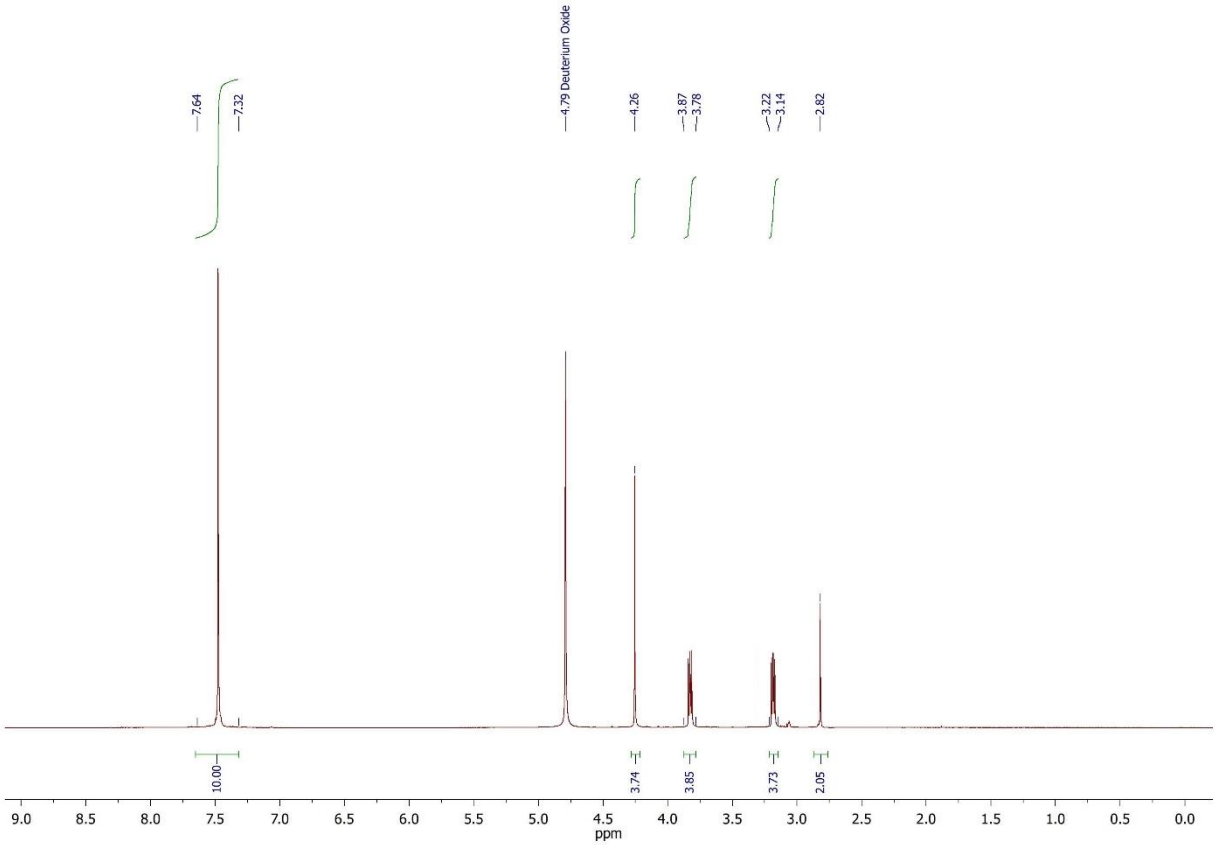

Figure S29 (a). ^{1}H NMR Spectrum of **14** (D_2O, δ, ppm, *J*, Hz)

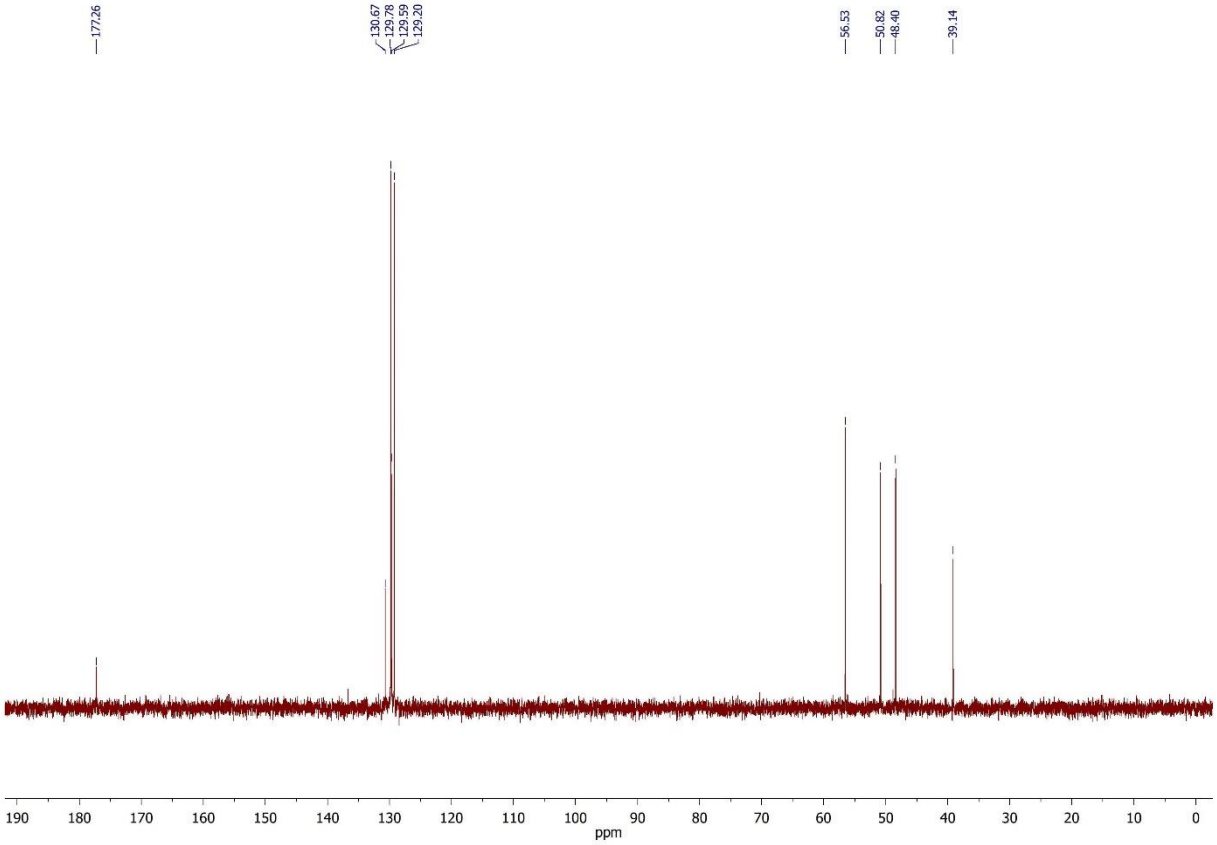

Figure S29 (b). ^{13}C NMR Spectrum of **14** (D_2O, δ, ppm)

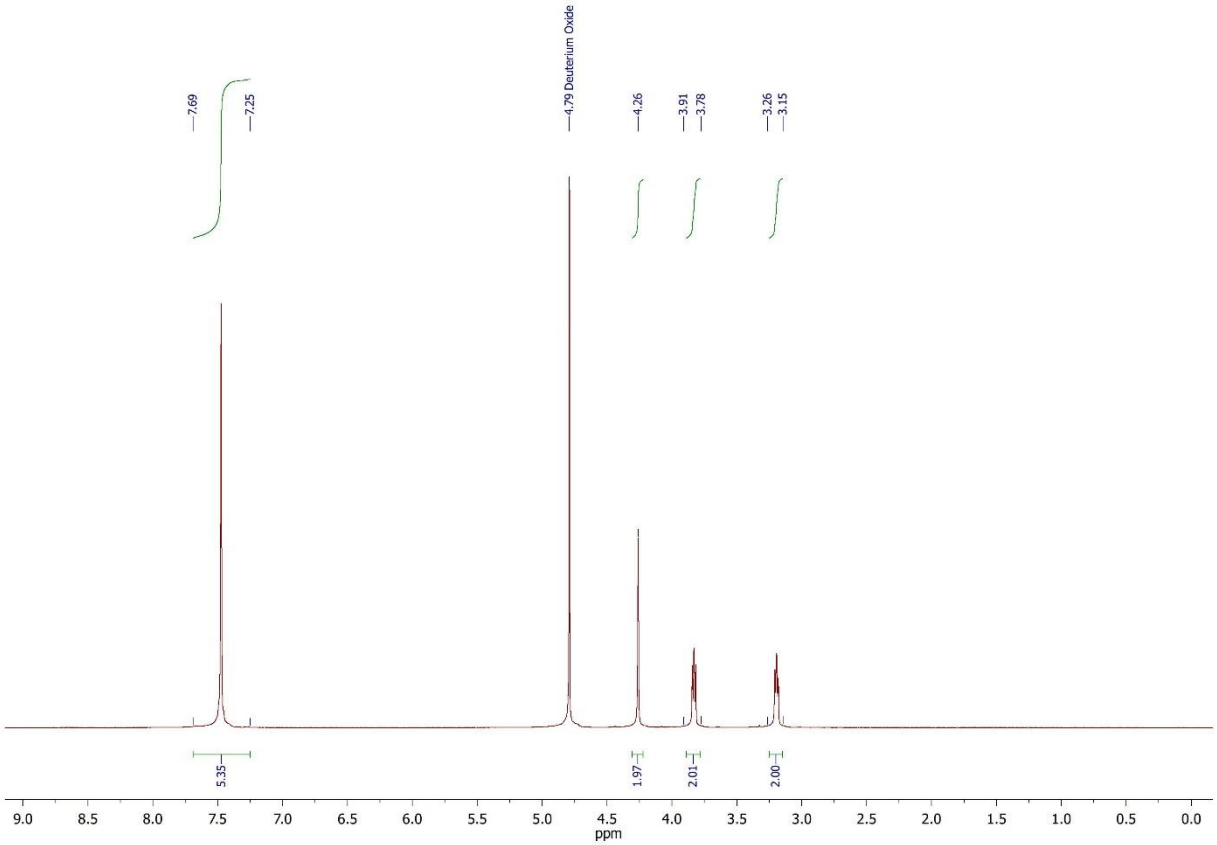

Figure S30 (a). ^{1}H NMR Spectrum of **15** (D_2O, δ, ppm, *J*, Hz)

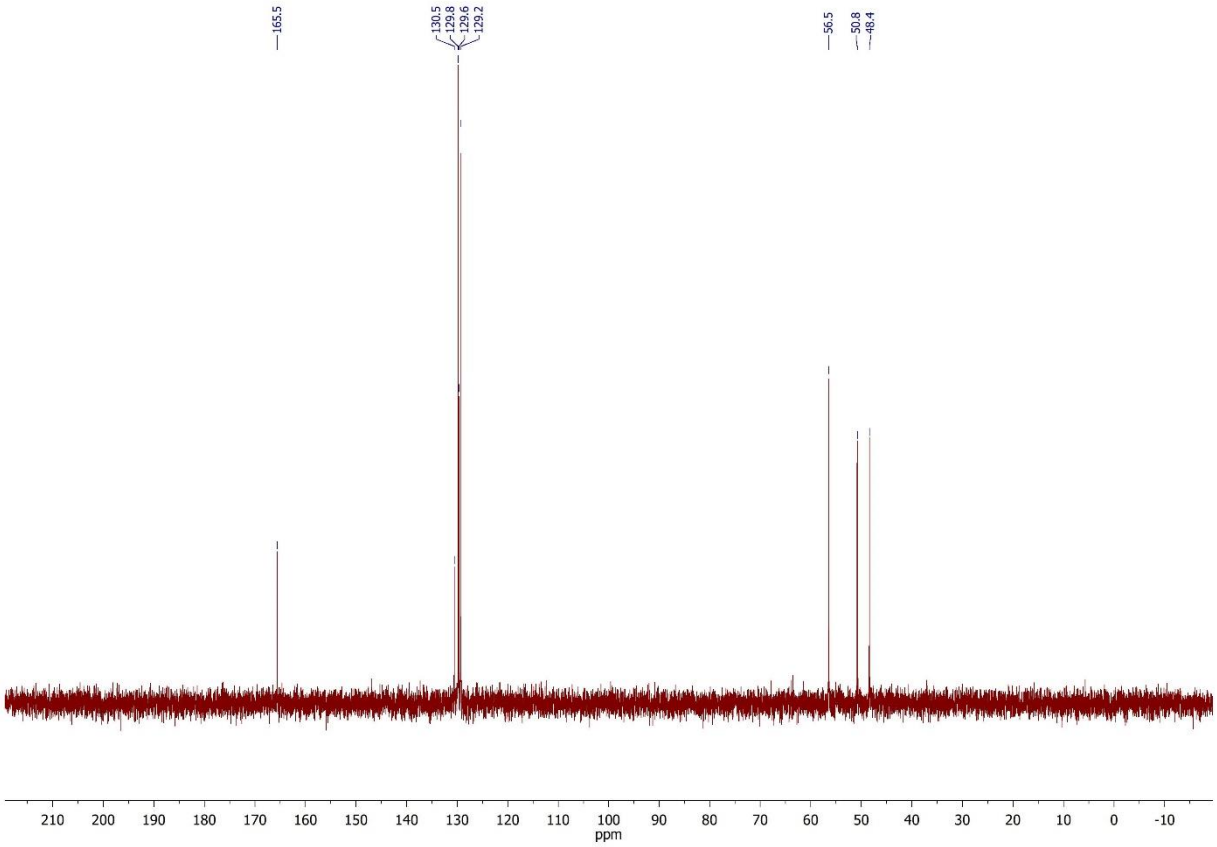

Figure S30 (b). ^{13}C NMR Spectrum of **15** (D_2O, δ, ppm)

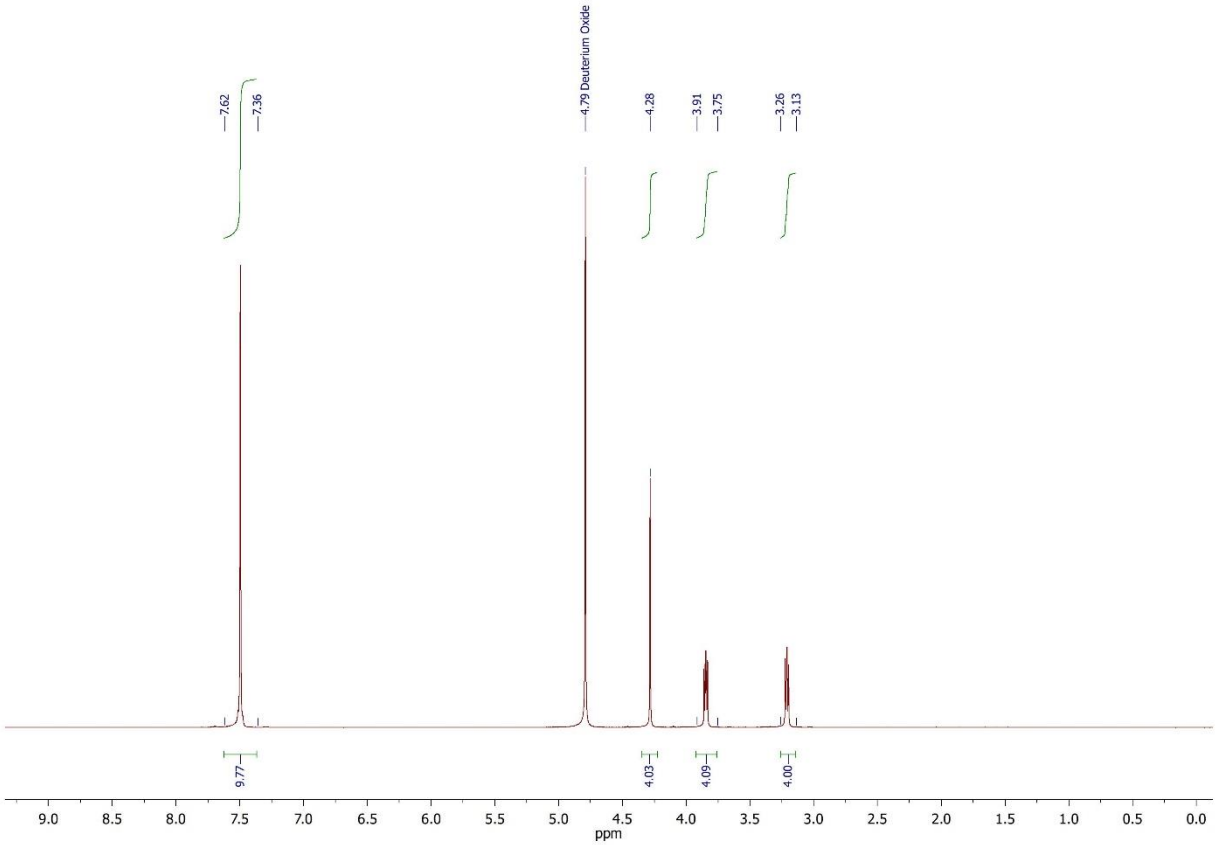

Figure S31 (a). ^{1}H NMR Spectrum of **16** (D_2O, δ, ppm, *J*, Hz)

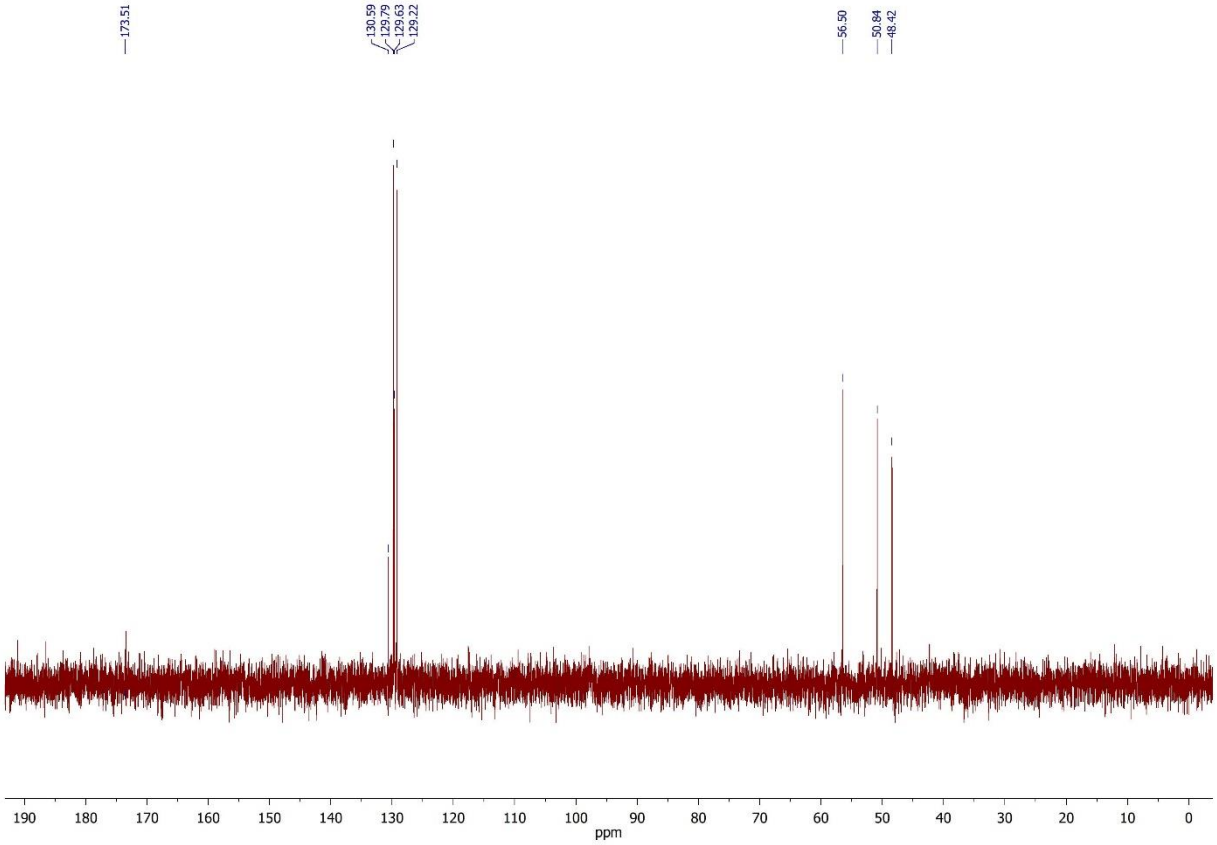

Figure S31 (b). ^{13}C NMR Spectrum of **16** (D_2O, δ, ppm)

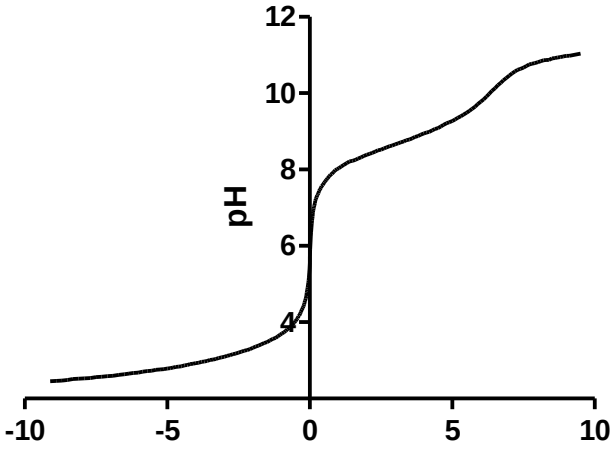

Figure S32. pH profile of buffer **3**

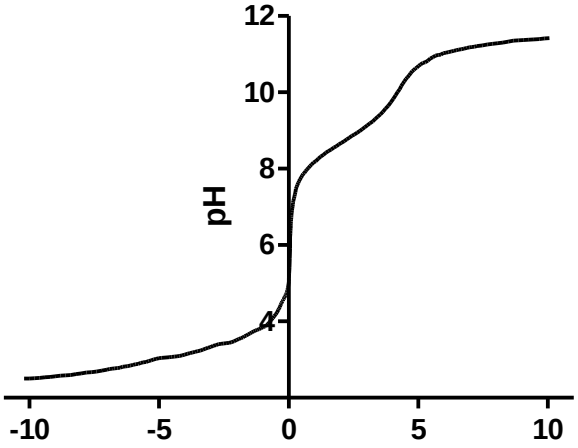

Figure S33. pH profile of buffer **4**

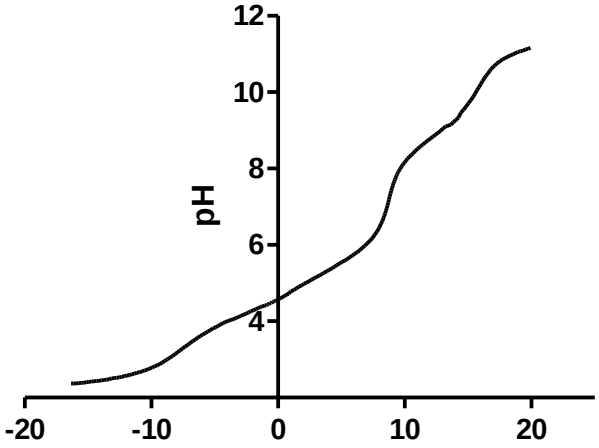

Figure S34. pH profile of buffer **12**

NMR (^{1}H, ^{13}C) spectroscopy data of BEA salts 1-16:

1) N-benzylethanolammonium benzoate (1)

^{1}H NMR spectrum of **1** (D_2O, ppm): 3.12-3.25 m (2H, C_6H_5-CH_2-NH_2^+-C<u>H</u>$_2$-CH_2-OH); 3.77-3.88 m (2H, C_6H_5-CH_2-NH_2^+-CH_2-C<u>H</u>$_2$-OH); 4.25 s (2H, C_6H_5-C<u>H</u>$_2$-NH_2^+-CH_2-CH_2-OH); 7.39-7.59 m ($8H_{Ar}$); 7.81-7.94 m ($2H_{Ar}$).

^{13}C NMR spectrum of **1** (D_2O, ppm): 48.4 (C_6H_5-CH_2-NH_2^+-<u>C</u>H_2-CH_2-OH); 50.8 (C_6H_5-<u>C</u>H_2-NH_2^+-CH_2-CH_2-OH); 56.5 (C_6H_5-CH_2-NH_2^+-CH_2-<u>C</u>H_2-OH); 128.3 (<u>C</u>$_{Ar}$H); 128.8 (<u>C</u>$_{Ar}$H); 129.2 (<u>C</u>$_{Ar}$H); 129.6 (<u>C</u>$_{Ar}$H); 129.8 (<u>C</u>$_{Ar}$H); 130.5 (<u>C</u>$_{Ar}$); 131.5 (<u>C</u>$_{Ar}$H); 135.3(<u>C</u>$_{Ar}$); 175.1 (<u>C</u>O_2^-).

2) N-benzylethanolammonium cinnamate (2)

^{1}H NMR spectrum of **2** (D_2O, ppm): 3.07-3.20 m (2H, C_6H_5-CH_2-NH_2^+-C<u>H</u>$_2$-CH_2-OH); 3.72-3.84 m (2H, C_6H_5-CH_2-NH_2^+-CH_2-C<u>H</u>$_2$-OH); 4.19 s (2H, C_6H_5-C<u>H</u>$_2$-NH_2^+-CH_2-CH_2-OH); 6.37-6.52 m (1H, C_6H_5-CH=C<u>H</u>-CO_2^-); 7.29-7.34 m (1H, C_6H_5-CH=C<u>H</u>-CO_2); 7.36-7.47 m ($8H_{Ar}$); 7.51-7.56 м ($2H_{Ar}$).

^{13}C NMR spectrum of **2** (D_2O, ppm): 48.4 (C_6H_5-CH_2-NH_2^+-<u>C</u>H_2-CH_2-OH); 50.8 (C_6H_5-<u>C</u>H_2-NH_2^+-CH_2-CH_2-OH); 56.5 (C_6H_5-CH_2-NH_2^+-CH_2-<u>C</u>H_2-OH); 123.9 (C_6H_5CH=<u>C</u>H-CO_2^-); 127.6 (<u>C</u>$_{Ar}$H); 128.9 (<u>C</u>$_{Ar}$H); 129.2 (<u>C</u>$_{Ar}$H); 129.6 (<u>C</u>$_{Ar}$H); 129.7 (<u>C</u>$_{Ar}$H); 130.5 (<u>C</u>$_{Ar}$); 135.0 (<u>C</u>$_{Ar}$); 140.8 (C_6H_5<u>C</u>H=CH-CO_2^-); 175.5 (C_6H_5-CH=CH-<u>C</u>O_2^-).

3) N-benzylethanolammonium salicylate (3)

^{1}H NMR spectrum of **3** (D_2O, ppm): 3.07-3.19 m (2H, C_6H_5-CH_2-NH_2^+-C<u>H</u>$_2$-CH_2-OH); 3.73-3.86 m (2H, C_6H_5-CH_2-NH_2^+-CH_2-C<u>H</u>$_2$-OH); 4.19 s (2H, C_6H_5-C<u>H</u>$_2$-NH_2^+-CH_2-CH_2-OH); 6.79-6.97 m ($2H_{Ar}$); 7.30-7.49 m ($6H_{Ar}$); 7.67-7.82 m ($1H_{Ar}$).

^{13}C NMR spectrum of **3** (D_2O, ppm): 48.4 (C_6H_5-CH_2-NH_2^+-<u>C</u>H_2-CH_2-OH); 50.8 (C_6H_5-<u>C</u>H_2-NH_2^+-CH_2-CH_2-OH); 56.5 (C_6H_5-CH_2-NH_2^+-CH_2-<u>C</u>H_2-OH); 116.2 (<u>C</u>$_{Ar}$H); 118.0 (<u>C</u>$_{Ar}$); 119.3 (<u>C</u>$_{Ar}$H); 129.2 (<u>C</u>$_{Ar}$H); 129.6 (<u>C</u>$_{Ar}$H); 129.7 (<u>C</u>$_{Ar}$H); 130.4 (<u>C</u>$_{Ar}$H); 130.4 (<u>C</u>$_{Ar}$H); 133.9 (<u>C</u>$_{Ar}$); 159.5 (<u>C</u>$_{Ar}$); 175.5 (<u>C</u>O_2^-).

4) N-benzylethanolammonium 2-methylpnenoxyacetate (5)

^{1}H NMR spectrum of **5** (D_2O, ppm): 2.22 с (3H, *o*-C<u>H</u>$_3$-C_6H_4-O-CH_2-CO_2^-); 3.06-3.27 m (2H, C_6H_5- CH_2-NH_2^+-C<u>H</u>$_2$-CH_2-OH); 3.70-3.92 m (2H, C_6H_5- CH_2-

NH_2^+-CH_2-C<u>H_2</u>-OH); 4.22 s (2H, C_6H_5-C<u>H_2</u>-NH_2^+-CH_2-CH_2-OH); 4.43 s (2H, *o*-CH_3-C_6H_4-O-C<u>H_2</u>-CO_2^-); 6.68-6.82 m ($1H_{Ar}$); 6.84-6.98 m ($1H_{Ar}$); 7.07-7.27 m ($2H_{Ar}$); 7.35-7.57 m ($5H_{Ar}$).

^{13}C NMR spectrum of **5** (D_2O, ppm): 15.5 (*o*-<u>C</u>H_3-C_6H_4-O-CH_2- CO_2^-); 48.4 (C_6H_5-CH_2-NH_2^+-<u>C</u>H_2-CH_2-OH); 50.8 (C_6H_5-<u>C</u>H_2-NH_2^+-CH_2-CH_2-OH); 56.5 (C_6H_5-CH_2-NH_2^+-CH_2-<u>C</u>H_2-OH); 67.0 (*o*-CH_3-C_6H_4-O-<u>C</u>H_2-CO_2^-); 111.5 (<u>C</u>$_{Ar}$H); 121.1 (<u>C</u>$_{Ar}$H); 126.8 (<u>C</u>$_{Ar}$); 127.0 (<u>C</u>$_{Ar}$H); 129.2 (<u>C</u>$_{Ar}$H); 129.6 (<u>C</u>$_{Ar}$H); 129.8 (<u>C</u>$_{Ar}$H); 130.5 (<u>C</u>$_{Ar}$); 130.9 (<u>C</u>$_{Ar}$H); 156.0 (<u>C</u>$_{Ar}$); 177.0 (<u>C</u>O_2^-).

5) N-benzylethanolammonium 4-chloro-2-methylpnenoxyacetate (6)

^{1}H NMR spectrum of **6** (D_2O, ppm): 2.19 s (3H, (Cl)(C<u>H_3</u>)C_6H_4-O-CH_2- CO_2^-); 3.08-3.22 m (2H, C_6H_5- CH_2-NH_2^+-C<u>H_2</u>-CH_2-OH); 3.75-3.86 m (2H, C_6H_5- CH_2-NH_2^+-CH_2-C<u>H_2</u>-OH); 4.23 s (2H, C_6H_5-C<u>H_2</u>-NH_2^+-CH_2-CH_2-OH); 4.42 s (2H, (Cl)(CH_3)C_6H_4-O-C<u>H_2</u>-CO_2^-); 6.60-6.74 m ($1H_{Ar}$); 7.05-7.21 m ($2H_{Ar}$); 7.33-7.54 m ($5H_{Ar}$).

^{13}C NMR spectrum of **6** (D_2O, ppm): 15.4 ((Cl)(<u>C</u>H_3)C_6H_4-O-CH_2-CO_2^-); 48.4 (C_6H_5-CH_2-NH_2^+-<u>C</u>H_2-CH_2-OH); 50.8 (C_6H_5-<u>C</u>H_2-NH_2^+-CH_2-CH_2-OH); 56.5 (C_6H_5-CH_2-NH_2^+-CH_2-<u>C</u>H_2-OH); 67.1 ((Cl)(CH_3)C_6H_4-O-<u>C</u>H_2-CO_2^-); 112.6 (<u>C</u>$_{Ar}$H); 124.9 (<u>C</u>$_{Ar}$); 126.3 (<u>C</u>$_{Ar}$H); 128.9 (<u>C</u>$_{Ar}$); 129.2 (<u>C</u>$_{Ar}$H); 129.6 (<u>C</u>$_{Ar}$H); 129.8 (<u>C</u>$_{Ar}$H); 130.3 (<u>C</u>$_{Ar}$H); 130.5 (<u>C</u>$_{Ar}$); 154.6 (<u>C</u>$_{Ar}$); 176.7 (<u>C</u>O_2^-).

6) N-benzylethanolammonium hydrogen phthalate (7)

^{1}H NMR spectrum of **7** (D_2O, ppm): 3.08-3.19 m (2H, C_6H_5-CH_2-NH_2^+-C<u>H_2</u>-CH_2-OH); 3.68-3.87 m (2H, C_6H_5- CH_2-NH_2^+-CH_2-C<u>H_2</u>-OH); 4.20 s (2H, C_6H_5-C<u>H_2</u>-NH_2^+-CH_2-CH_2-OH); 7.37-7.47 m ($5H_{Ar}$); 7.47-7.55 m ($2H_{Ar}$); 7.65-7.70 m ($2H_{Ar}$).

^{13}C NMR spectrum of **7** (D_2O, ppm): 48.4 (C_6H_5-CH_2-NH_2^+-<u>C</u>H_2-CH_2-OH); 50.8 (C_6H_5-<u>C</u>H_2-NH_2^+-CH_2-CH_2-OH); 56.5 (C_6H_5-CH_2-NH_2^+-CH_2-<u>C</u>H_2-OH); 128.7 (<u>C</u>$_{Ar}$H); 129.2 (<u>C</u>$_{Ar}$H); 129.6 (<u>C</u>$_{Ar}$H); 129.7 (<u>C</u>$_{Ar}$H); 130.5 (<u>C</u>$_{Ar}$); 130.7 (<u>C</u>$_{Ar}$H); 133.7 (<u>C</u>$_{Ar}$); 174.0 (HO_2<u>C</u>-C_6H_4-<u>C</u>O_2^-).

7) N-benzylethanolammonium phthalate (8)

^{1}H NMR spectrum of **8** (D_2O, ppm): 3.09-3.25 m (4H, C_6H_5-CH_2-NH_2^+-$C\underline{H_2}$-CH_2-OH); 3.75-3.89 m (4H, C_6H_5- CH_2-NH_2^+-CH_2-$C\underline{H_2}$-OH); 4.22 s (4H, C_6H_5-$C\underline{H_2}$-NH_2^+-CH_2-CH_2-OH); 7.38-7.44 m ($12H_{Ar}$); 7.70-7.79 m ($2H_{Ar}$).

^{13}C NMR spectrum of **8** (D_2O, ppm): 48.8 (C_6H_5-CH_2-NH_2^+-$\underline{C}H_2$-CH_2-OH); 50.4 (C_6H_5-$\underline{C}H_2$-NH_2^+-CH_2-CH_2-OH); 56.8 (C_6H_5-CH_2-NH_2^+-CH_2-$\underline{C}H_2$-OH); 129.2 ($\underline{C}_{Ar}H$); 129.5 ($\underline{C}_{Ar}H$); 130.5 ($\underline{C}_{Ar}H$); 131.0 ($\underline{C}_{Ar}H$); 131.2 ($\underline{C}_{Ar}$); 132.3 ($\underline{C}_{Ar}H$); 134.5 ($\underline{C}_{Ar}$); 168.8 ($^{-}O_2\underline{C}$-C_6H_4-$\underline{C}O_2^-$).

8) N-benzylethanolammonium trihydrogen pyromellitate (9)

^{1}H NMR spectrum of **9** (D_2O, ppm): 3.12-3.19 m (2H, C_6H_5-CH_2-NH_2^+-$C\underline{H_2}$-CH_2-OH); 3.77-3.84 m (2H, C_6H_5-CH_2-NH_2^+-CH_2-$C\underline{H_2}$-OH); 4.21 s (2H, C_6H_5-$C\underline{H_2}$-NH_2^+-CH_2-CH_2-OH); 7.37-7.49 m ($5H_{Ar}$); 7.97-8.04 m ($2H_{Ar}$).

^{13}C NMR spectrum of **9** (D_2O, ppm): 48.4 (C_6H_5-CH_2-NH_2^+-$\underline{C}H_2$-CH_2-OH); 50.8 (C_6H_5-$\underline{C}H_2$-NH_2^+-CH_2-CH_2-OH); 56.5 (C_6H_5-CH_2-NH_2^+-CH_2-$\underline{C}H_2$-OH); 129.1 ($\underline{C}_{Ar}H$); 129.2 ($\underline{C}_{Ar}H$); 129.6 ($\underline{C}_{Ar}H$); 129.7 ($\underline{C}_{Ar}H$); 130.5 ($\underline{C}_{Ar}$); 134.9 ($\underline{C}_{Ar}$); 171.0 (($HO_2\underline{C}$)$_3$-C_6H_5-$\underline{C}O_2^-$).

9) N-benzylethanolammonium dihydrogen pyromellitate (10)

^{1}H NMR spectrum of **10** (D_2O, ppm): 3.13-3.20 m (4H, C_6H_5-CH_2-NH_2^+-$C\underline{H_2}$-CH_2-OH); 3.76-3.85 m (4H, C_6H_5-CH_2-NH_2^+-CH_2-$C\underline{H_2}$-OH); 4.22 s (2H, C_6H_5-$C\underline{H_2}$-NH_2^+-CH_2-CH_2-OH); 7.36-7.50 m ($10H_{Ar}$); 7.87-7.95 m ($2H_{Ar}$).

^{13}C NMR spectrum of **10** (D_2O, ppm): 48.4 (C_6H_5-CH_2-NH_2^+-$\underline{C}H_2$-CH_2-OH); 50.8 (C_6H_5-$\underline{C}H_2$-NH_2^+-CH_2-CH_2-OH); 56.5 (C_6H_5-CH_2-NH_2^+-CH_2-$\underline{C}H_2$-OH); 129.0 ($\underline{C}_{Ar}H$); 129.2 ($\underline{C}_{Ar}H$); 129.6 ($\underline{C}_{Ar}H$); 129.7 ($\underline{C}_{Ar}H$); 130.5 ($\underline{C}_{Ar}$); 135.6 ($\underline{C}_{Ar}$); 172.2 (($HO_2\underline{C}$)$_2$-C_6H_5-($\underline{C}O_2^-$)$_2$).

10) N-benzylethanolammonium hydrogen succinate (11)

^{1}H NMR spectrum of **11** (D_2O, ppm): 2.49 s (4H, COOH-$C\underline{H_2}$-$C\underline{H_2}$-CO_2^-); 3.12-3.23 m (2H, C_6H_5- CH_2-NH_2^+-$C\underline{H_2}$-CH_2-OH); 3.76-3.90 m (2H, C_6H_5- CH_2-NH_2^+-CH_2-$C\underline{H_2}$-OH); 4.26 s (2H, C_6H_5-$C\underline{H_2}$-NH_2^+-CH_2-CH_2-OH); 7.31-7.69 m ($5H_{Ar}$).

^{13}C NMR spectrum of **11** (D_2O, ppm): 31.2 (COOH-$\underline{C}H_2$-$\underline{C}H_2$-CO_2^-); 48.4 (C_6H_5-CH_2-NH_2^+-$\underline{C}H_2$-CH_2-OH); 50.8 (C_6H_5-$\underline{C}H_2$-NH_2^+-CH_2-CH_2-OH); 56.5

(C_6H_5-CH_2-NH_2^+-CH_2-$\underline{C}H_2$-OH); 129.2 ($\underline{C}_{Ar}H$); 129.6 ($\underline{C}_{Ar}H$); 129.8 ($\underline{C}_{Ar}H$); 130.6 ($\underline{C}_{Ar}$); 179.6 ($\underline{C}OOH$-CH_2-CH_2-$\underline{C}O_2^-$).

11) N-benzylethanolammonium succinate (12)

^{1}H NMR spectrum of **12** (D_2O, ppm): 2.53 s (4H, ^-O_2C-$C\underline{H}_2$-$C\underline{H}_2$-CO_2^-); 3.11-3.28 m (4H, C_6H_5- CH_2-NH_2^+-$C\underline{H}_2$-CH_2-OH); 3.77-3.91 m (4H, C_6H_5- CH_2-NH_2^+-CH_2-$C\underline{H}_2$-OH); 4.27 s (4H, C_6H_5-$C\underline{H}_2$-NH_2^+-CH_2-CH_2-OH); 7.25-7.77 m ($10H_{Ar}$).

^{13}C NMR spectrum of **12** (D_2O, ppm): 30.8 (^-O_2C-$\underline{C}H_2$-$\underline{C}H_2$-CO_2^-); 48.4 (C_6H_5-CH_2-NH_2^+-$\underline{C}H_2$-CH_2-OH); 50.8 (C_6H_5-$\underline{C}H_2$-NH_2^+-CH_2-CH_2-OH); 56.5 (C_6H_5-CH_2-NH_2^+-CH_2-$\underline{C}H_2$-OH); 129.2 ($\underline{C}_{Ar}H$); 129.6 ($\underline{C}_{Ar}H$); 129.8 ($\underline{C}_{Ar}H$); 130.6 ($\underline{C}_{Ar}$); 179.2 ($^-O_2\underline{C}$-CH_2-CH_2-$\underline{C}O_2^-$).

12) N-benzylethanolammonium hydrogen malonate (13)

^{1}H NMR spectrum of **13** (D_2O, ppm): 2.89-3.01 m (2H, HO_2C-$C\underline{H}_2$-CO_2^-); 3.13-3.23 m (2H, C_6H_5-CH_2-NH_2^+-$C\underline{H}_2$-CH_2-OH); 3.77-3.88 m (2H, C_6H_5-CH_2-NH_2^+-CH_2-$C\underline{H}_2$-OH); 4.26 s (2H, C_6H_5-$C\underline{H}_2$-NH_2^+-CH_2-CH_2-OH); 7.40-7.67 m ($5H_{Ar}$).

^{13}C NMR spectrum of **13** (D_2O, ppm): 39.6 (HO_2C-$\underline{C}H_2$-CO_2^-); 48.4 (C_6H_5-CH_2-NH_2^+-$\underline{C}H_2$-CH_2-OH); 50.8 (C_6H_5-$\underline{C}H_2$-NH_2^+-CH_2-CH_2-OH); 56.5 (C_6H_5-CH_2-NH_2^+-CH_2-$\underline{C}H_2$-OH); 129.2 ($\underline{C}_{Ar}H$); 129.6 ($\underline{C}_{Ar}H$); 129.8 ($\underline{C}_{Ar}H$); 130.6 ($\underline{C}_{Ar}$); 174.6 ($HO_2\underline{C}$-CH_2-$\underline{C}O_2^-$).

13) N-benzylethanolammonium malonate (14)

^{1}H NMR spectrum of **14** (D_2O, ppm): 2.82 s (2H, ^-O_2C-$C\underline{H}_2$-CO_2^-); 3.14-3.22 m (4H, C_6H_5-CH_2-NH_2^+-$C\underline{H}_2$-CH_2-OH); 3.78-3.87 m (4H, C_6H_5-CH_2-NH_2^+-CH_2-$C\underline{H}_2$-OH); 4.26 s (4H, C_6H_5-$C\underline{H}_2$-NH_2^+-CH_2-CH_2-OH); 7.32-7.64 m ($10H_{Ar}$).

^{13}C NMR spectrum of **14** (D_2O, ppm): 39.1 (^-O_2C-$\underline{C}H_2$-CO_2^-); 48.4 (C_6H_5-CH_2-NH_2^+-$\underline{C}H_2$-CH_2-OH); 50.8 (C_6H_5-$\underline{C}H_2$-NH_2^+-CH_2-CH_2-OH); 56.5 (C_6H_5-CH_2-NH_2^+-CH_2-$\underline{C}H_2$-OH); 129.2 ($\underline{C}_{Ar}H$); 129.6 ($\underline{C}_{Ar}H$); 129.8 ($\underline{C}_{Ar}H$); 130.6 ($\underline{C}_{Ar}$); 177.3 ($^-O_2\underline{C}$-CH_2-$\underline{C}O_2^-$).

14) N-benzylethanolammonium hydrogen oxalate (15)

^{1}H NMR spectrum of **15** (D_2O, ppm): 3.15-3.26 m (2H, C_6H_5- CH_2-NH_2^+-$C\underline{H_2}$-CH_2-OH); 3.78-3.91 m (2H, C_6H_5- CH_2-NH_2^+-CH_2-$C\underline{H_2}$-OH); 4.26 s (2H, C_6H_5-$C\underline{H_2}$-NH_2^+-CH_2-CH_2-OH); 7.25-7.69 m ($5H_{Ar}$).

^{13}C NMR spectrum of **15** (D_2O, ppm): 48.4 (C_6H_5-CH_2-NH_2^+-$\underline{C}H_2$-CH_2-OH); 50.8 (C_6H_5-$\underline{C}H_2$-NH_2^+-CH_2-CH_2-OH); 56.5 (C_6H_5-CH_2-NH_2^+-CH_2-$\underline{C}H_2$-OH); 129.2 ($\underline{C}_{Ar}H$); 129.6 ($\underline{C}_{Ar}H$); 129.8 ($\underline{C}_{Ar}H$); 130.5 ($\underline{C}_{Ar}$); 165.5 ($HO_2\underline{C}$-$\underline{C}O_2^-$).

15) N-benzylethanolammonium oxalate (16)

^{1}H NMR spectrum of **16** (D_2O, ppm): 3.13-3.26 m (4H, C_6H_5-CH_2-NH_2^+-$C\underline{H_2}$-CH_2-OH); 3.75-3.91 m (4H, C_6H_5-CH_2-NH_2^+-CH_2-$C\underline{H_2}$-OH); 4.28 s (4H, C_6H_5-$C\underline{H_2}$-NH_2^+-CH_2-CH_2-OH); 7.36-7.62 m ($10H_{Ar}$).

^{13}C NMR spectrum of **16** (D_2O, ppm): 48.4 (C_6H_5-CH_2-NH_2^+-$\underline{C}H_2$-CH_2-OH); 50.8 (C_6H_5-$\underline{C}H_2$-NH_2^+-CH_2-CH_2-OH); 56.5 (C_6H_5-CH_2-NH_2^+-CH_2-$\underline{C}H_2$-OH); 129.2 ($\underline{C}_{Ar}H$); 129.6 ($\underline{C}_{Ar}H$); 129.8 ($\underline{C}_{Ar}H$); 130.6 ($\underline{C}_{Ar}$); 173.5 ($^{-}O_2\underline{C}$-$\underline{C}O_2^-$).

Table S1. pH value of reaction mixtures for ^{68}Ga- and Al^{18}F-radiolabeling reactions

BEA Salt	pH of reaction mixture	
	^{68}Ga-radiolabeling	Al^{18}F-radiolabeling
1	4.1	6.1
2	5.4	6.3
3	3.0	5.5
4	5.1	5.4
5	4.3	5.8
6	3.9	5.7
7	2.6	5.4
8	2.9	4.3
9	1.8	3.6
10	2.7	4.7
11	3.9	6.0
12	4.2	5.8
13	2.8	5.5
14	5.5	7.5
15	1.6	4.6
16	4.1	4.3