

# Designing Thermally Stable Organocatalysts for Poly(ethylene terephthalate) Synthesis

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Supporting Information

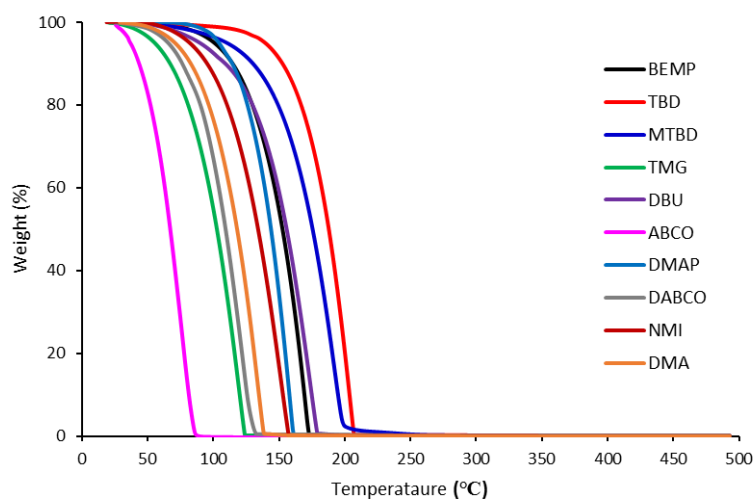
**Designing thermally stable organocatalysts for  
poly(ethylene terephthalate) synthesis: Towards a  
one-pot, closed-loop chemical recycling system for  
PET**

Shu Kaiho,<sup>a,b</sup> Ali Al Rida Hmayed,<sup>a</sup> Kayla R. Delle Chiaie,<sup>a</sup> Joshua C. Worch<sup>a</sup> and Andrew P. Dove<sup>a\*</sup>

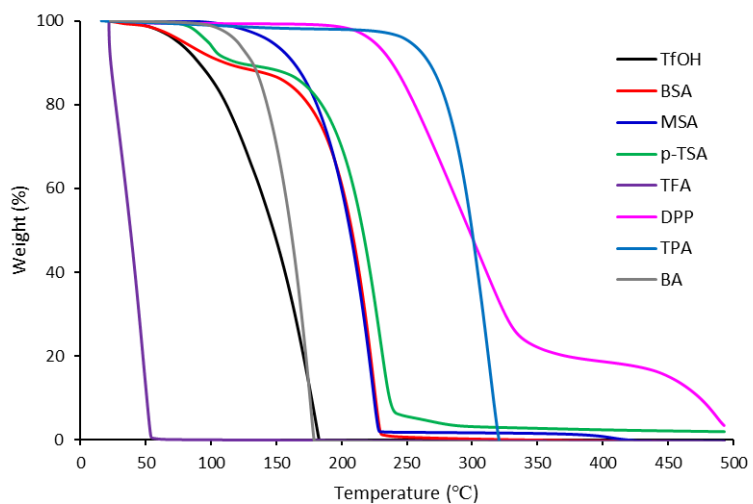
<sup>a</sup> School of Chemistry, University of Birmingham, Edgbaston, Birmingham, B15 2TT, U.K.

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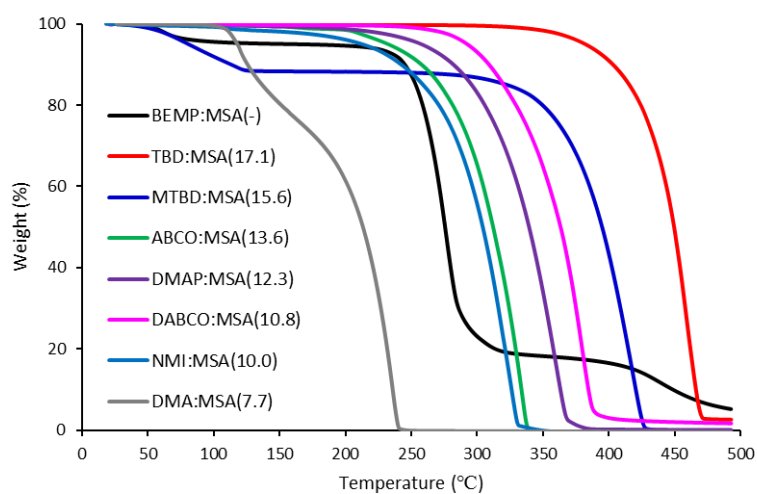
## 1. Thermal stability of salts



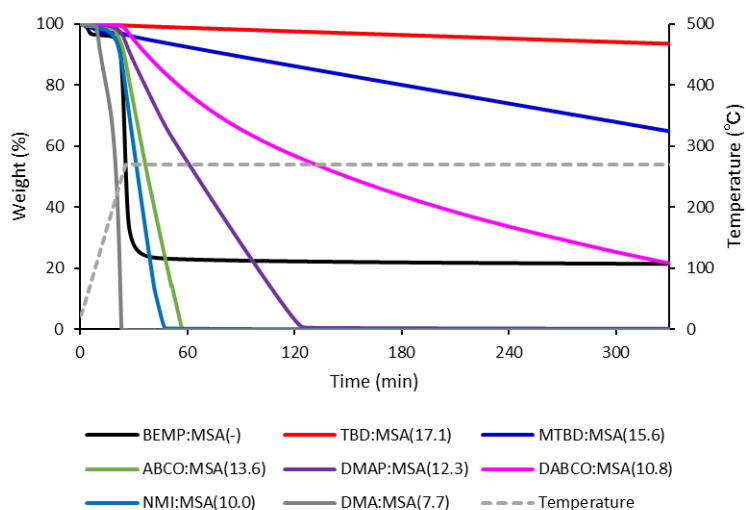
**Figure S1.** TGA thermograms of organic bases conducted under programmed heating condition from room temperature to 500 °C at a rate of 10 °C/min.



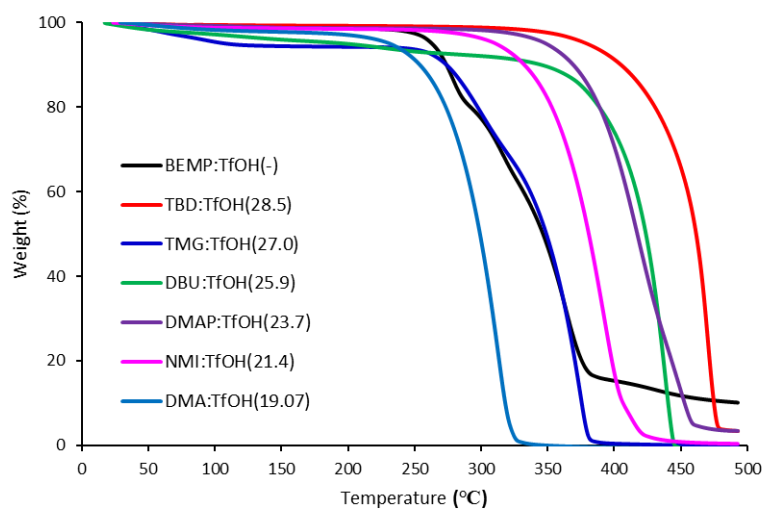
**Figure S2.** TGA thermograms of organic acids conducted under programmed heating condition from room temperature to 500 °C at a rate of 10 °C/min.



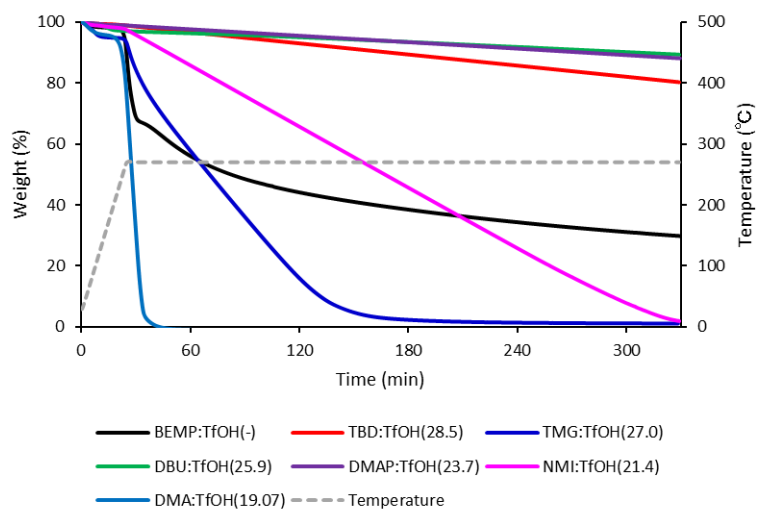
**Figure S3.** TGA thermograms of MSA salts conducted under programmed heating condition from room temperature to 500 °C at a rate of 10 °C/min. Data in parentheses indicate  $\Delta pK_a$  values in water.



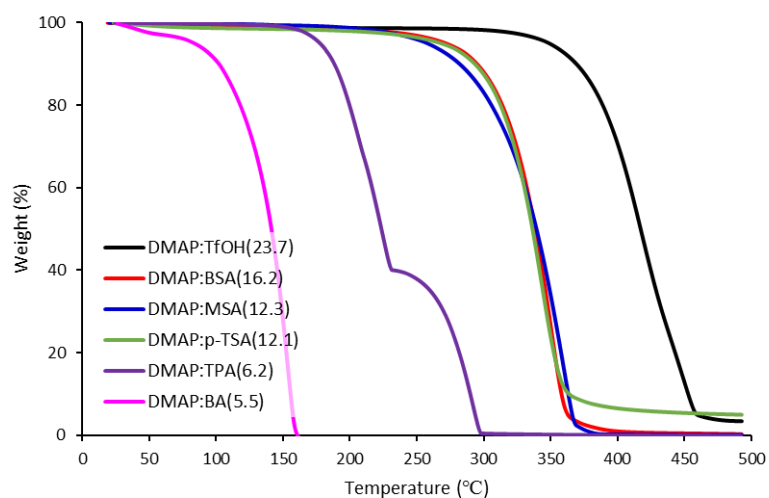
**Figure S4.** Isothermal TGA analyses of MSA salts conducted under the programmed heating condition from room temperature to 270 °C at a rate of 10 °C/min followed by the isothermal heating condition at 270 °C for 5 h. Data in parentheses indicate  $\Delta pK_a$  values in water.



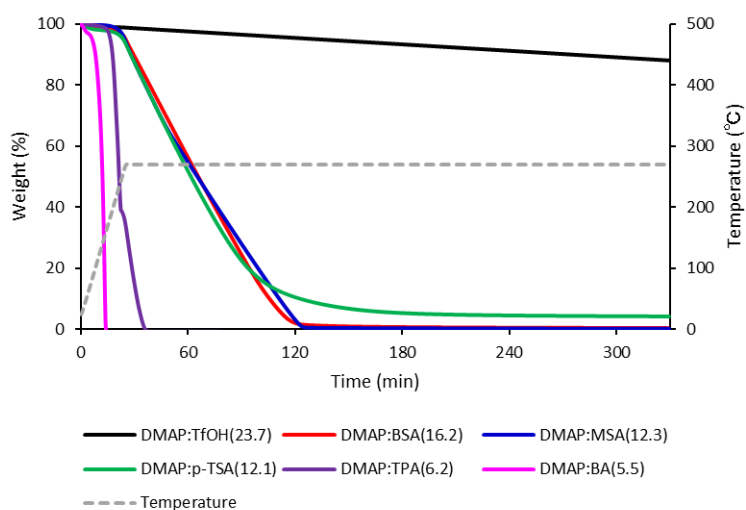
**Figure S5.** TGA thermograms of TfOH salts conducted under programmed heating condition from room temperature to 500 °C at a rate of 10 °C/min. Data in parentheses indicate  $\Delta pK_a$  values in water.



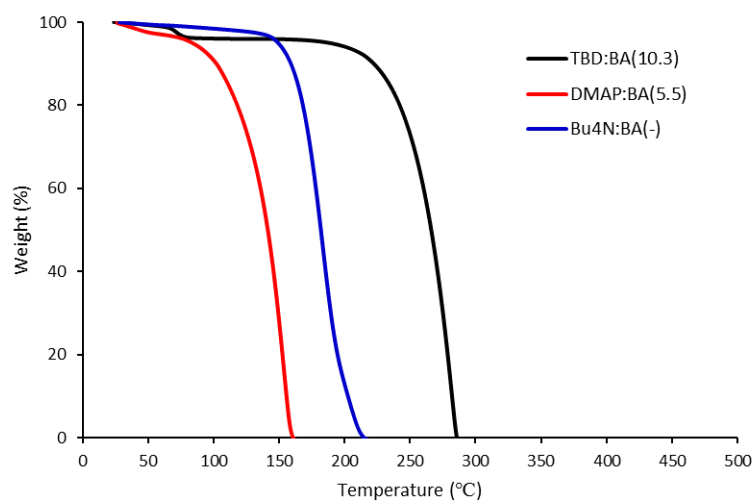
**Figure S6.** Isothermal TGA analyses of TfOH salts conducted under the programmed heating condition from room temperature to 270 °C at a rate of 10 °C/min followed by the isothermal heating condition at 270 °C for 5 h. Data in parentheses indicate  $\Delta pK_a$  values in water.



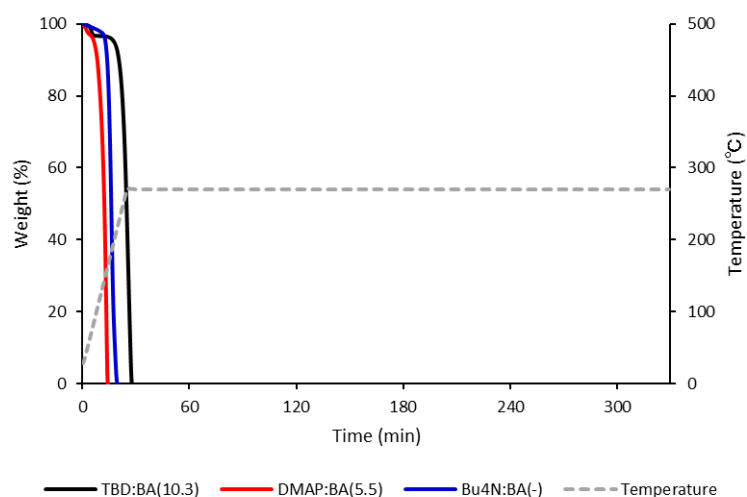
**Figure S7.** TGA thermograms of DMAP salts conducted under programmed heating condition from room temperature to 500 °C at a rate of 10 °C/min. Data in parentheses indicate  $\Delta pK_a$  values in water.



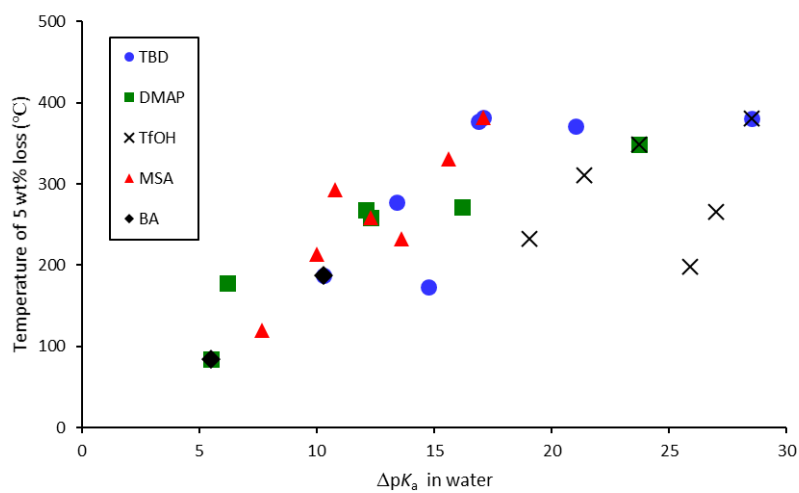
**Figure S8.** Isothermal TGA analyses of DMAP salts conducted under the programmed heating condition from room temperature to 270 °C at a rate of 10 °C/min followed by the isothermal heating condition at 270 °C for 5 h. Data in parentheses indicate  $\Delta pK_a$  values in water.



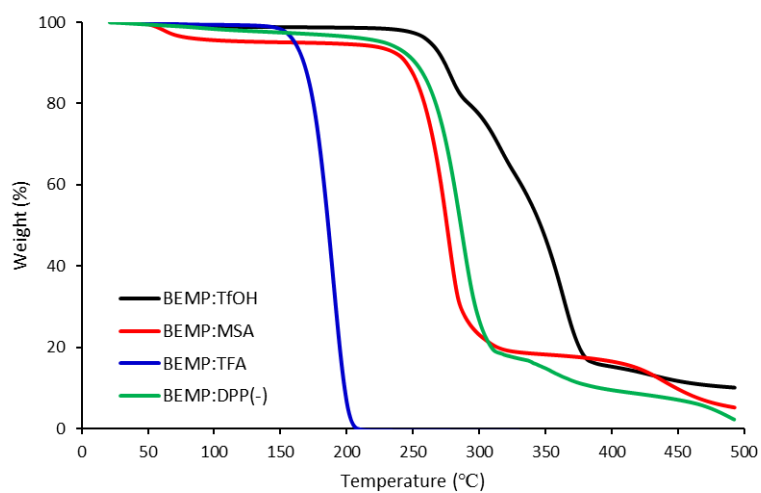
**Figure S9.** TGA thermograms of BA salts conducted under programmed heating condition from room temperature to 500 °C at a rate of 10 °C/min. Data in parentheses indicate  $\Delta pK_a$  values in water.



**Figure S10.** Isothermal TGA analyses of BA salts conducted under the programmed heating condition from room temperature to 270 °C at a rate of 10 °C/min followed by the isothermal heating condition at 270 °C for 5 h. Data in parentheses indicate  $\Delta pK_a$  values in water.

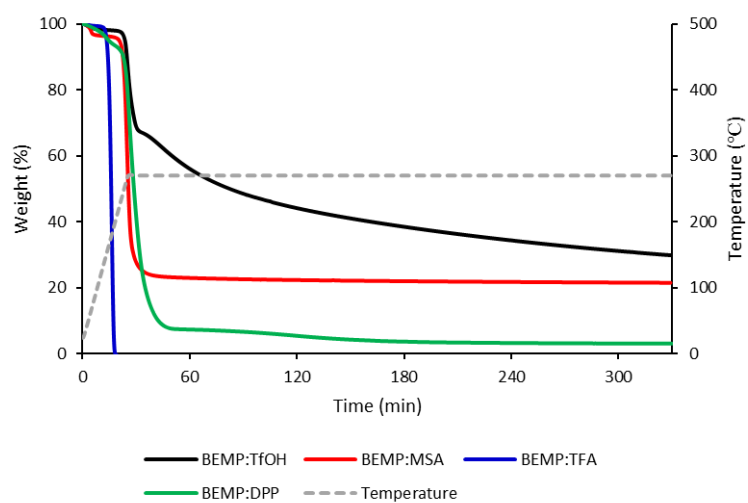


**Figure S11.** Temperatures of 5 wt% loss of the salts as a function of  $\Delta pK_a$  of the constituent bases and acids.



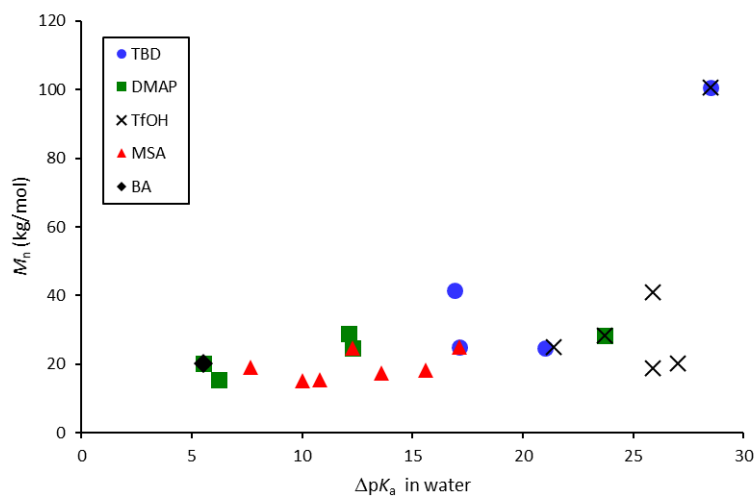
**Figure S12.** TGA analyses of BEMP salts conducted under programmed heating condition from room temperature to 500 °C at a rate of 10 °C/min.



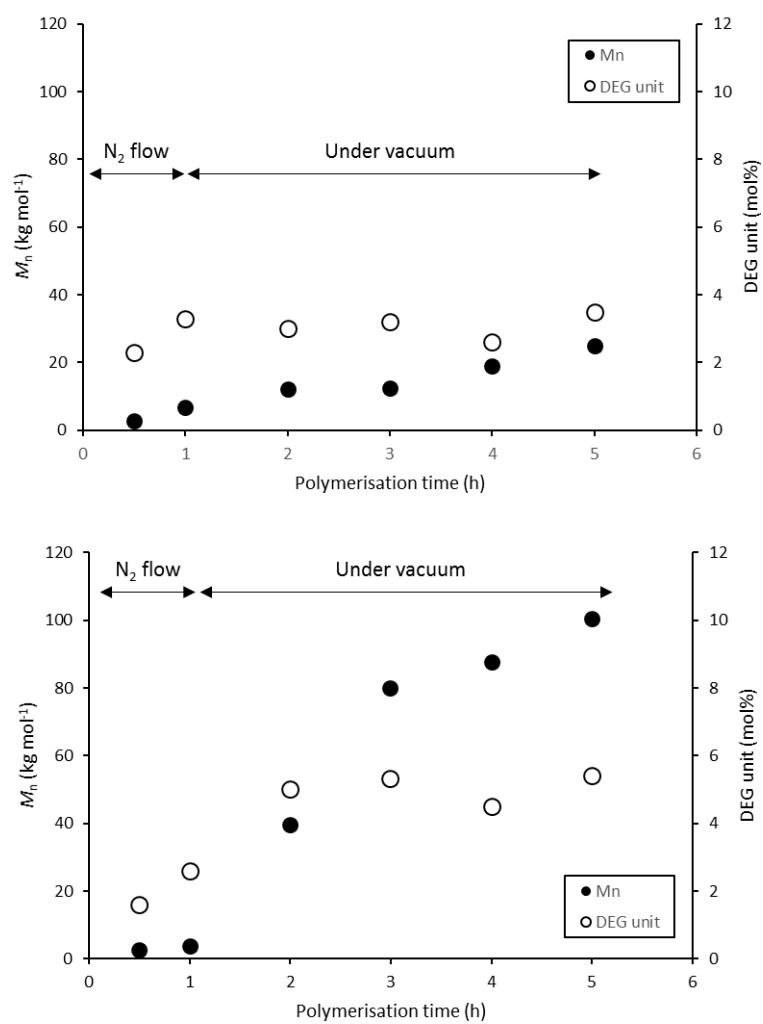


**Figure S13.** Isothermal TGA analyses of BEMP salts conducted under the programmed heating condition from room temperature to 270 °C at a rate of 10 °C/min followed by the isothermal heating condition at 270 °C for 5 h.

## 2. Polymer data



**Figure S14.** Number average molecular weights as a function of  $\Delta pK_a$  of the constituent bases and acids of the salts.



**Figure S15.** Relationships between polymerisation times and molecular weights, and polymerisation times and DEG units (catalyst; 5 mol% of TBD:MSA salt (above) and 5 mol% of TBD:TfOH salt (below)).

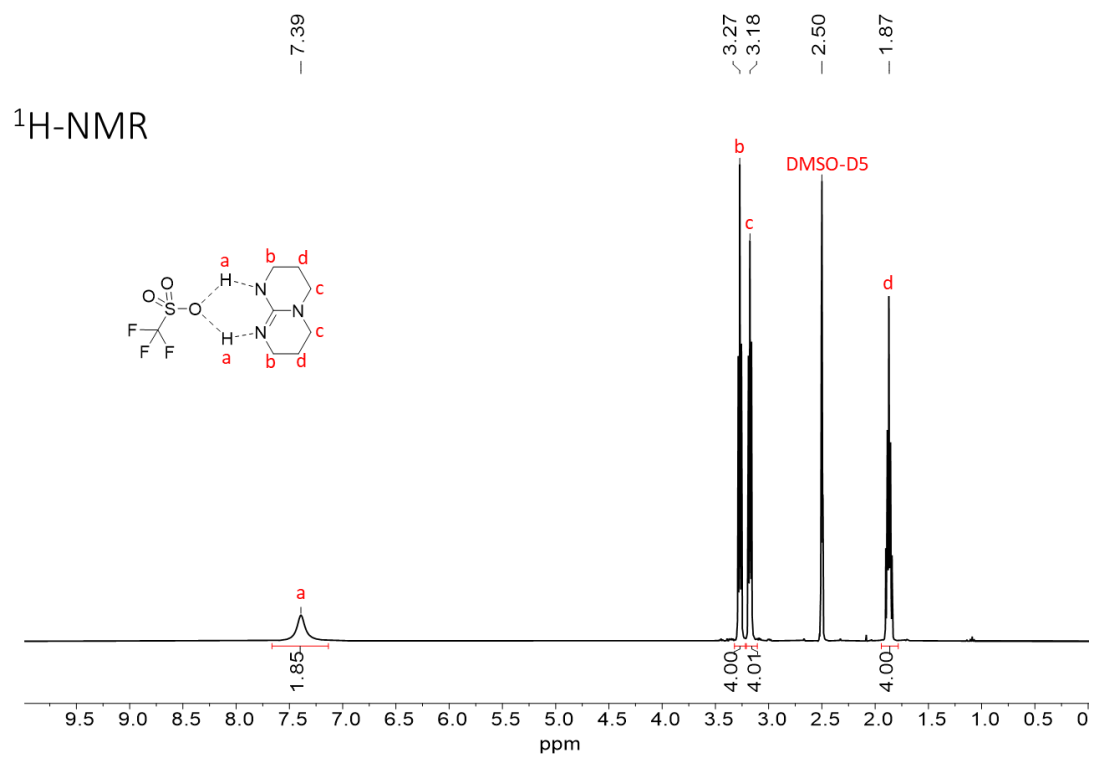
**Table S1.** Molecular weight, DEG unit content, and colourimetry analyses of PET synthesised using salts.

Base	Acid	Molar ratio (Base:Acid)	$pK_a$ of base in water	$pK_a$ of acid** in water	$\Delta pK_a$ in water	Salt amount (mol%)	$M_n^{a)}$ ( $kg\ mol^{-1}$ )	DEG unit <sup>b)</sup> (mol%)	Colourimetry <sup>c)</sup>		
									$L^*$	$a^*$	$b^*$
TBD	TfOH	1:1	14.5	-14	28.5	5	100.6 <sup>d)</sup>	5.4	100.0	-0.1	0.2
TBD	BSA	1:1	14.5	-6.5	21	5	24.8	4.8	99.9	-0.1	0.2
TBD	MSA	1:1	14.5	-2.6	17.1	5	25	3.5	99.6	0.0	0.4
TBD	<i>p</i> -TSA	1:1	14.5	-2.4	16.9	5	41.4	5	99.9	-0.1	0.4
TBD	TFA	1:1	14.5	-0.25	14.75	5	Insoluble	-	-	-	-
TBD	DPP	1:1	14.5	1.1	13.4	5	Insoluble	-	-	-	-
TBD	BA	1:1	14.5	4.2	10.3	5	Insoluble	-	-	-	-
TBD	-	-	14.5	-	-	5	Insoluble	-	-	-	-
MTBD	MSA	1:1	13	-2.6	15.6	5	18.2	7.2	99.2	-0.1	0.6
TMG	TfOH	1:1	13	-14	27	5	20.3	36.5	89.8	-0.5	20.7
DBU	TfOH	1:1	11.9	-14	25.9	5	18.7 <sup>d)</sup>	38.5	90.5	-1.1	7.6
ABCO	MSA	1:1	11	-2.6	-	5	17.4	40.6	95.5	-0.6	8.9
DMAP	TfOH	1:1	9.7	-14	23.7	5	28.4	41.5	99.6	-0.2	1.1
DMAP	BSA	1:1	9.7	-6.5	16.2	-	-	-	-	-	-
DMAP	MSA	1:1	9.7	-2.6	12.3	5	24.8	21	94.5	-1.3	10.6
DMAP	<i>p</i> -TSA	1:1	9.7	-2.4	12.1	5	28.9	29.4	93.4	-5.3	24.4
DMAP	TPA	2:1	9.7	3.51	6.19	2.5	15.5	1.2	99.2	0.0	1.2
DMAP	BA	1:1	9.7	4.2	5.5	5	20.3	1.4	96.7	0.0	4.1
DMAP	-	-	9.7	-	-	5	15.6	1.3	99.0	0.0	1.7
DABCO	MSA	1:2	8.2	-2.6	-	2.5	15.5	51.9	90.9	-0.5	15.1
NMI	TfOH	1:1	7.4	-14	21.4	5	25.1 <sup>d)</sup>	39.4	99.1	-0.1	1.5
NMI	BSA	1:1	7.4	-6.5	13.9	-	-	-	-	-	-
NMI	MSA	1:1	7.4	-2.6	10	5	15.3	42.5	92.5	-0.7	13.0
DMA	TfOH	1:1	5.07	-14	19.07	5	40.0 <sup>d)</sup>	6.8	56.7	8.2	47.0
DMA	MSA	1:1	5.07	-2.6	7.67	5	19.1	57.9	97.2	-0.4	4.2
BEMP	TfOH	1:1	-	-14	-	5	27.5	15.8	60.3	9.9	50.5
BEMP	MSA	1:1	-	-2.6	-	5	29.1	22.3	79.8	2.5	29.9
BEMP	TFA	1:1	-	-0.25	-	5	66.8 <sup>d)</sup>	3.7	88.6	0.4	18.0
BEMP	DPP	1:1	-	1.1	-	5	NA <sup>d)</sup>	8.8	81.7	1.3	30.9
Bu <sub>4</sub> N	BA	1:1	-	4.2	-	5	18	1.6	99.3	-0.2	1.4
-	MSA	-	-	-2.6	-	5	13.3	50.8	99.7	0.0	0.3
-	BA	-	-	4.2	-	5	18.9	1.1	99.4	-0.5	2.0

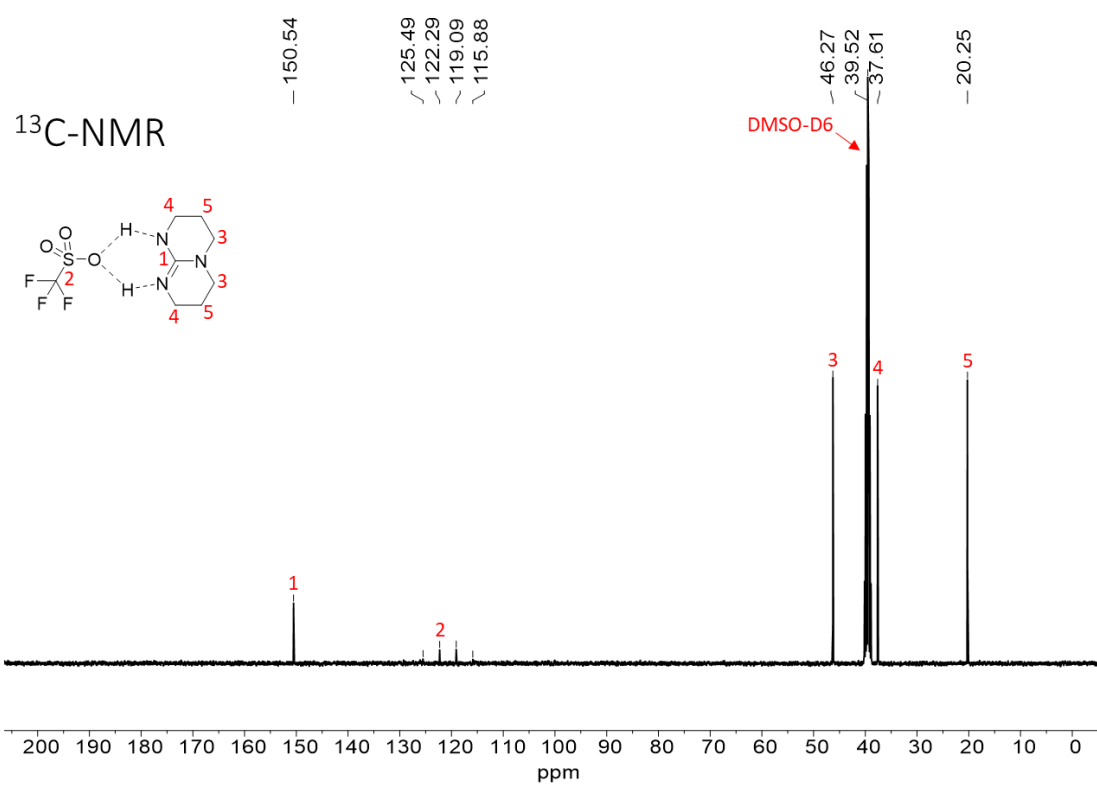
Polymerisation was conducted at 270 °C for for 1 h under N<sub>2</sub> flow, followed by 4 h under vacuum. <sup>a)</sup> Number average molecular weight measured by 1H NMR; <sup>b)</sup> Diethylene glycol content measured by 1H NMR; <sup>c)</sup> L\*a\*b\* values at concentrations of 5 mg mL<sup>-1</sup> using a mixture solvent of chloroform:trifluoroacetic acid (8:1), calculated under the condition of a standard illuminant D65 light source at 2°; <sup>d)</sup> Signals of the end oxyethylene unit were not clear.

\*\*The majority of the  $pK_a$  values are sourced from a compiled document<sup>1</sup>, which in itself lists  $pK_a$  values obtained from primary literature sources. This document is endorsed by the ACS organic division (most recently updated in July 2022). For any missing value from the compiled reference, we considered a  $pK_a$  value from a secondary reference: TPA<sup>2</sup>; DPP<sup>3</sup>; BSA/*p*-TSA<sup>4</sup>; TfOH<sup>5</sup>.

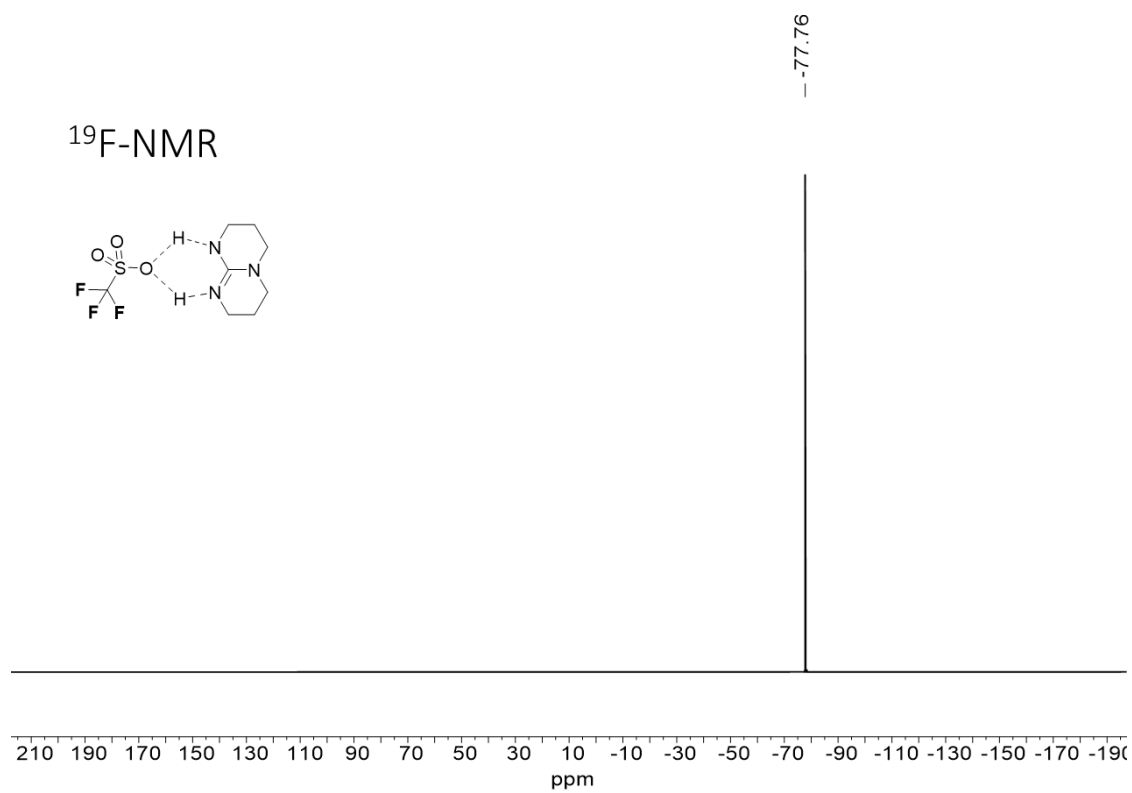
### 3. NMR spectra of the synthesized organic salts.



**Figure S16.** <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:TfOH salt.



**Figure S17.** <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:TfOH salt.



**Figure S18.** <sup>19</sup>F NMR (376.3 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:TfOH salt.

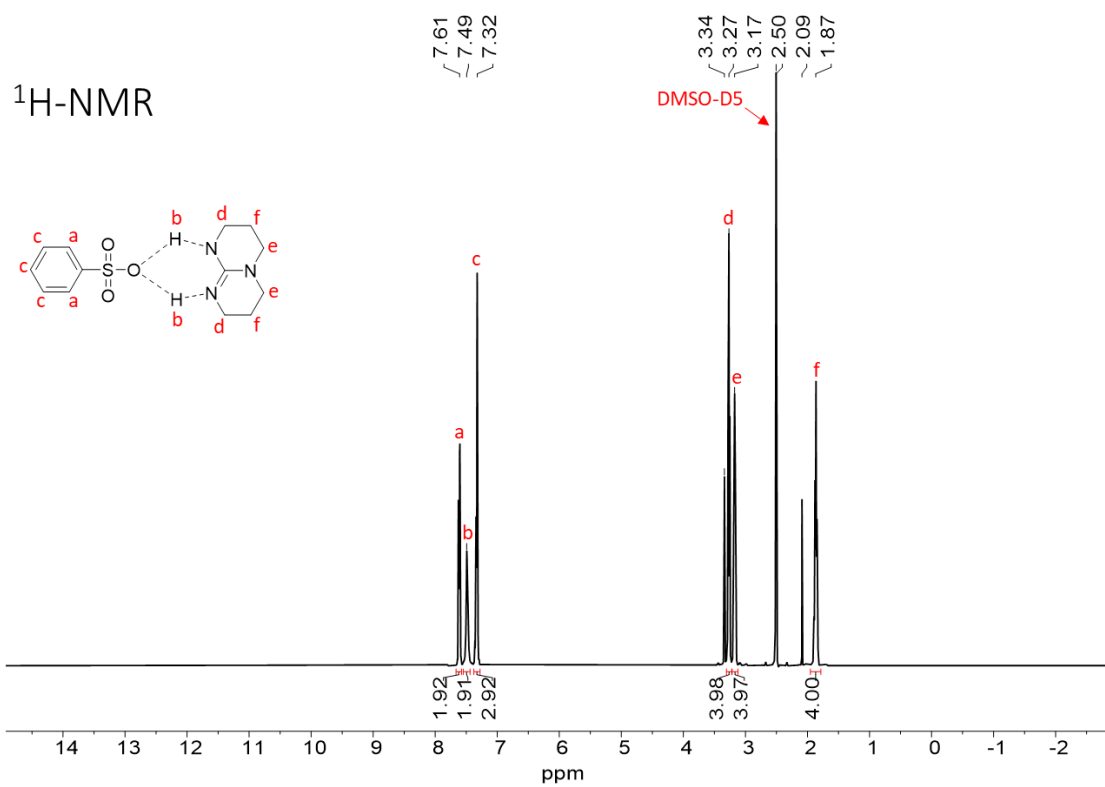


Figure S19. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:BSA salt.

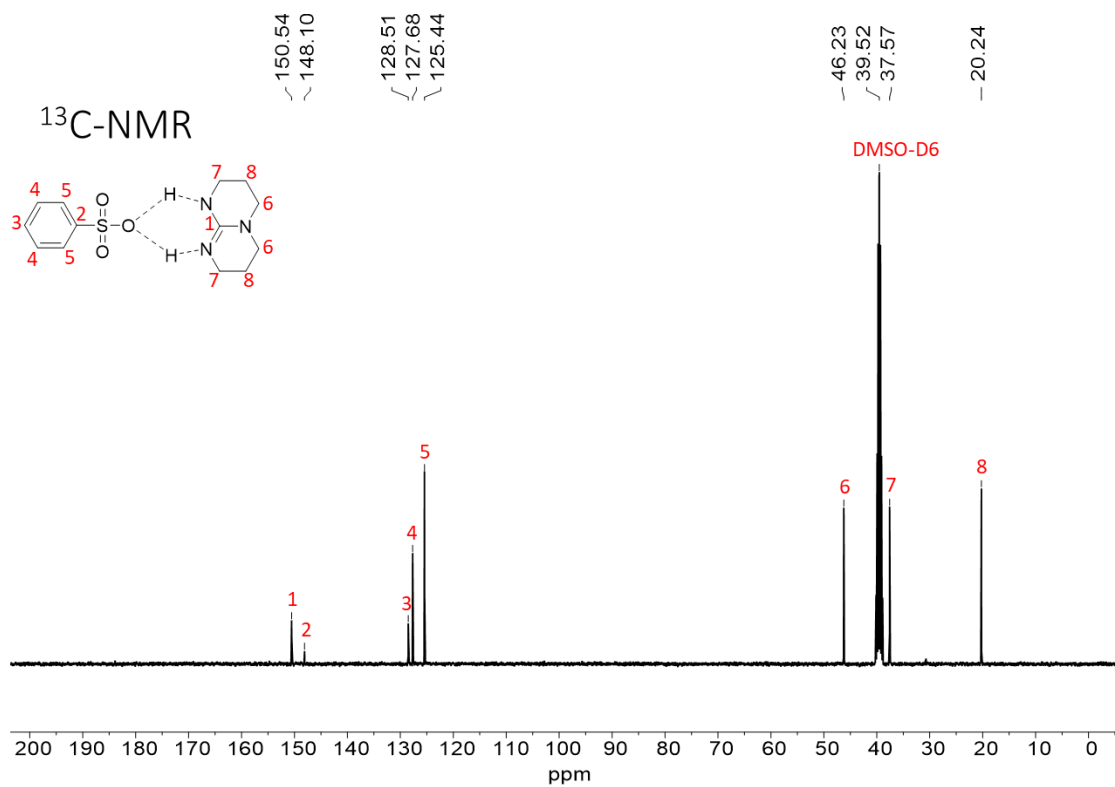


Figure S20. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:BSA salt.

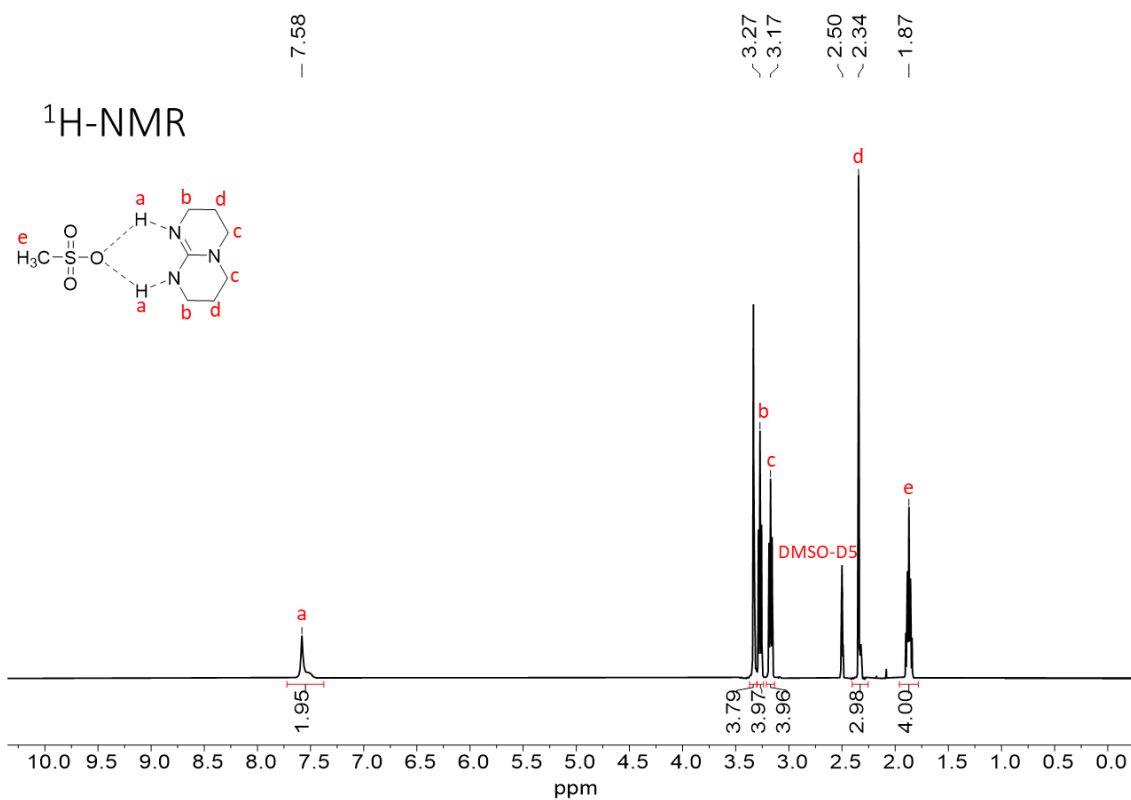


Figure S21. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:MSA salt.

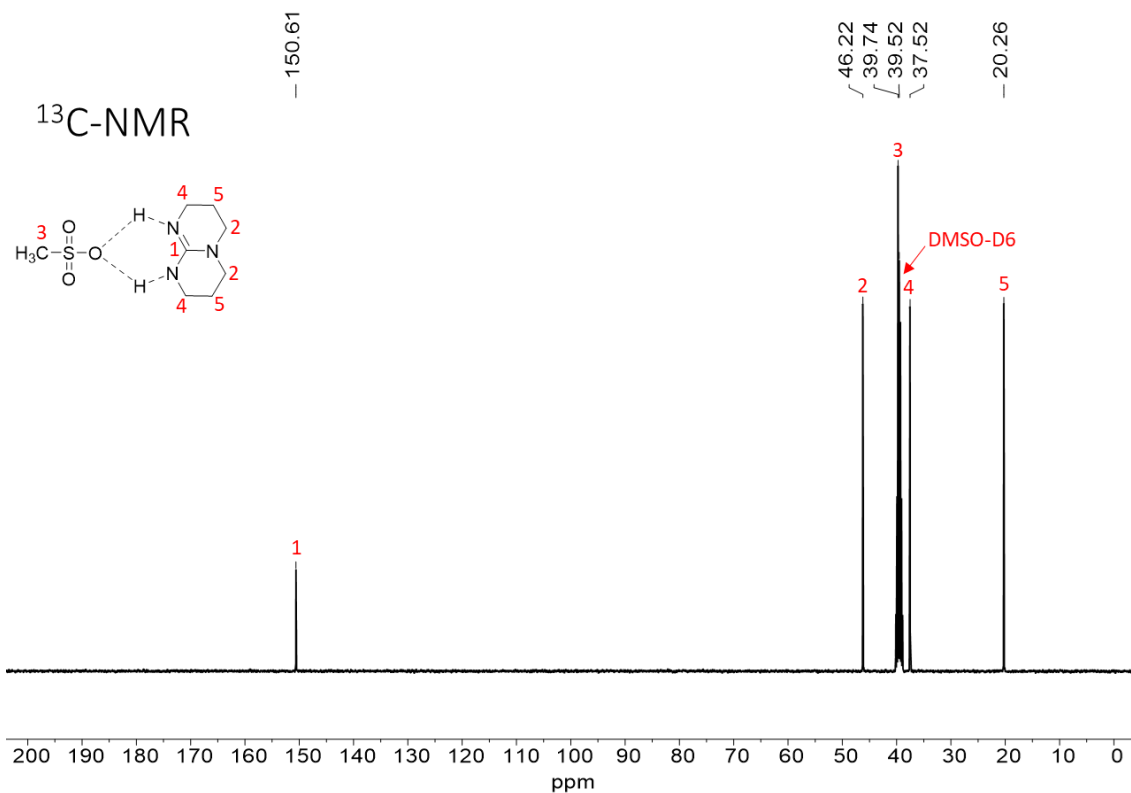


Figure S22. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:MSA salt.

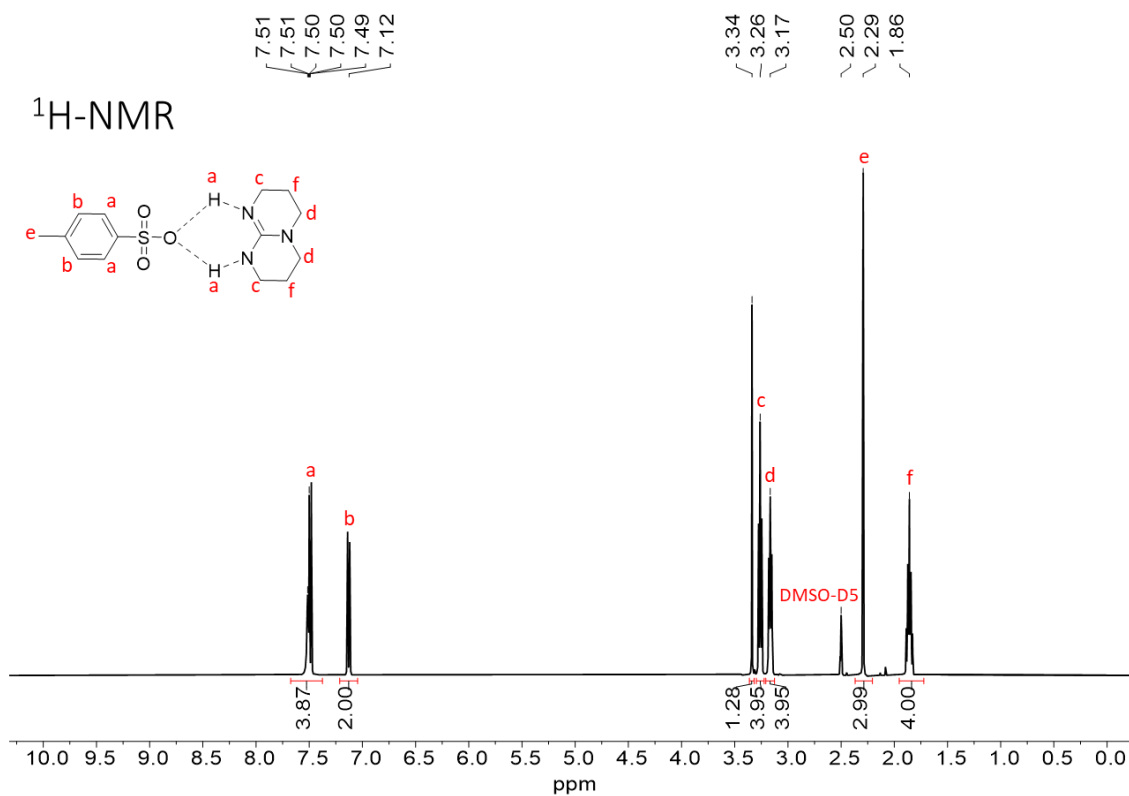


Figure S23. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:*p*-TSA salt.

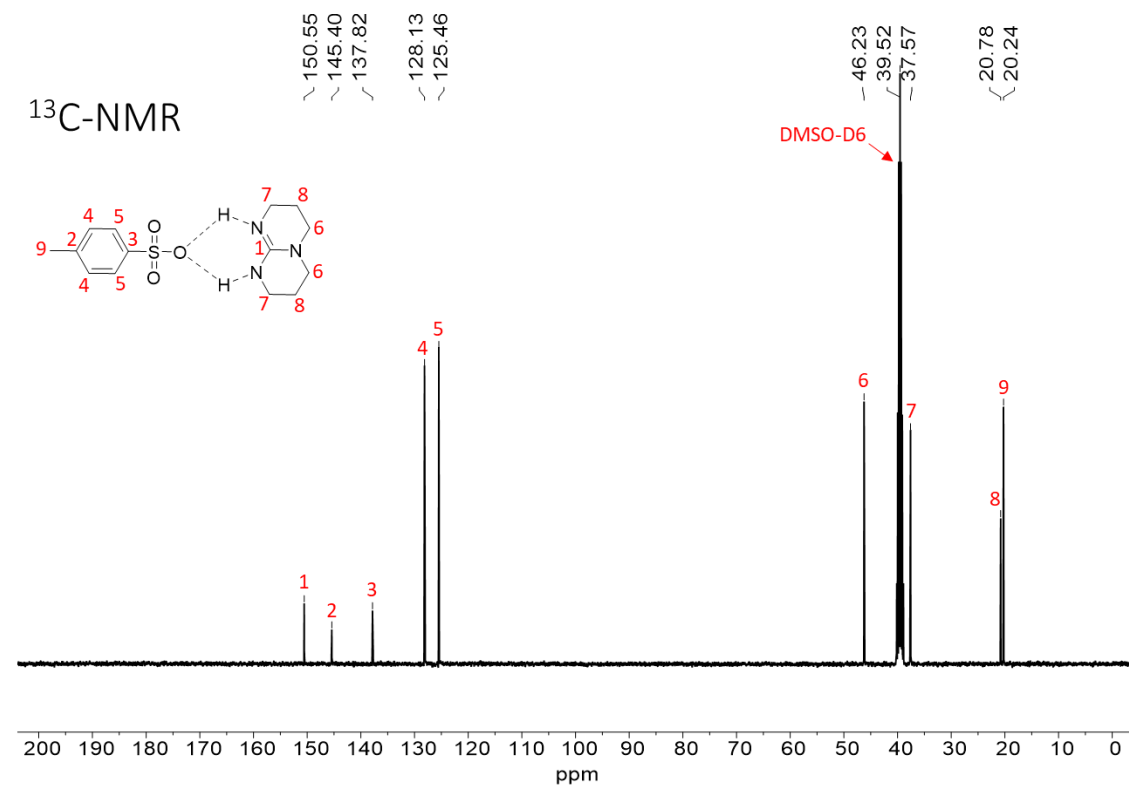


Figure S24. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:*p*-TSA salt.



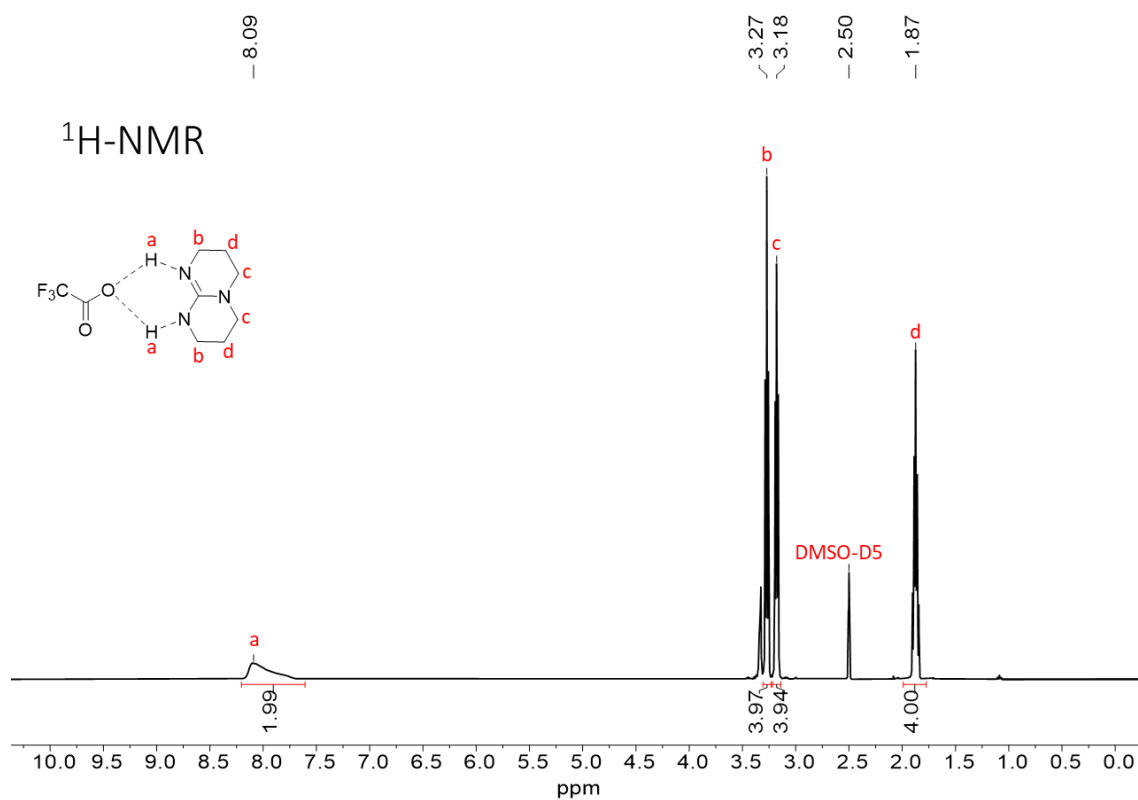


Figure S25. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:TFA salt.

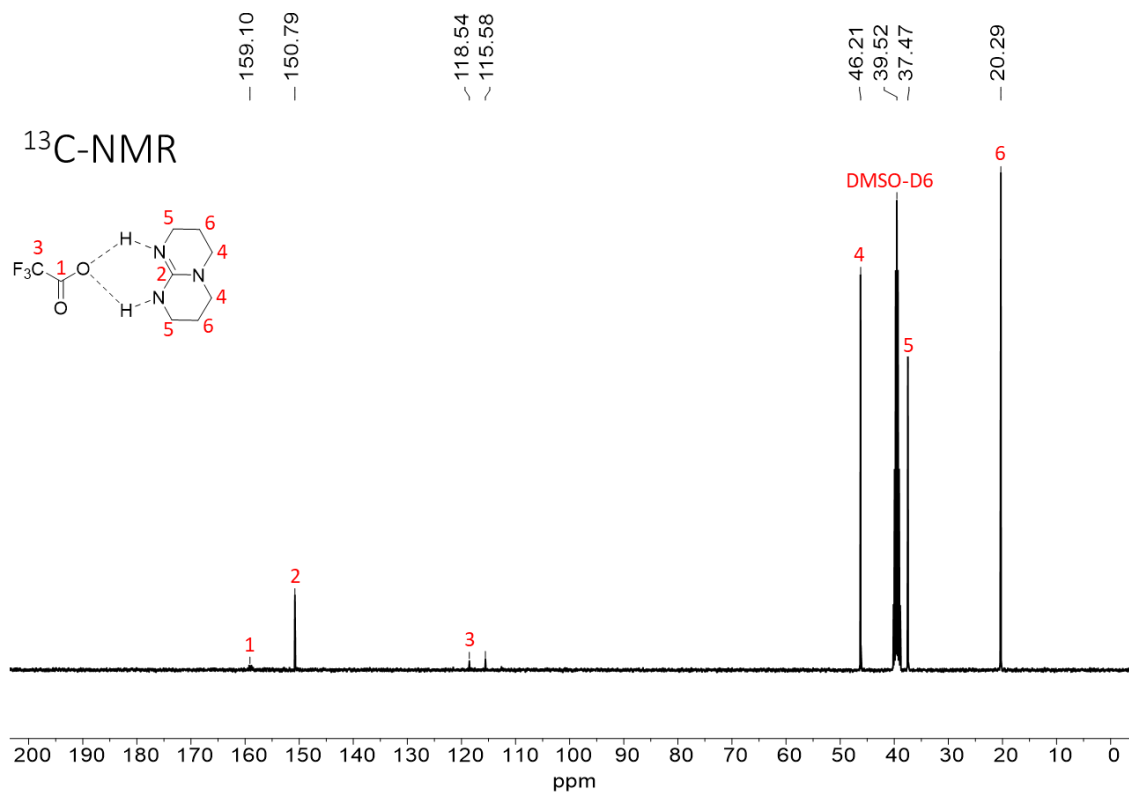


Figure S26. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:TFA salt.

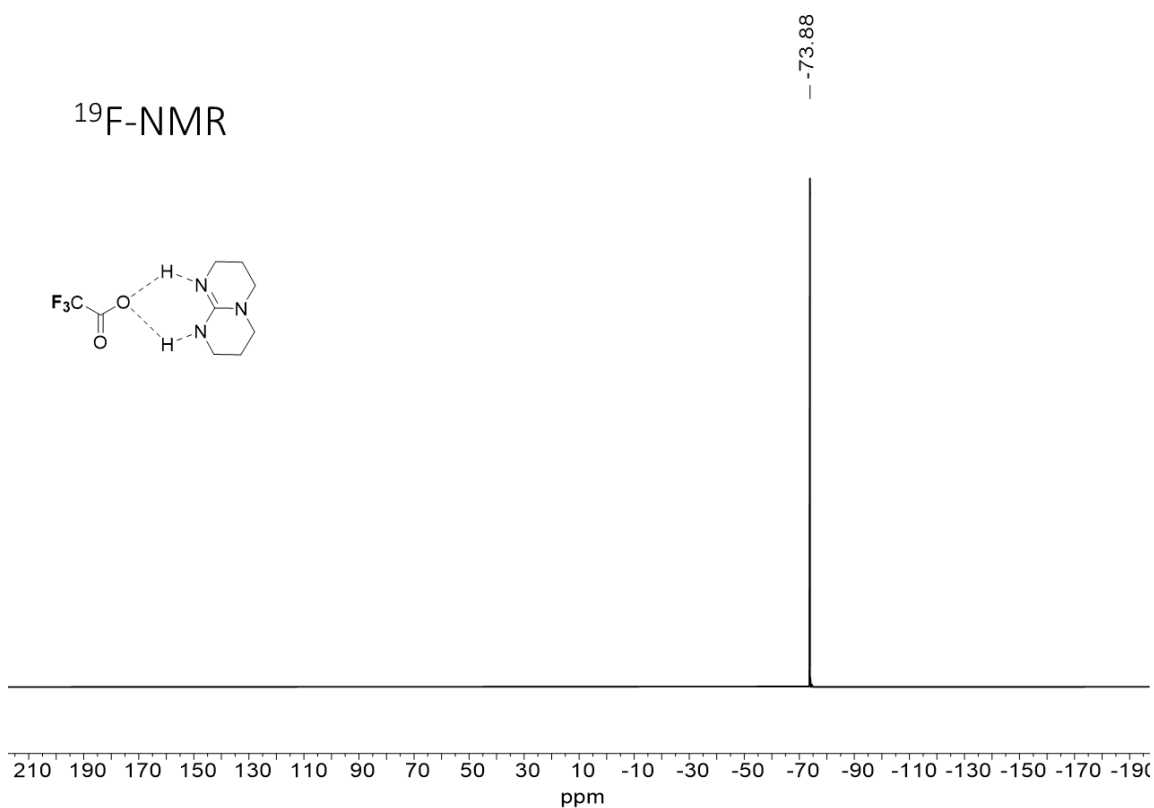


Figure S27. <sup>19</sup>F NMR (376.3 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:TFA salt.

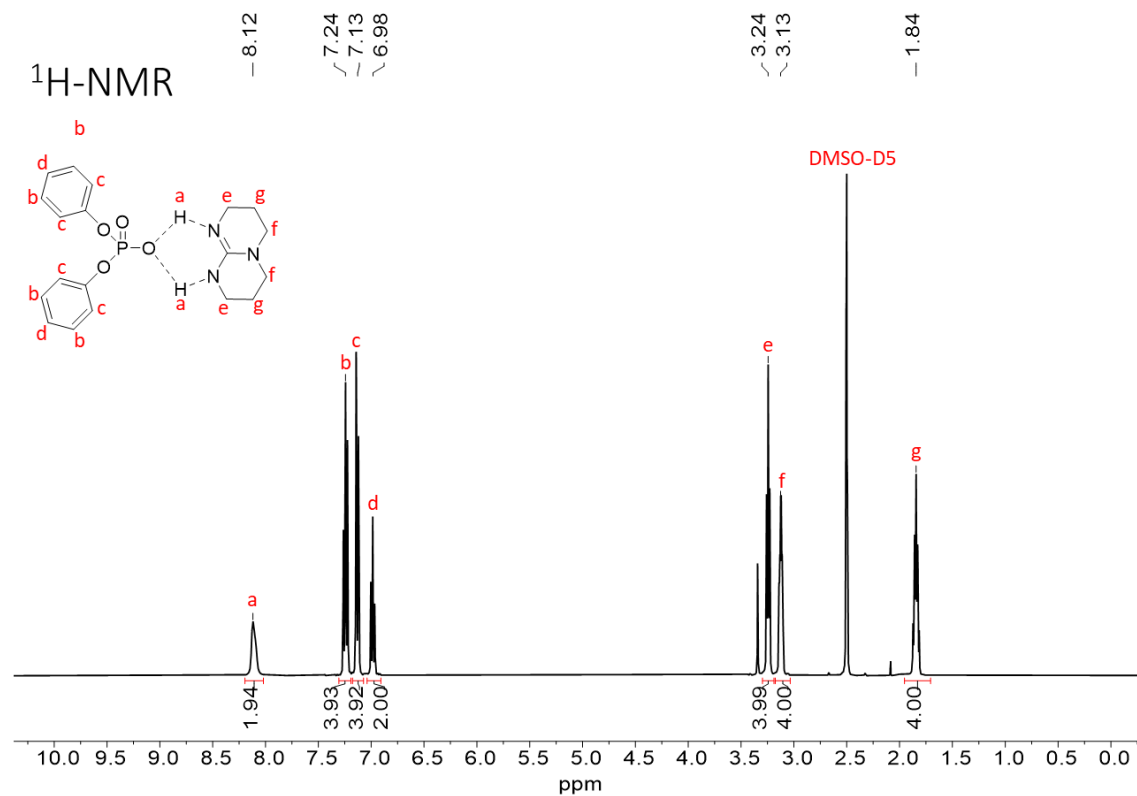
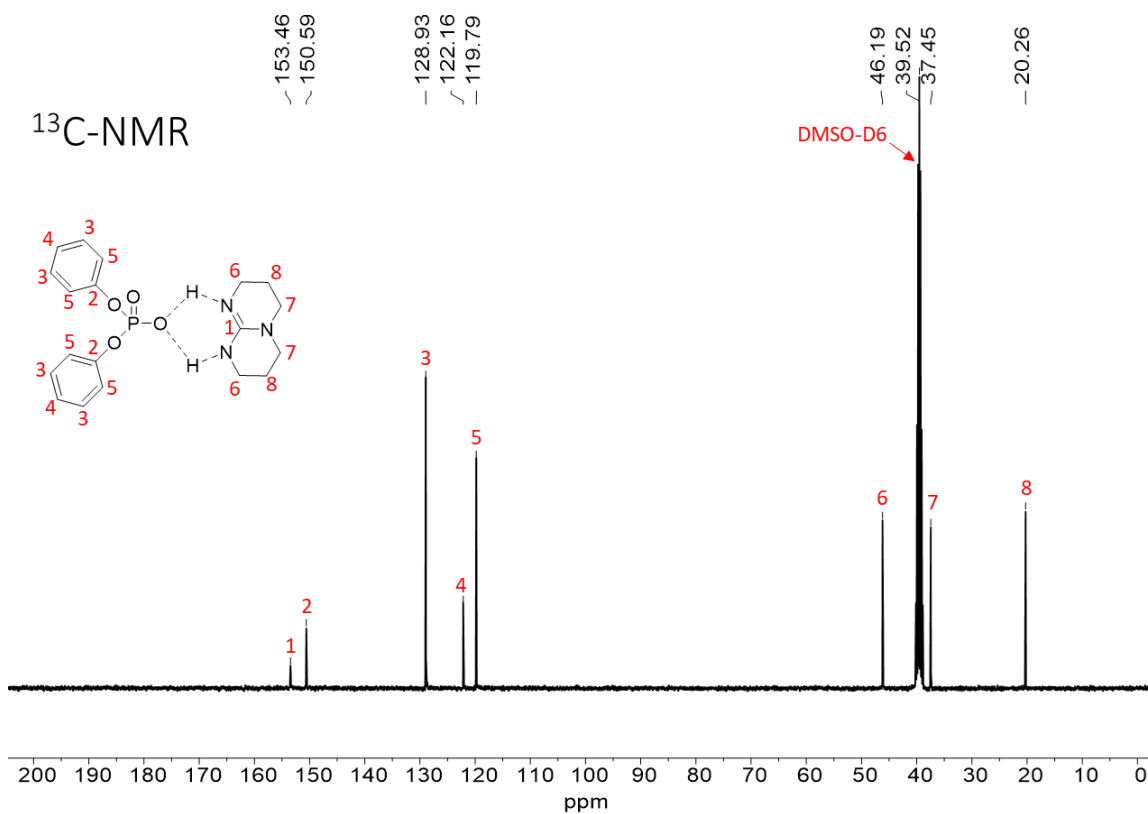
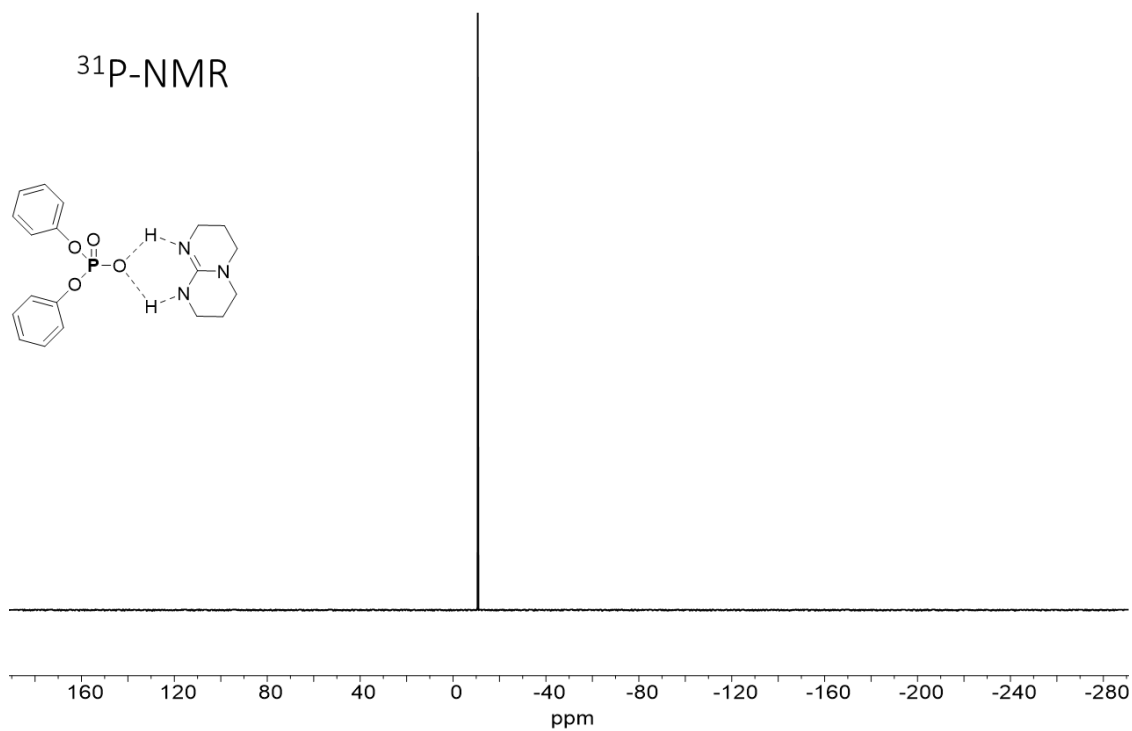


Figure S28. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:DPP salt.



**Figure S29.** <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:DPP salt.



**Figure S30.** <sup>31</sup>P NMR (161.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:DPP salt.

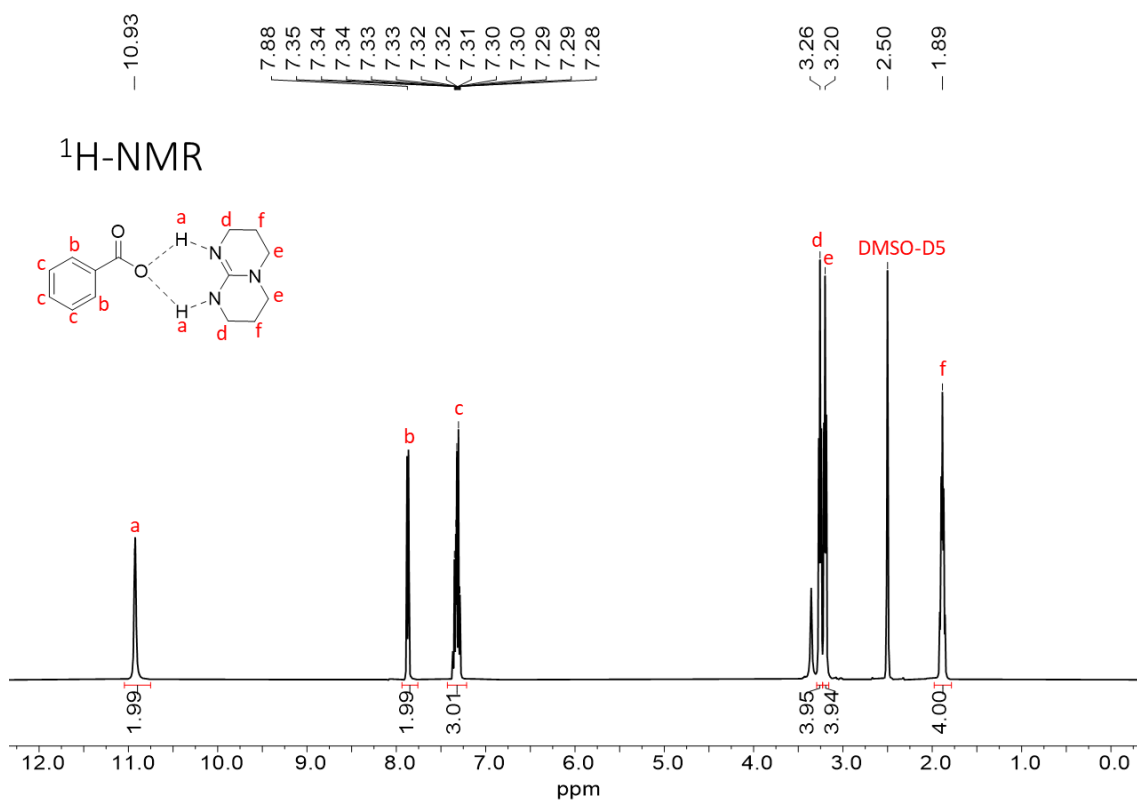


Figure S31. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:BA salt.

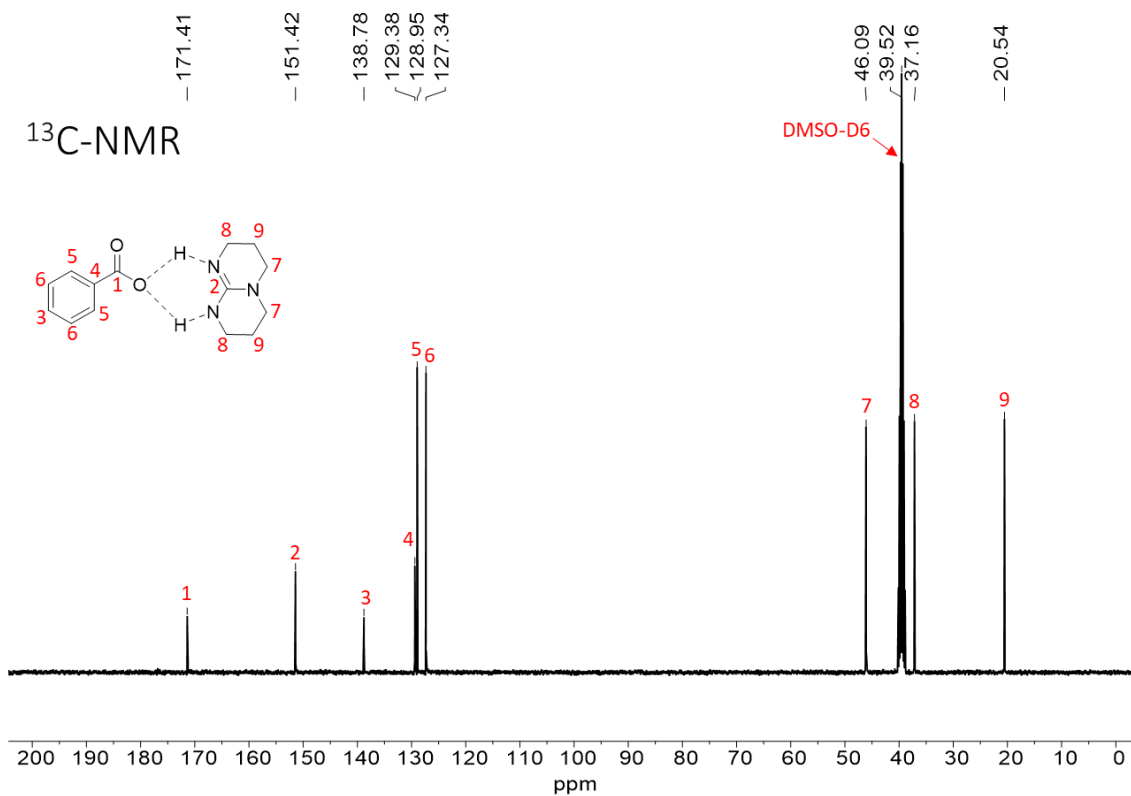


Figure S32. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TBD:BA salt.

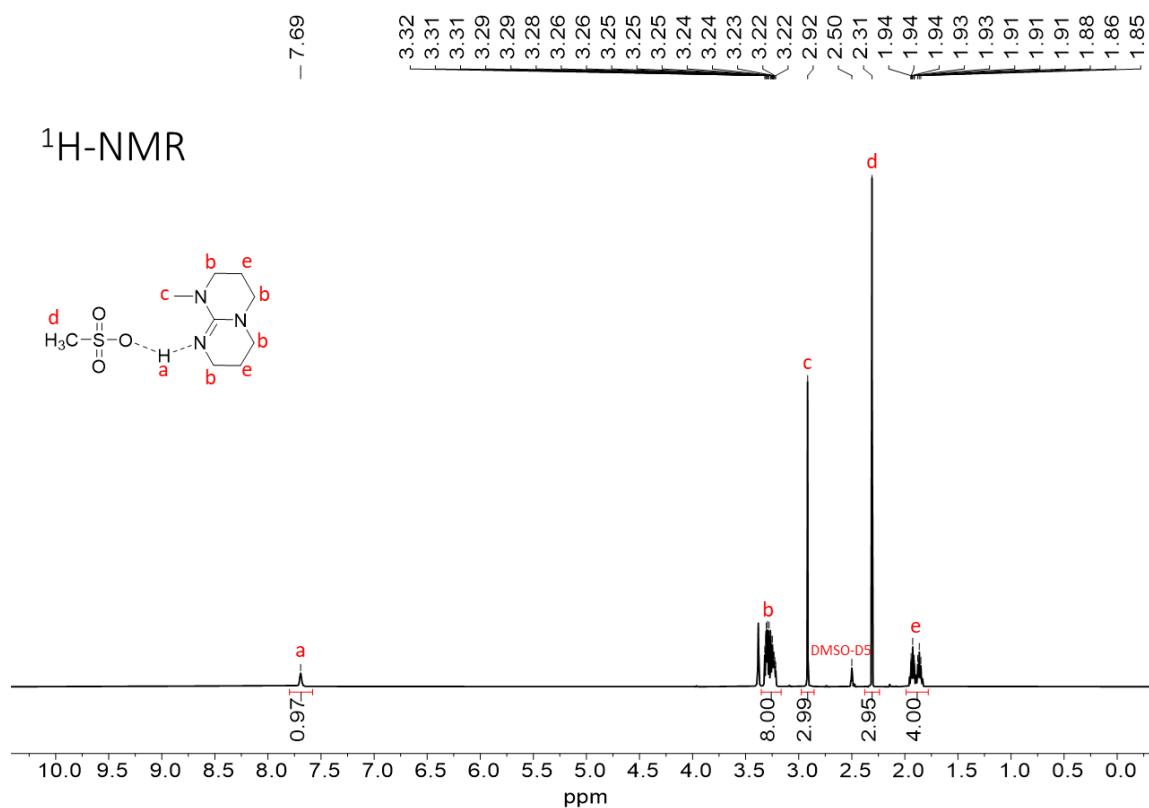


Figure S33. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for MTBD:MSA salt.

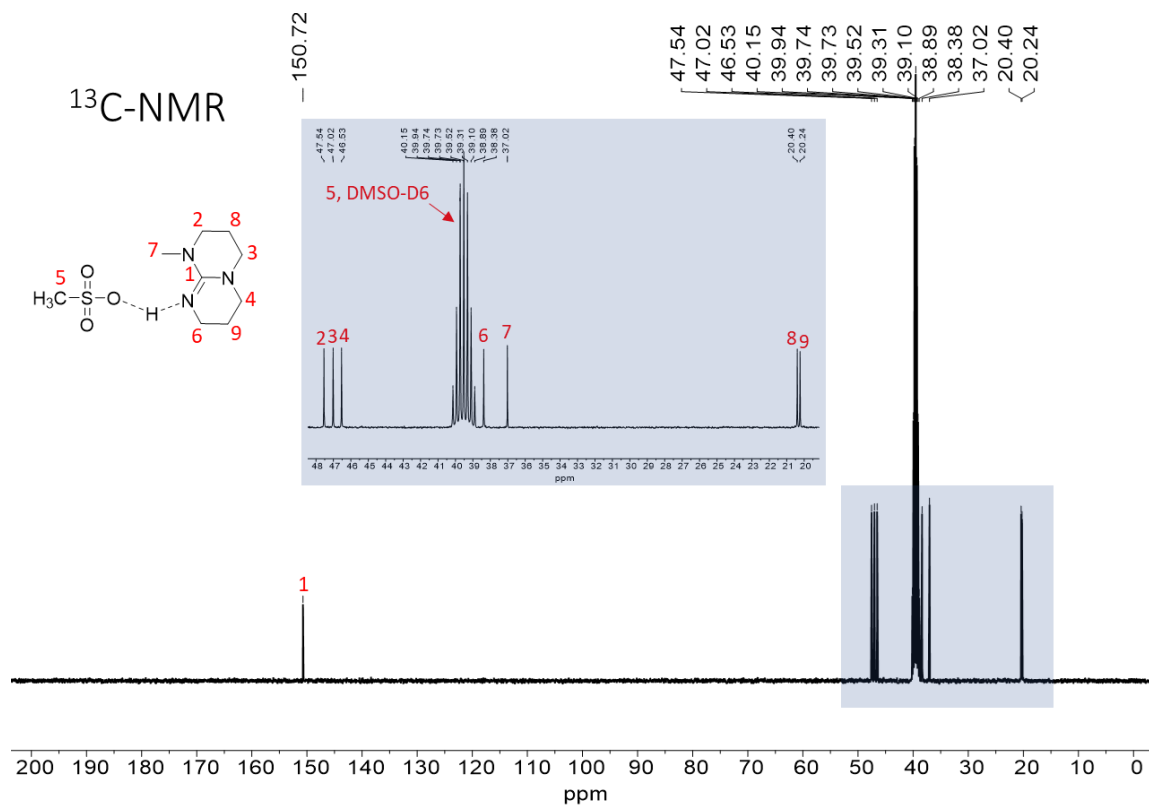


Figure S34. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for MTBD:MSA salt.

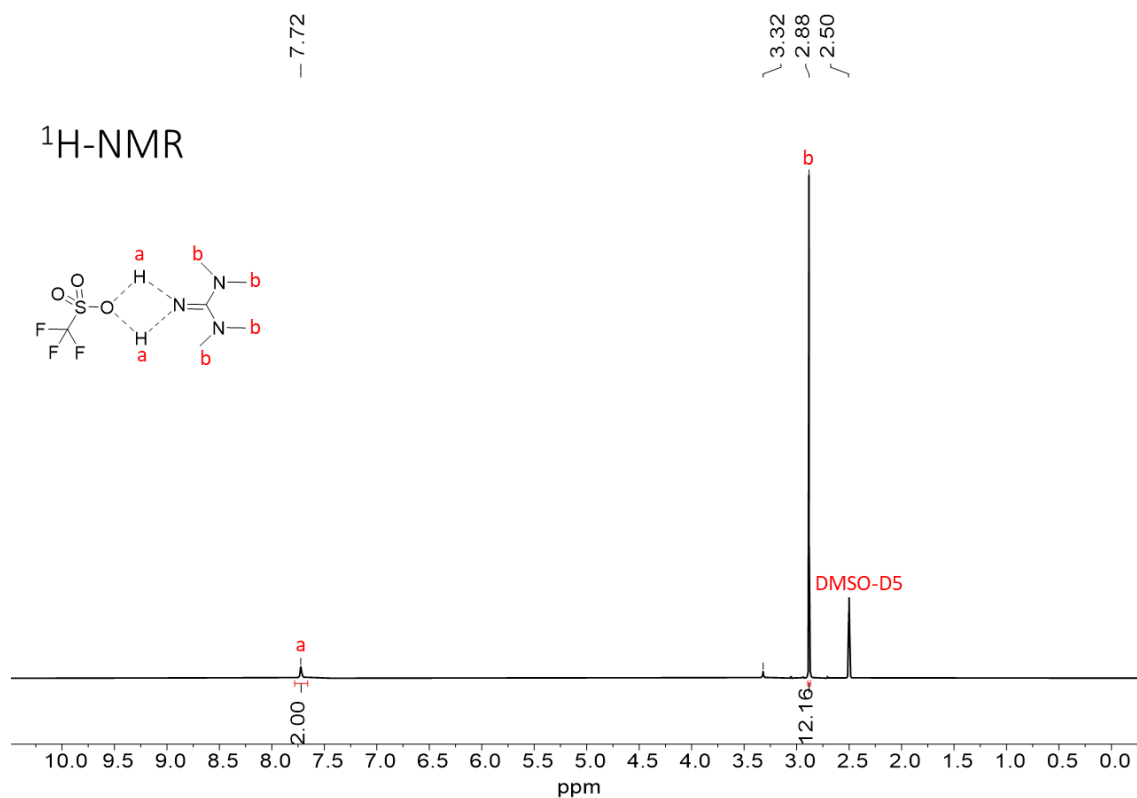


Figure S35. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TMG:TfOH salt.

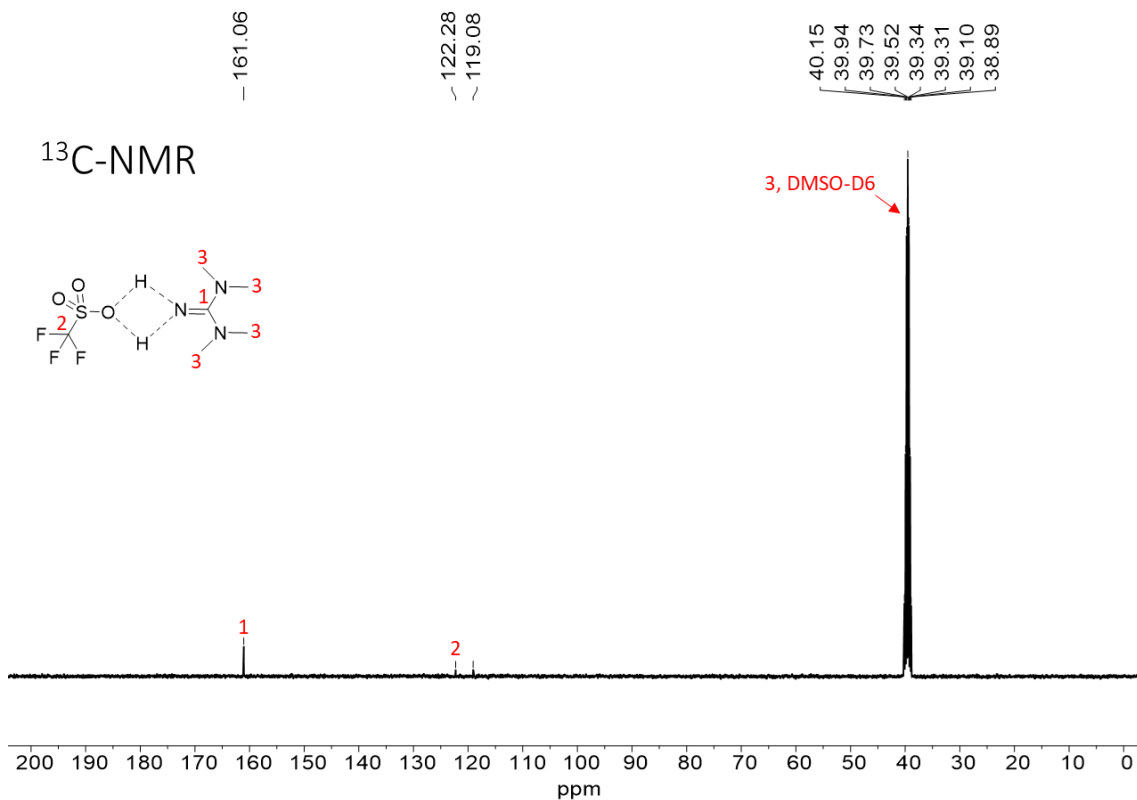


Figure S36. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TMG:TfOH salt.

# <sup>19</sup>F-NMR

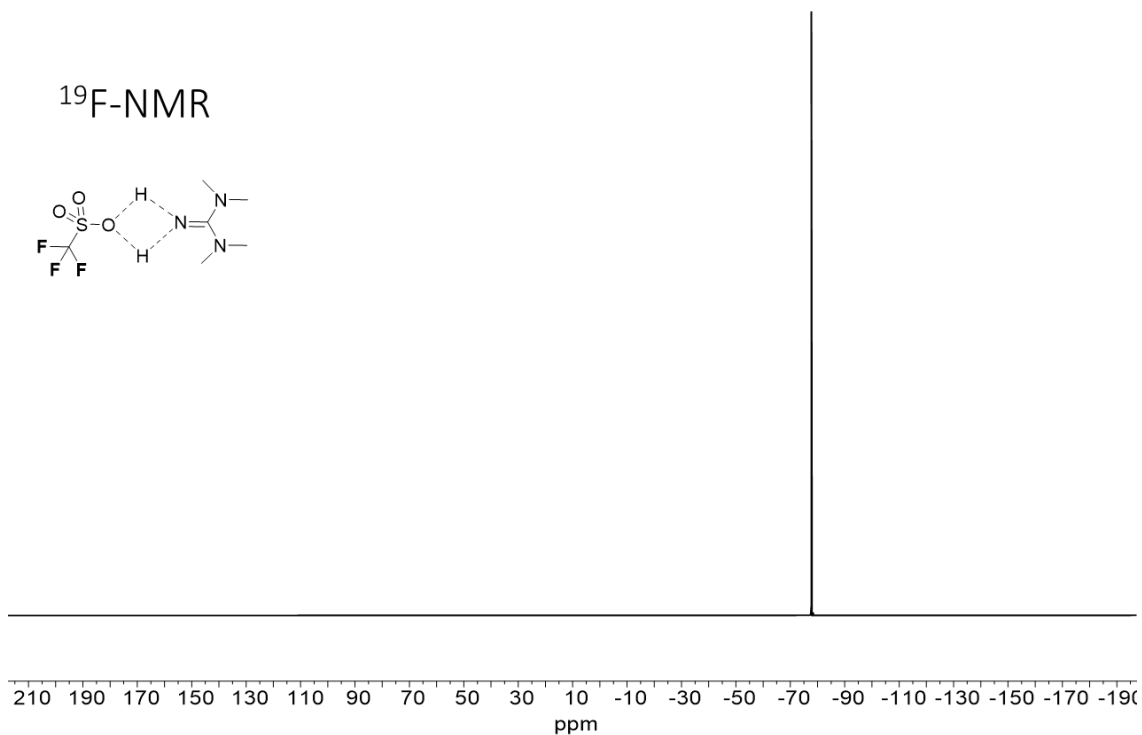
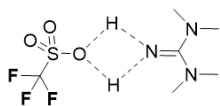


Figure S37. <sup>19</sup>F NMR (376.3 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for TMG:TfOH salt.

# <sup>1</sup>H-NMR

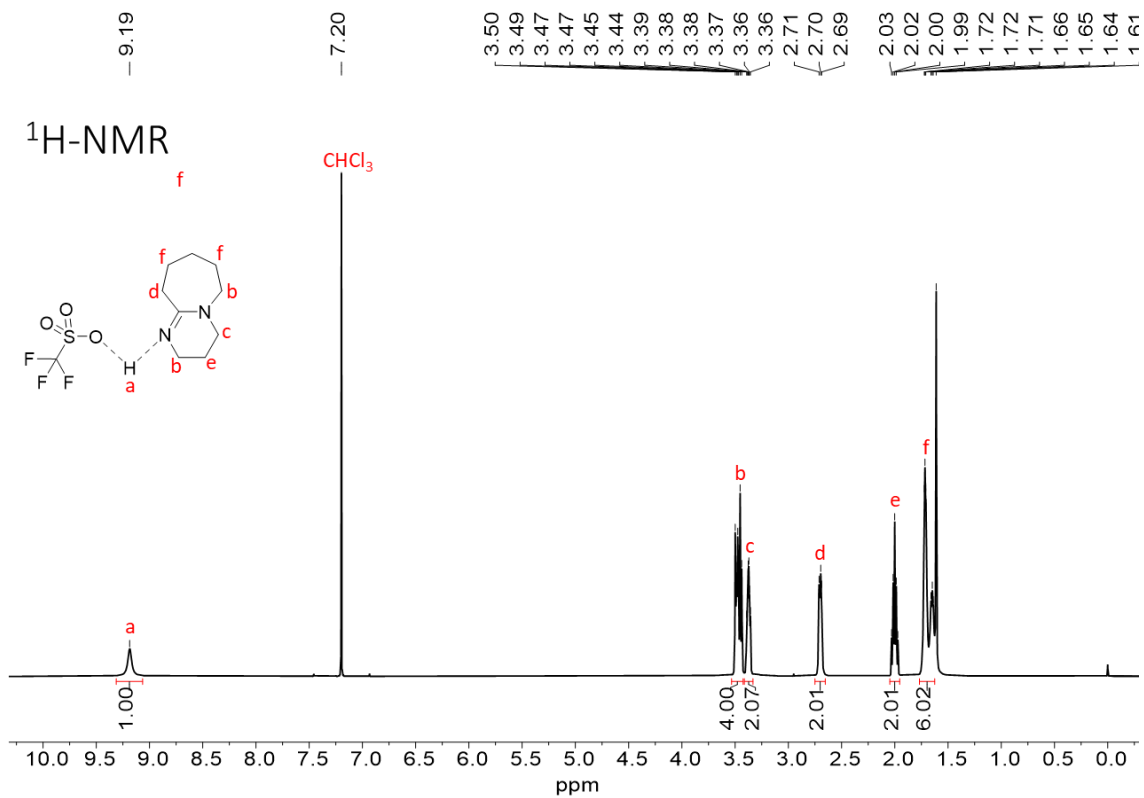
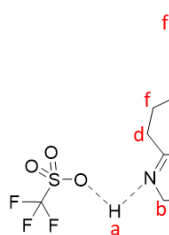


Figure S38. <sup>1</sup>H NMR (400 MHz; 298 K; CDCl<sub>3</sub>) spectrum for DBU:TfOH salt.

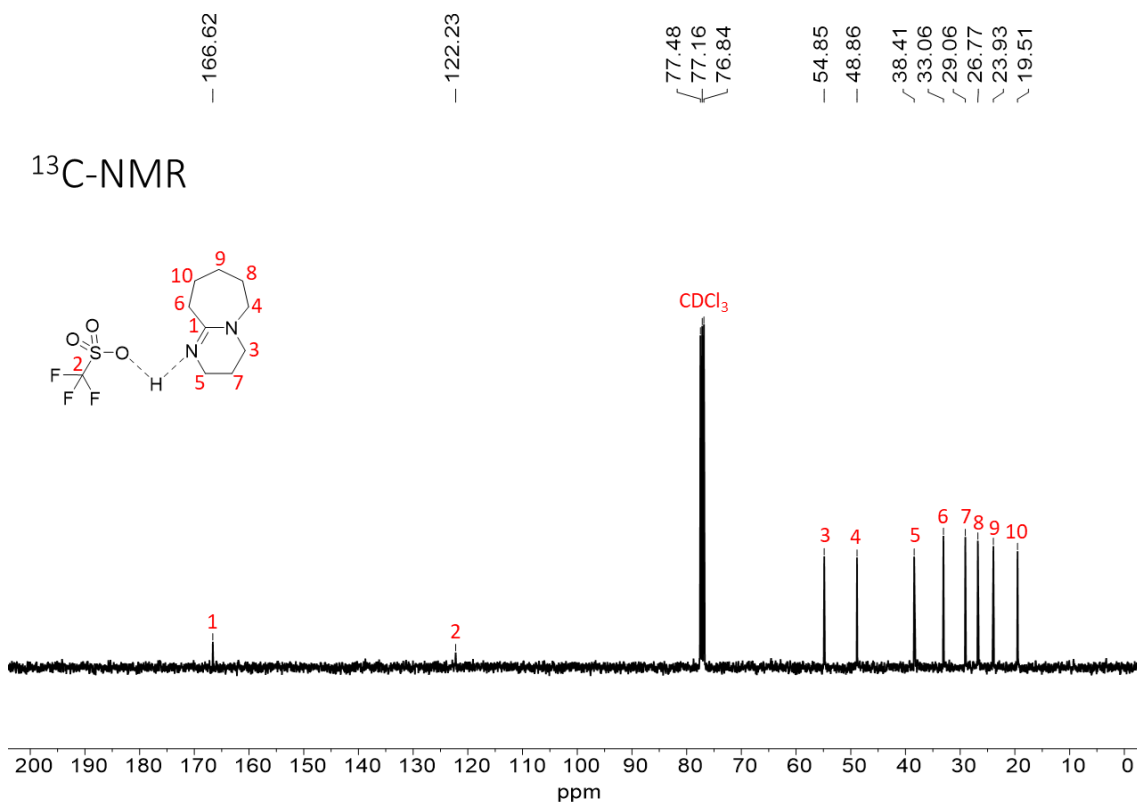


Figure S39. <sup>13</sup>C NMR (100.6 MHz; 298 K; CDCl<sub>3</sub>) spectrum for DBU:TfOH salt.

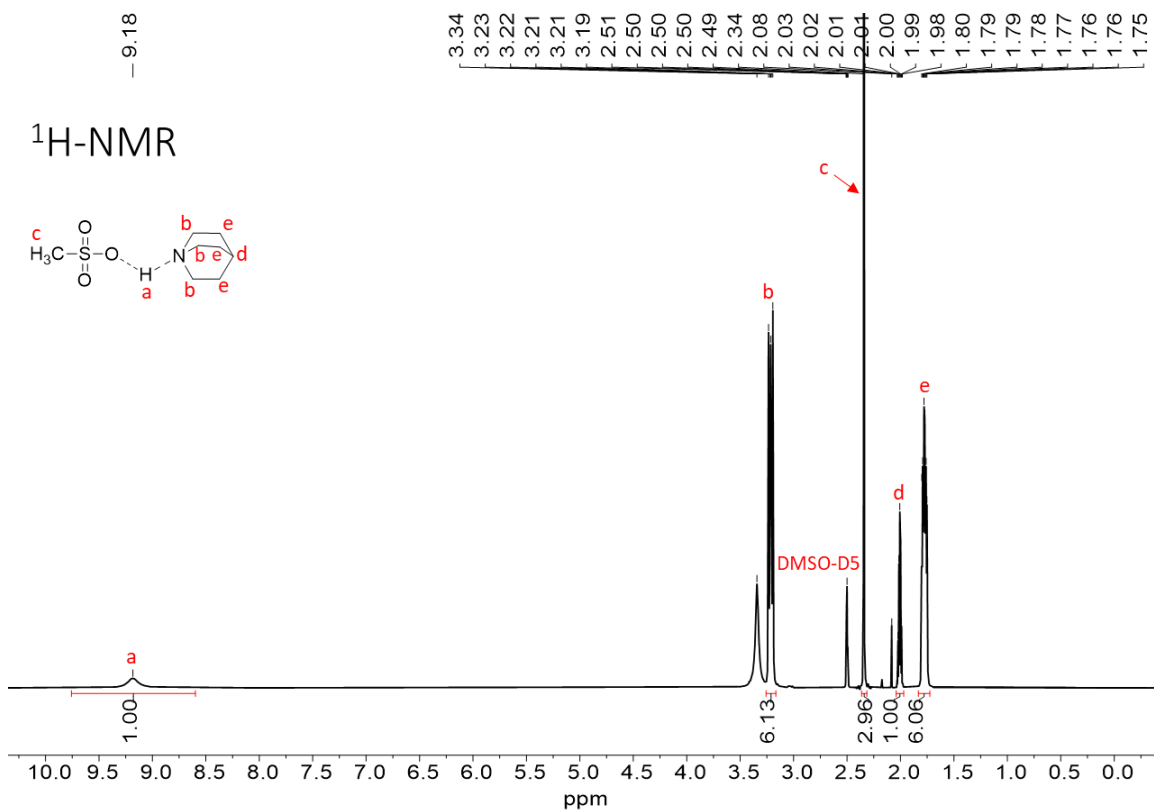
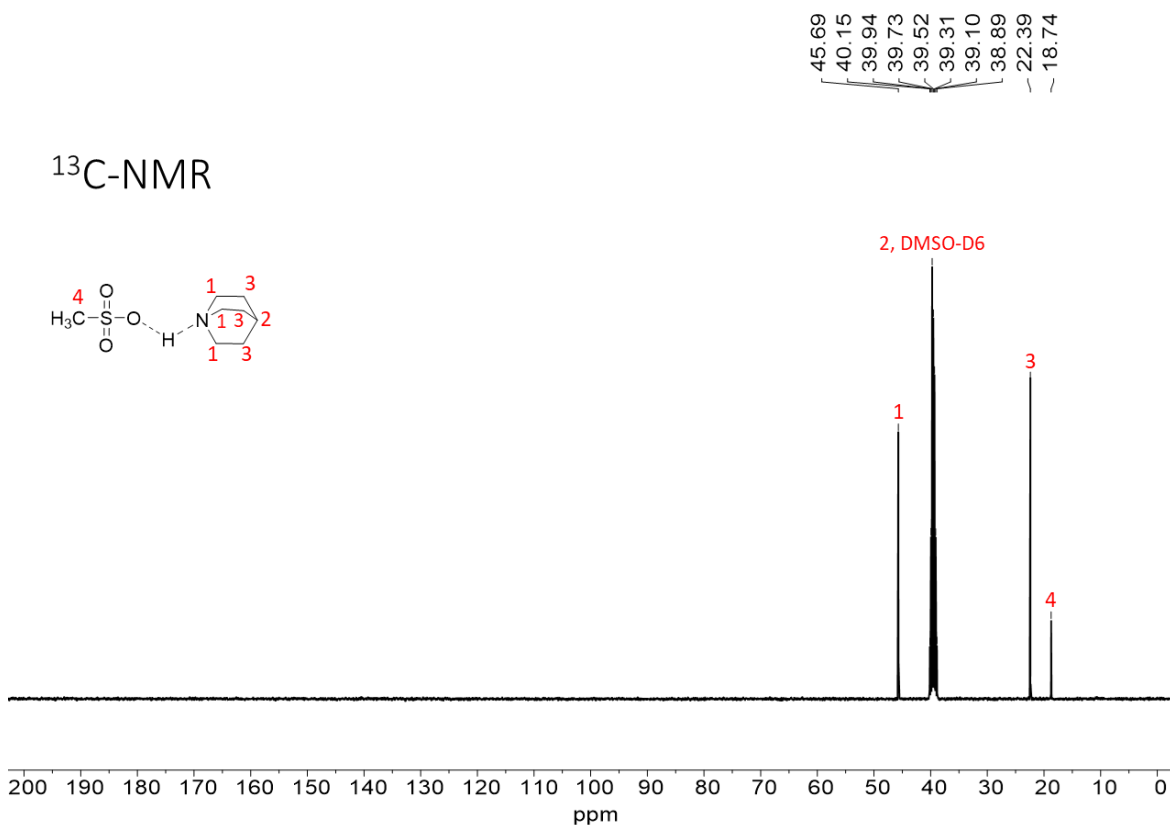
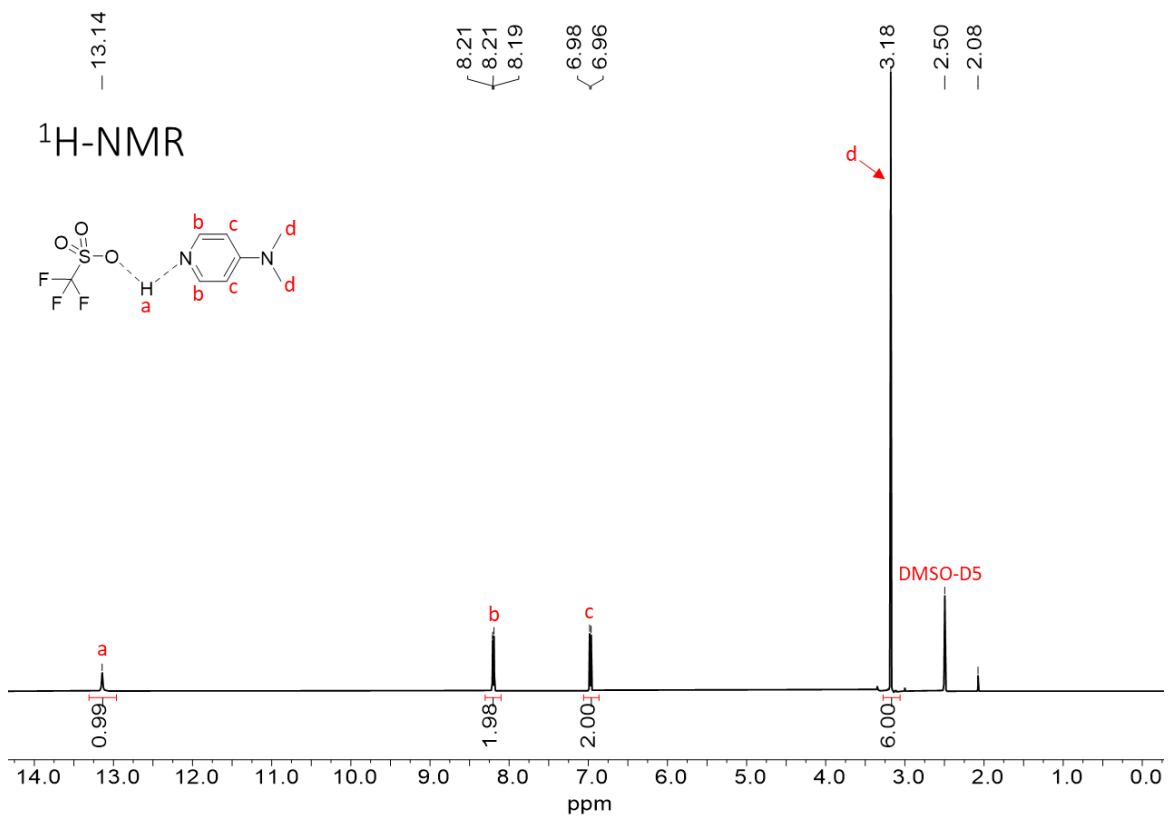


Figure S40. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for ABCO:MSA salt.

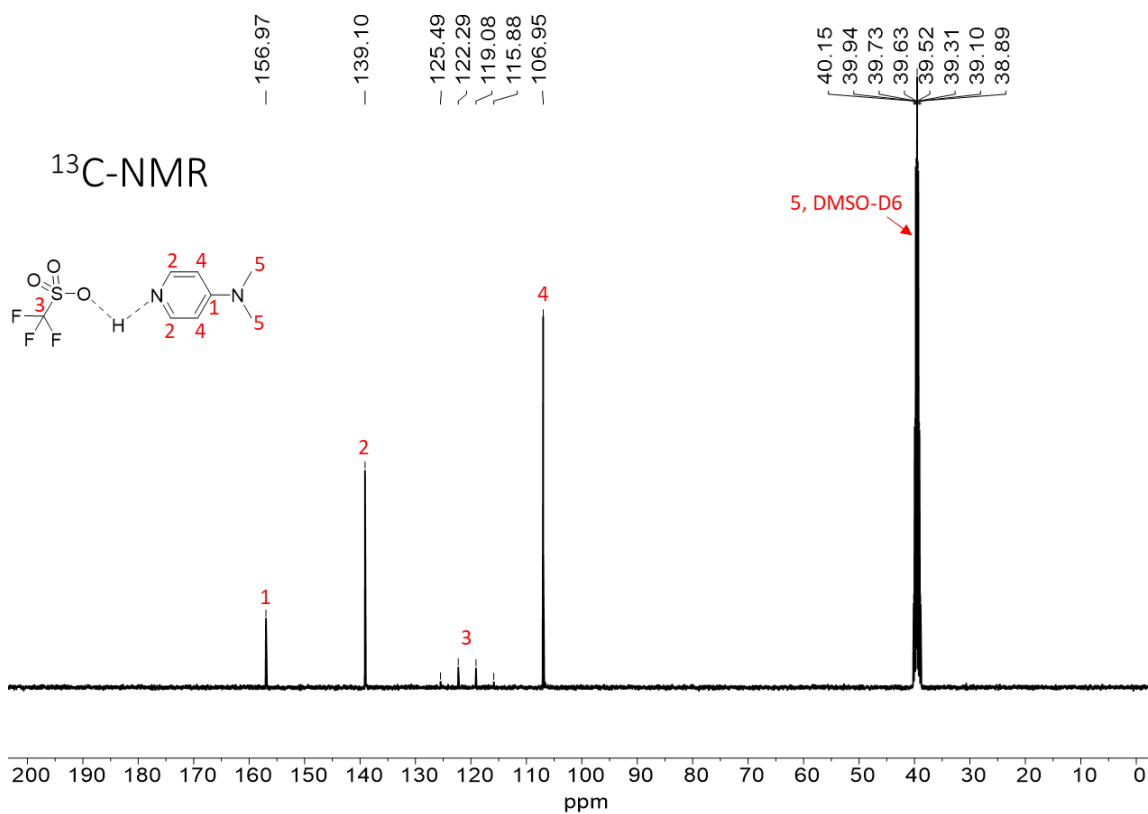




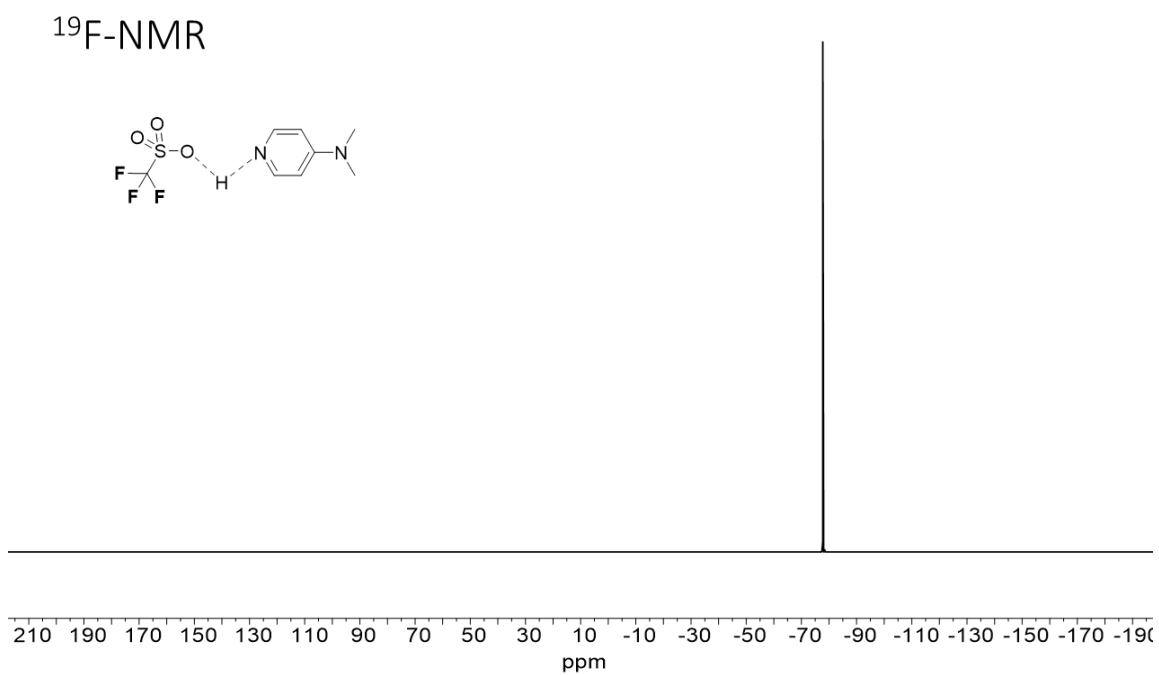
**Figure S41.** <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for ABCO:MSA salt.



**Figure S42.** <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DMAP:TfOH salt.



**Figure S43.** <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DMAP:TfOH salt.



**Figure S44.** <sup>19</sup>F NMR (376.3 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DMAP:TfOH salt.

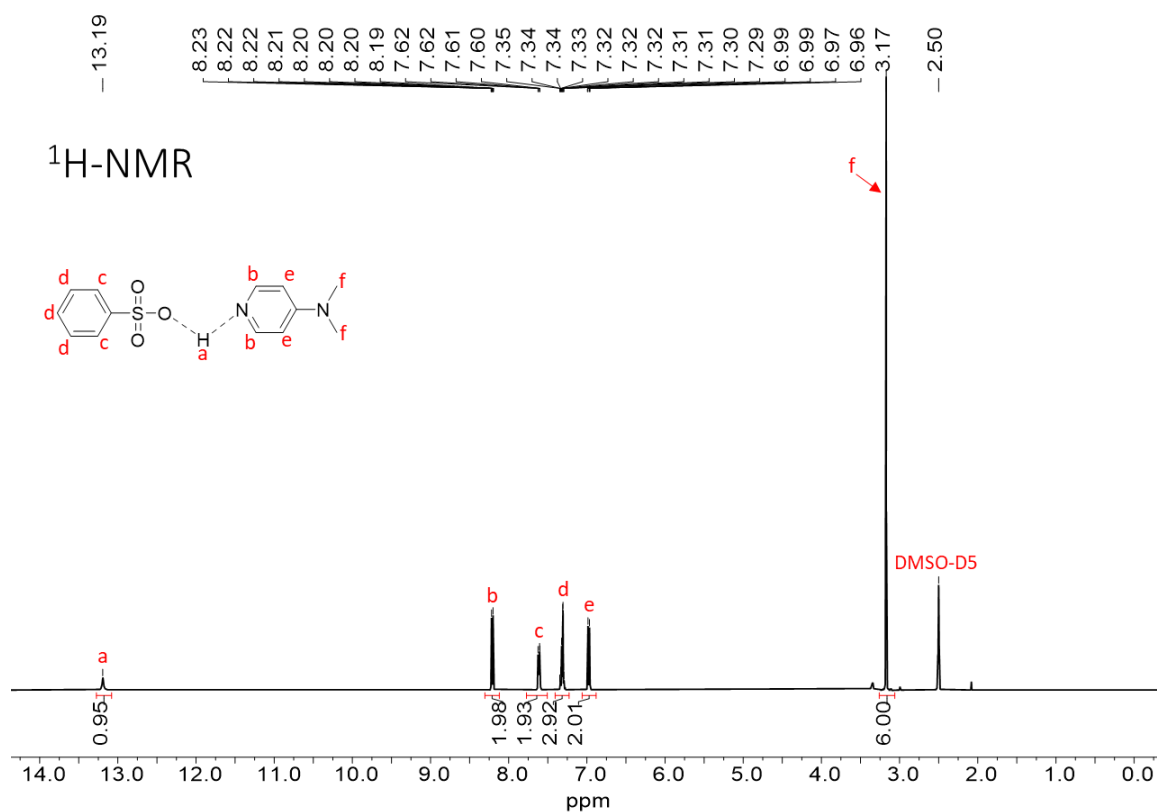


Figure S45. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DMAP:BSA salt.

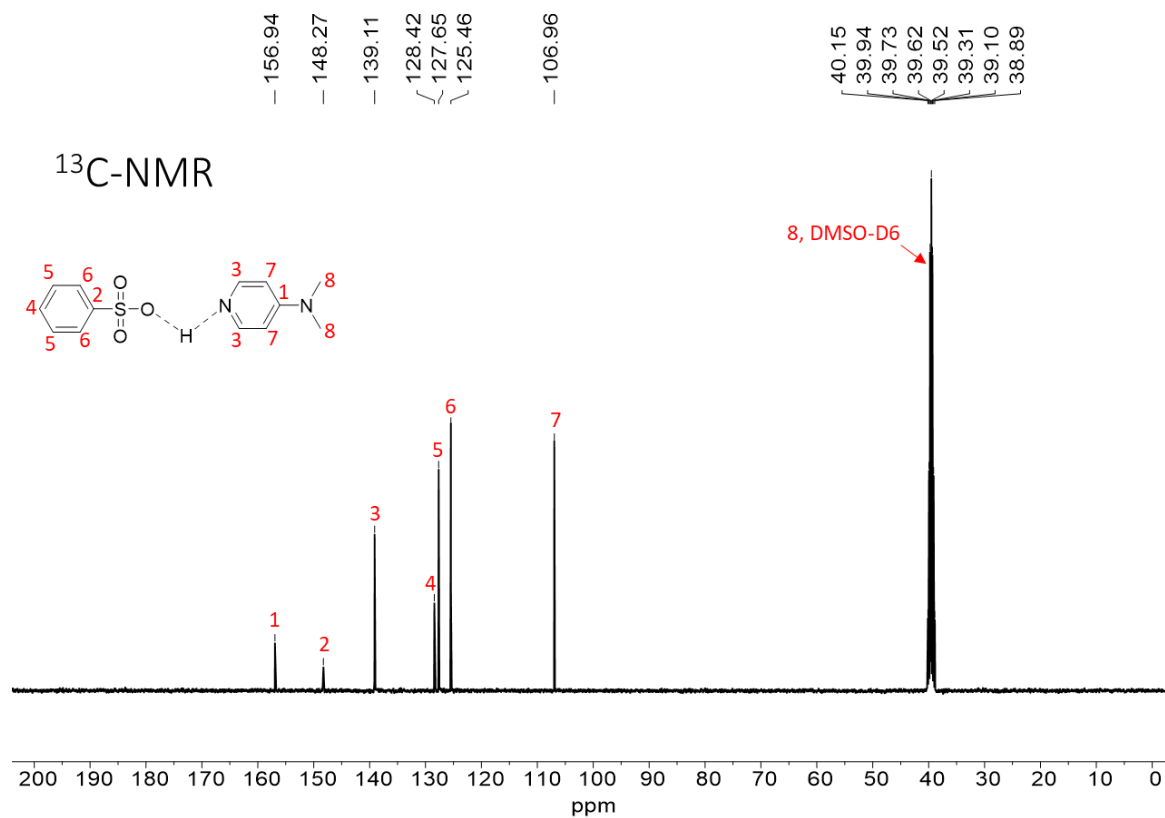


Figure S46. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DMAP:BSA salt.

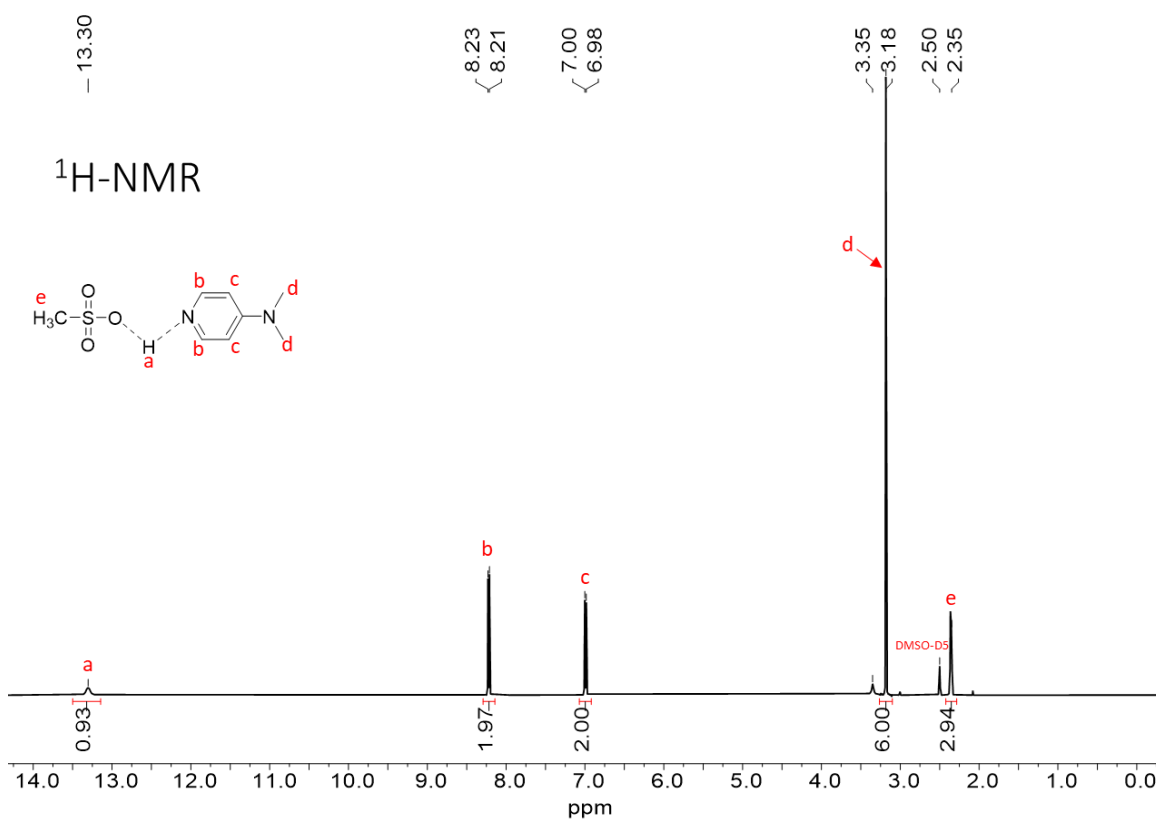


Figure S47. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DMAP:MSA salt.

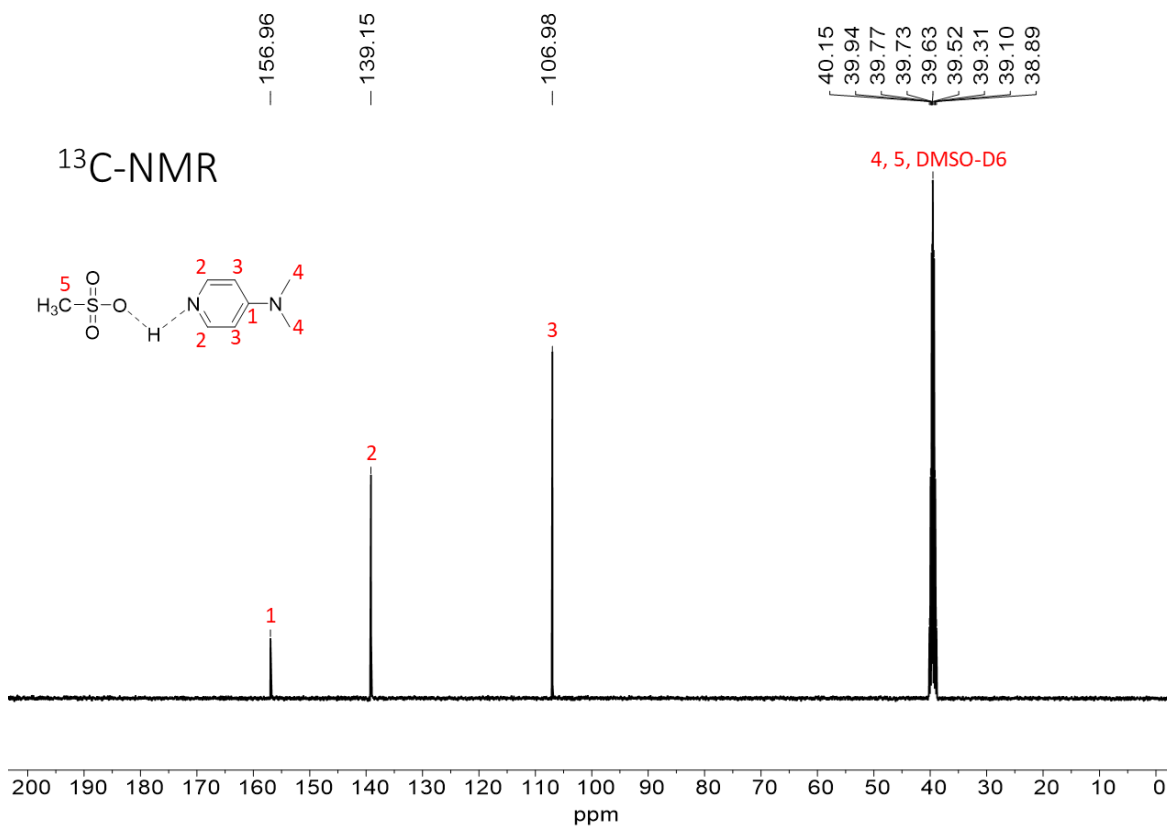


Figure S48. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DMAP:MSA salt.

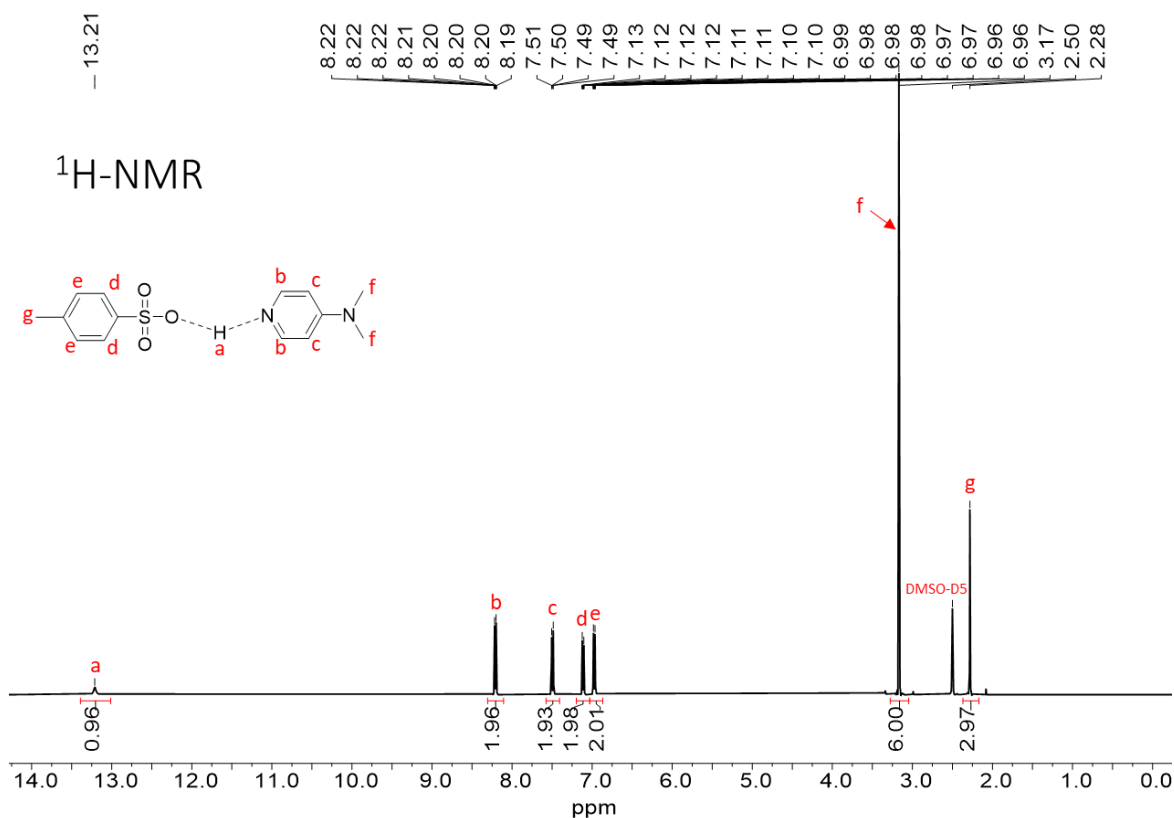


Figure S49. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DMAP:p-TSA salt.

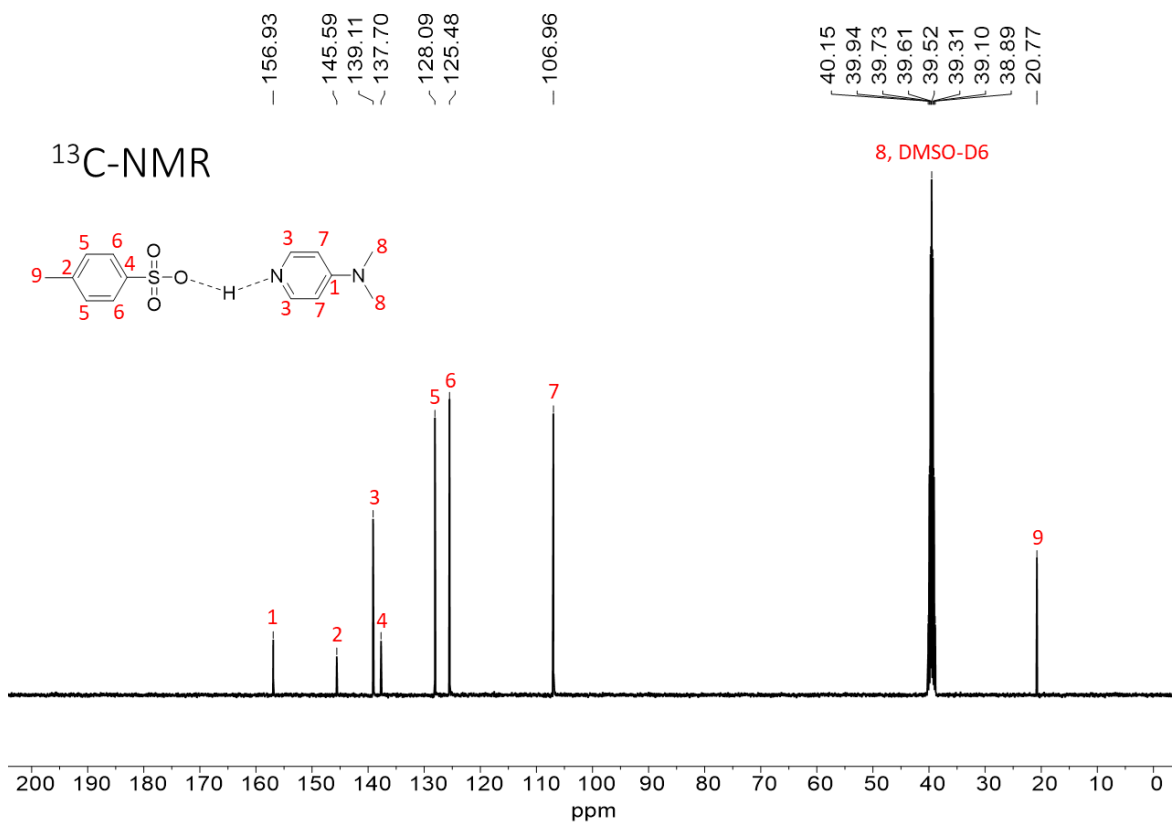


Figure S50. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DMAP:p-TSA salt.

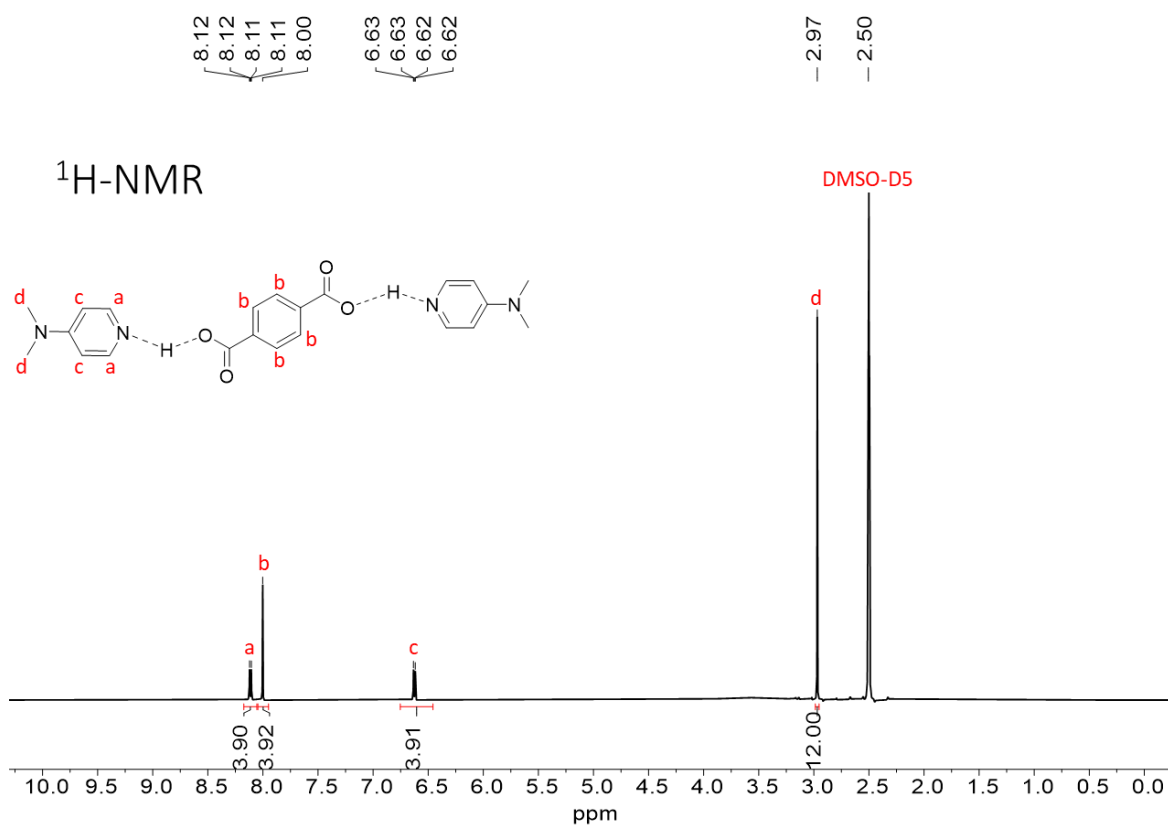


Figure S51. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DMAP:TPA salt.

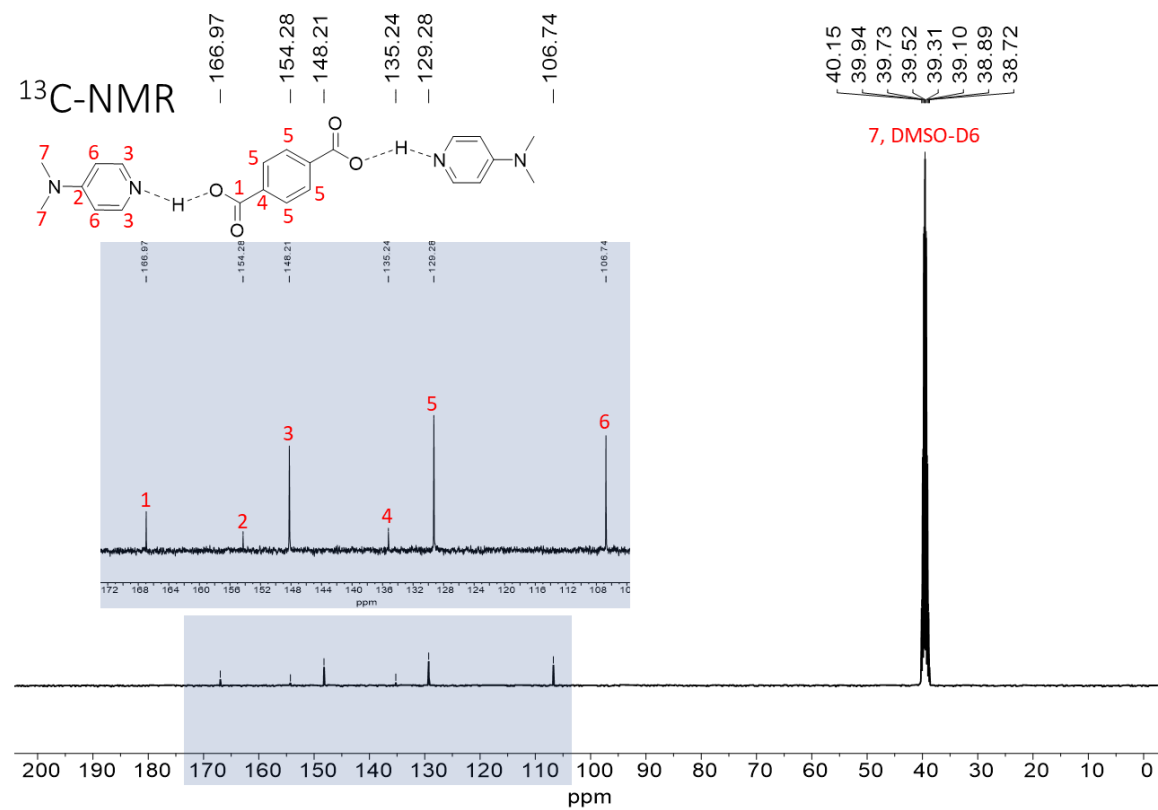


Figure S52. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DMAP:TPA salt.

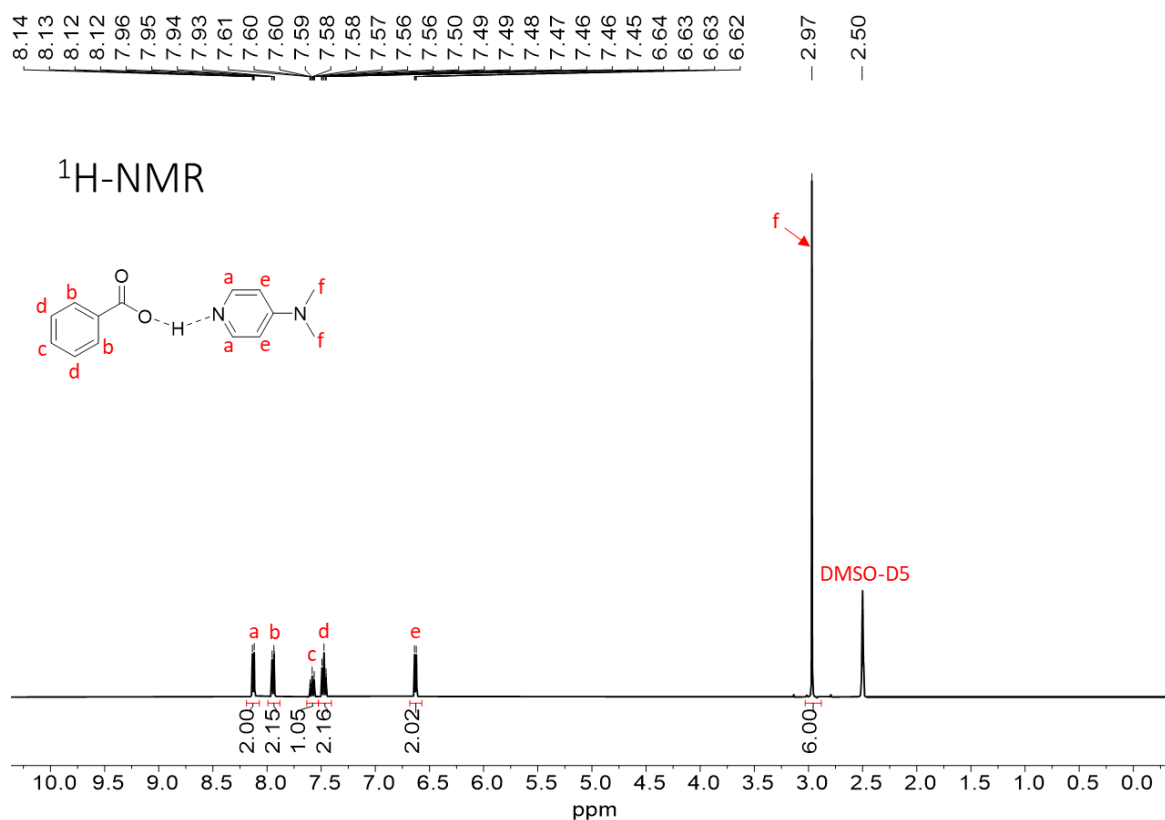


Figure S53. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DMAP:BA salt.

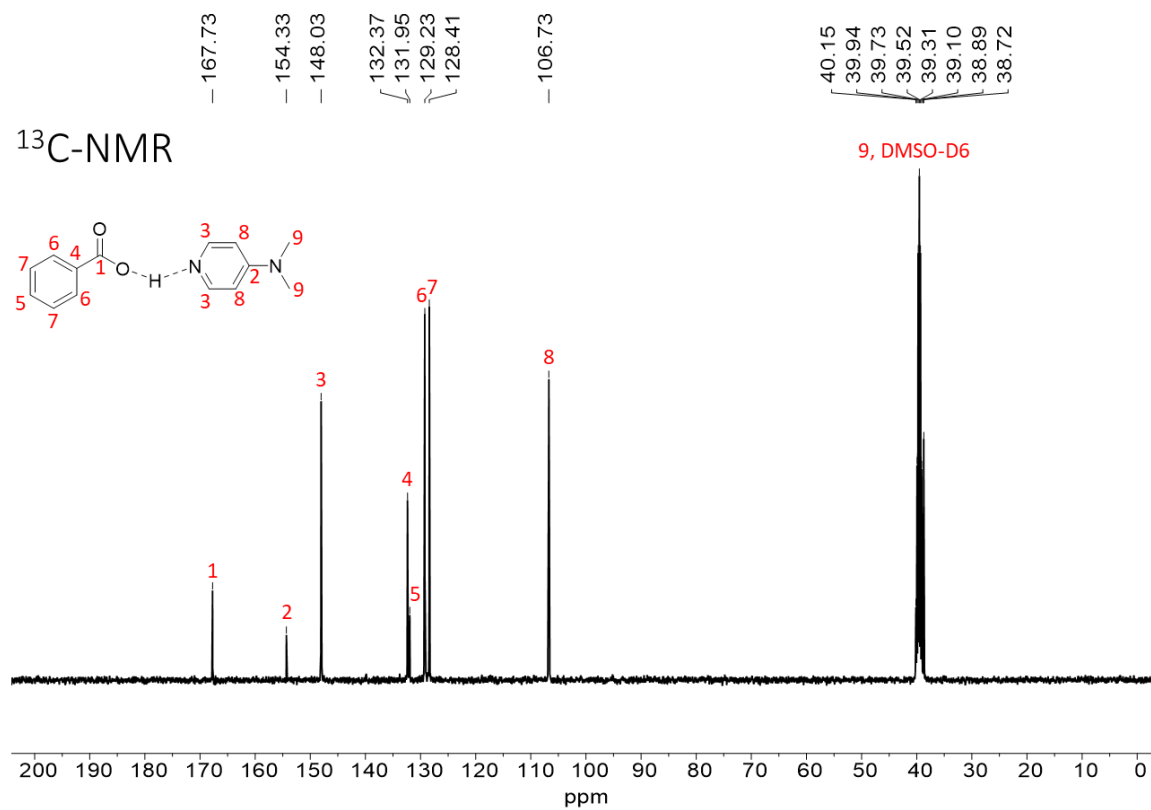


Figure S54. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DMAP:BA salt.

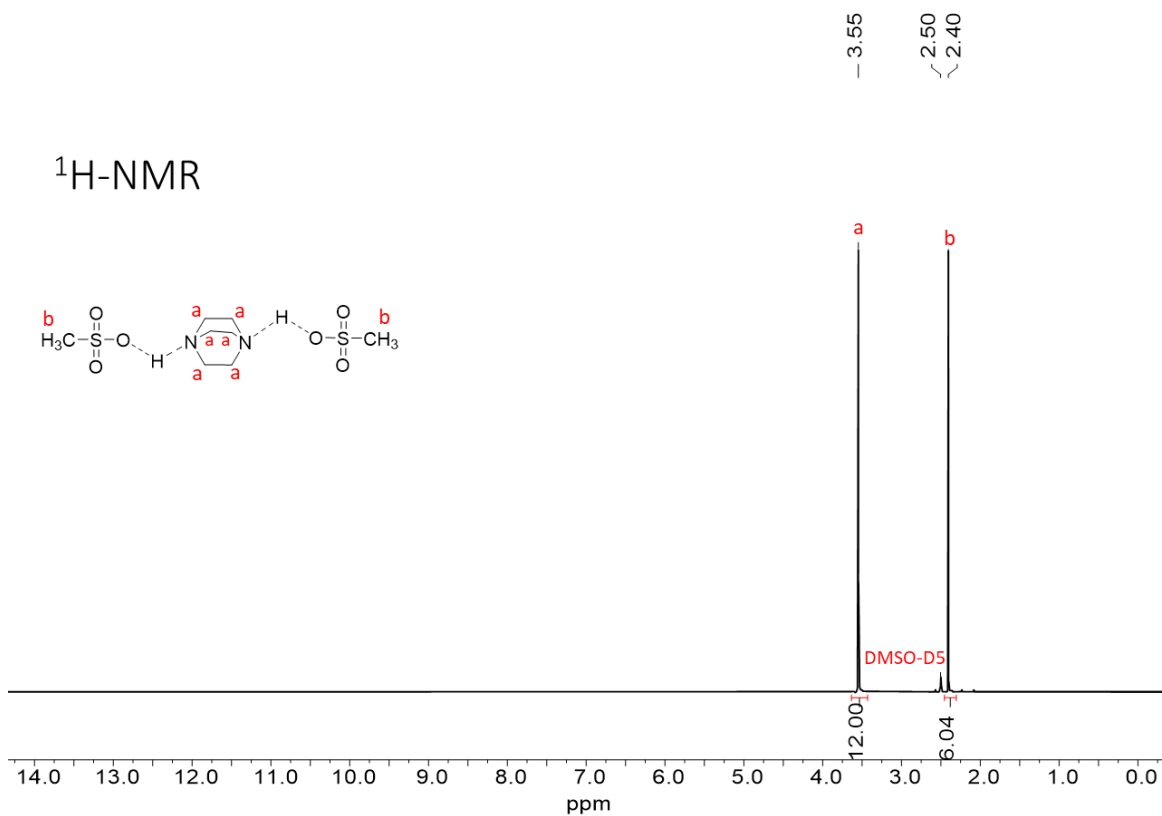


Figure S55. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DABCO:MSA (1:2) salt.

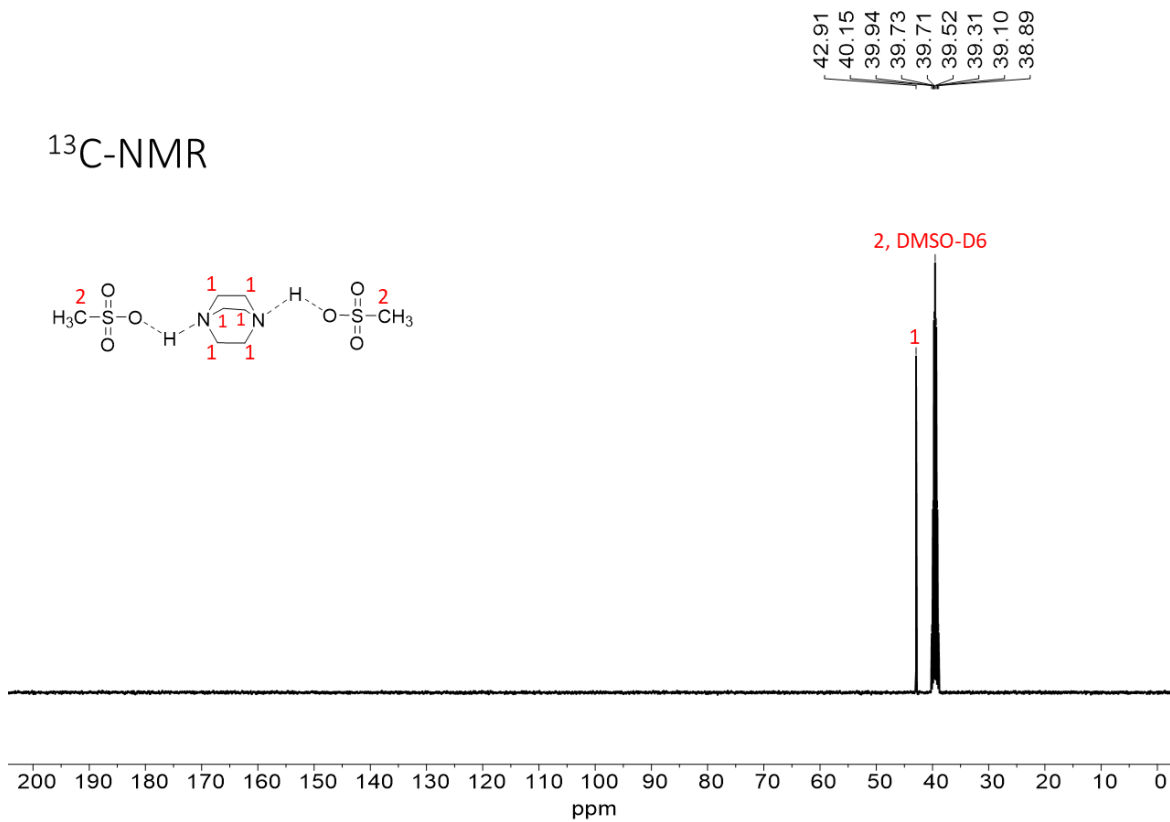


Figure S56. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DABCO:MSA (1:2) salt.



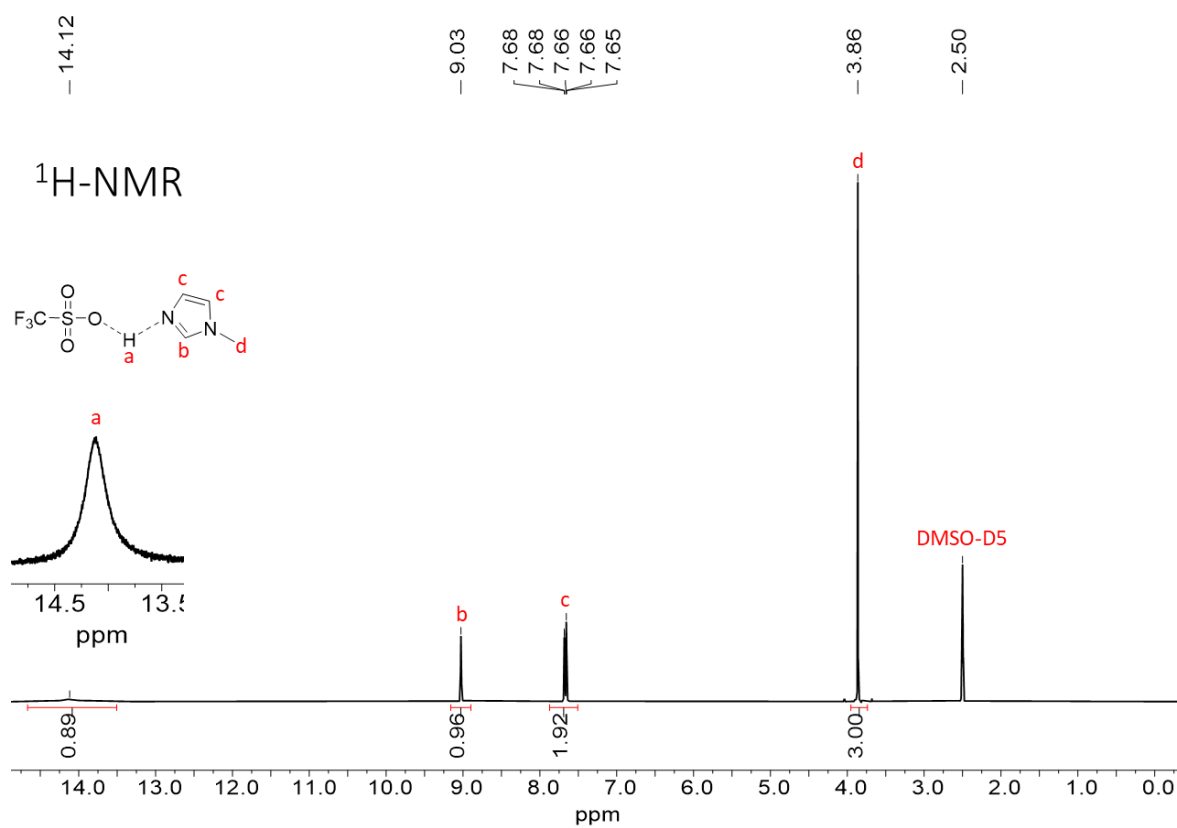


Figure S57. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for NMI:TfOH salt.

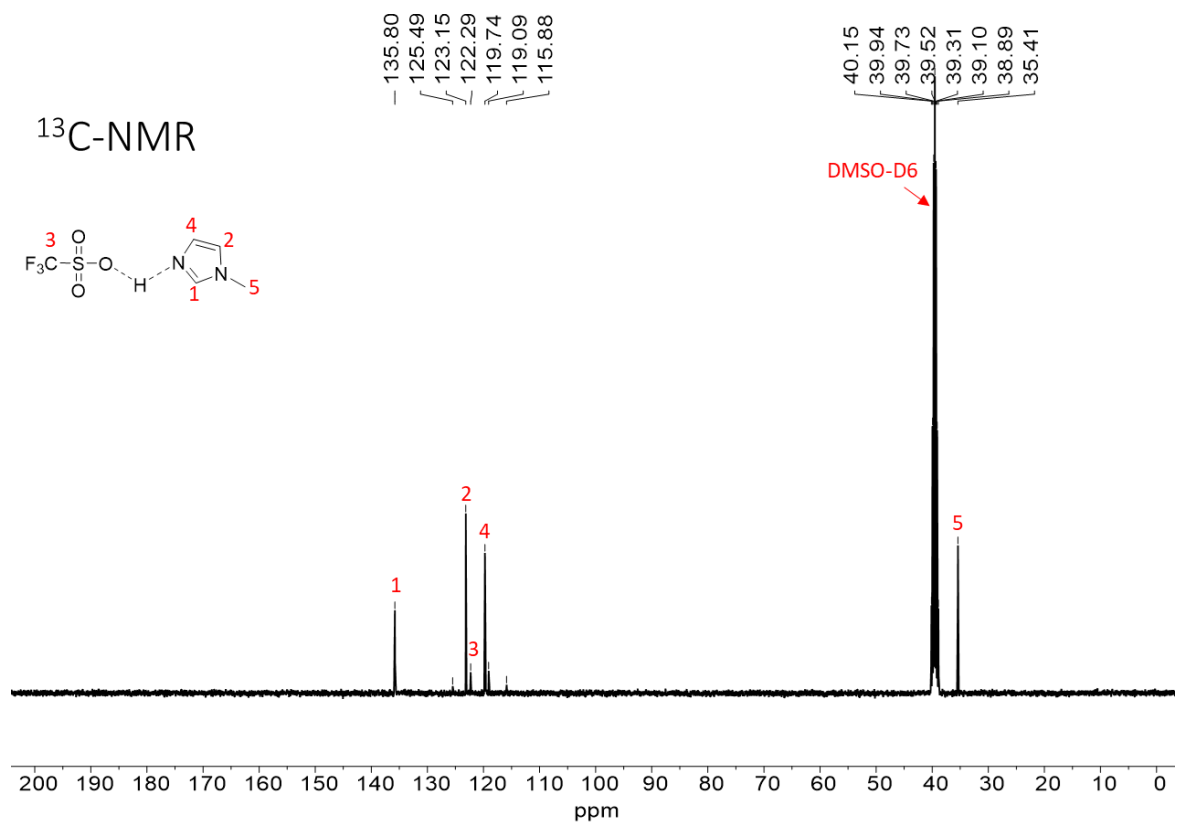


Figure S58. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for NMI:TfOH salt.

# <sup>19</sup>F-NMR

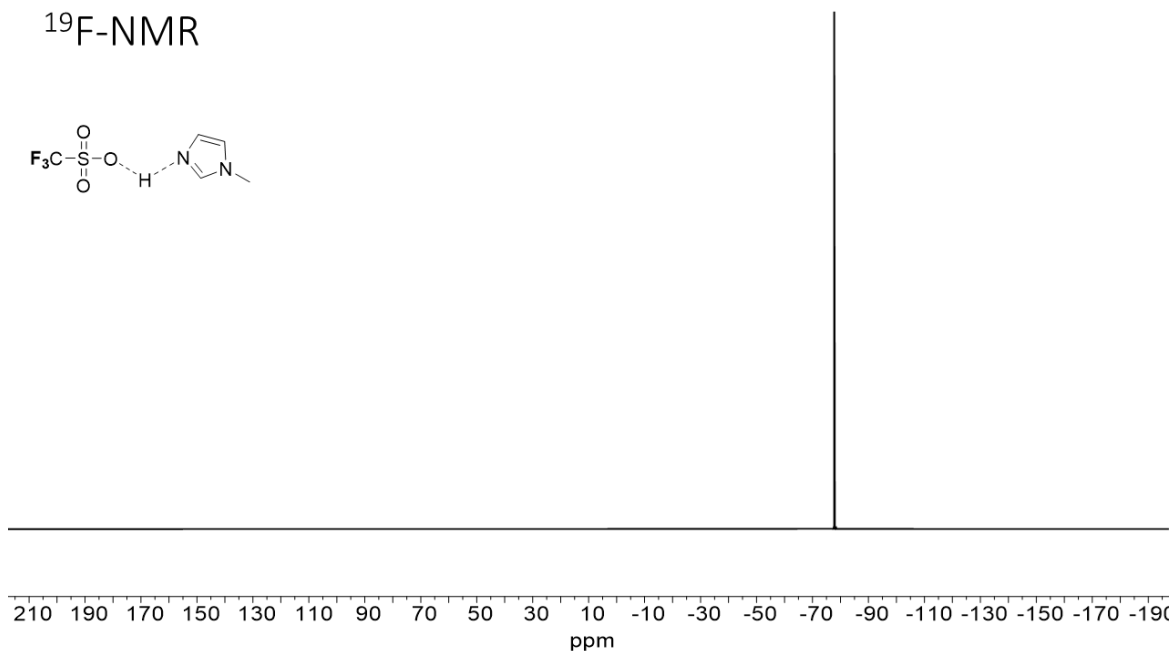
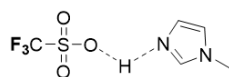


Figure S59. <sup>19</sup>F NMR (376.3 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for NMI:TfOH salt.

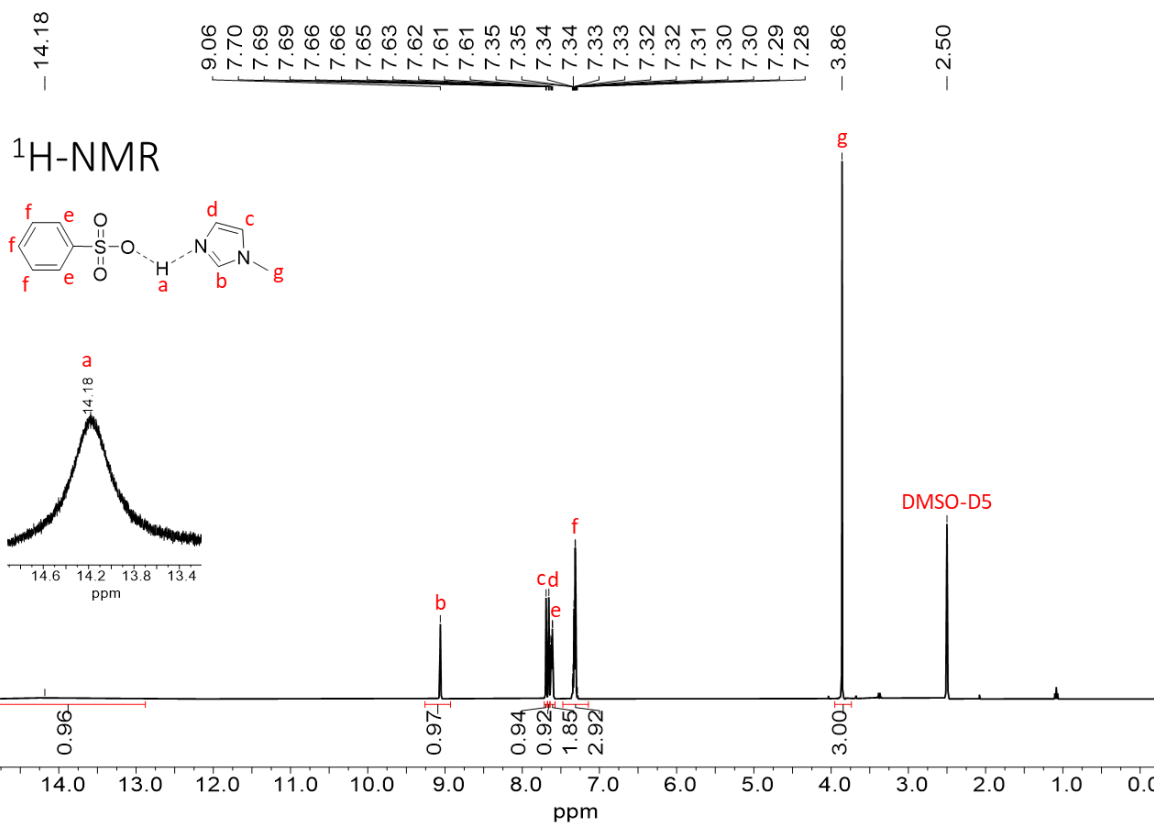


Figure S60. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for NMI:BSA salt.

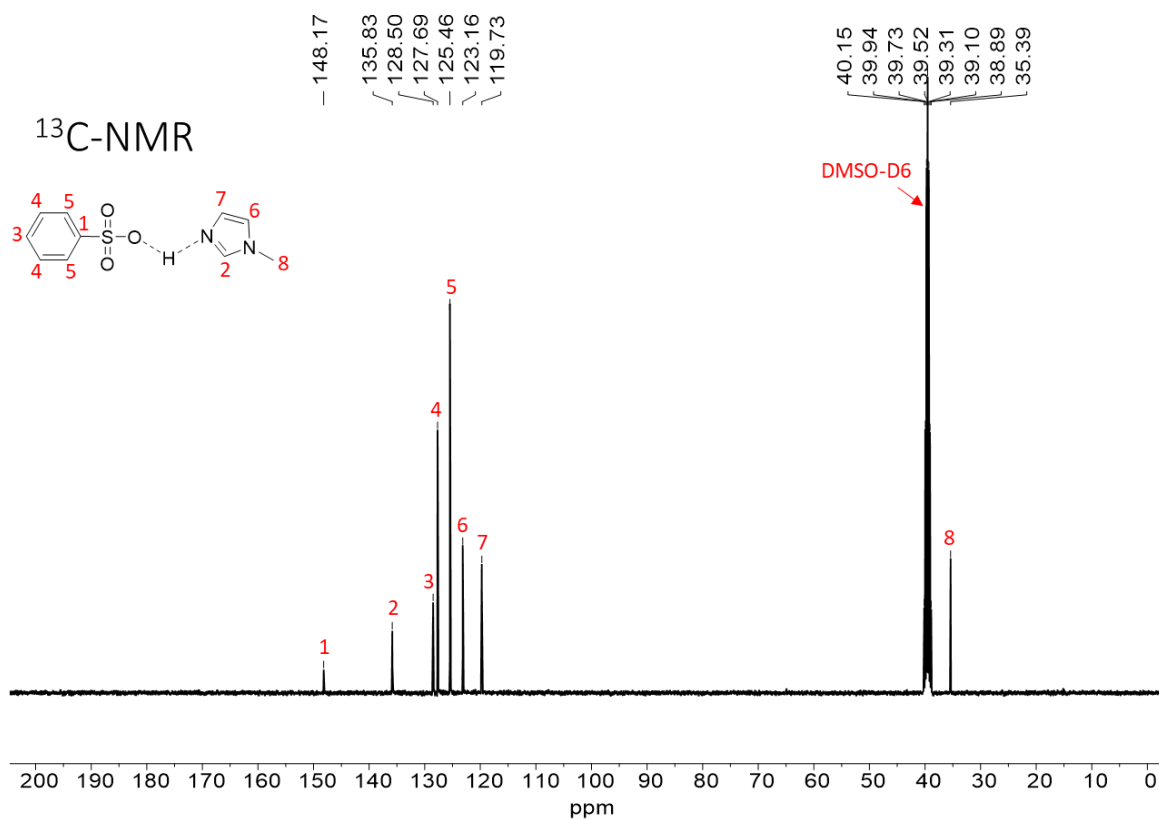


Figure S61. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for NMI:BSA salt.

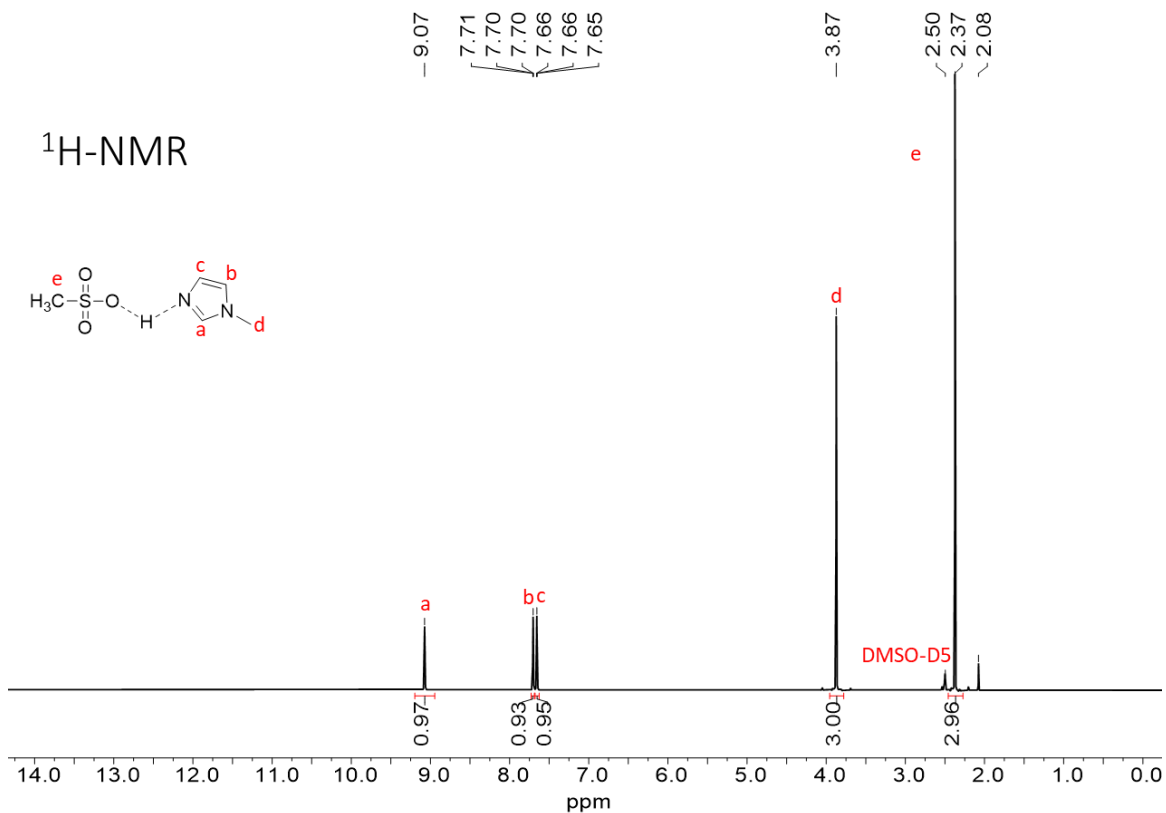
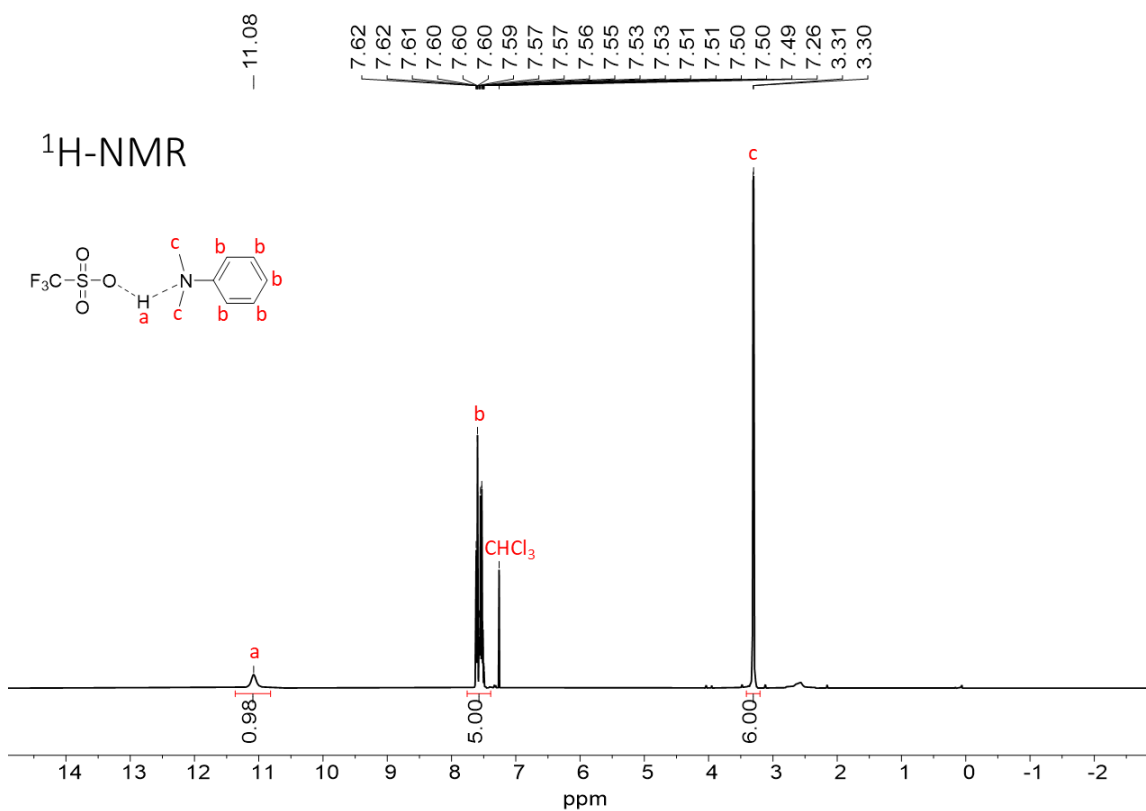
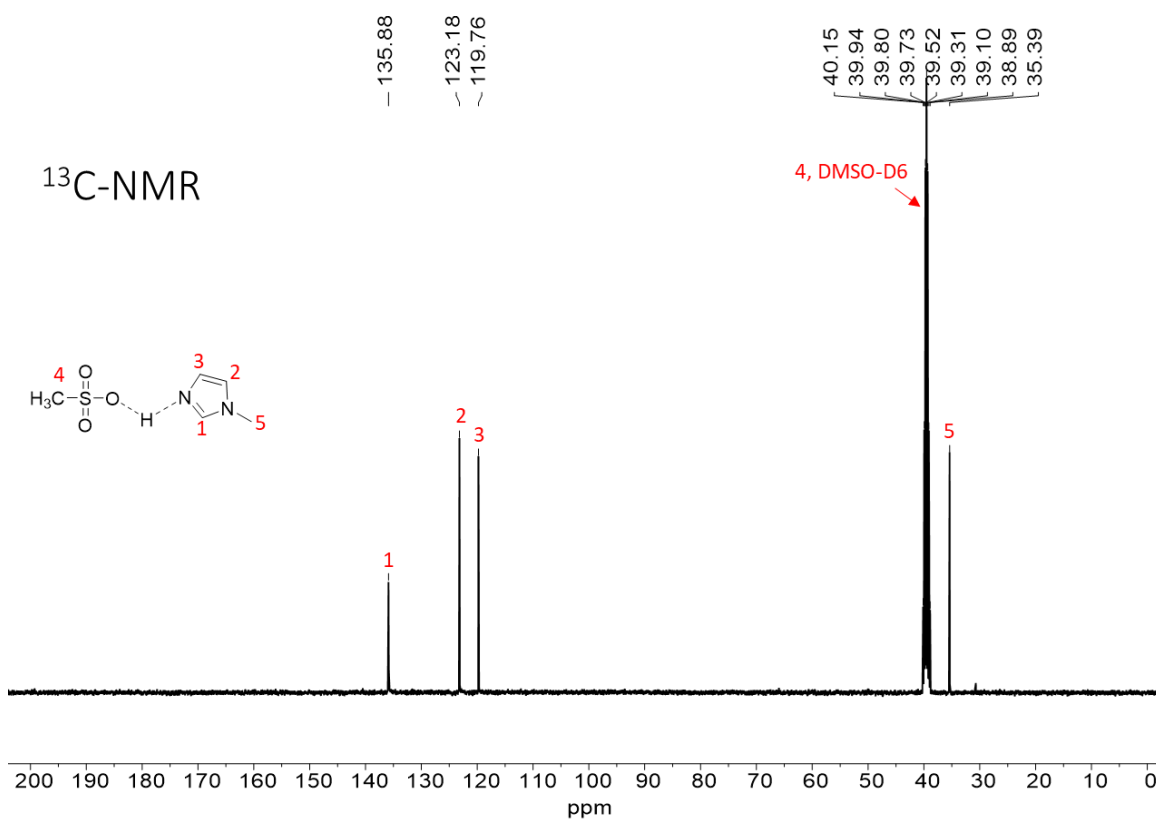
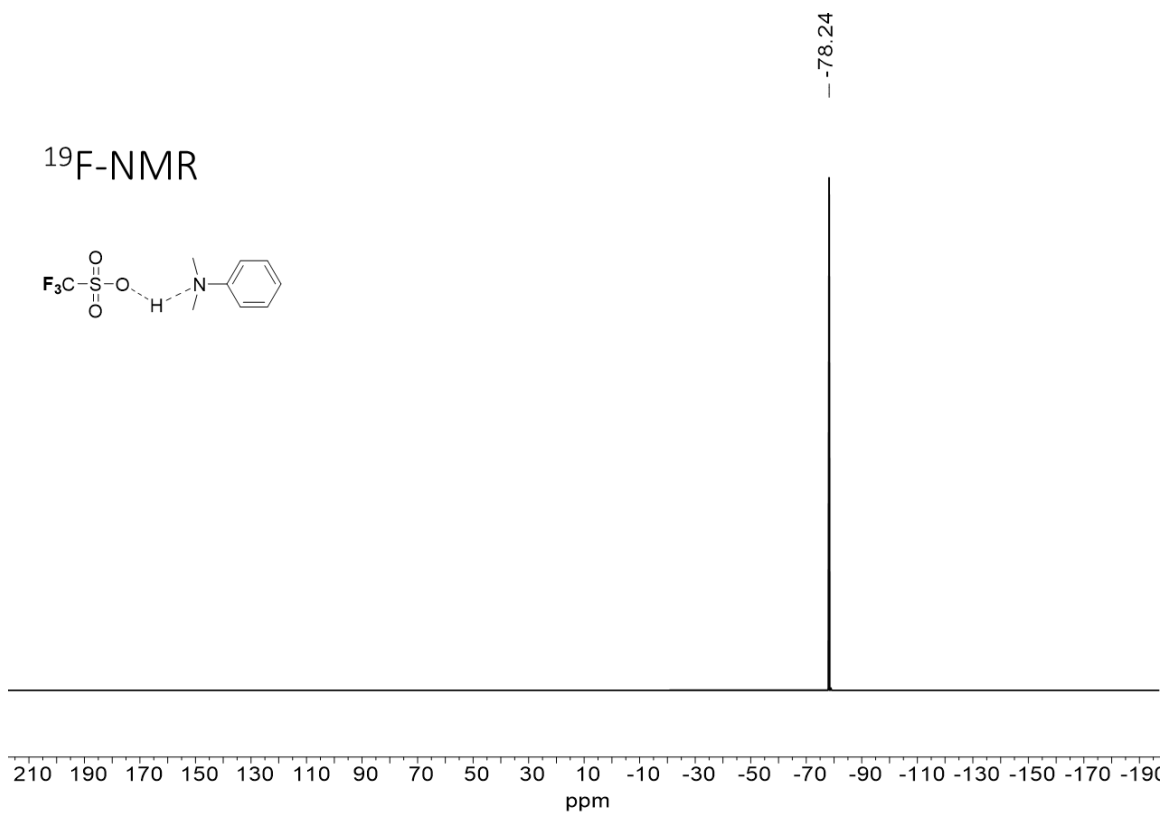
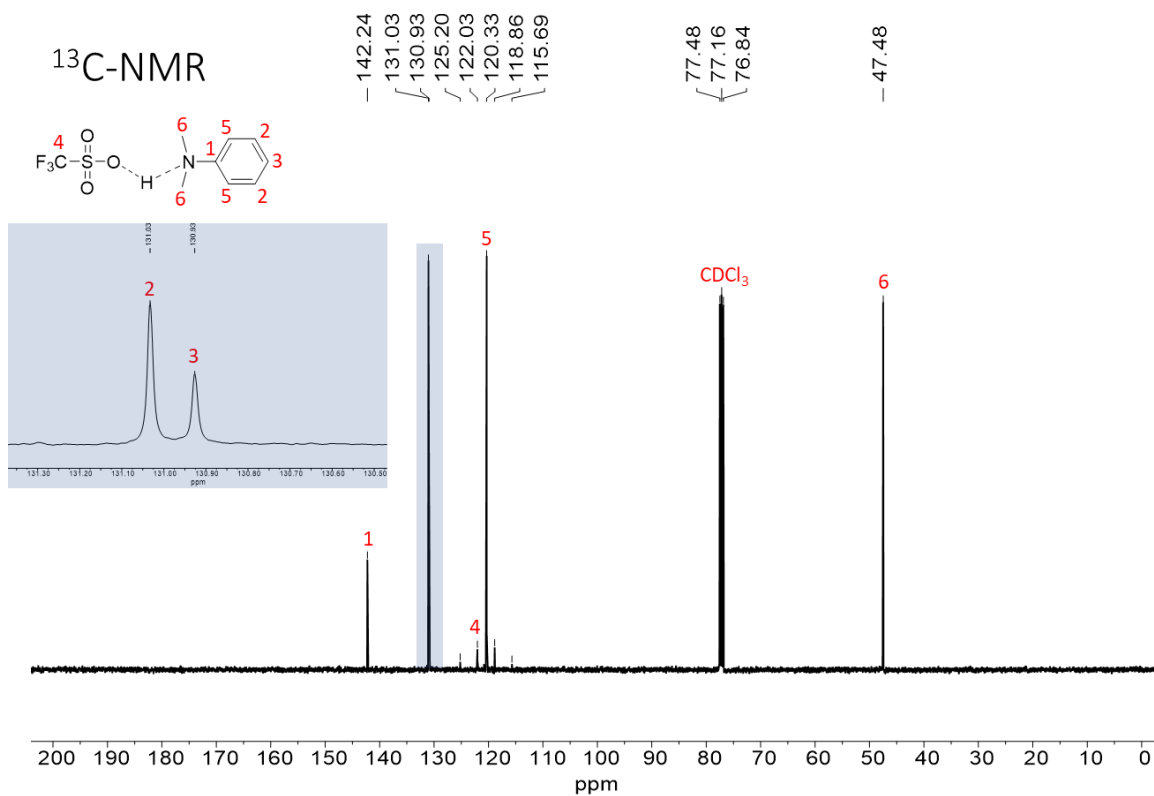


Figure S62. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for NMI:MSA salt.





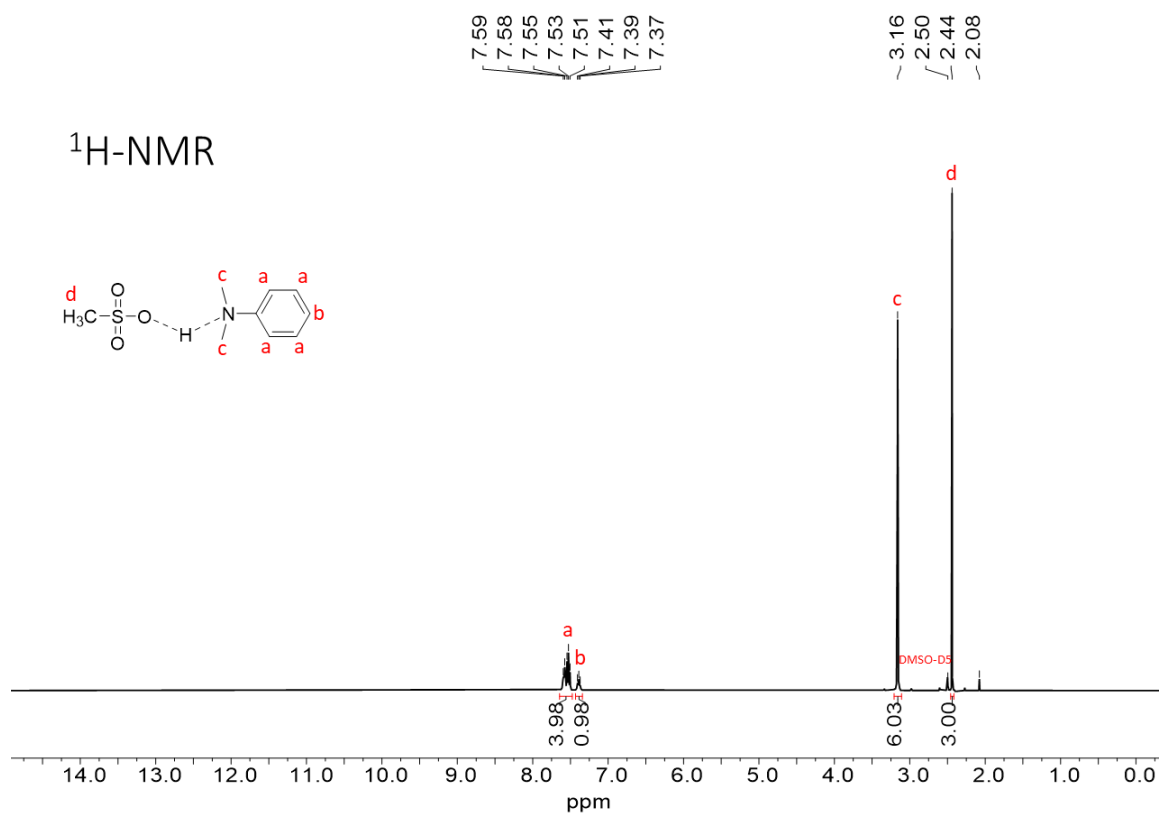


Figure S67. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DMA:MSA salt.

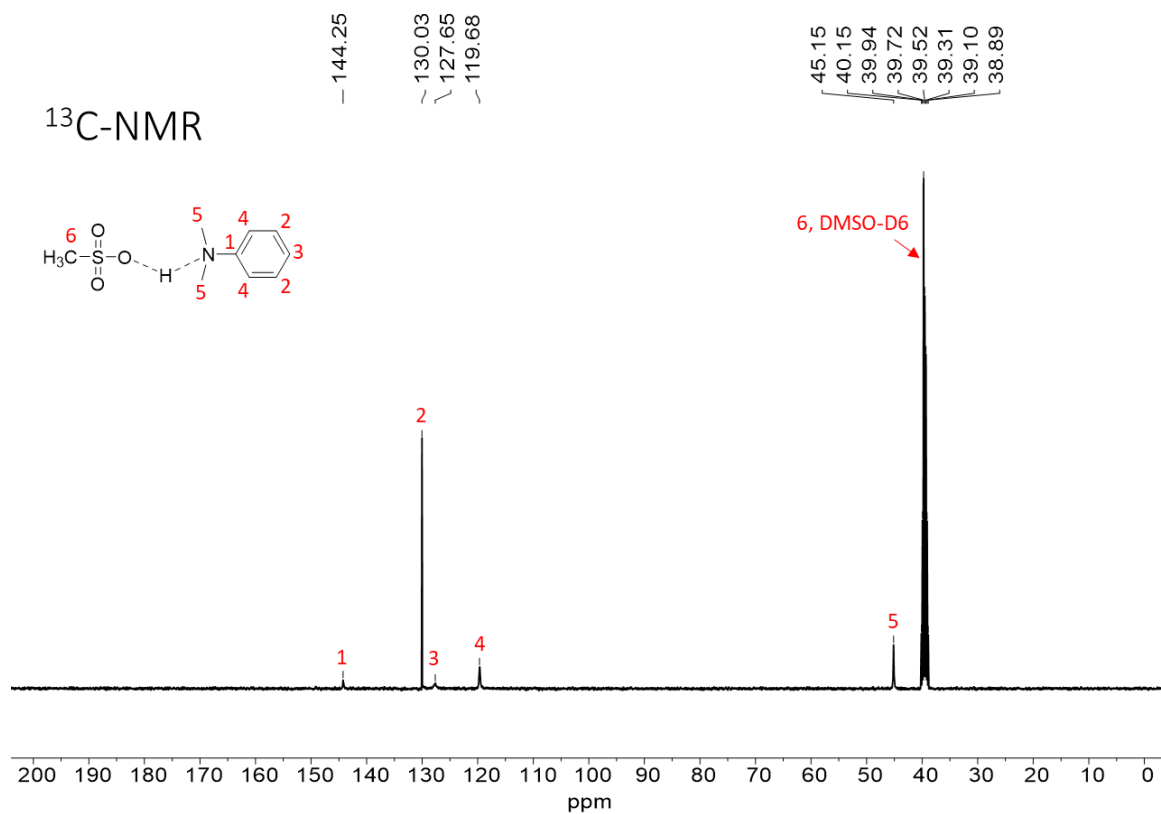


Figure S68. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for DMA:MSA salt.

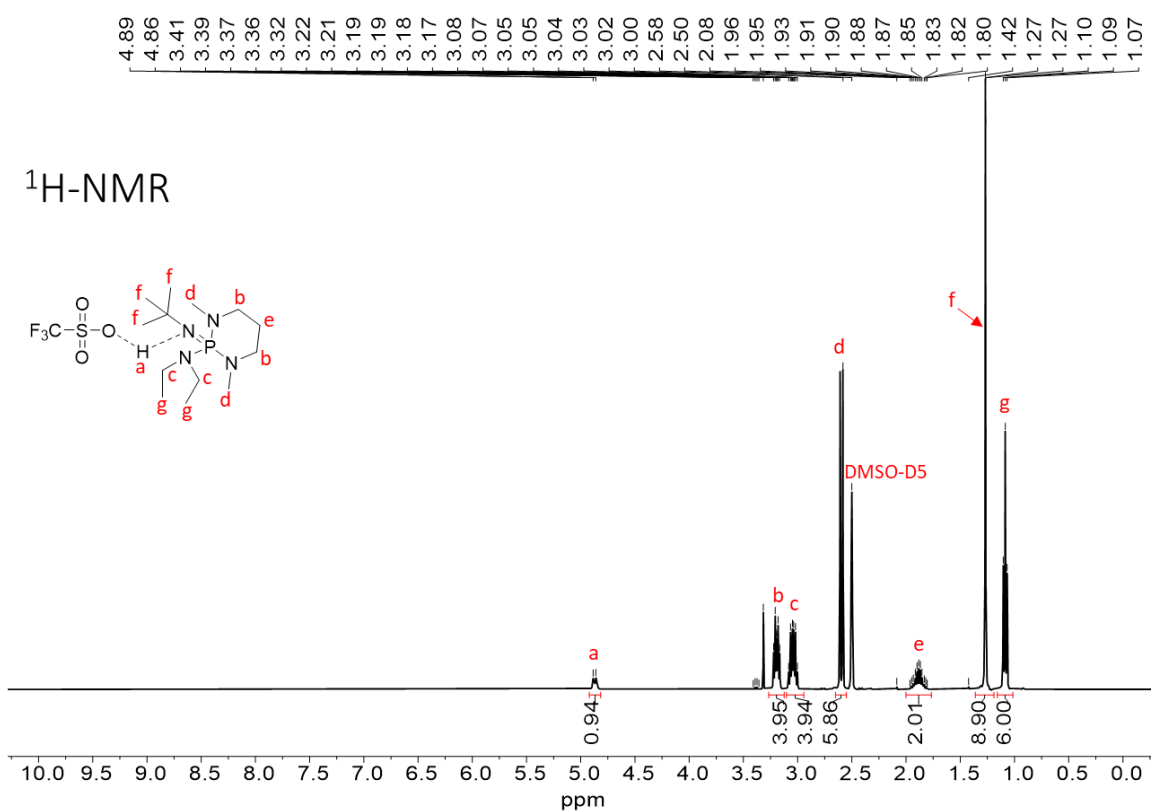


Figure S69. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for BEMP:TfOH salt.

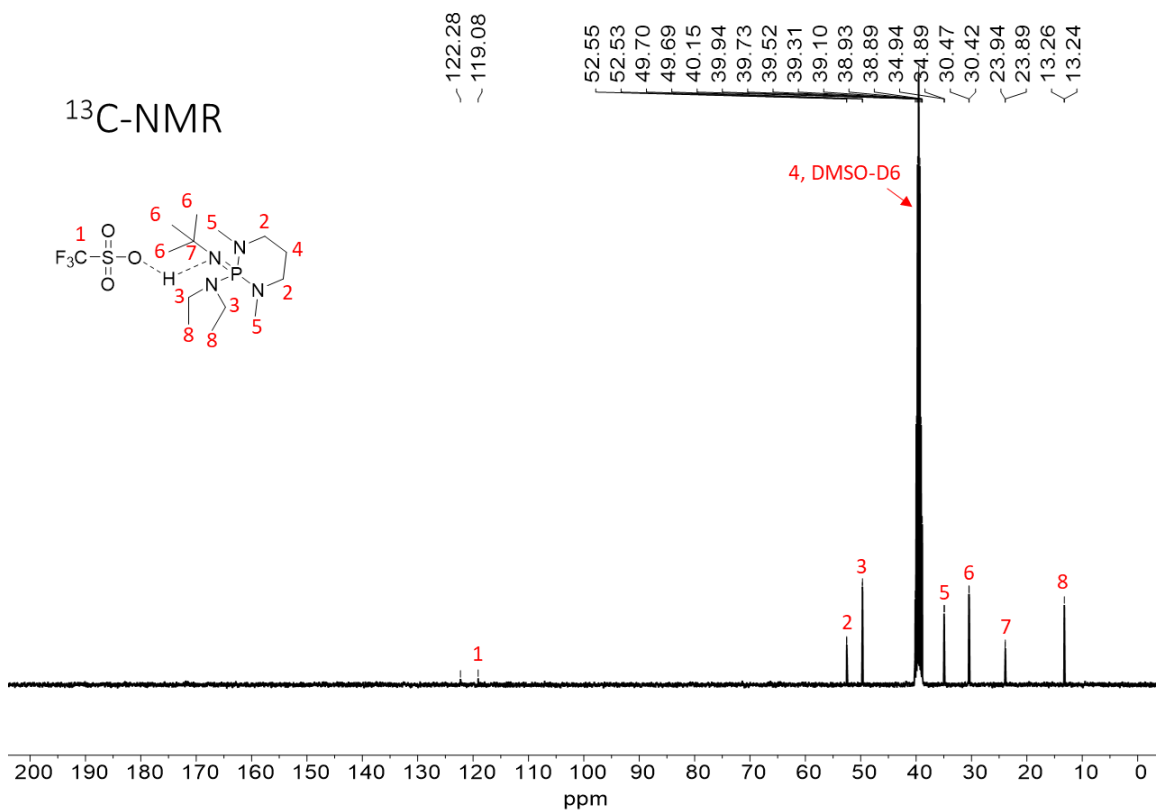


Figure S70. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for BEMP:TfOH salt.

# <sup>19</sup>F-NMR

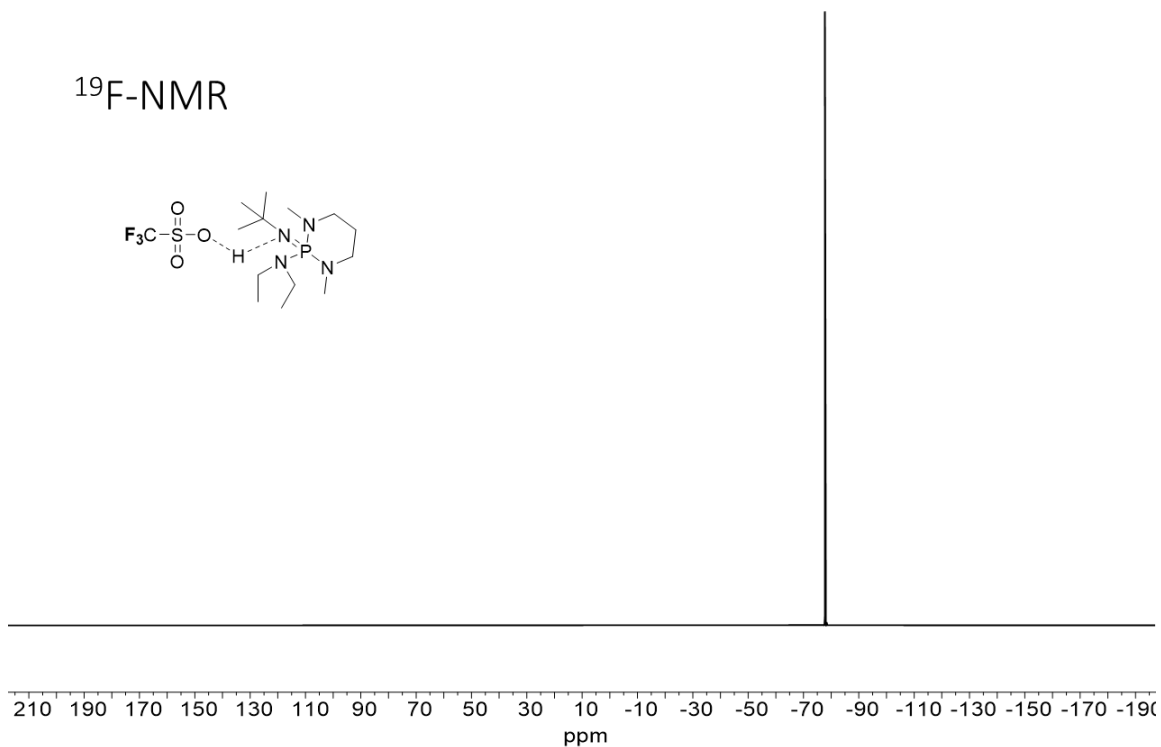
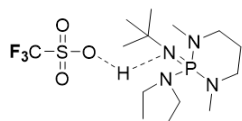
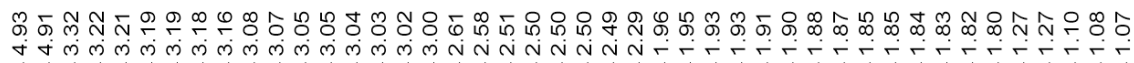


Figure S71. <sup>19</sup>F NMR (376.3 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for BEMP:TfOH salt.



# <sup>1</sup>H-NMR

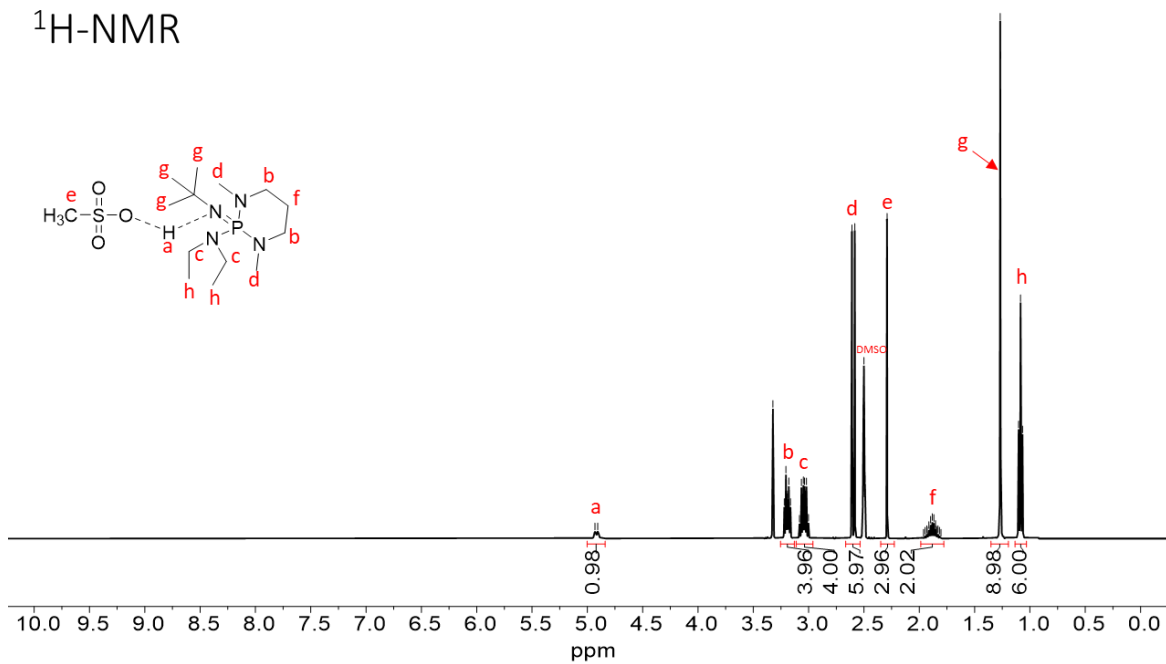
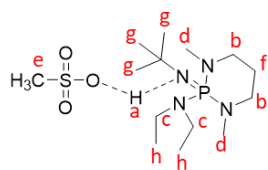
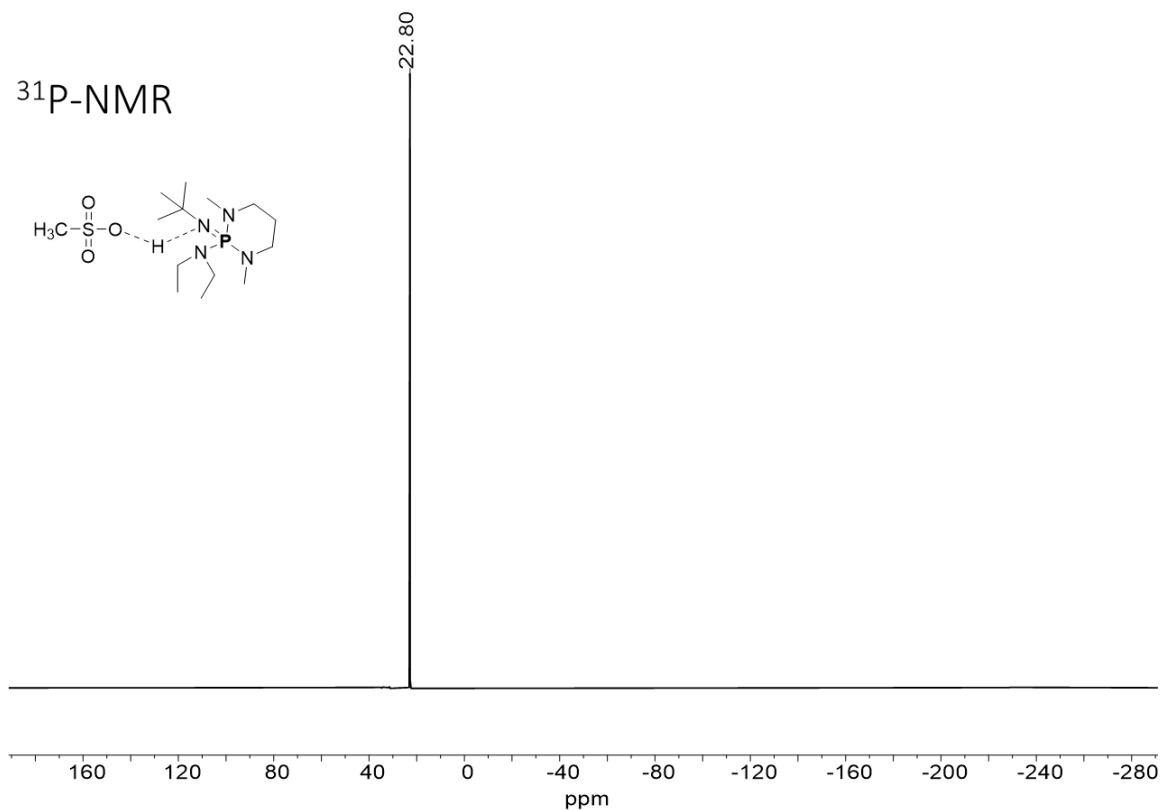
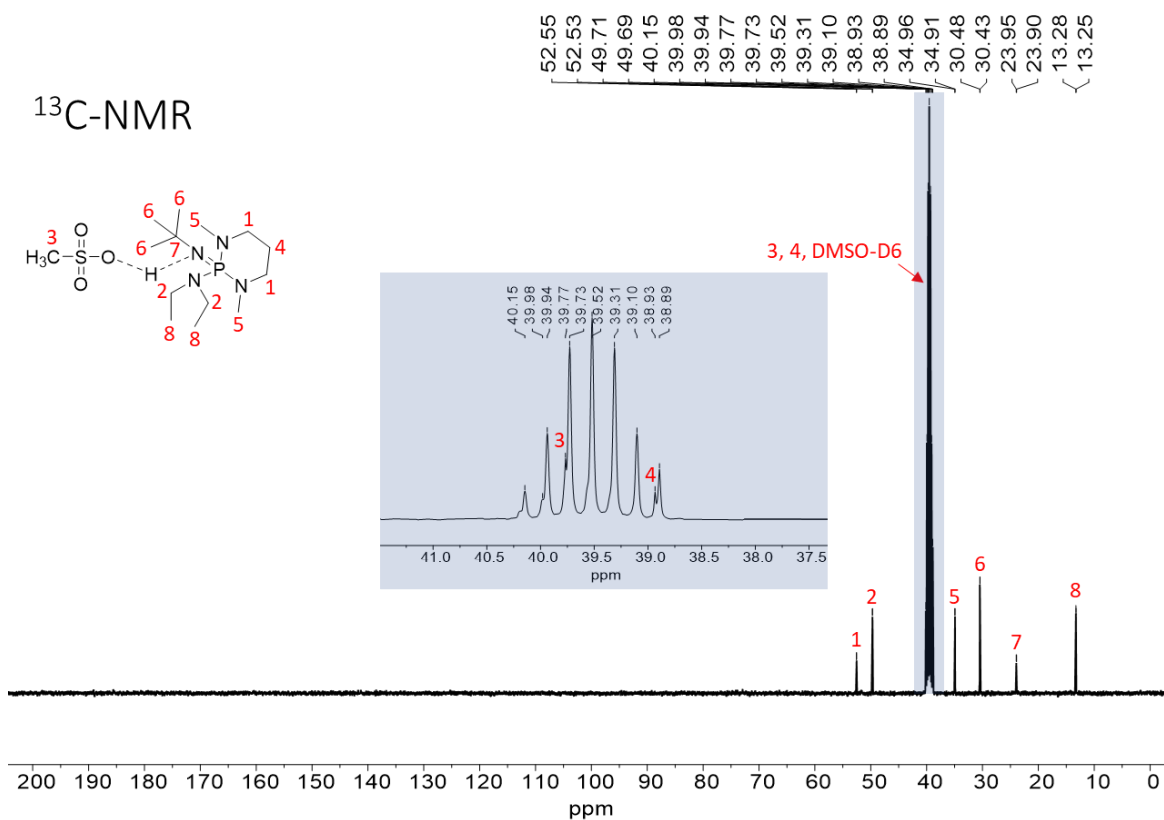


Figure S72. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for BEMP:MSA salt.





# $^1\text{H-NMR}$

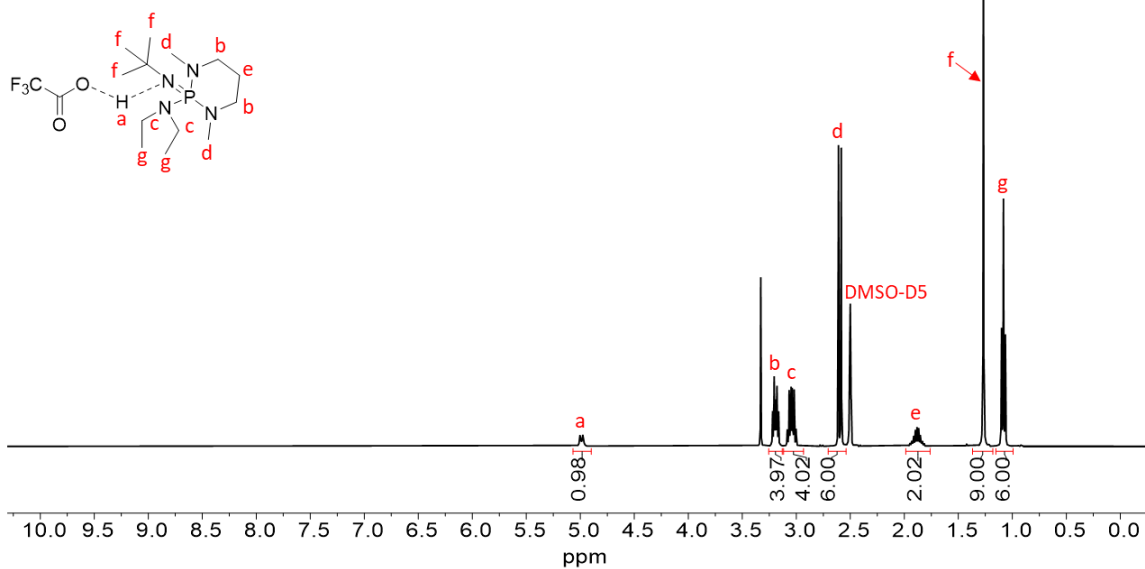


Figure S75.  $^1\text{H-NMR}$  (400 MHz; 298 K; DMSO- $d_6$ ) spectrum for BEMP:TFA salt.

# $^{13}\text{C-NMR}$

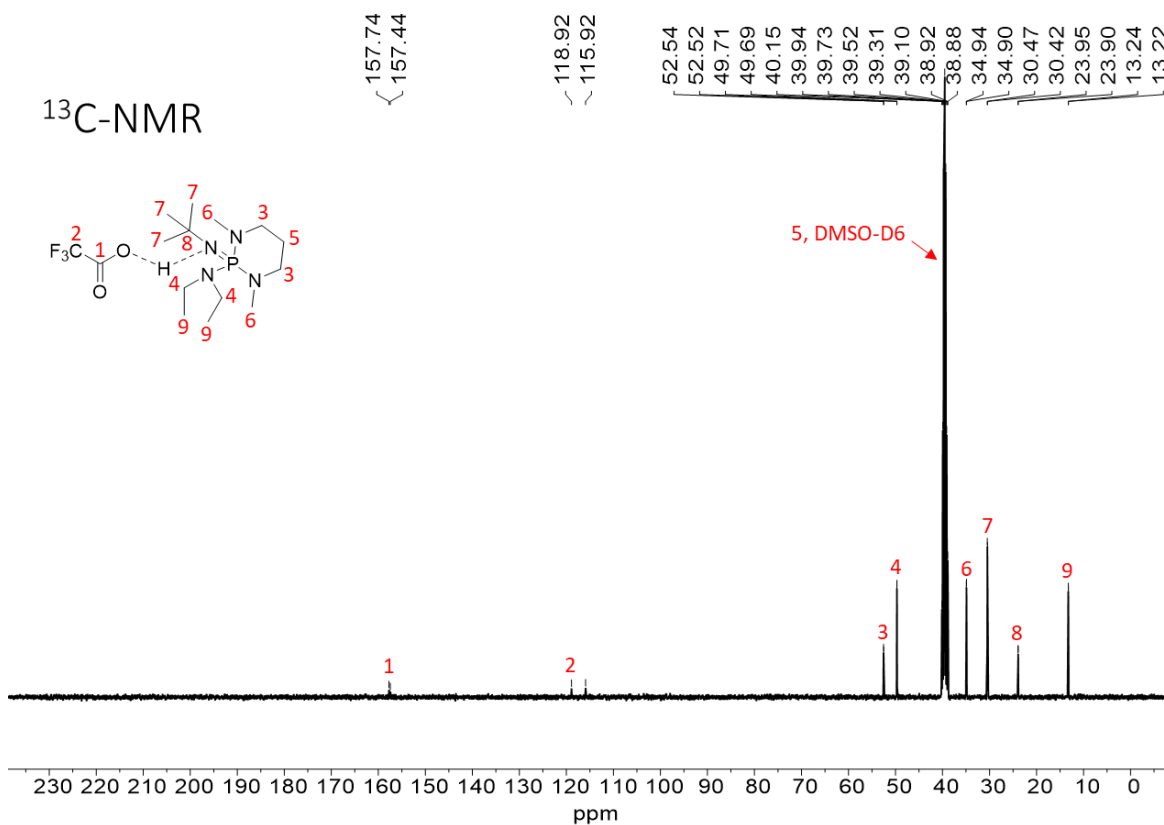
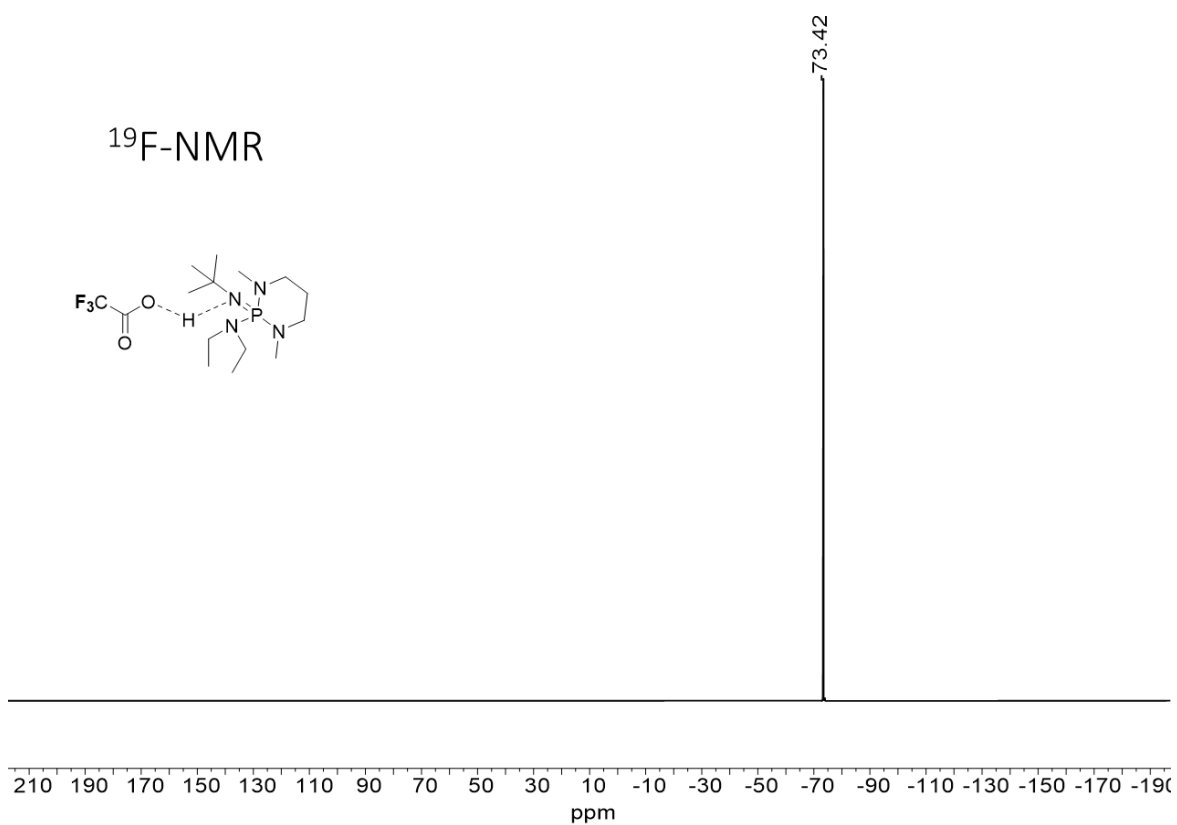
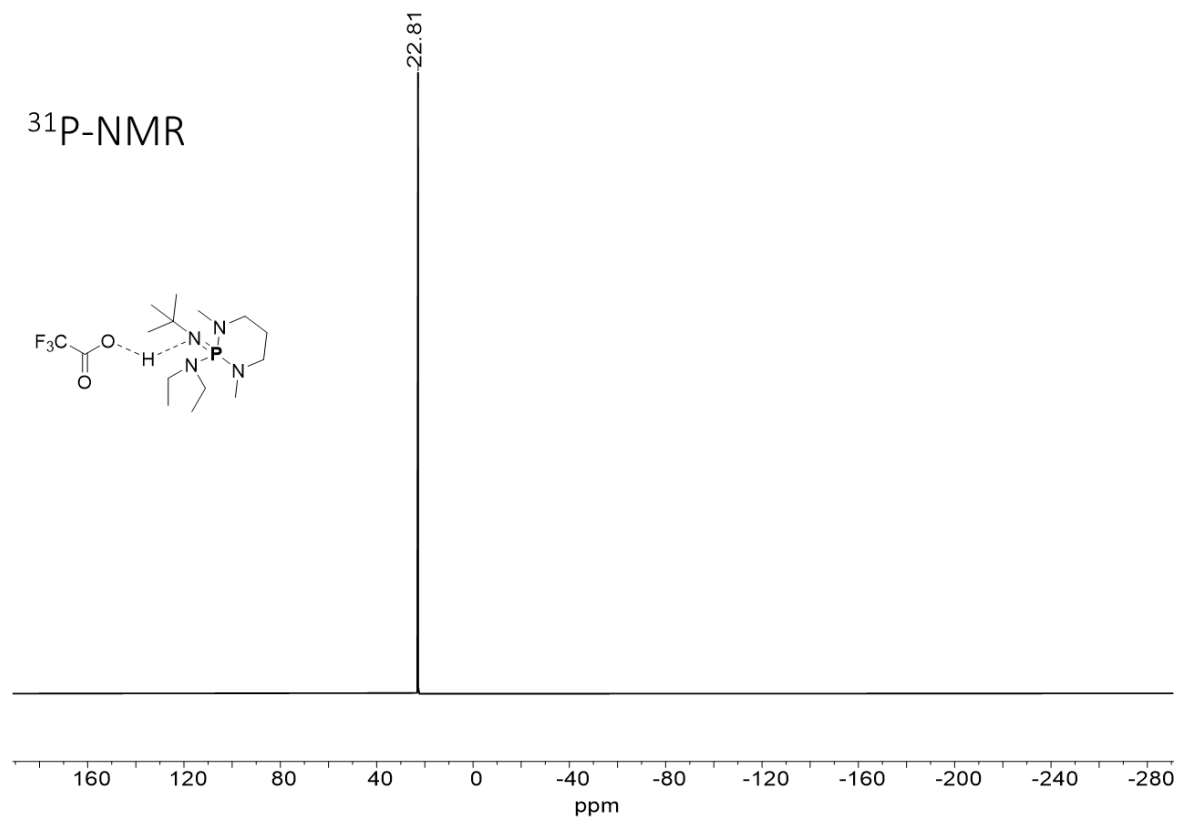


Figure S76.  $^{13}\text{C-NMR}$  (100.6 MHz; 298 K; DMSO- $d_6$ ) spectrum for BEMP:TFA salt.



**Figure S77.** <sup>19</sup>F NMR (376.3 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for BEMP:TFA salt.



**Figure S78.** <sup>31</sup>P NMR (161.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for BEMP:TFA salt.

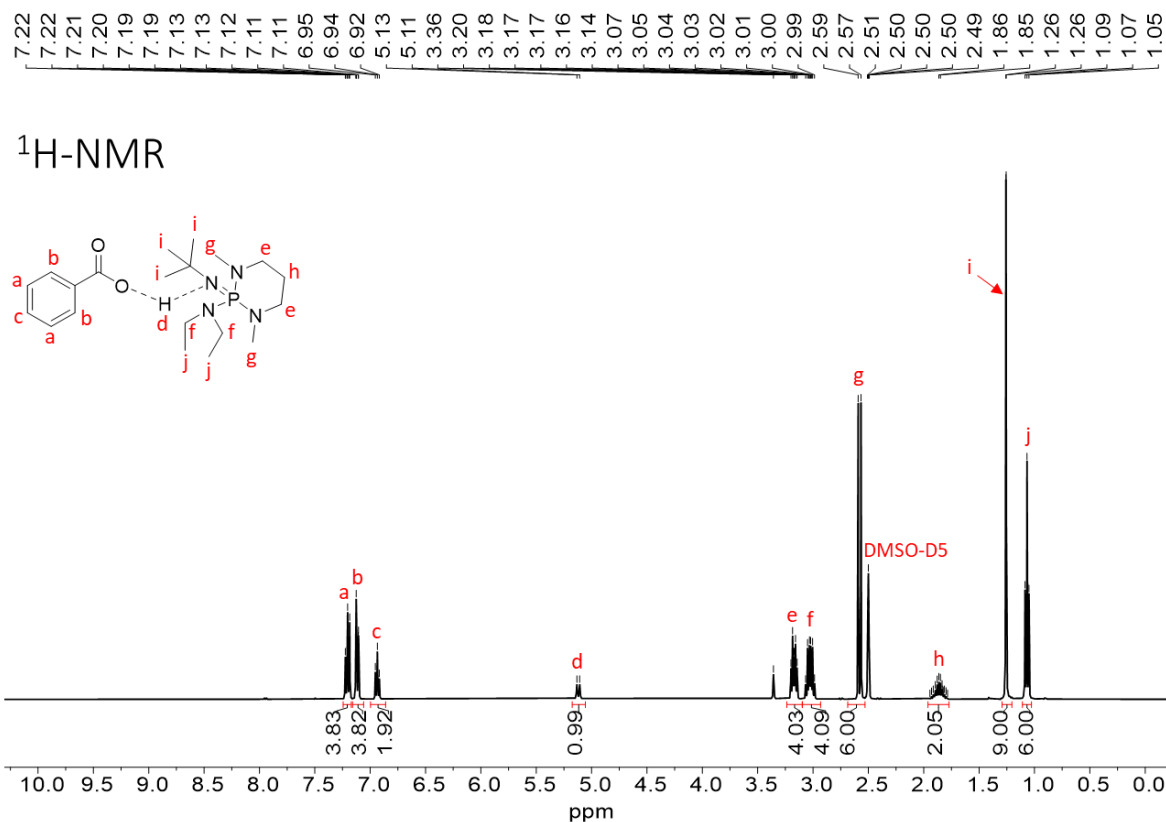


Figure S79. <sup>1</sup>H NMR (400 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for BEMP:DPP salt.

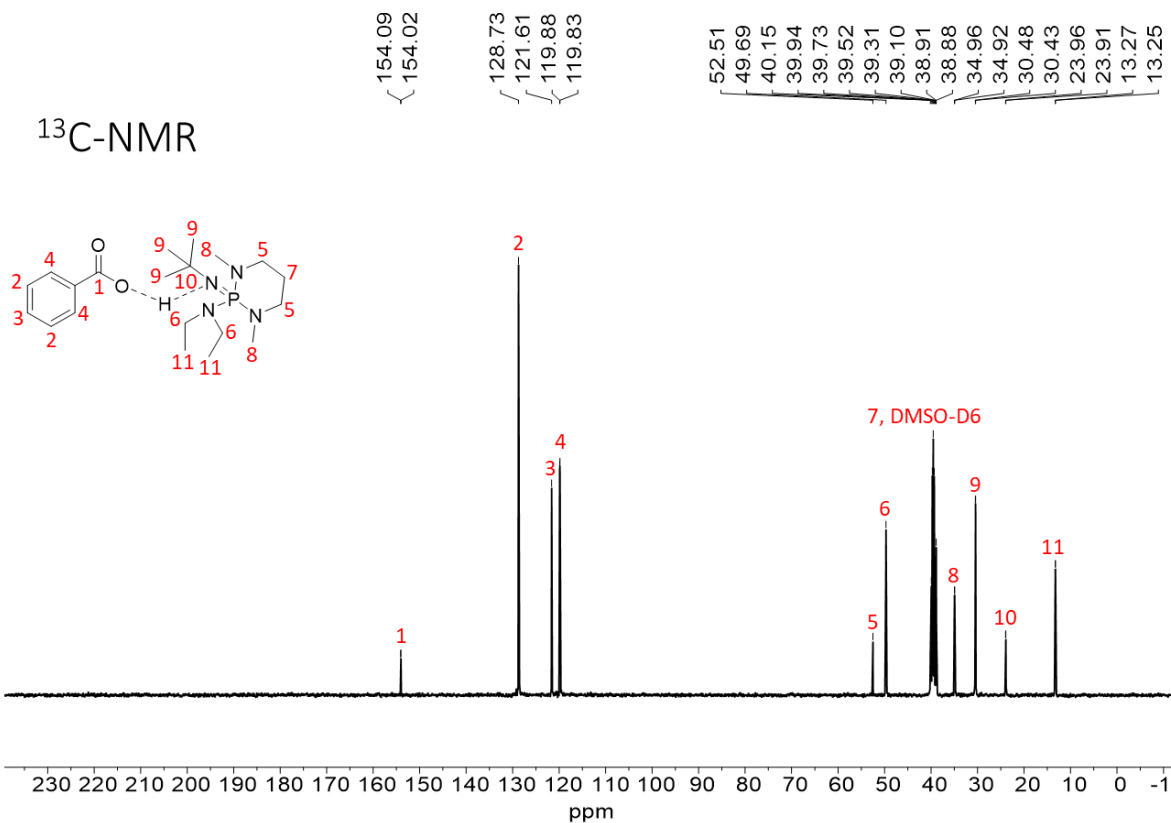


Figure S80. <sup>13</sup>C NMR (100.6 MHz; 298 K; DMSO-d<sub>6</sub>) spectrum for BEMP:DPP salt.

#### 4. References

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