

Supporting Information

Synthesis and Characterization of the Physicochemical and Magnetic Properties for Perfluoroalkyl Ester and Fe(III) Carboxylate-based Hydrophobic Magnetic Ionic Liquids

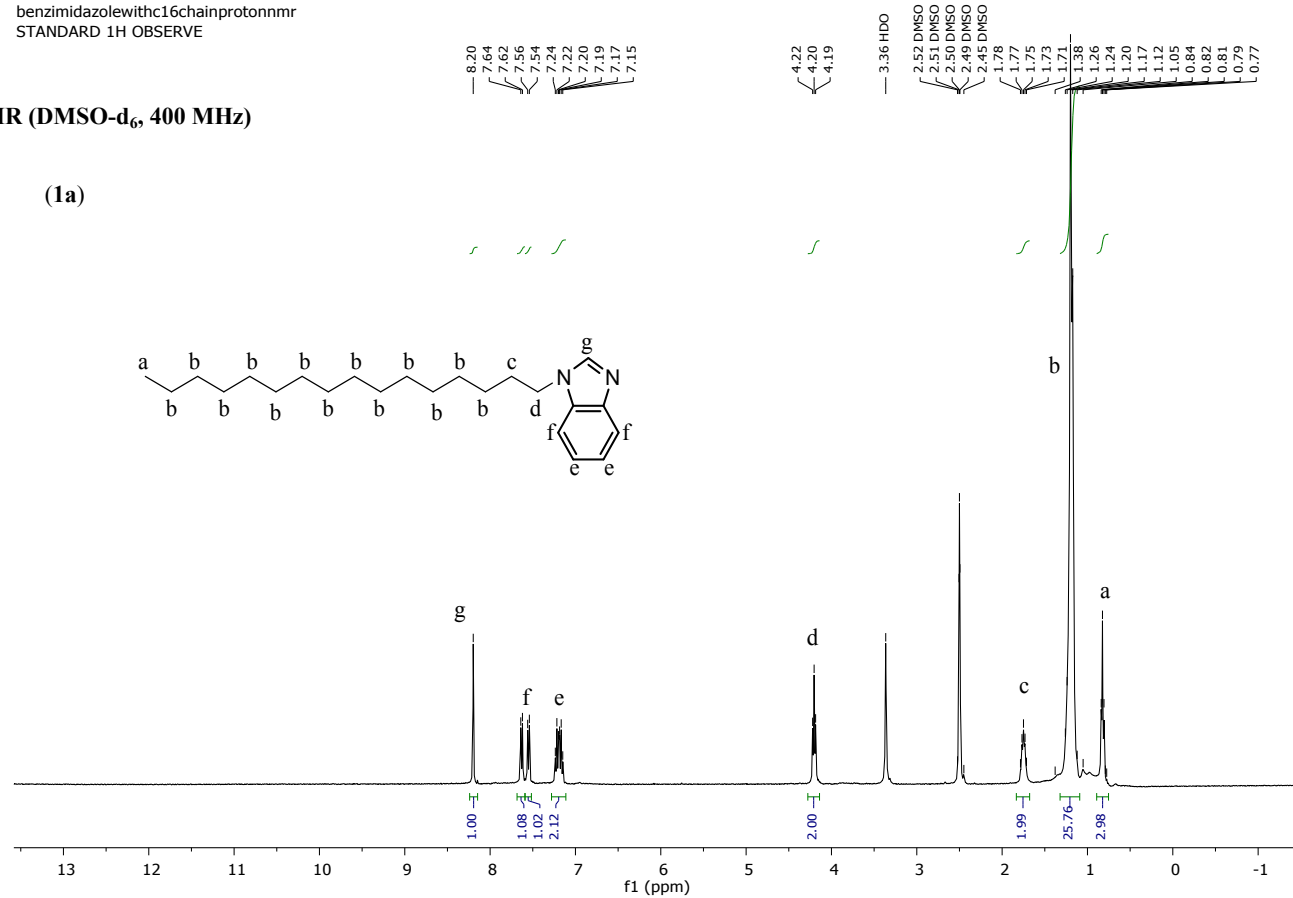
Omprakash Nacham, Kevin D. Clark, and Jared L. Anderson

Department of Chemistry, Iowa State University, Ames, IA 50011USA

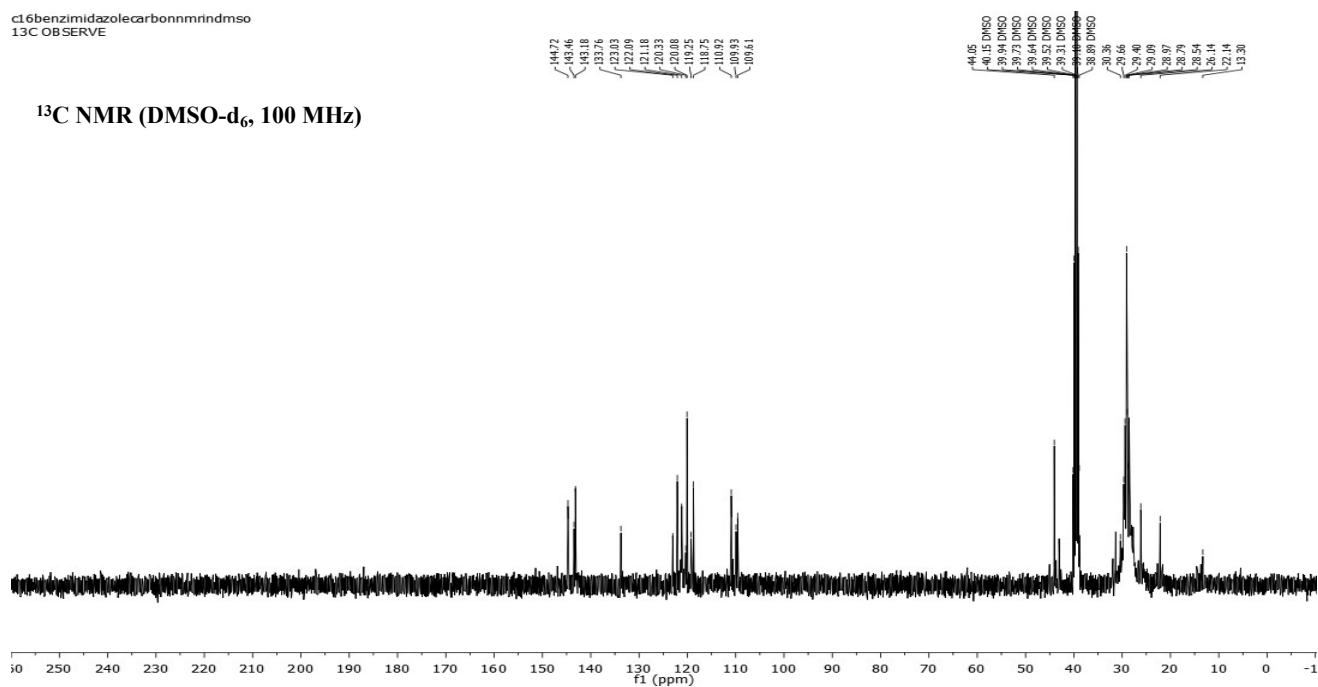
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benzimidazolewithc16chainprotonnmr
STANDARD 1H OBSERVE

¹H NMR (DMSO-d₆, 400 MHz)

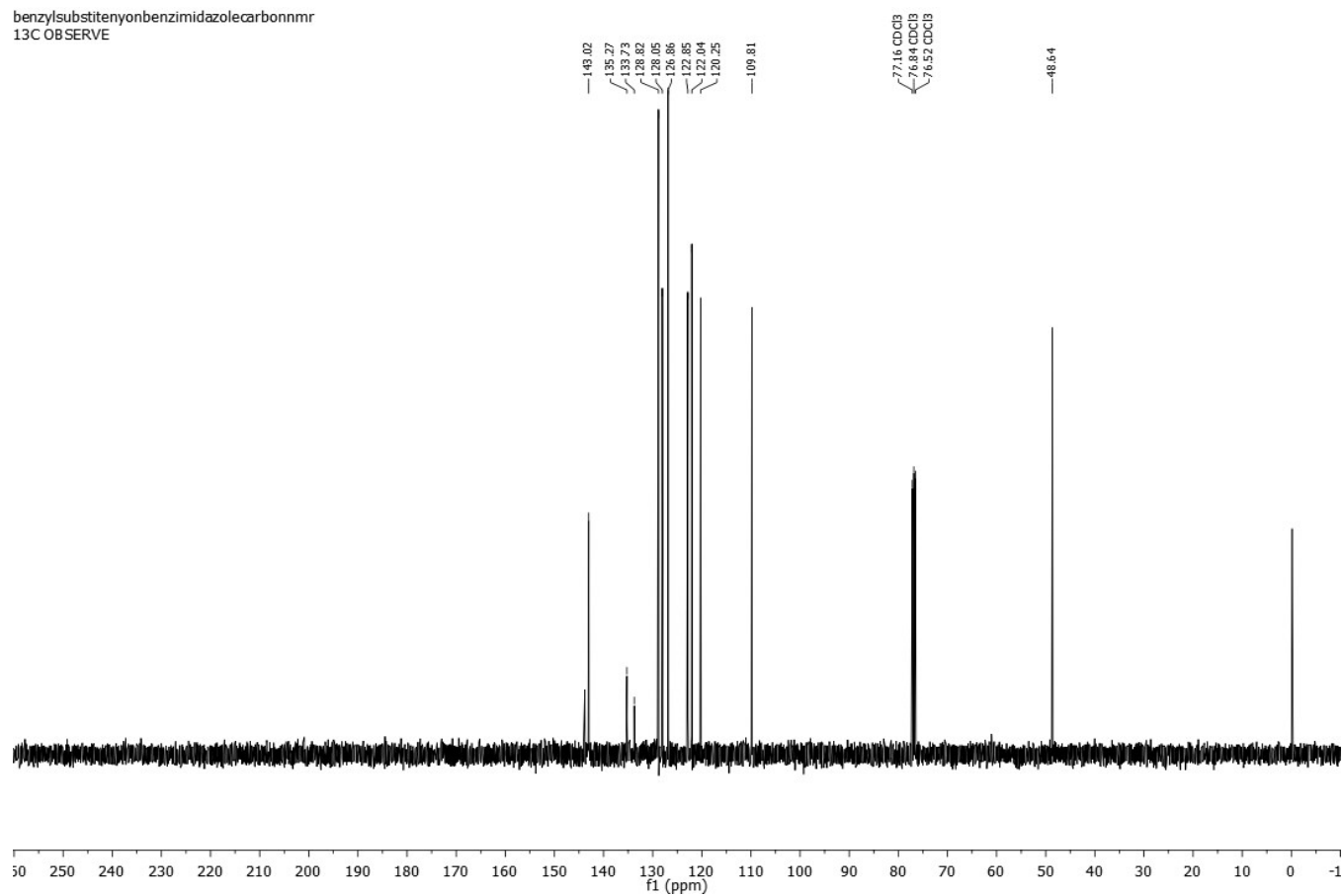


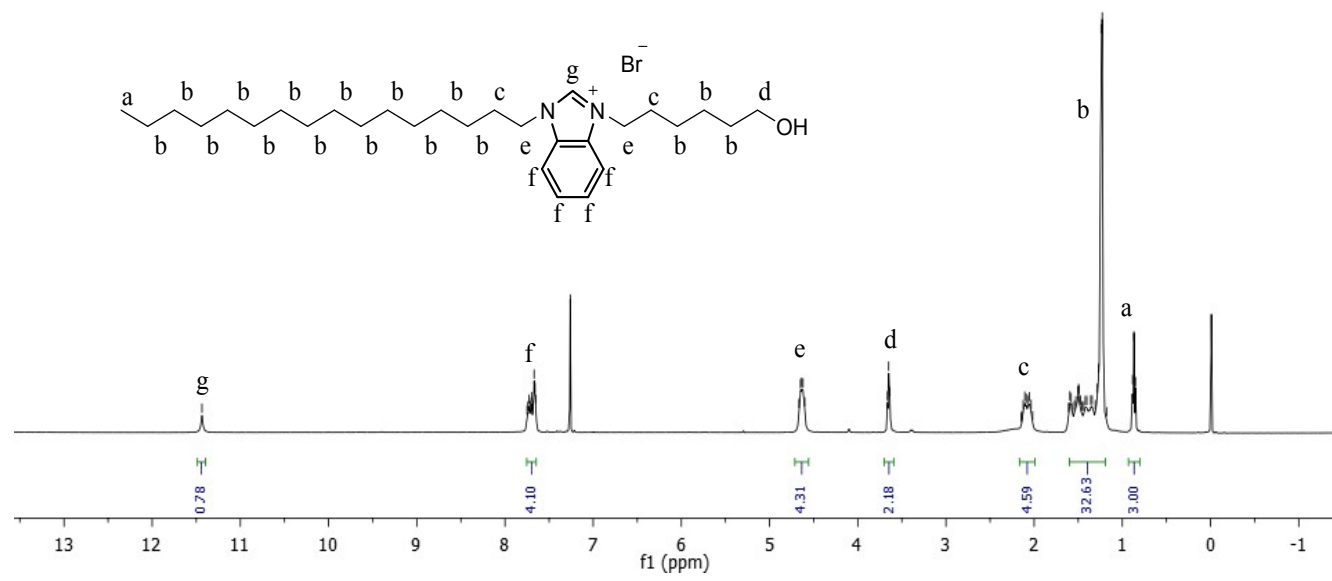
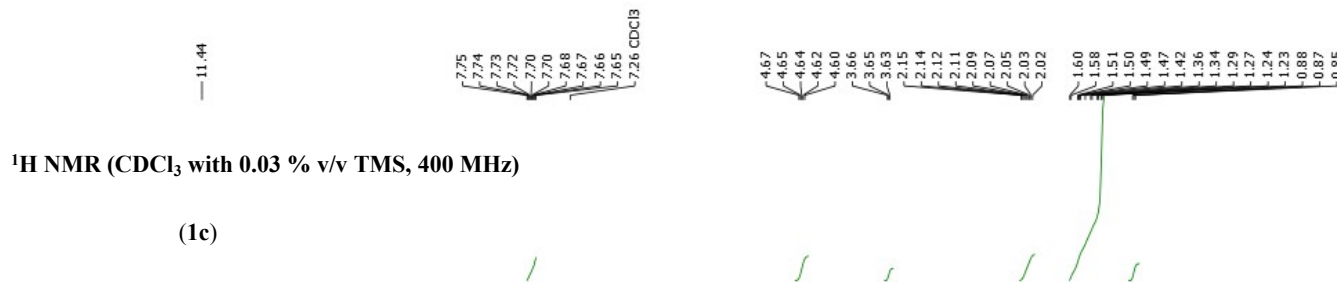
c16benzimidazolecarbonmndmsol
13C OBSERVE



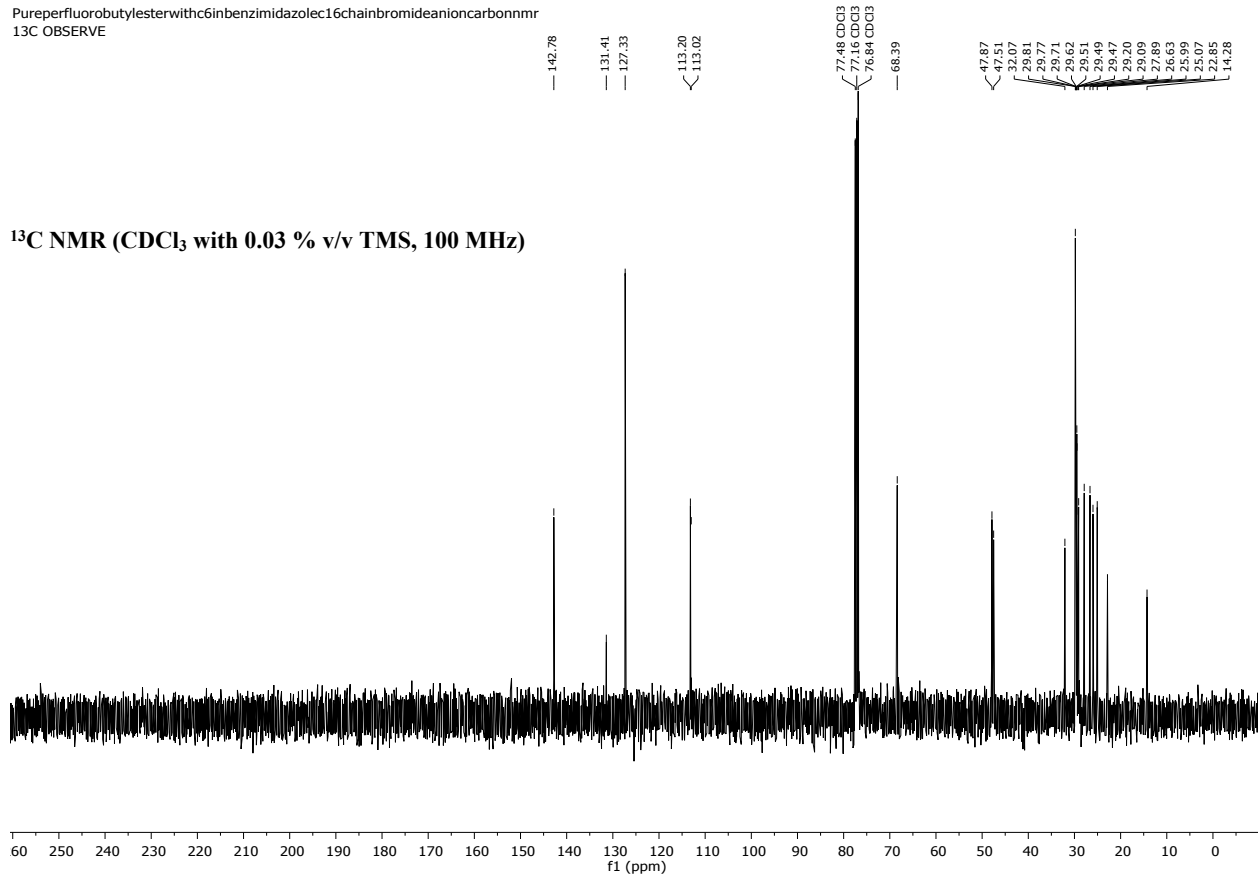
^{13}C NMR (CDCl₃ with 0.03 % v/v TMS, 100 MHz)

benzylsubstitenyonbenzimidazolecarbonmr
13C OBSERVE





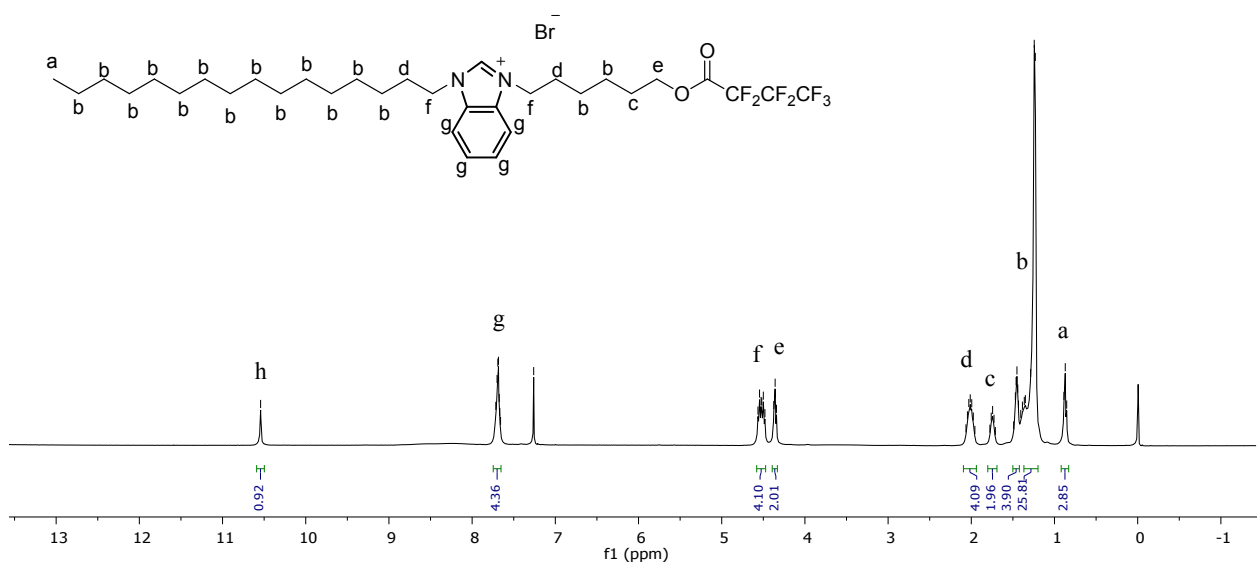
Pureperfluorobutylesterwithc6inbenzimidazolec16chainbromideanioncarbonnmr
13C OBSERVE



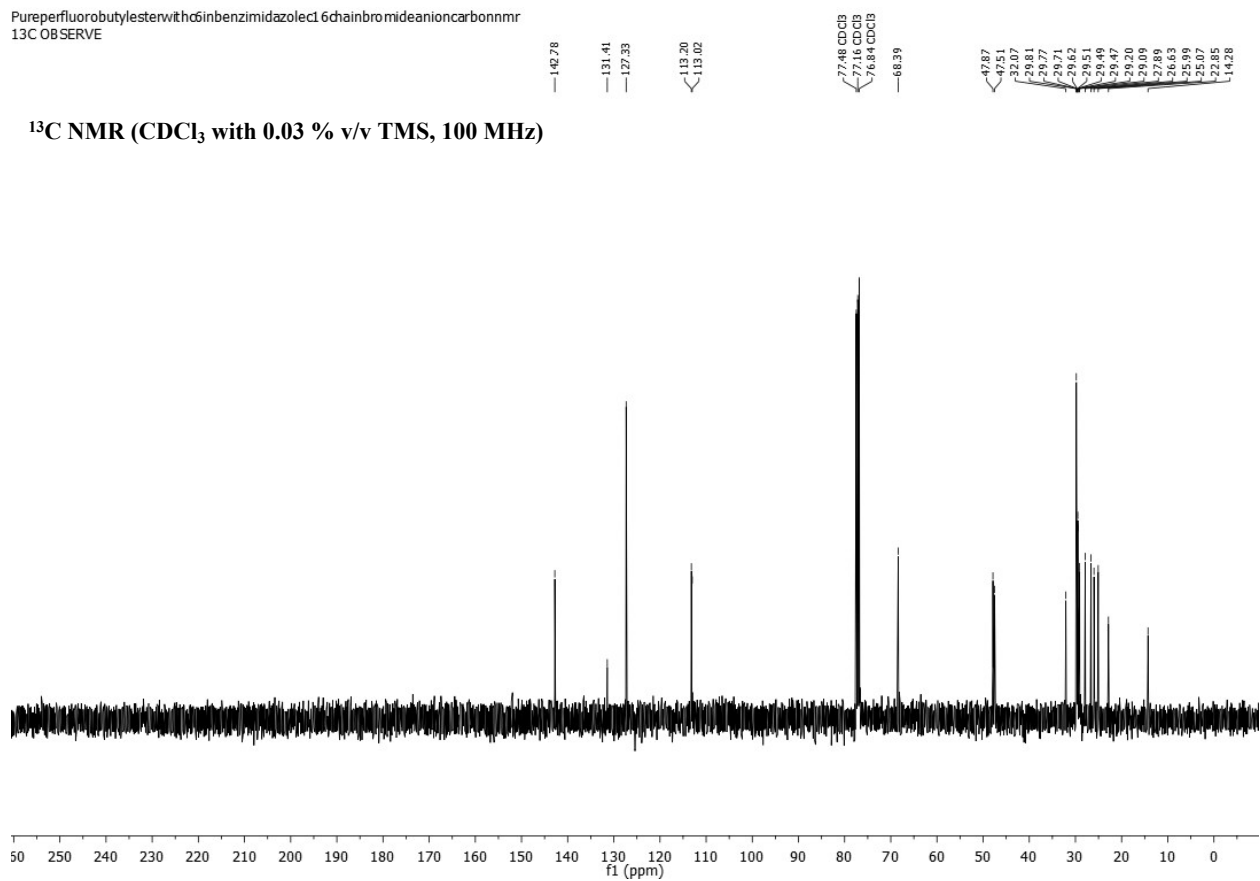
Pureperfluorobutylesterwithc6chaininc16benzimidazolewithbromideanion
STANDARD 1H OBSERVE

¹H NMR (CDCl₃ with 0.03 % v/v TMS, 400 MHz)

(1d)



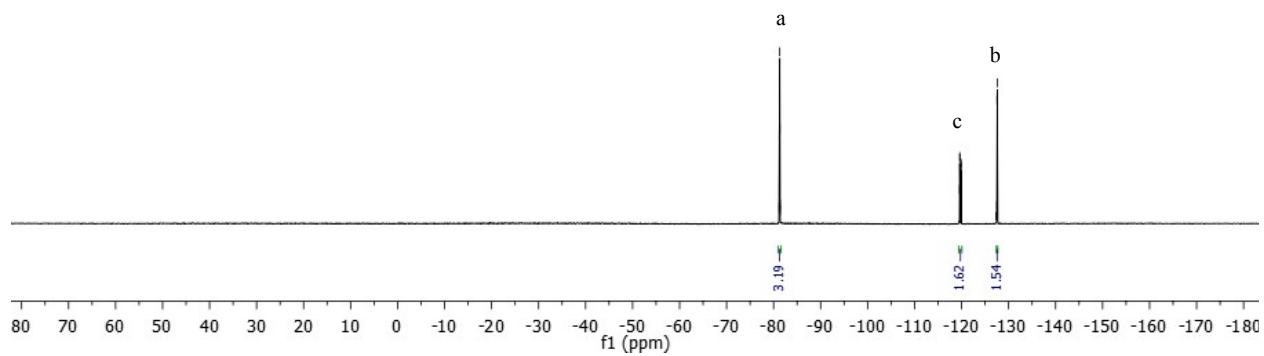
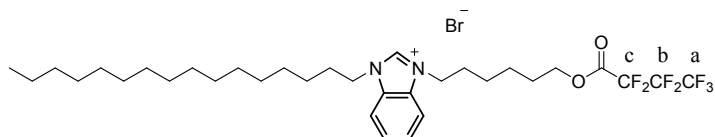
Pureperfluorobutylesterwithh6inbenzimidazolec16chainbromideanioncarbonnmr
13C OBSERVE



F19NMRforpurefluorobutylesterwithc6chaininbenzimidazolewithbromideanionfluorinenmr
 F19 OBSERVE
 STANDARD PARAMETERS

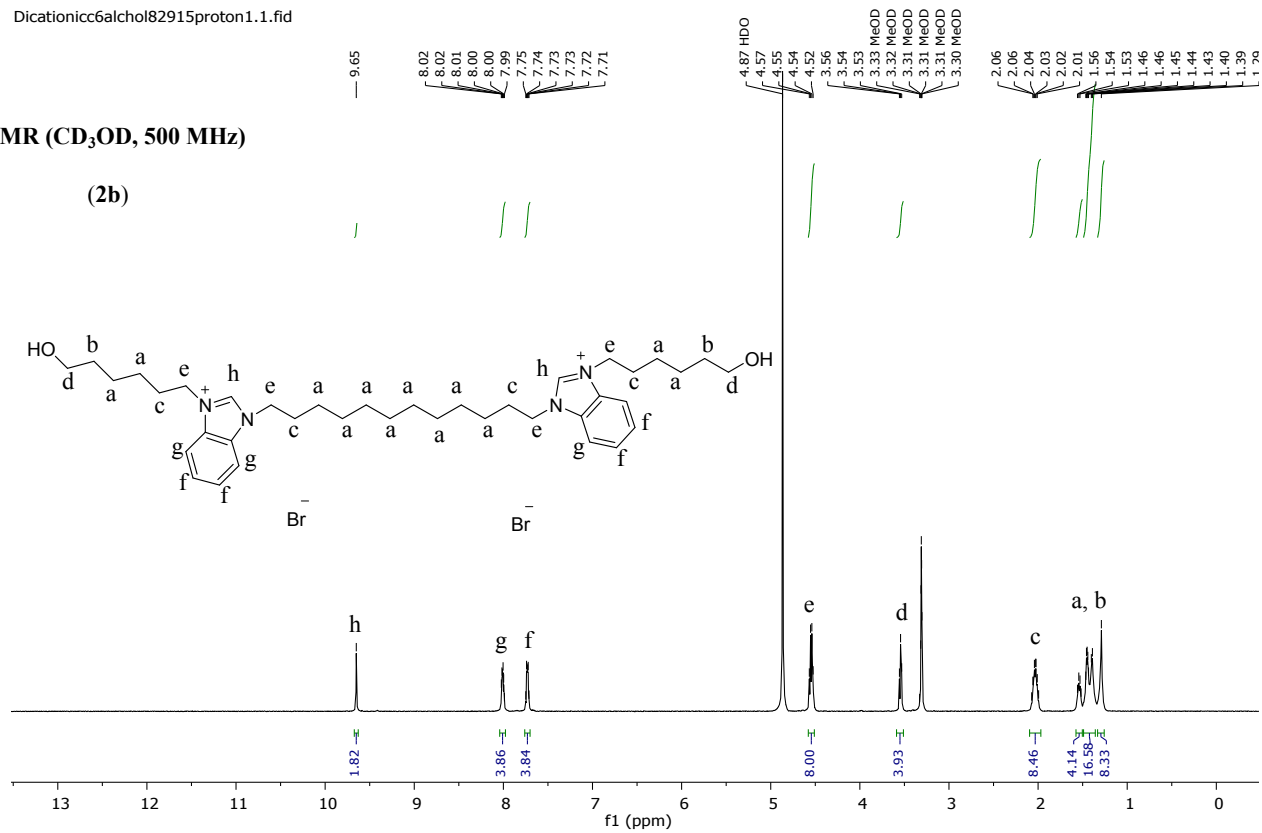
-81.202
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 -119.89
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 -127.50
 -127.53
 -127.59
 -127.64

¹⁹F NMR (1d)



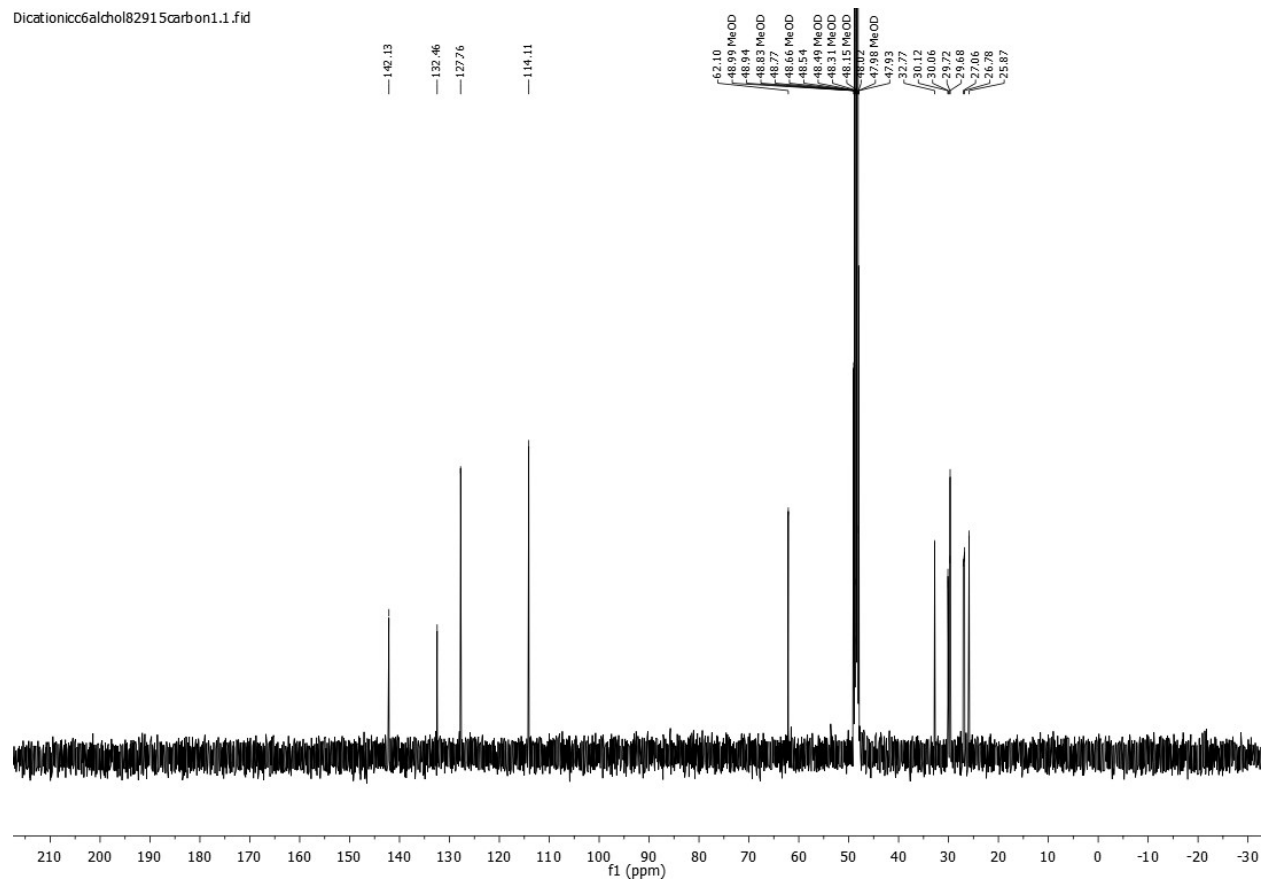
¹H NMR (CD₃OD, 500 MHz)

(2b)



¹³C NMR (CD₃OD, 400 MHz)

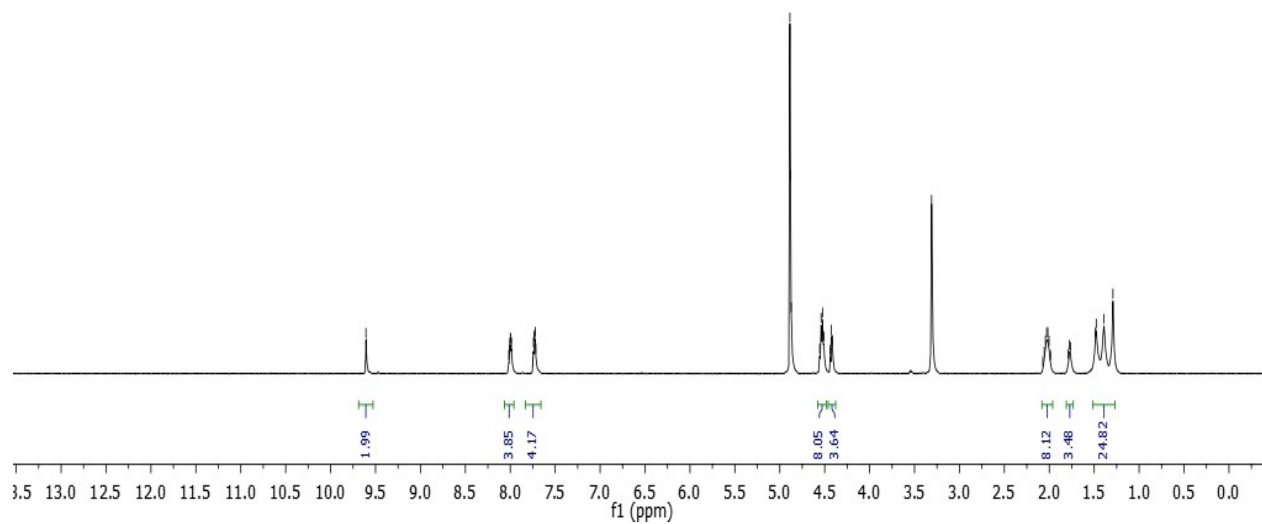
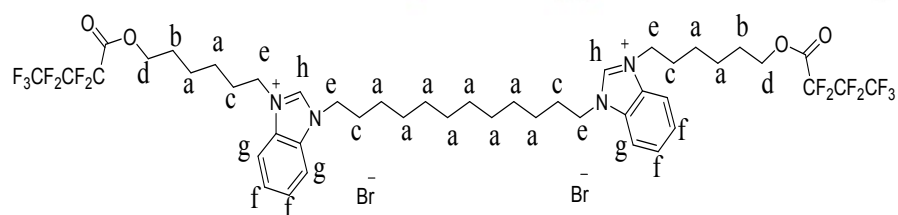
Dicationicc6alcohol82915carbon1.1.fid



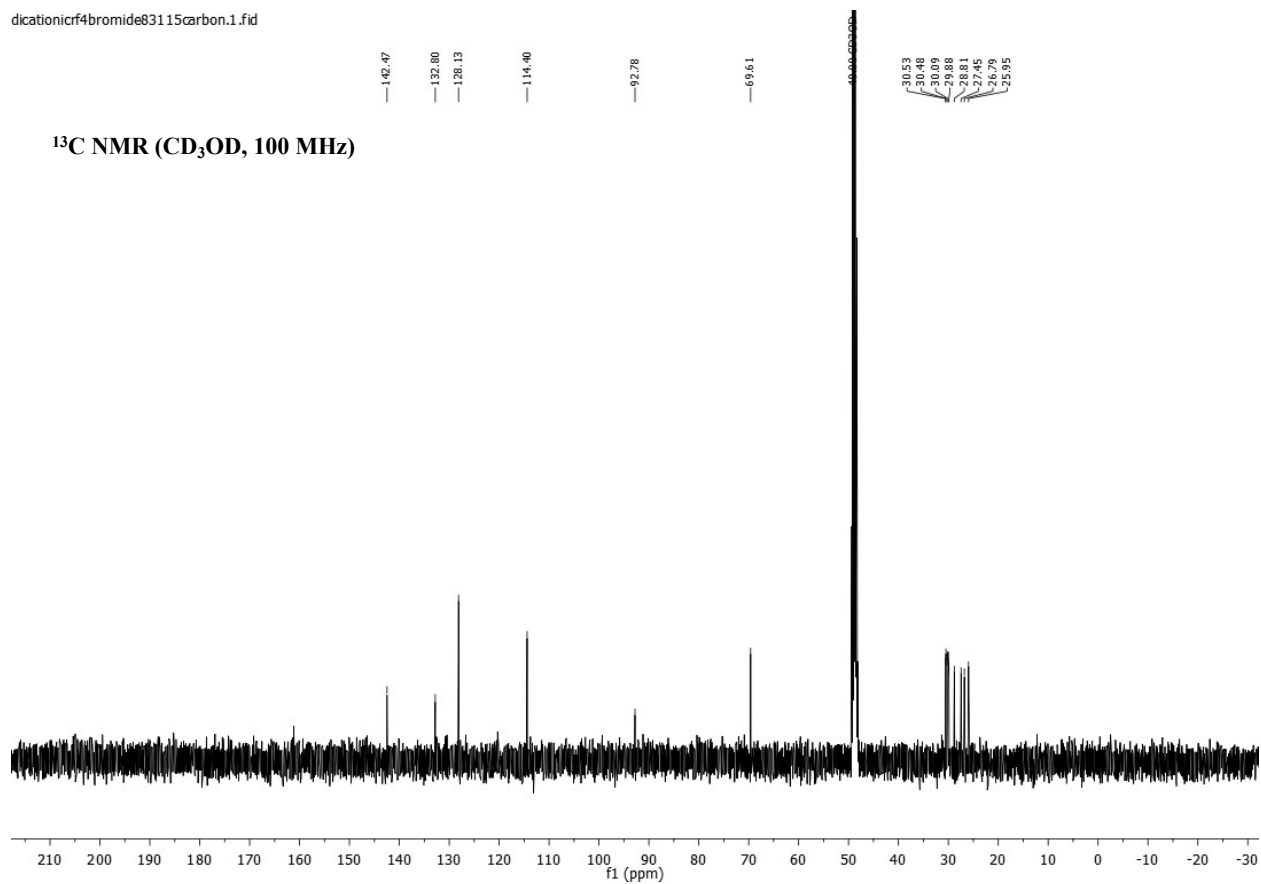
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¹H NMR (CD₃OD, 400 MHz)

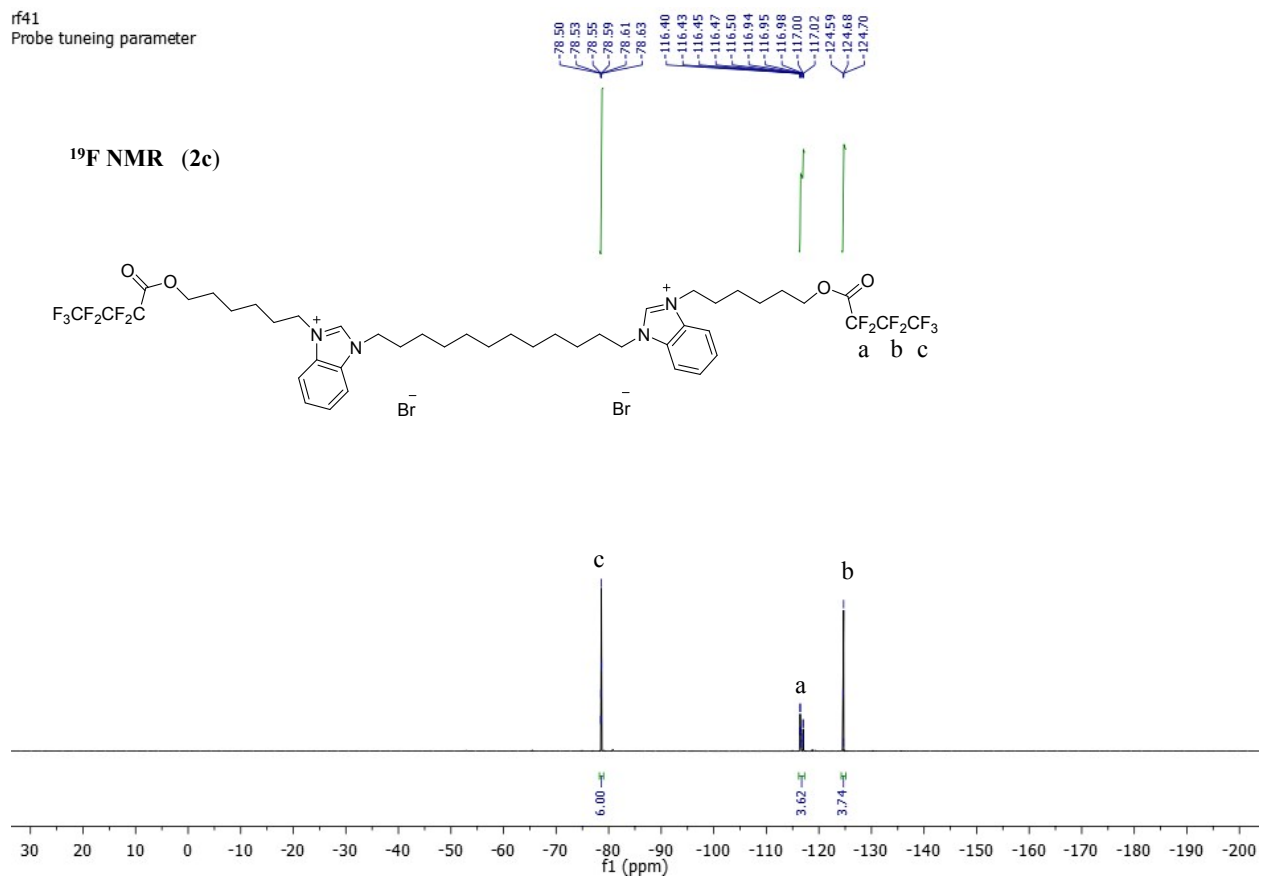
(2c)



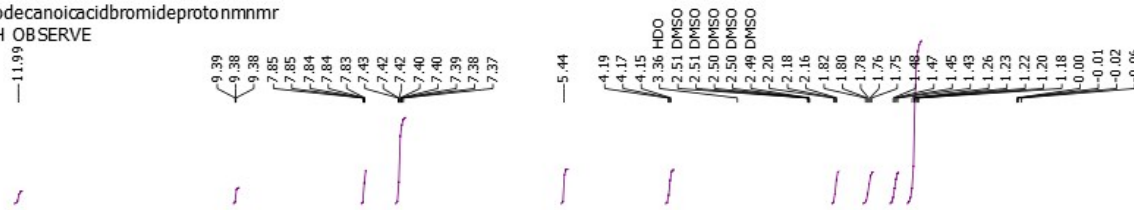
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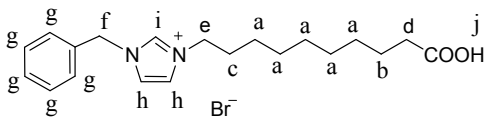
rf41
Probe tuning parameter



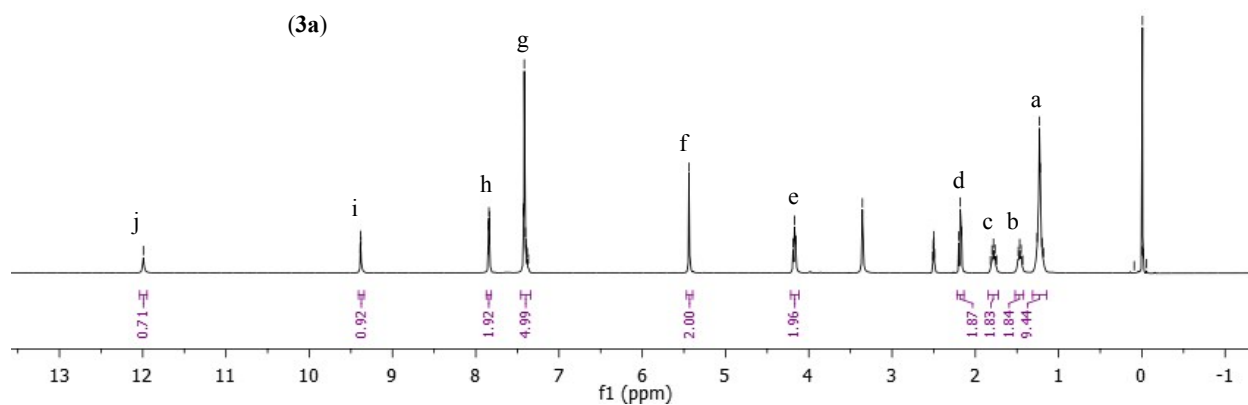
Nbenzylbromodecanoic acid bromide proton nmr
STANDARD 1H OBSERVE



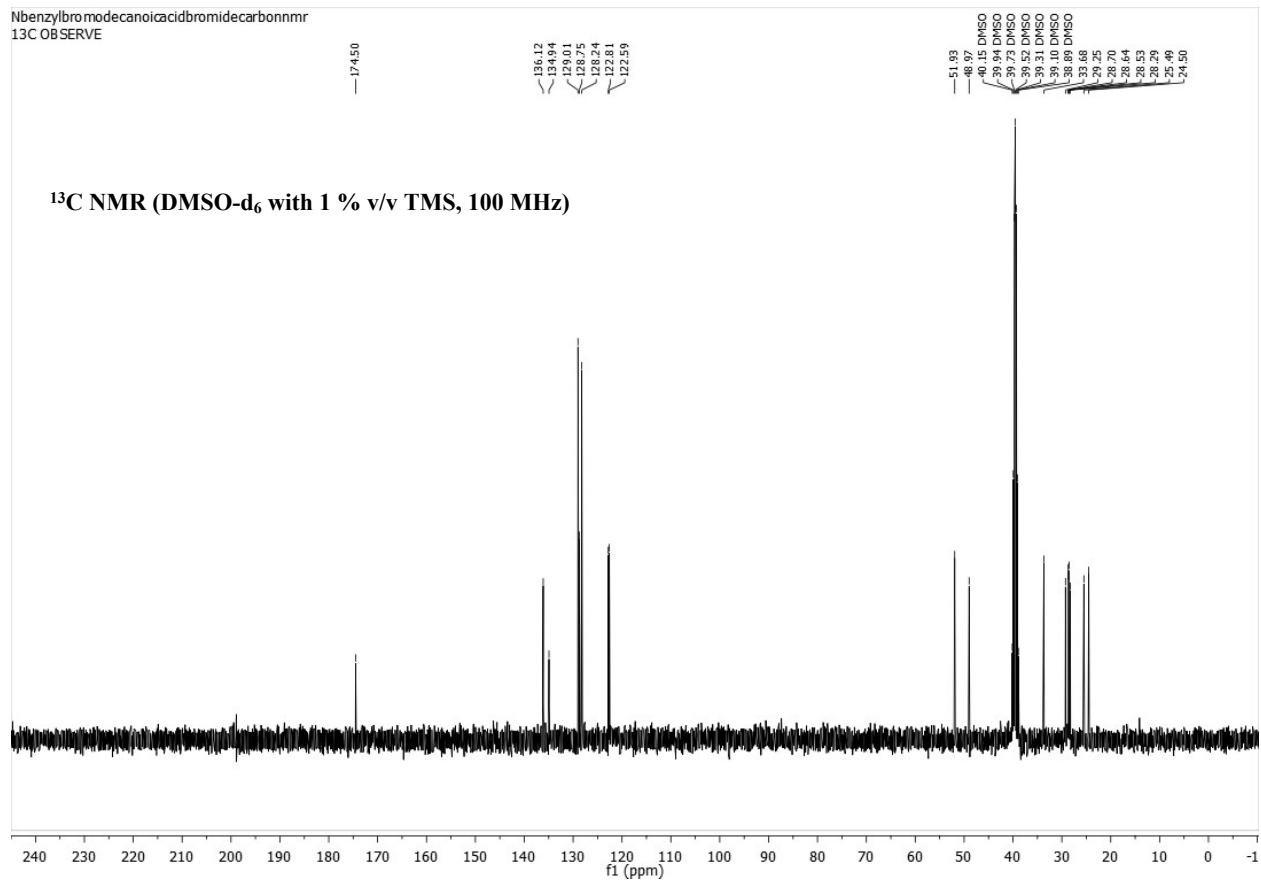
¹H NMR (DMSO-d₆ with 1 % v/v TMS, 400 MHz)



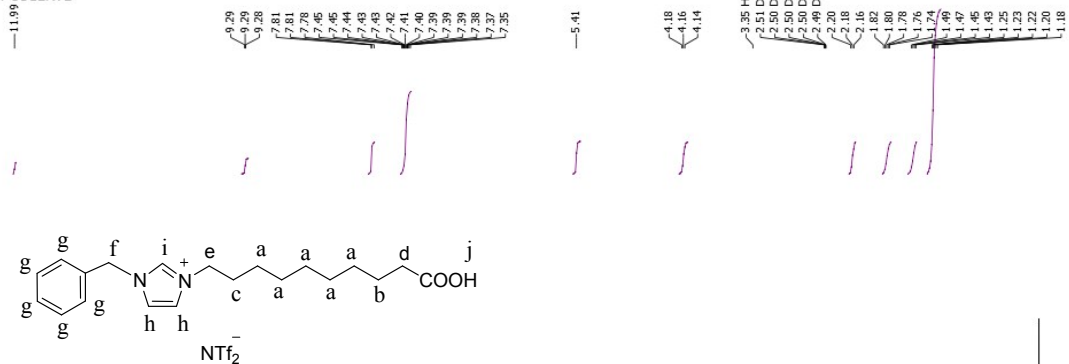
(3a)



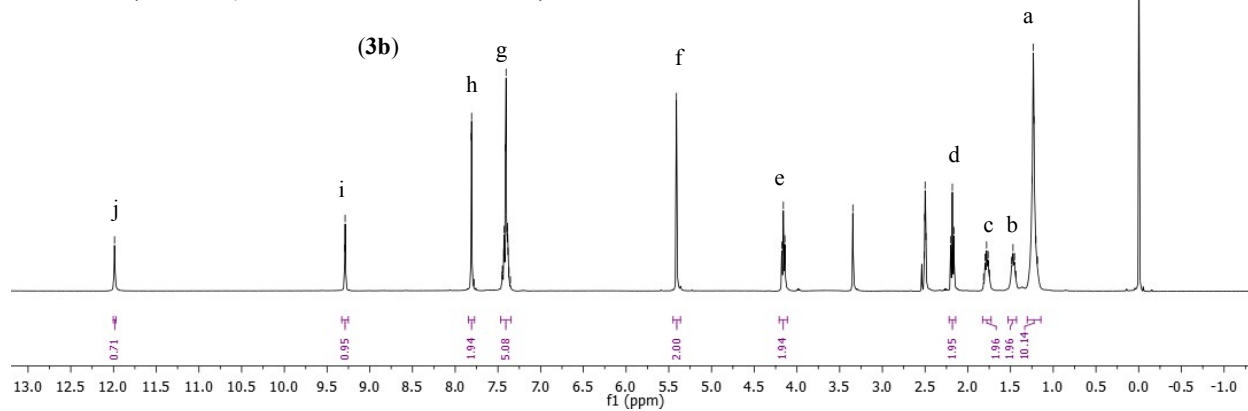
Nbenzylbromodecanoic acid bromide carbonmr
13C OBSERVE



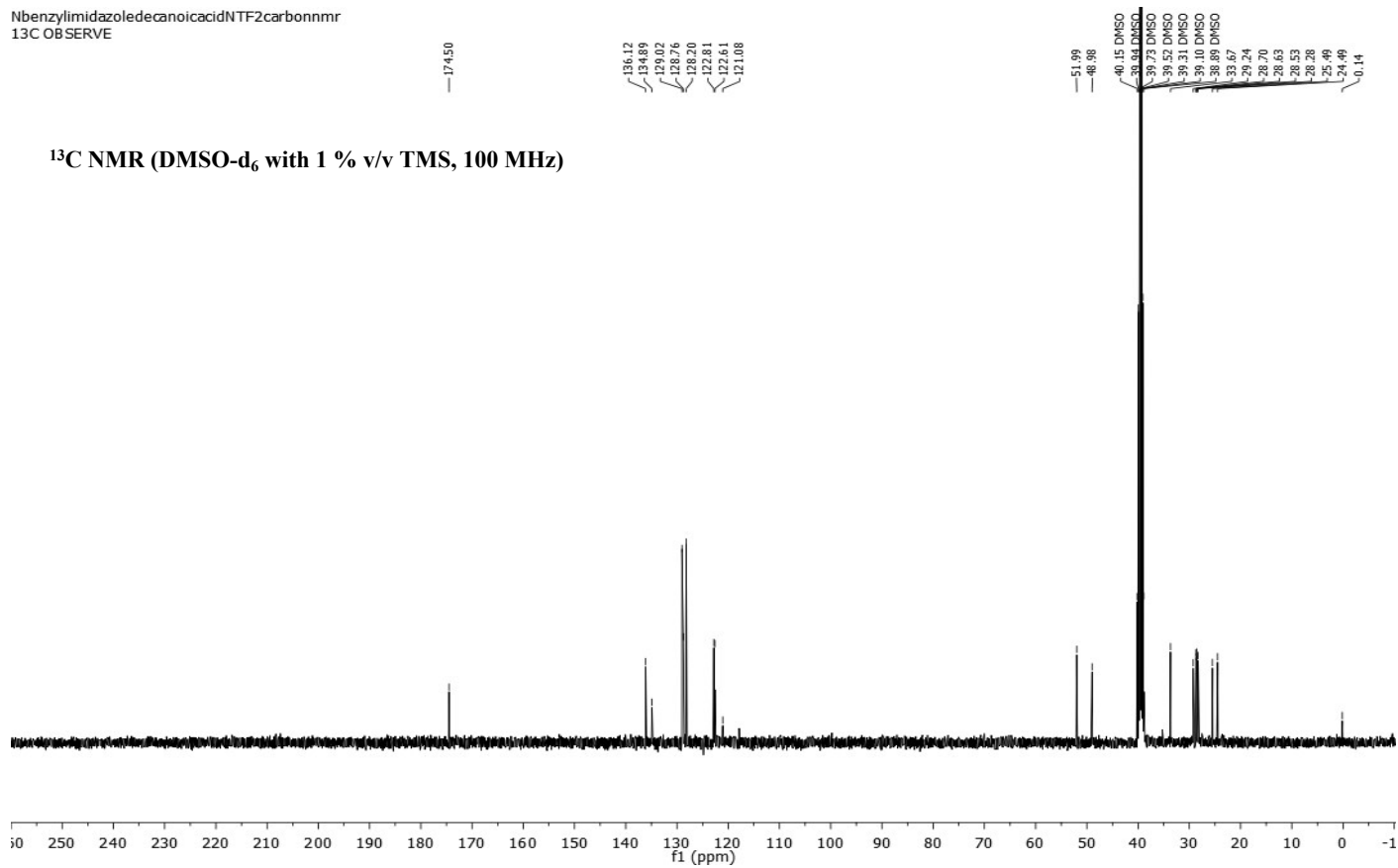
N-benzylimidazoledecanoic acidNTF2protonnmr
STANDARD 1H OBSERVE



¹H NMR (DMSO-d₆ with 1 % v/v TMS, 400 MHz)

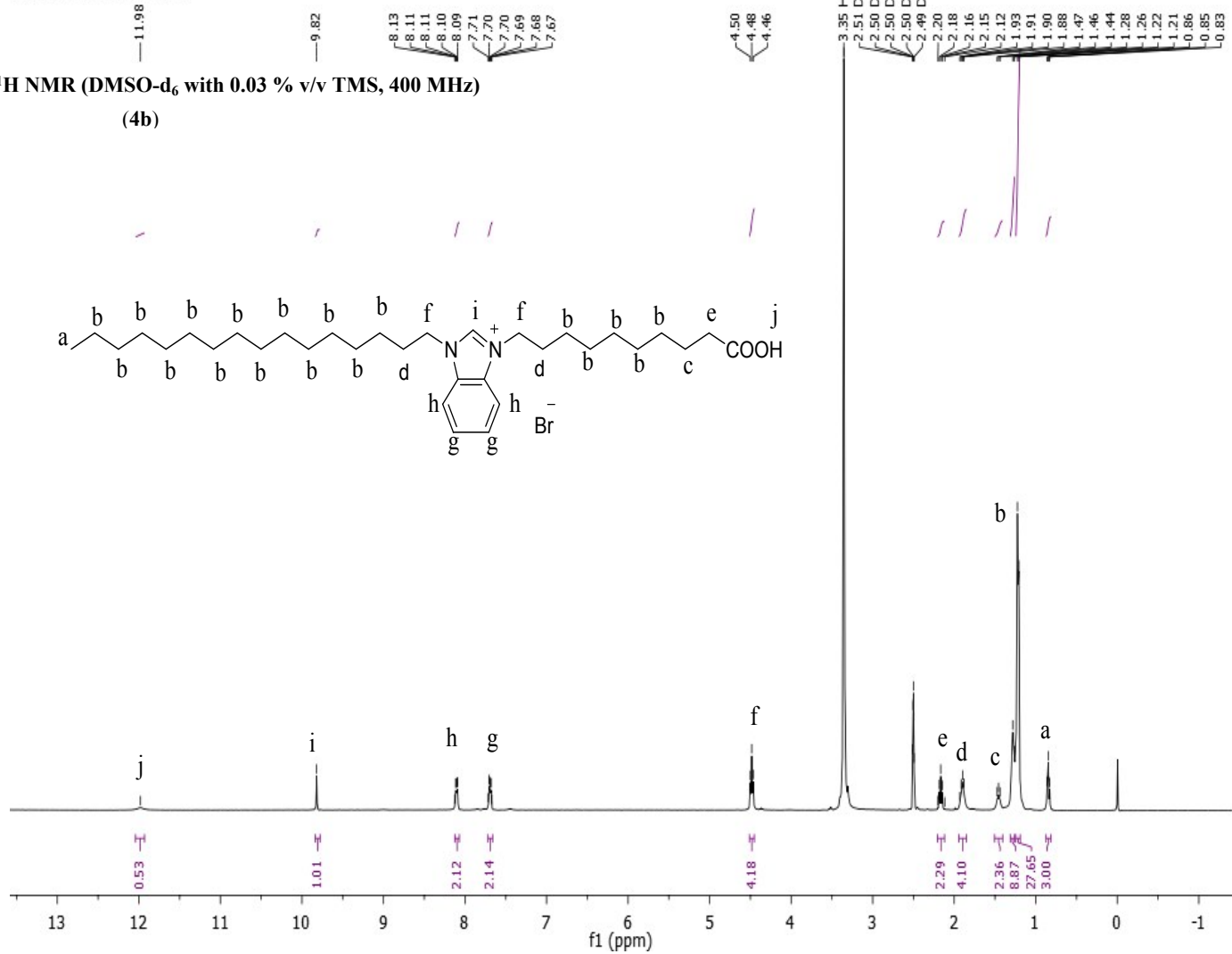


NbenzylimidazoledecanoicacidNTF2carbonnmr
13C OBSERVE

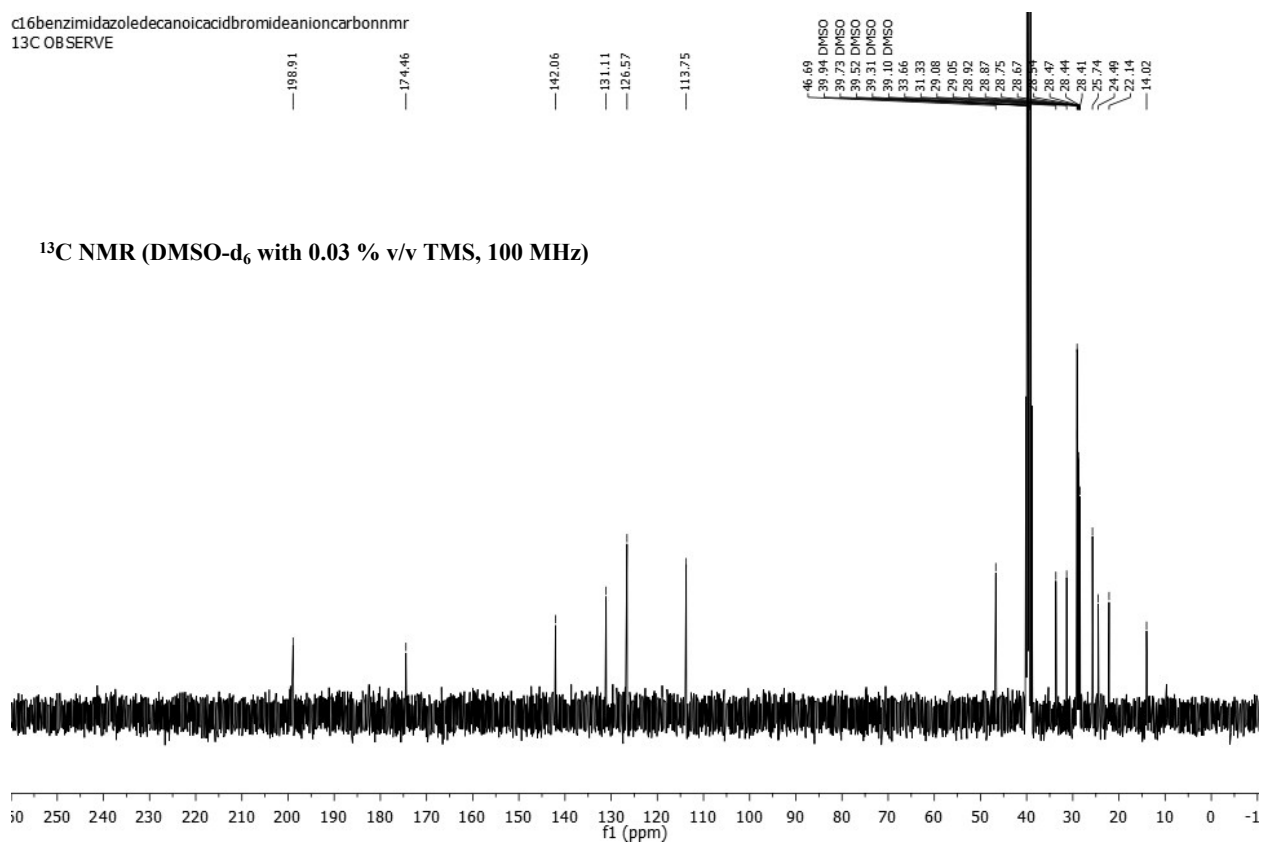


c16benzimidazolec10carboxyiacidbromideanionprotonmr
 STANDARD 1H OBSERVE

¹H NMR (DMSO-d₆ with 0.03 % v/v TMS, 400 MHz)
 (4b)



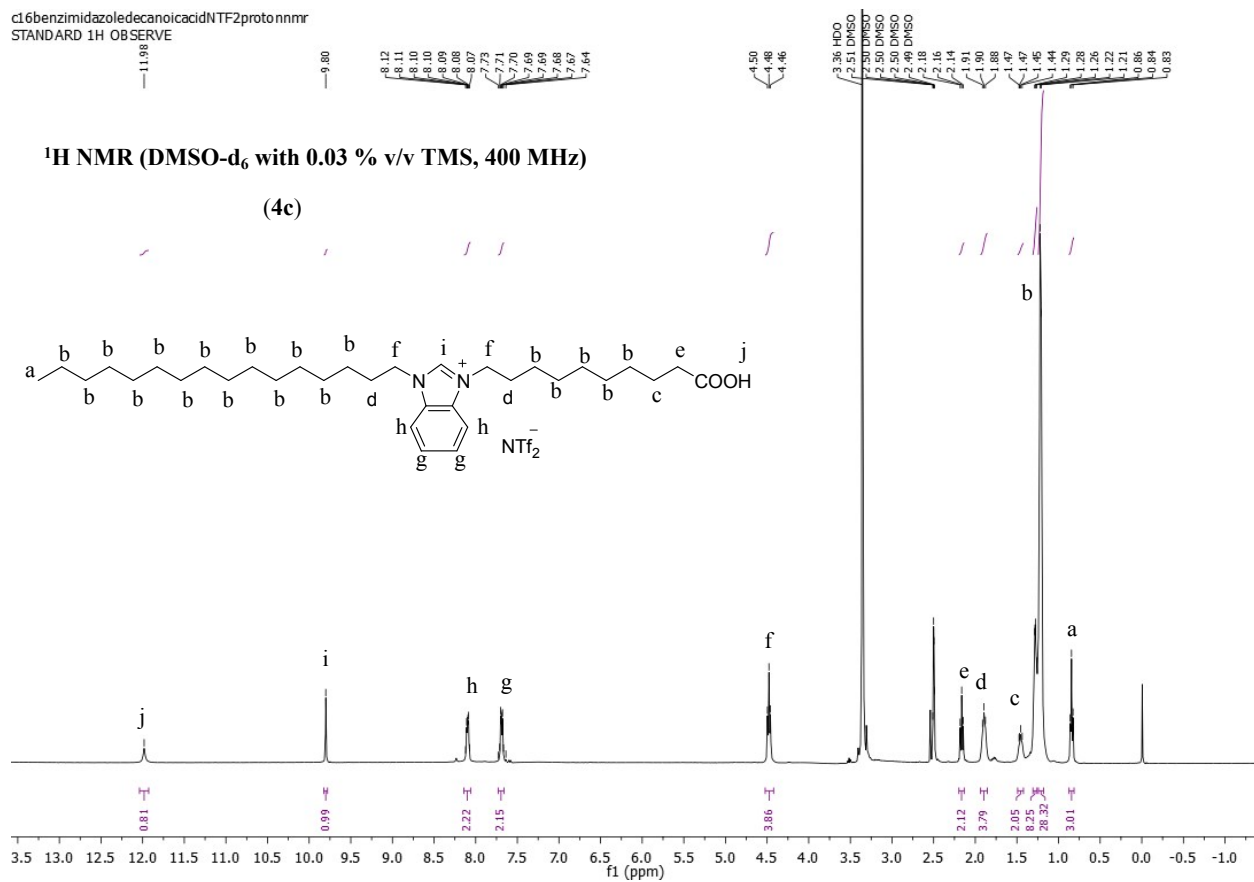
c16benzimidazoledecanoicacidbromideanioncarbonnmr
13C OBSERVE

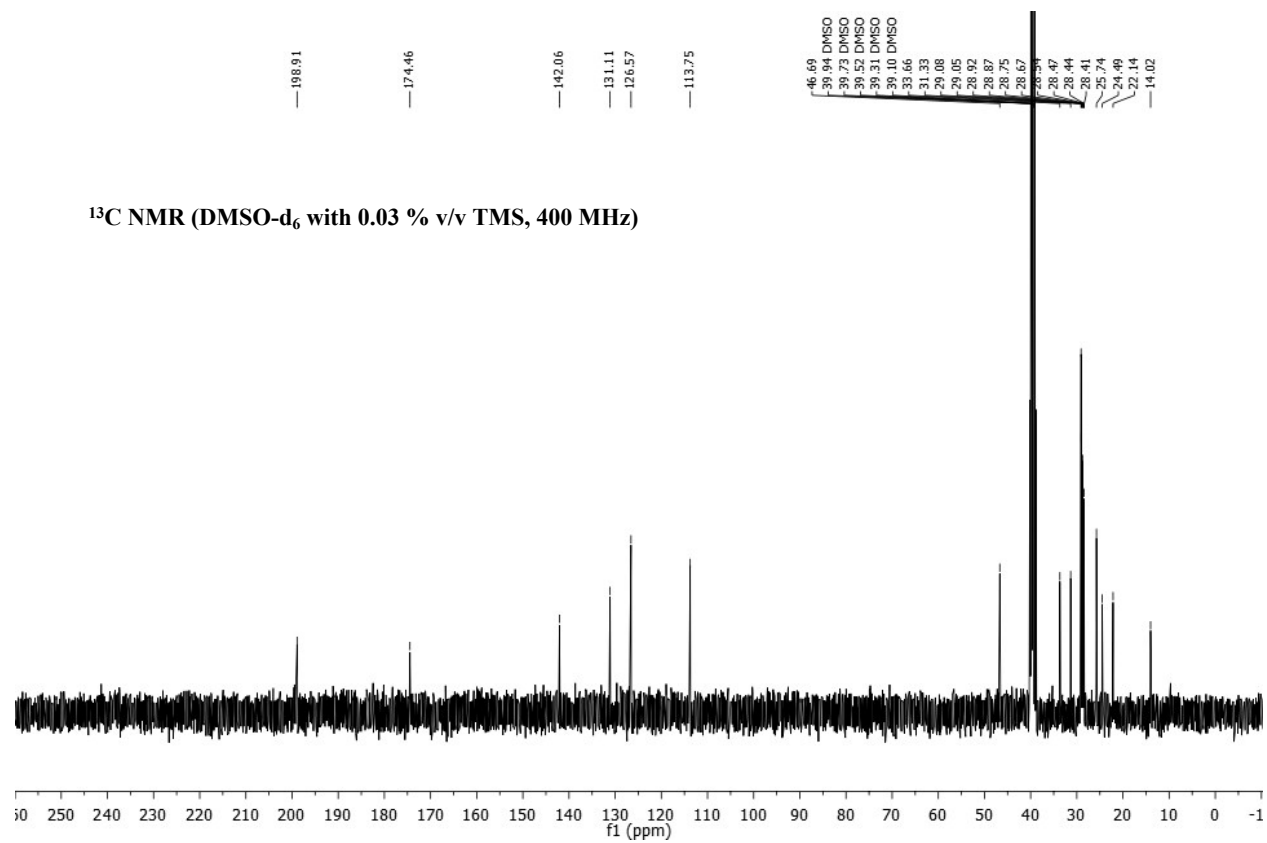


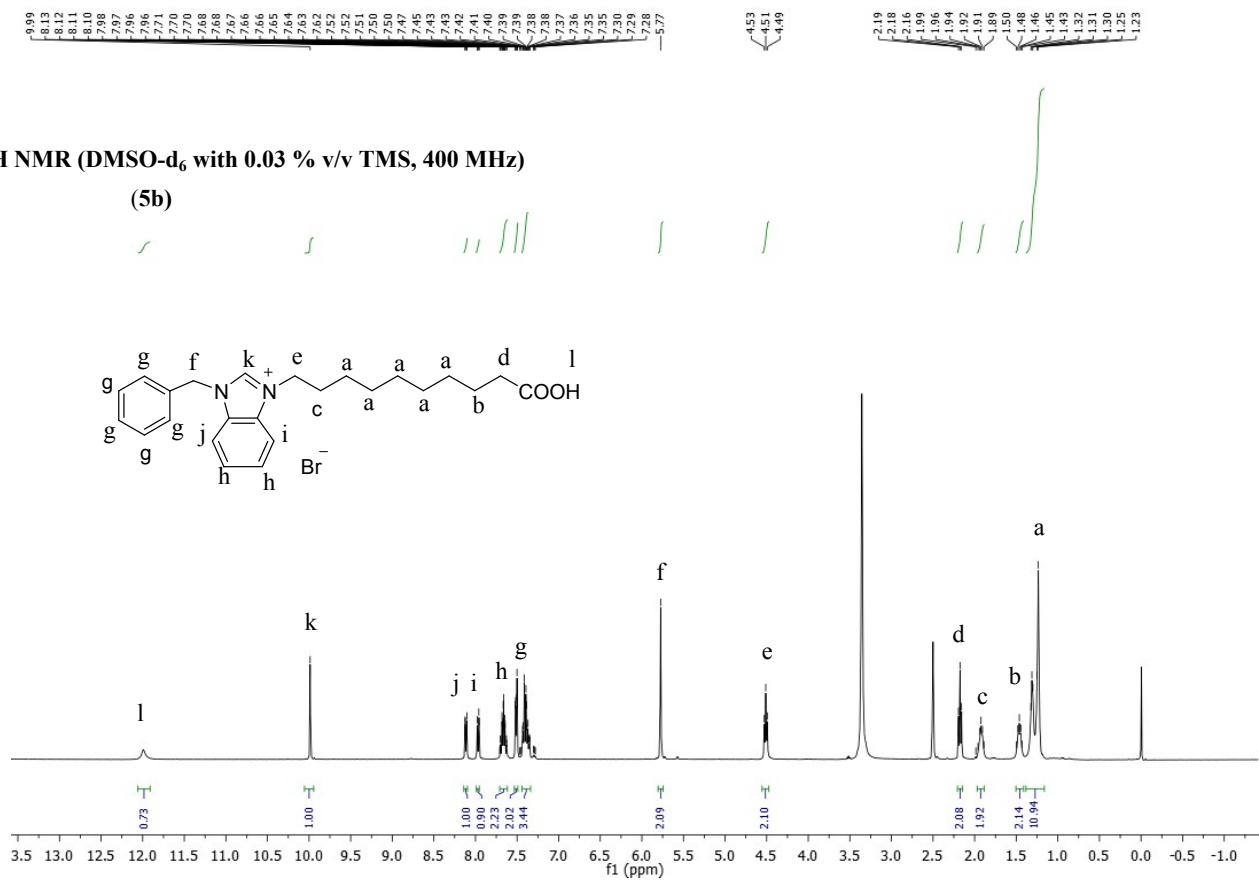
c16benzimidazoledecanoicacidNTF2proto nmr
STANDARD 1H OBSERVE

¹H NMR (DMSO-d₆ with 0.03 % v/v TMS, 400 MHz)

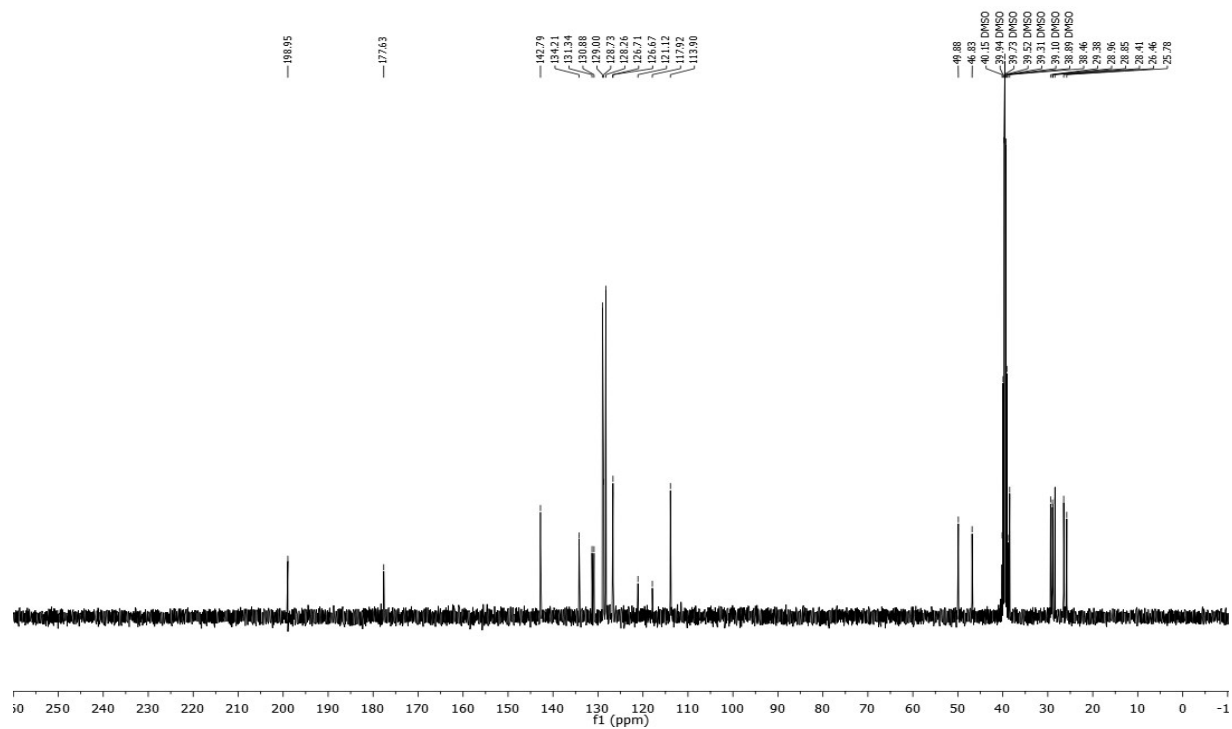
(4c)





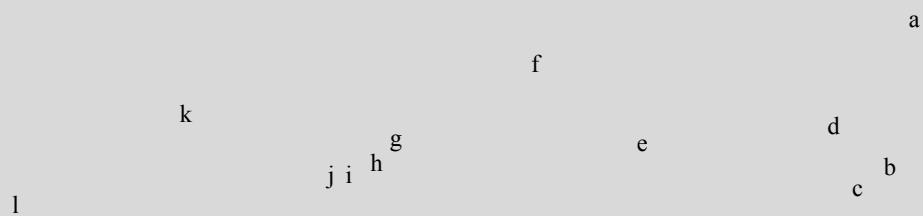
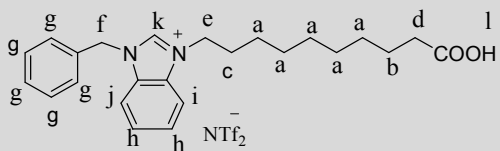


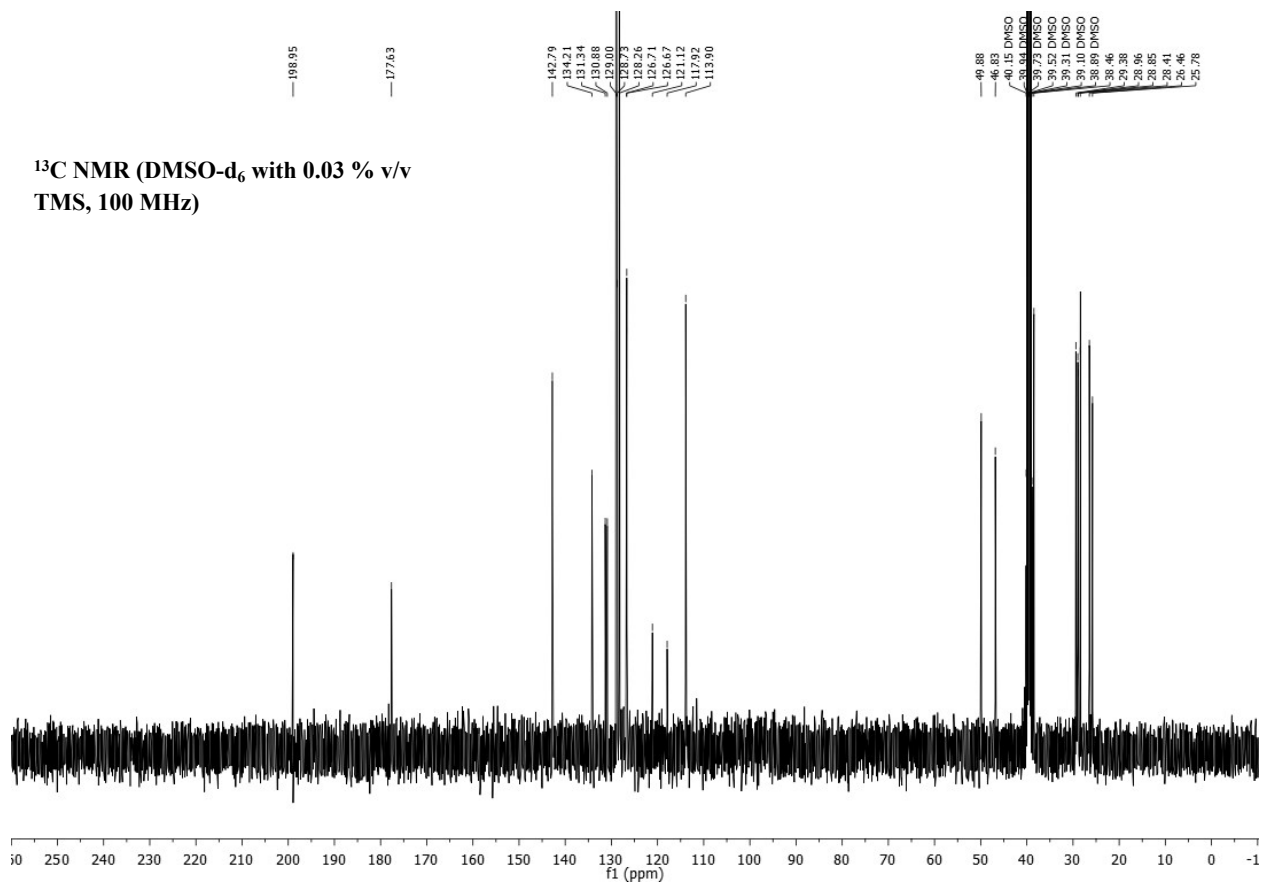
¹³C NMR (DMSO-d₆ with 0.03 % v/v TMS, 100 MHz)



¹H NMR (DMSO-d₆ with 0.03 % v/v TMS, 400 MHz)

(5c)





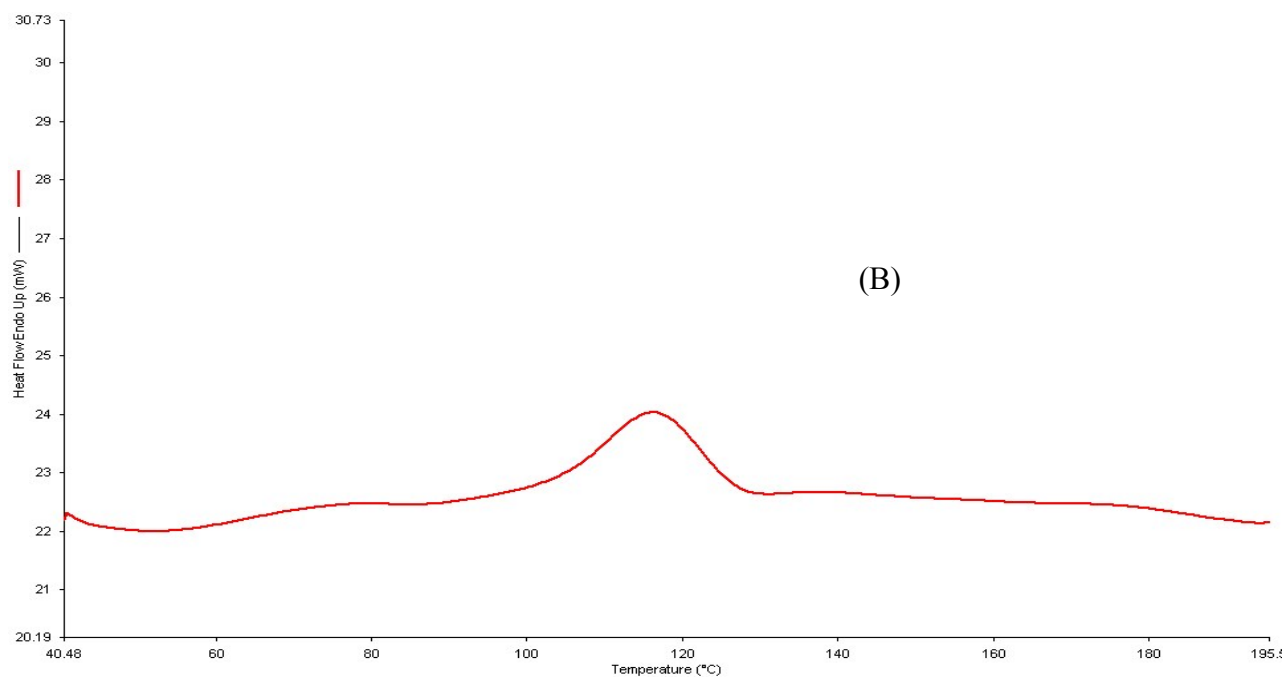
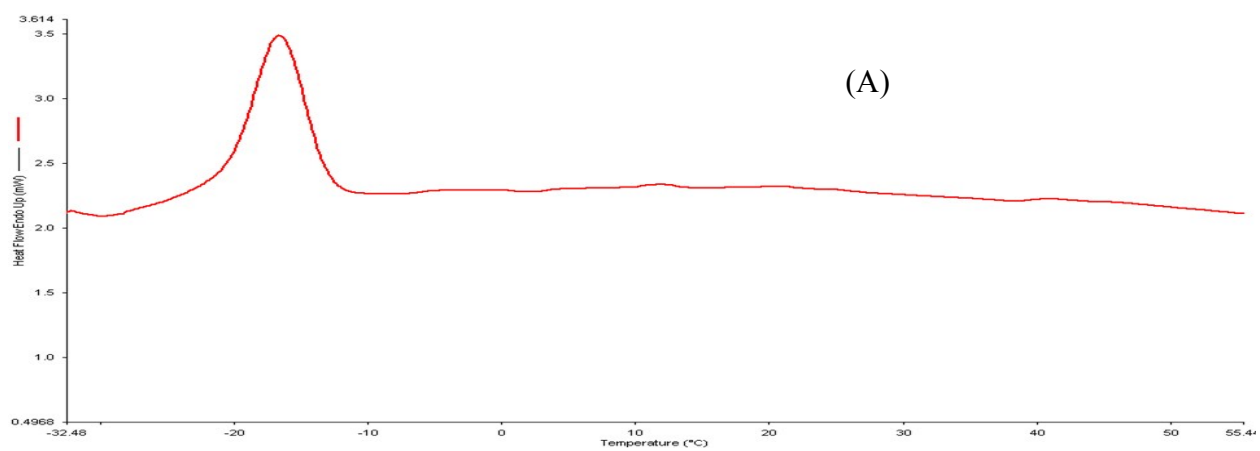


Figure S1. DSC traces of (A) MIL **1**; (B) dicationic MIL intermediate **2b**;

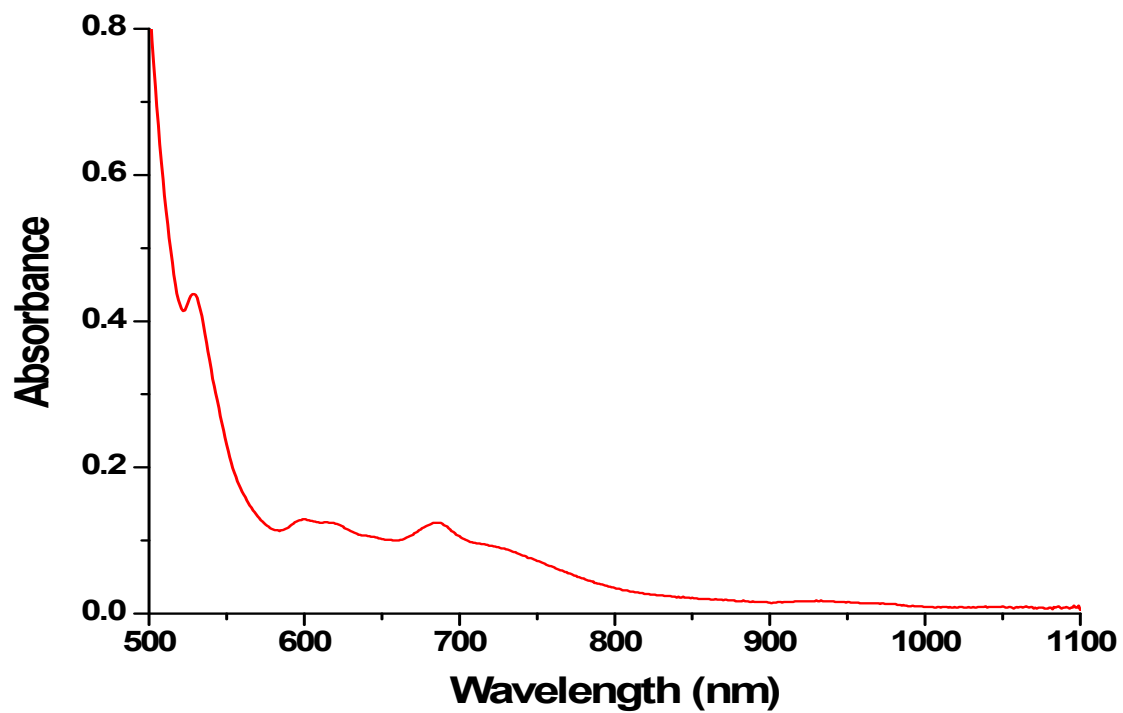


Figure S2. Absorbance spectrum of bromotrichloroferrate $[\text{FeCl}_3\text{Br}^-]$ anion

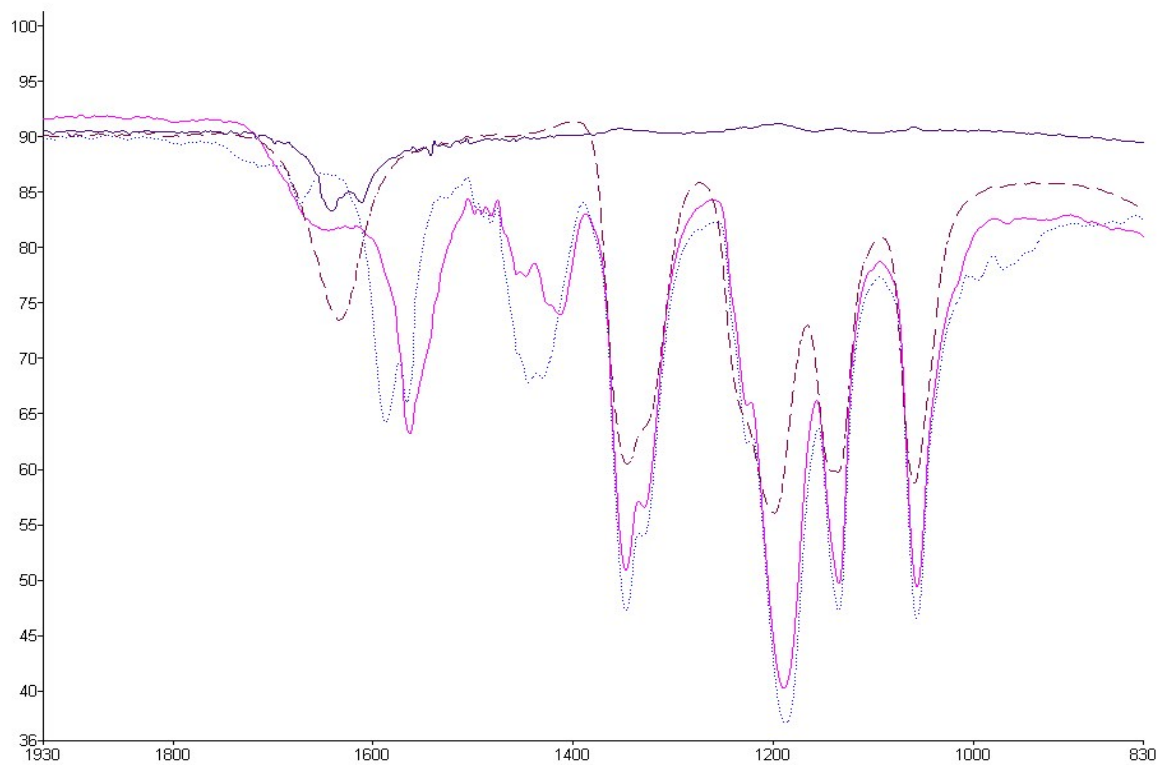


Figure S3. Representative IR overlay for Fe(III) carboxylate-based hydrophobic MIL 4 and compounds involved in its synthesis. FeCl₃·6H₂O (—); LiNTf₂ (- - -); Compound 4d (—); MIL 4 (.....)

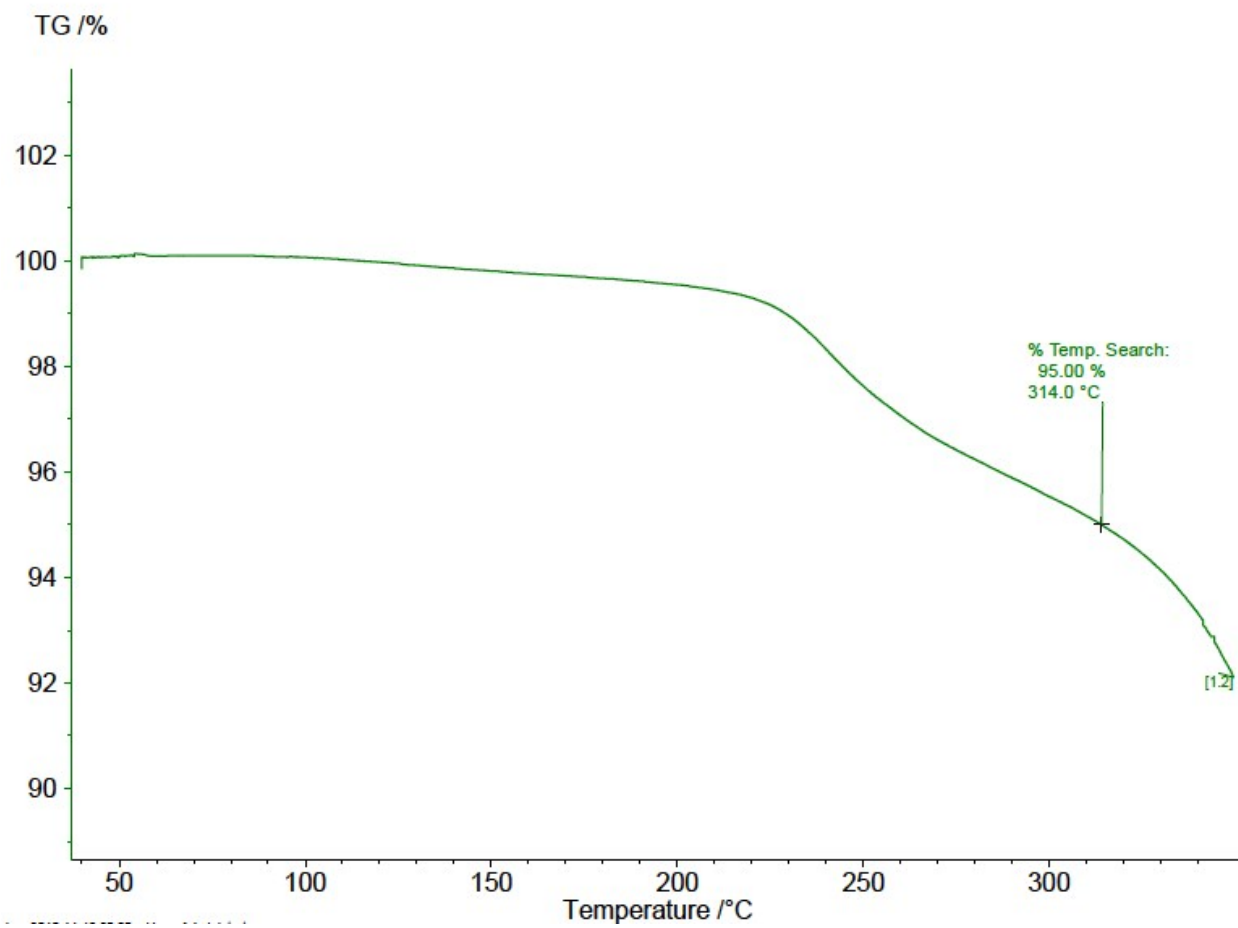


Figure S4. Representative TGA trace for hydrophobic MIL 3.

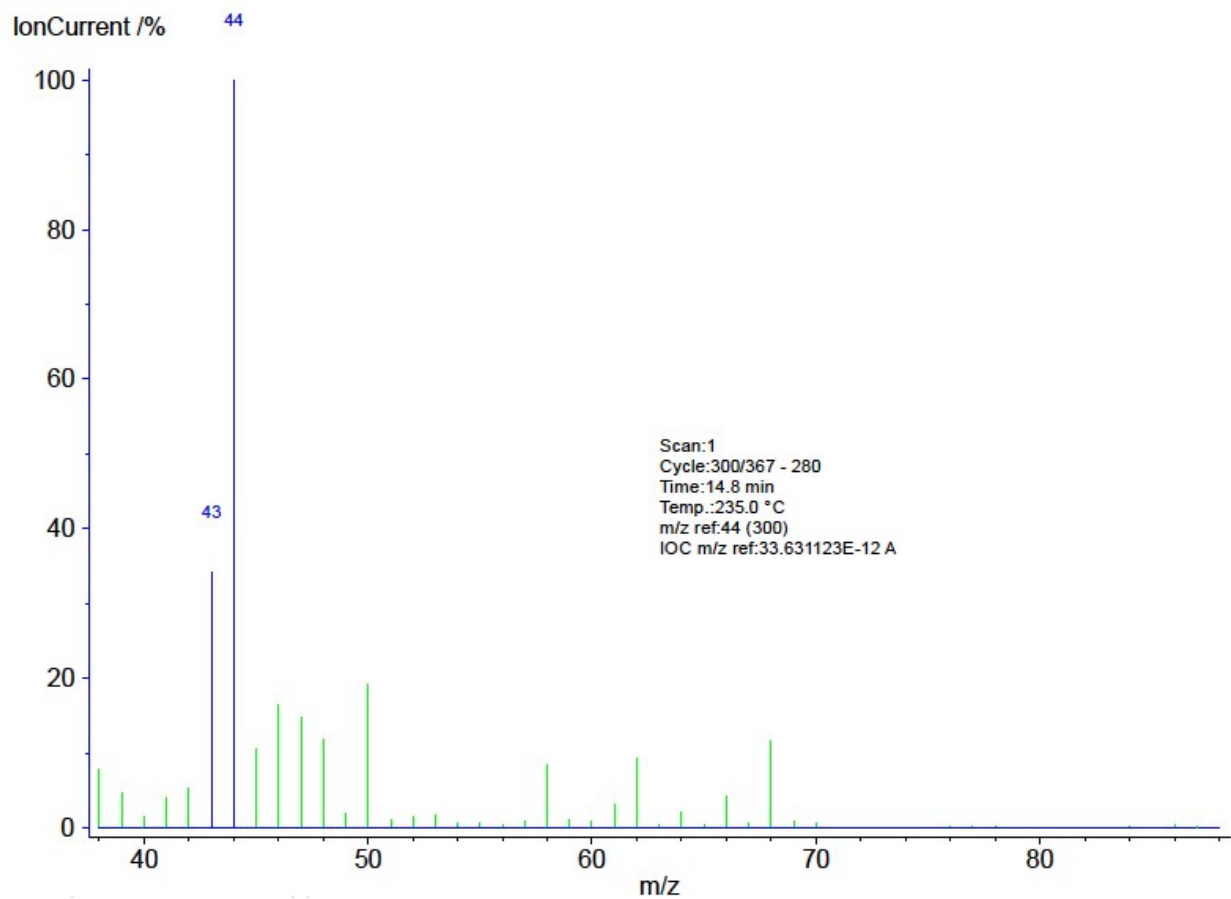


Figure S5. Mass spectrum of the evolved gases during the TGA experiment for the Fe(III) carboxylate-based MIL **3**. The spectrum shown was collected when the sample temperature was 235 °C.

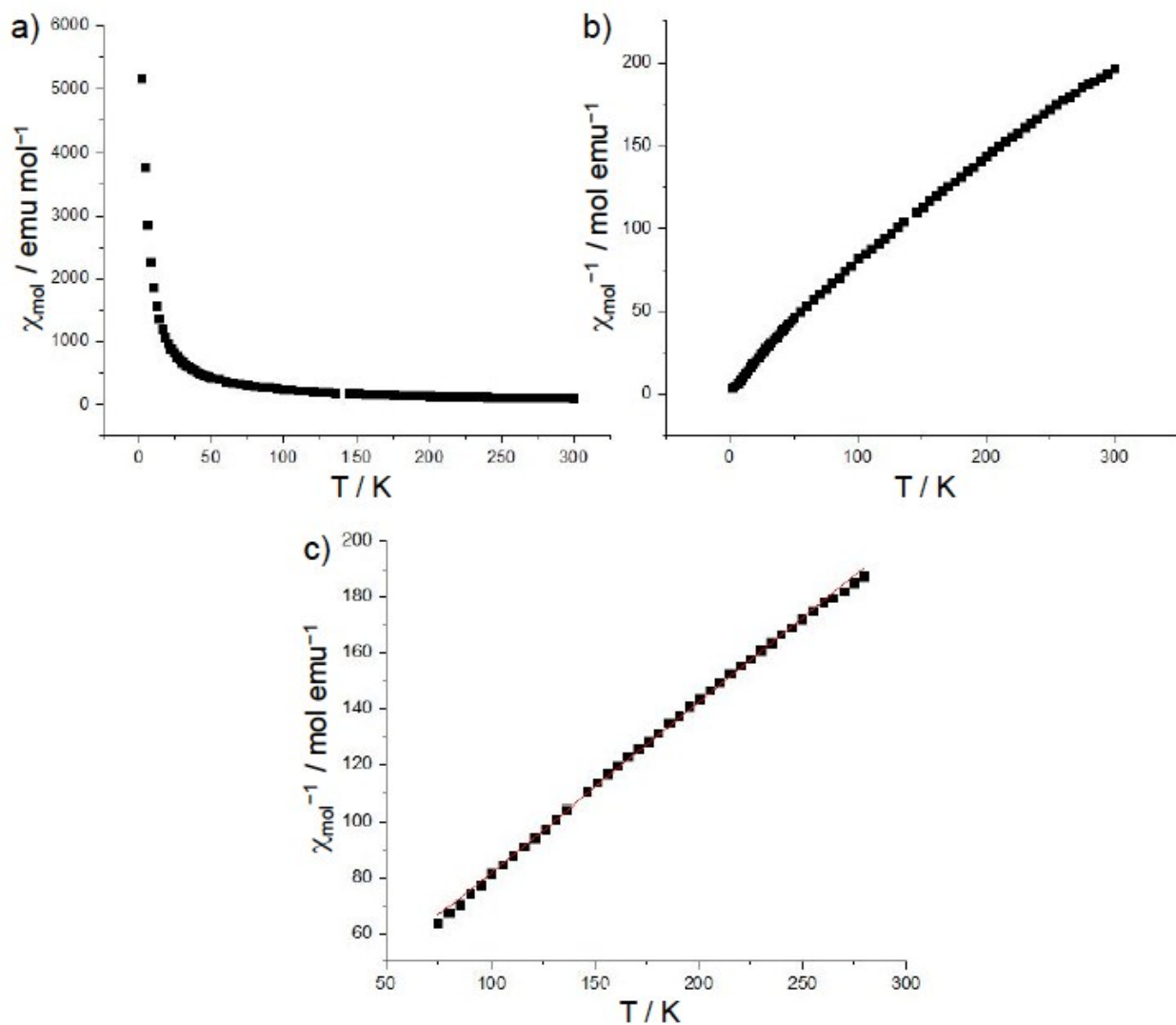


Figure S6. Temperature dependence of the (a) molar magnetic susceptibility and the (b) reciprocal molar susceptibility for MIL 3 using a field of 20,000 Oe. Panel (c) shows the linear fit for reciprocal molar susceptibility versus temperature from 280 K down to 75 K.

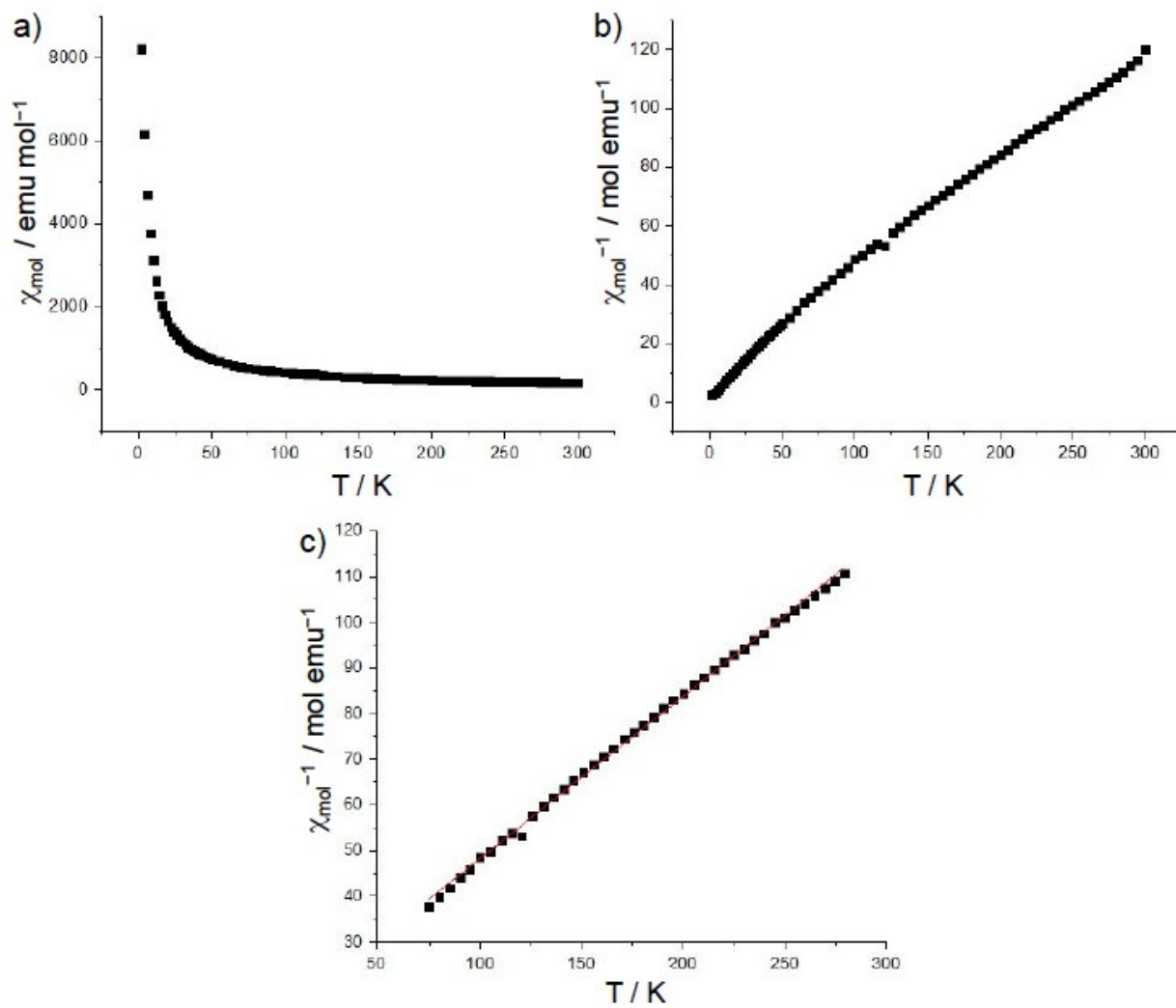


Figure S7. Temperature dependence of the (a) molar magnetic susceptibility, the (b) reciprocal molar susceptibility, and the (c) linear fit for reciprocal molar susceptibility versus temperature from 280 K down to 75 K for MIL **5** using a field of 20,000 Oe.