

Supporting Information

Synthesis of Dual Functional Pyrimidinium Ionic Liquids as Reaction Media and Antimicrobial Agents

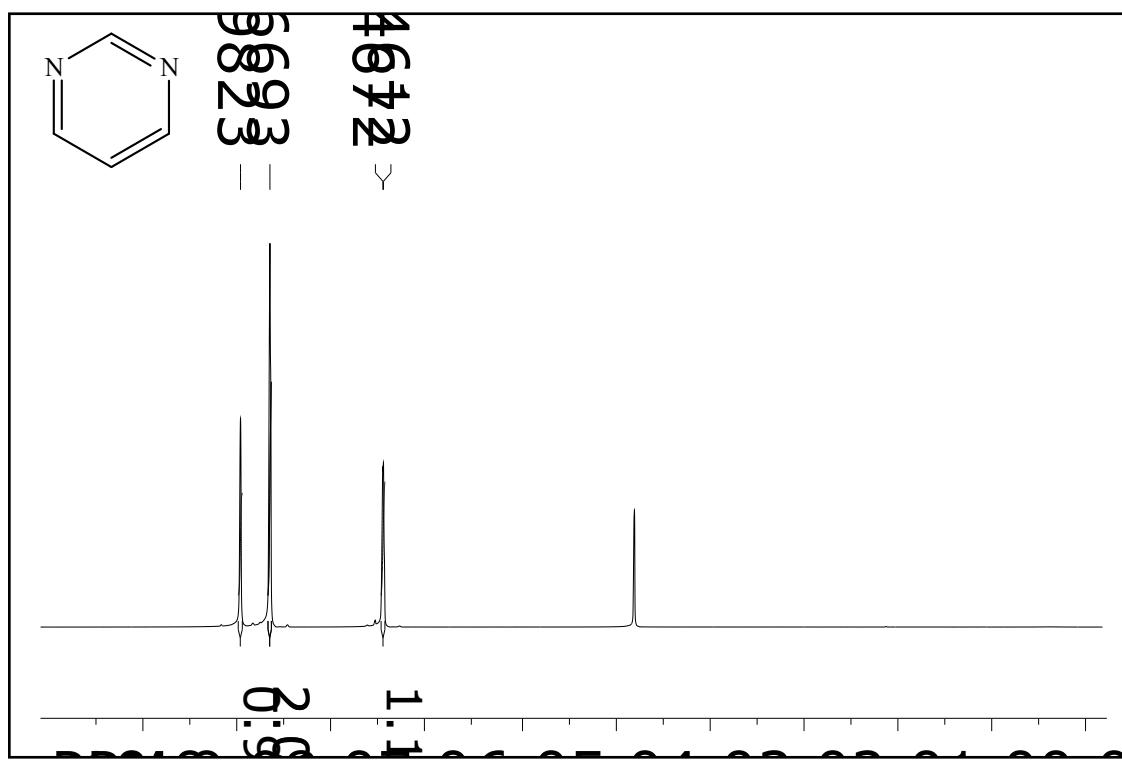
Kamna Goel, Smritilekha Bera, Man Singh, and Dhananjoy Mondal*

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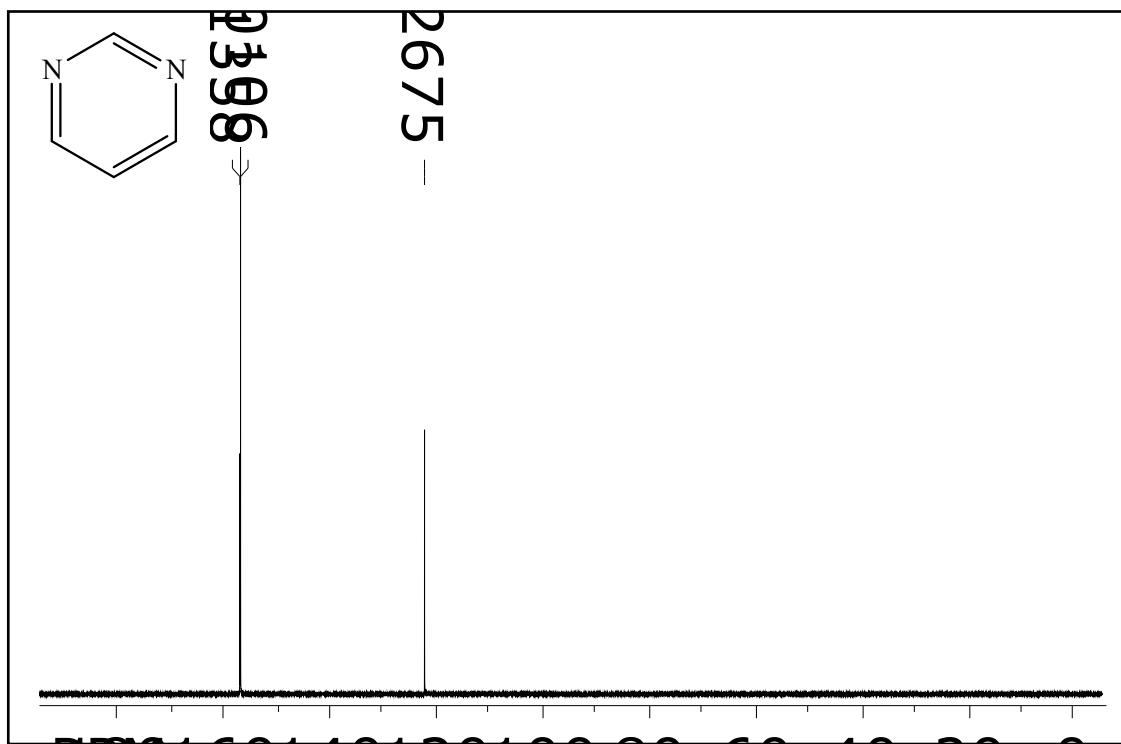
dhananjoym@yahoo.com

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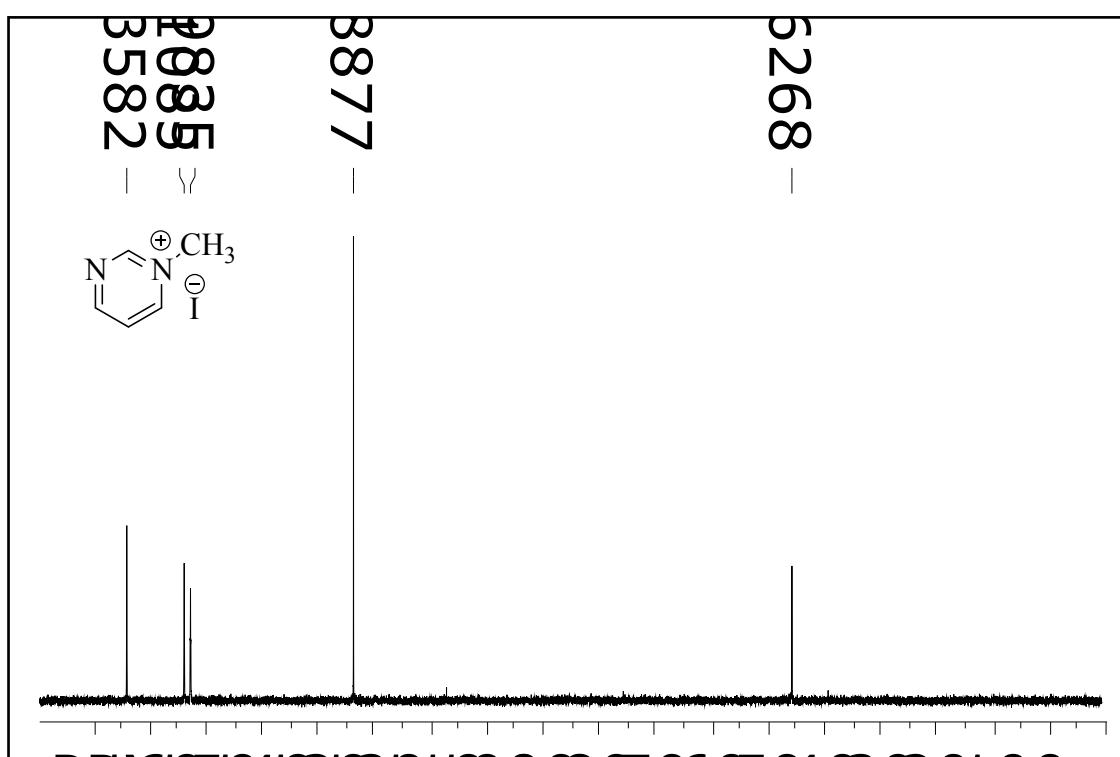
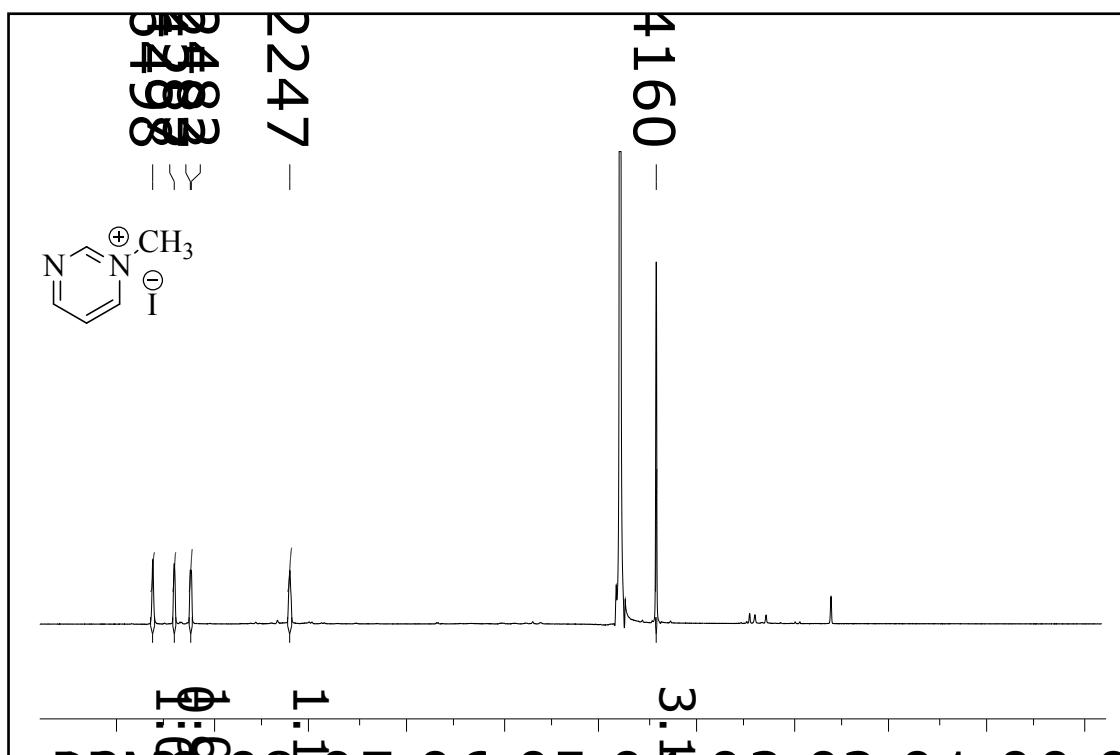
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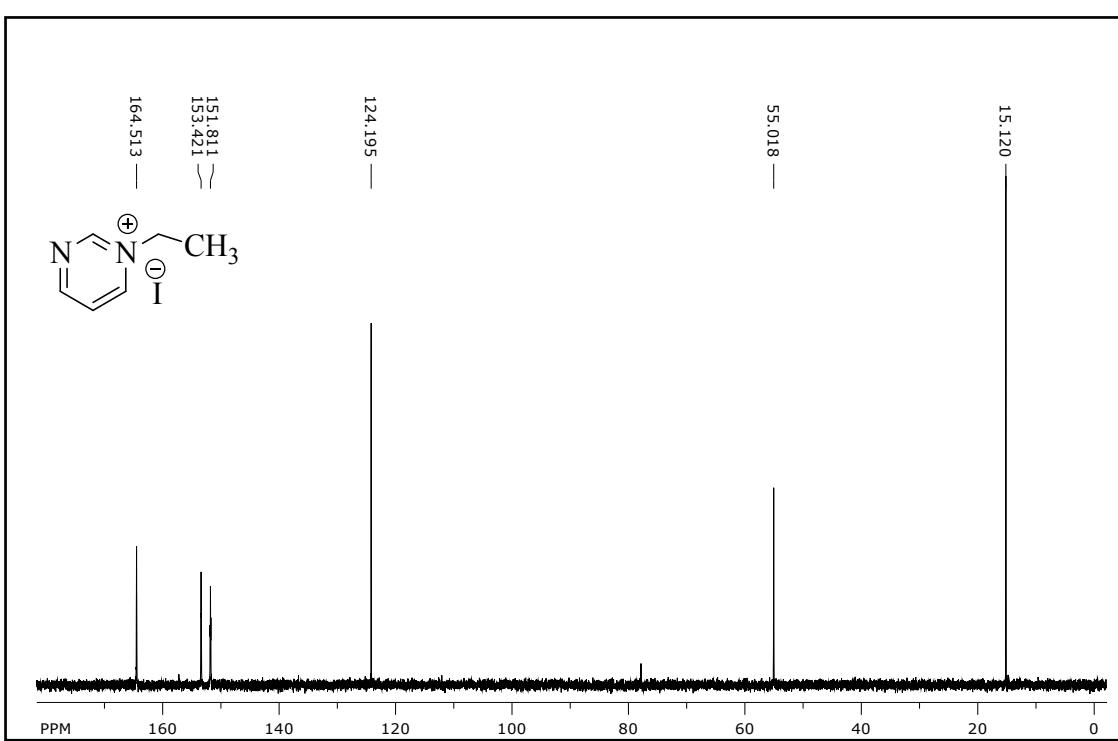
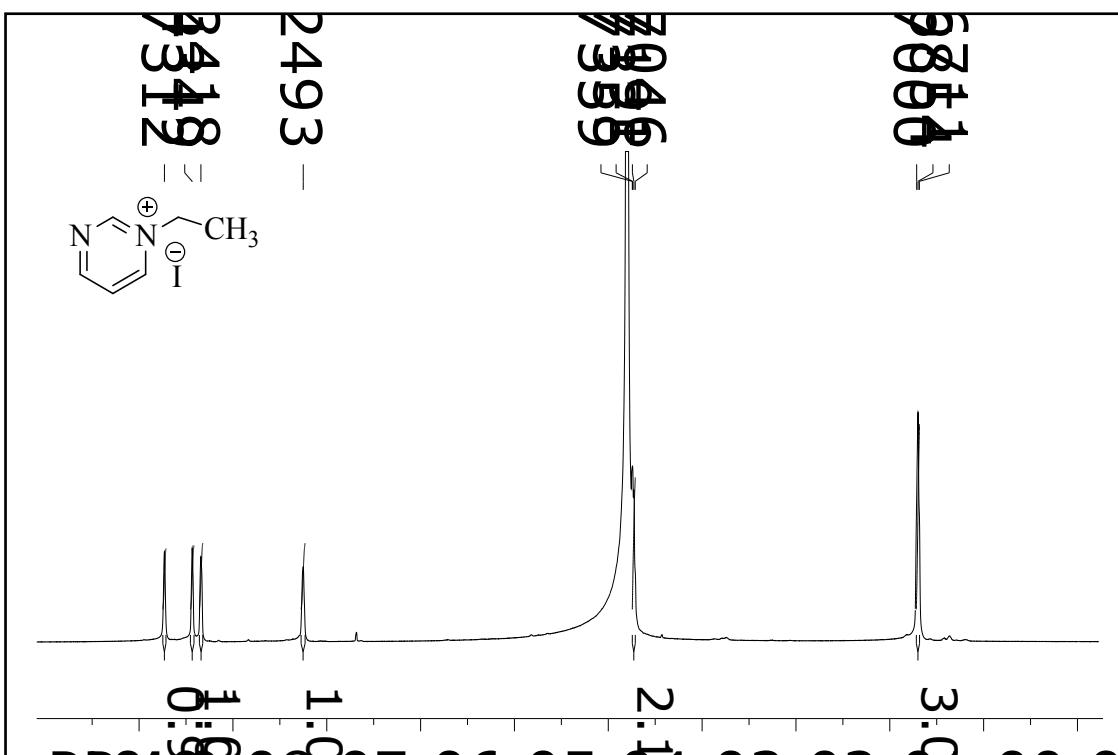


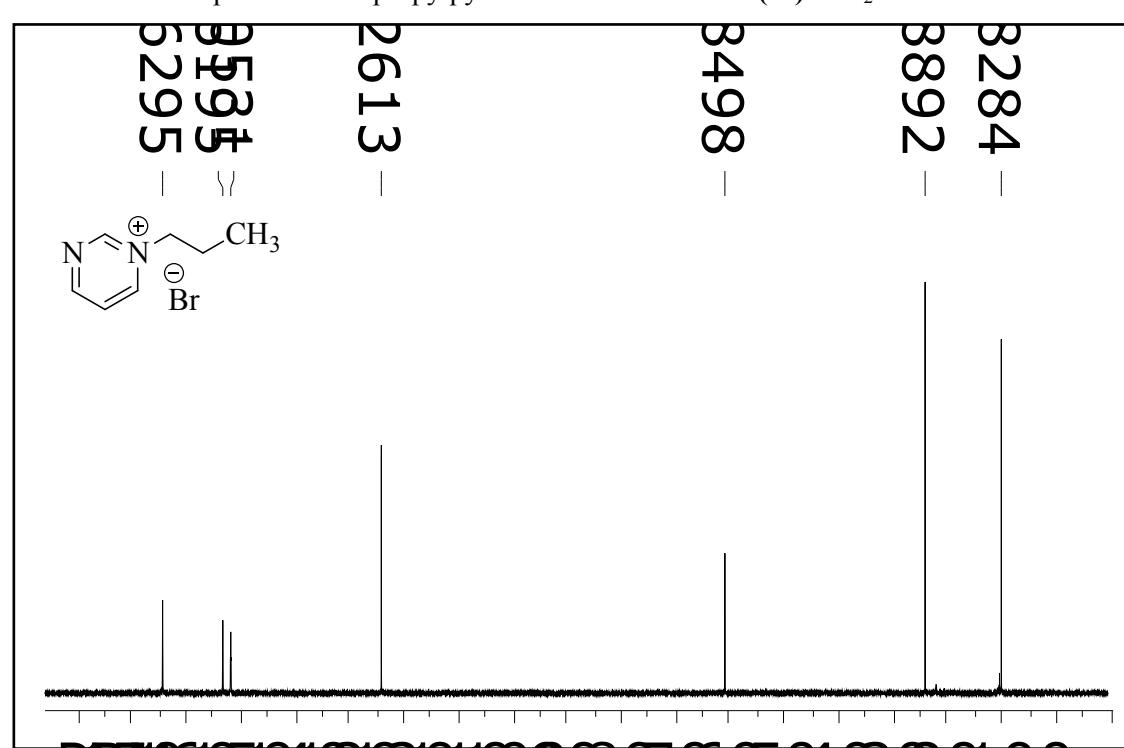
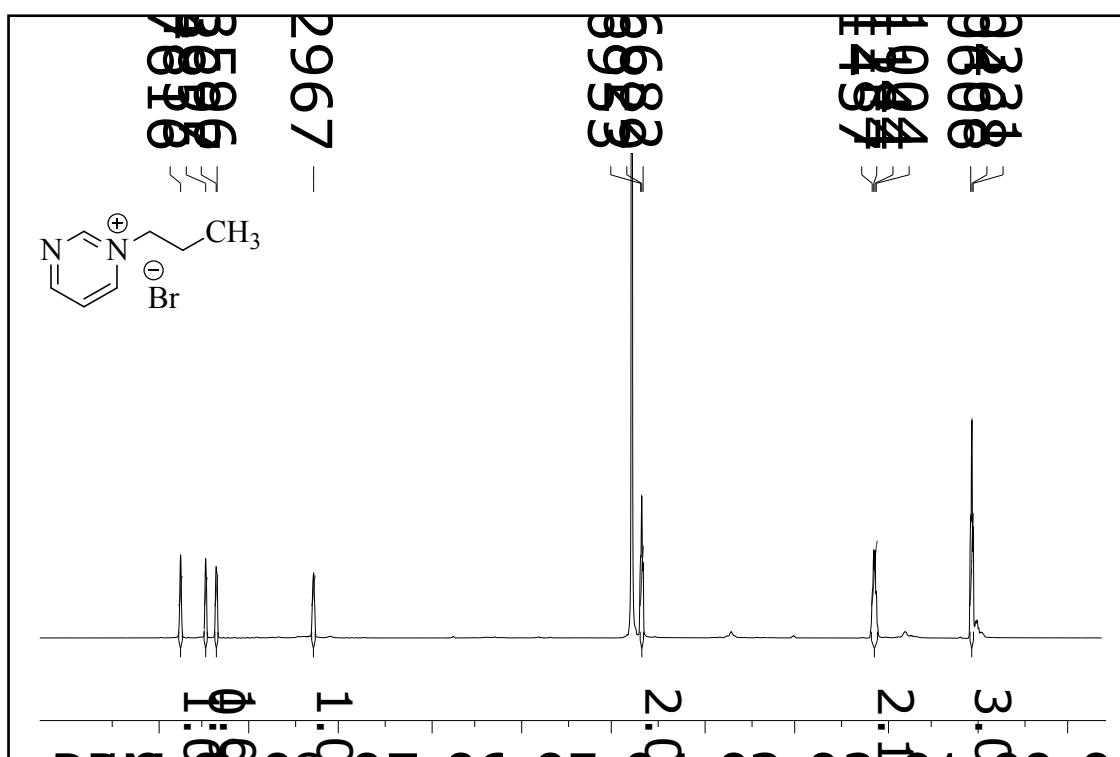
¹H NMR spectrum of pyrimidine (**1a**) in D_2O at 500 MHz

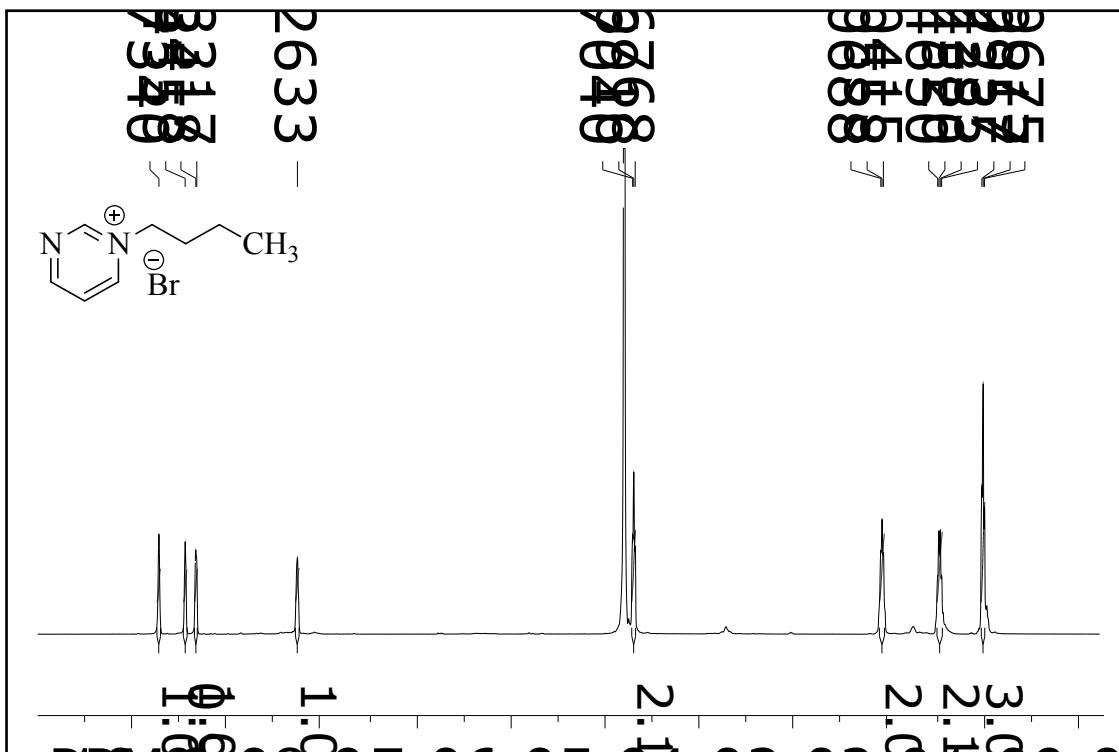


¹³C NMR spectrum of pyrimidine (**1a**) in D_2O at 500 MHz

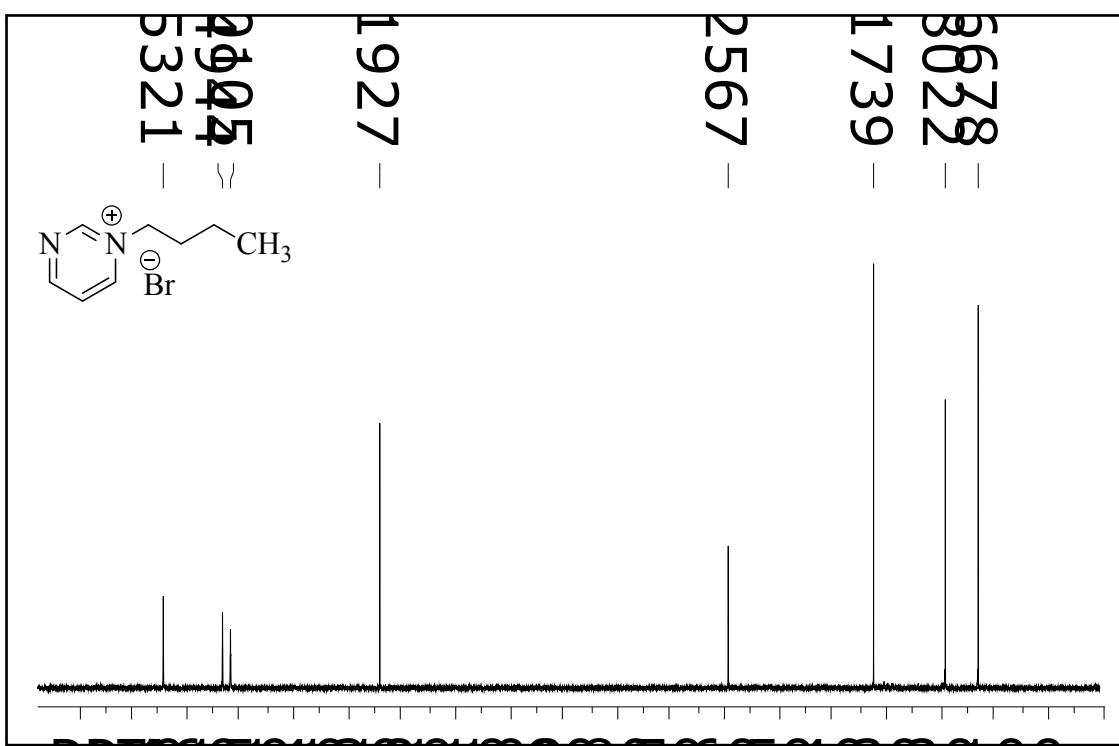




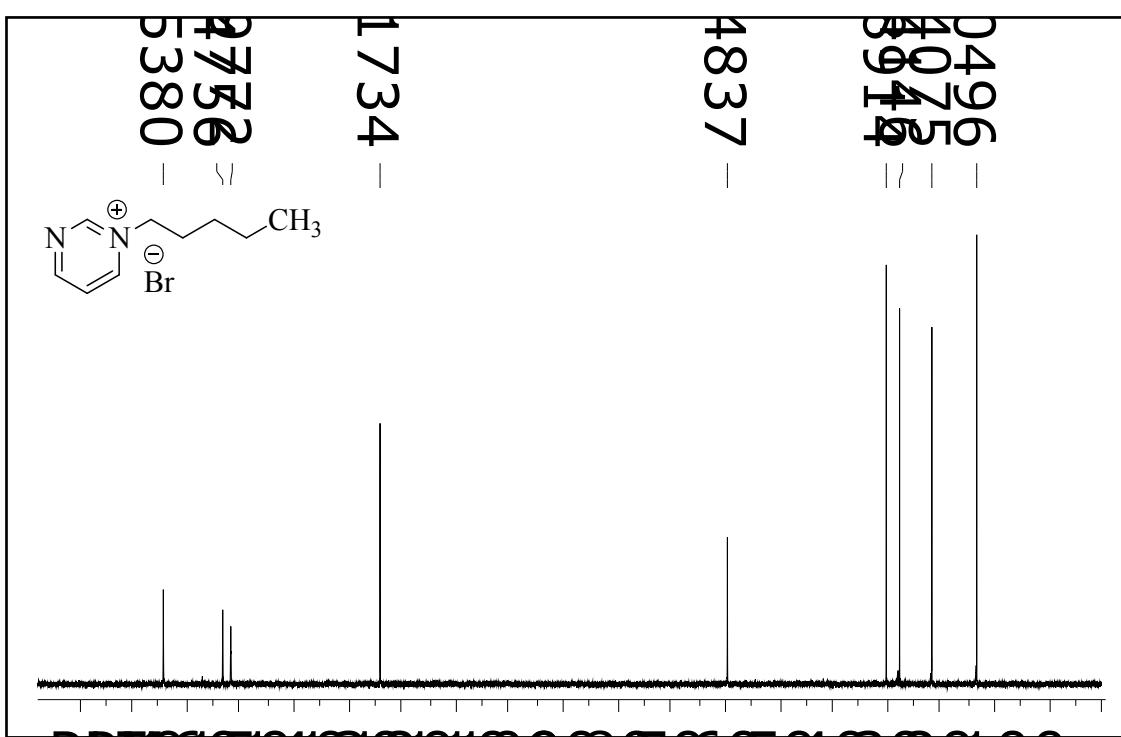
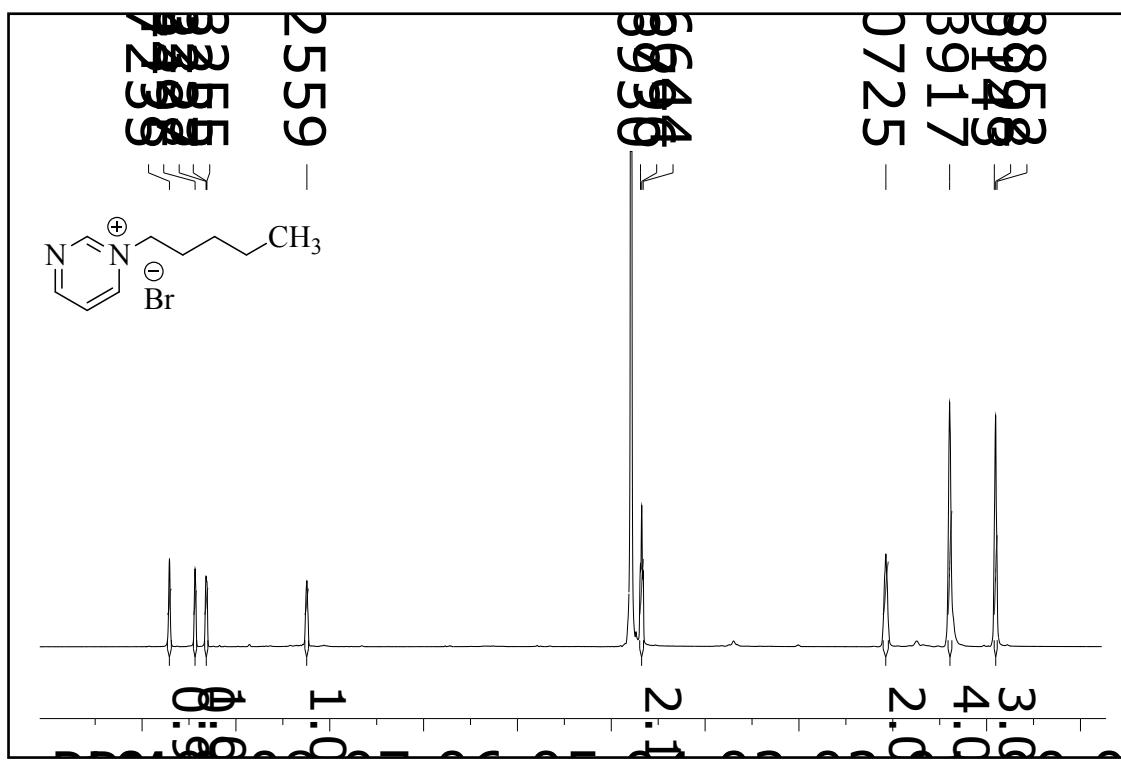


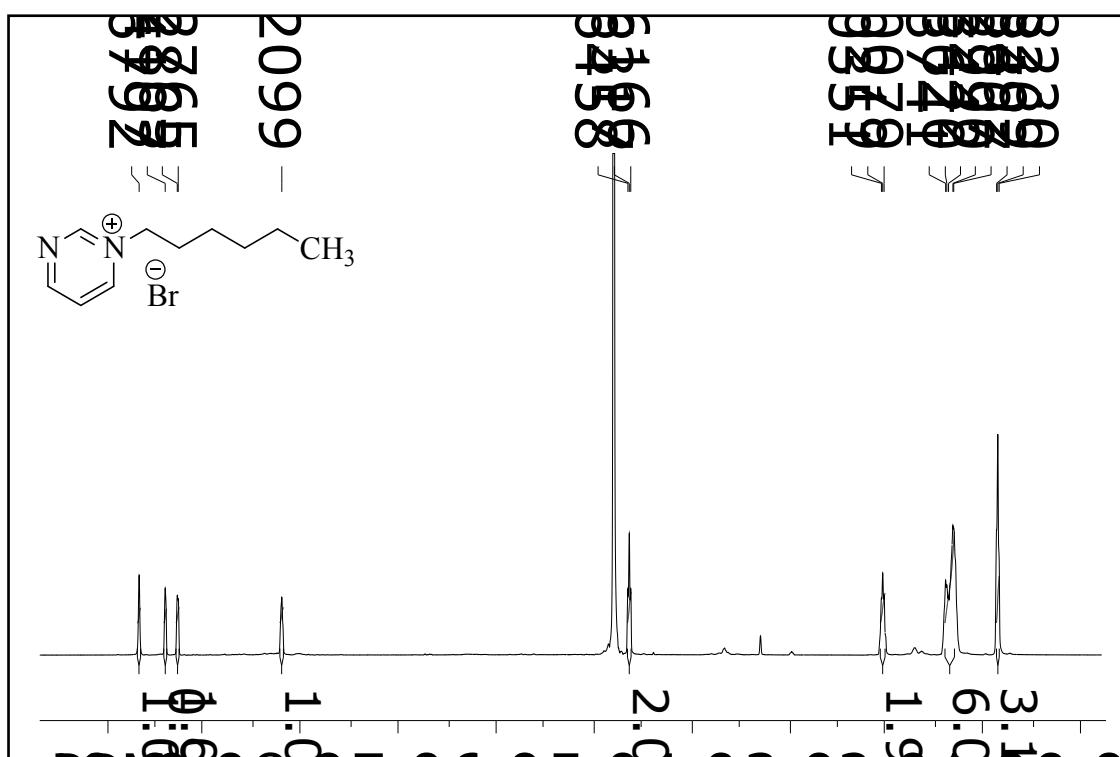


¹H NMR spectrum of 1-butylpyrimidin-1-ium bromide (**2d**) in D₂O at 500 MHz

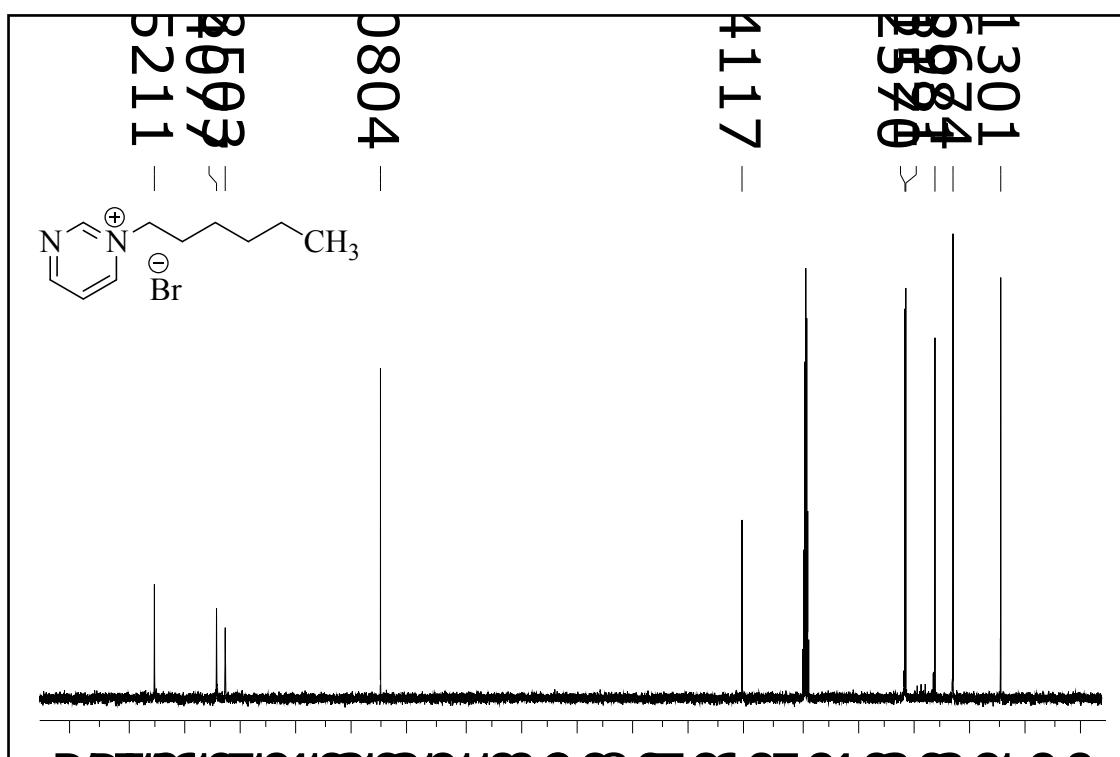


¹³C NMR spectrum of 1-butylpyrimidin-1-i um bromide (**2d**) in D₂O at 500 MHz

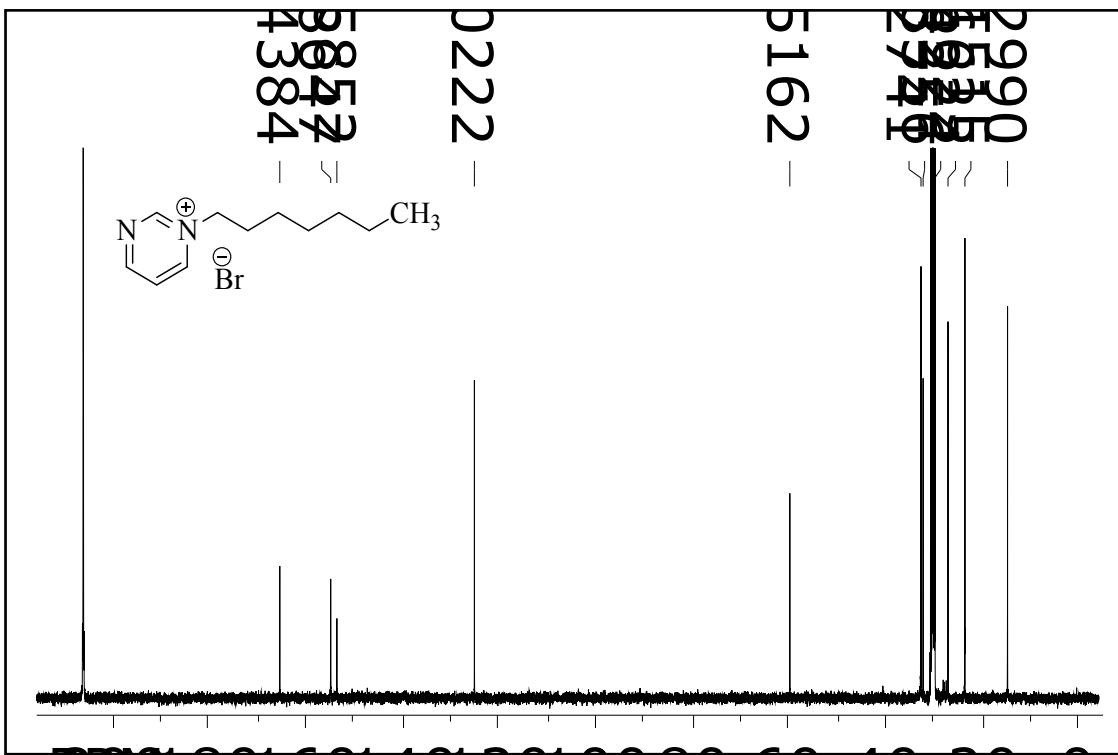
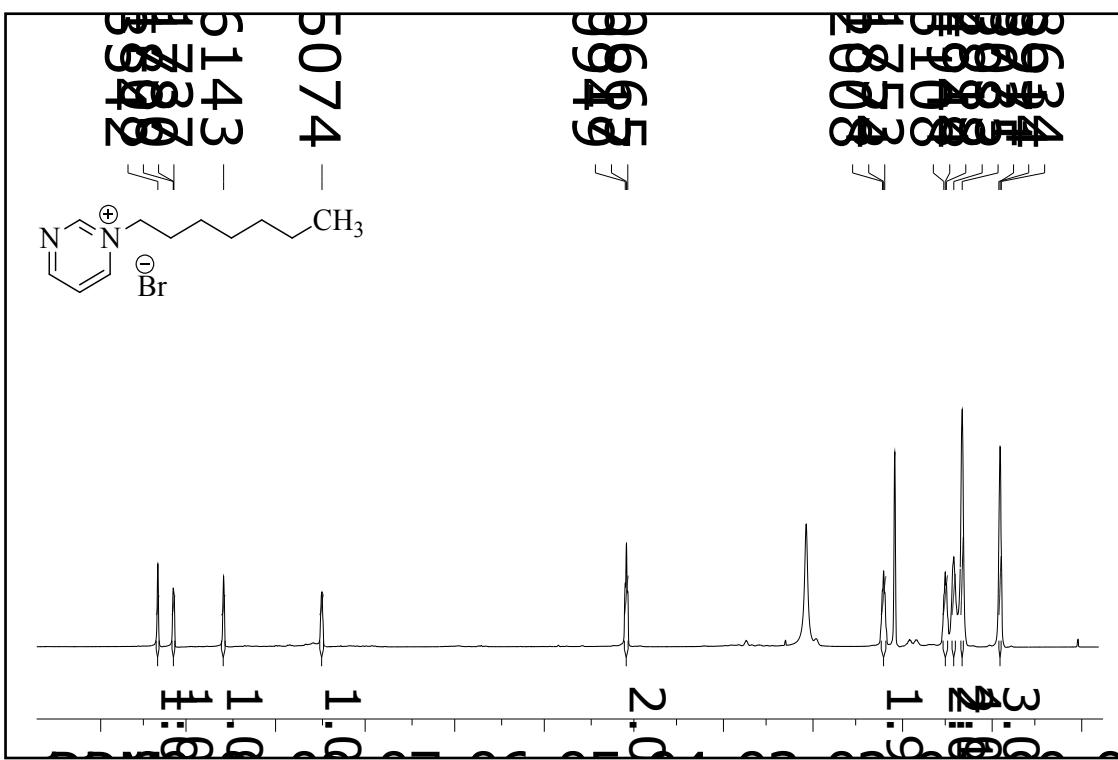


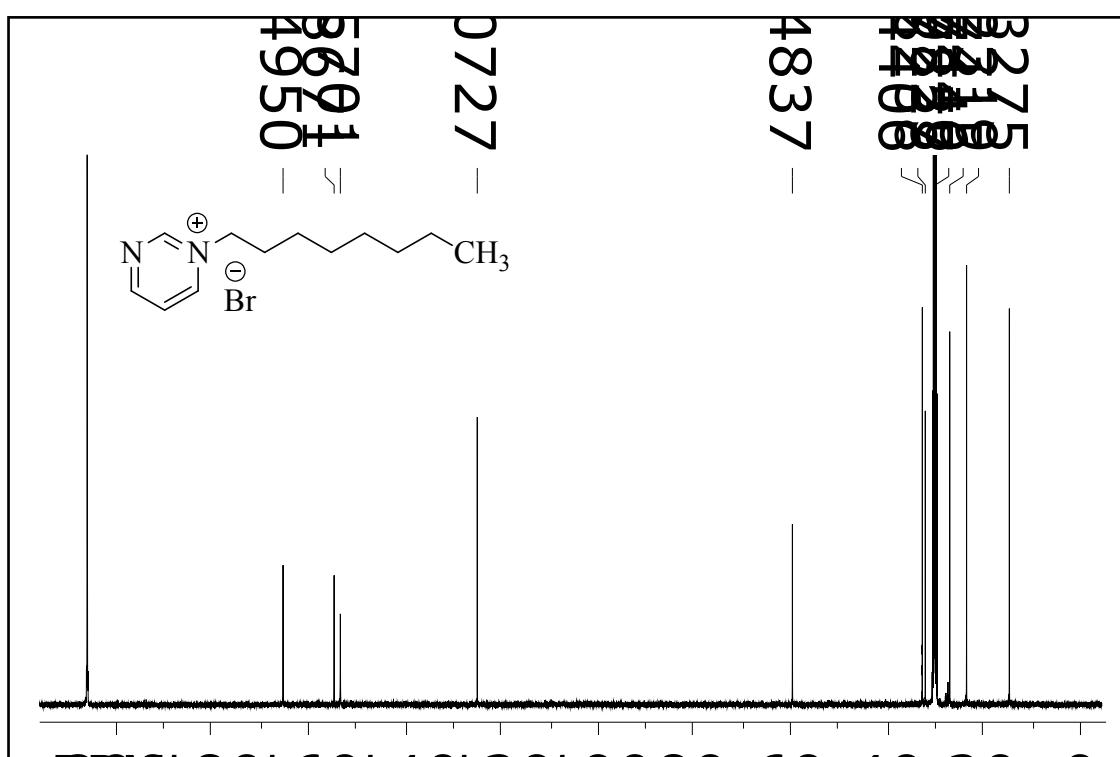
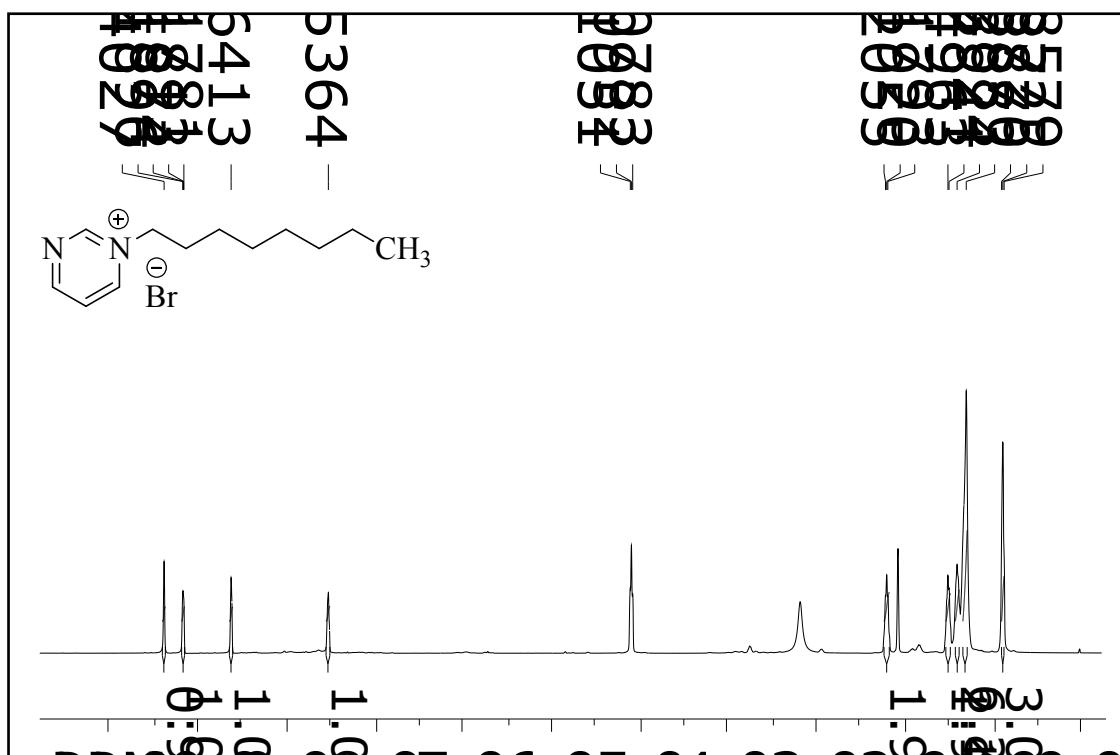


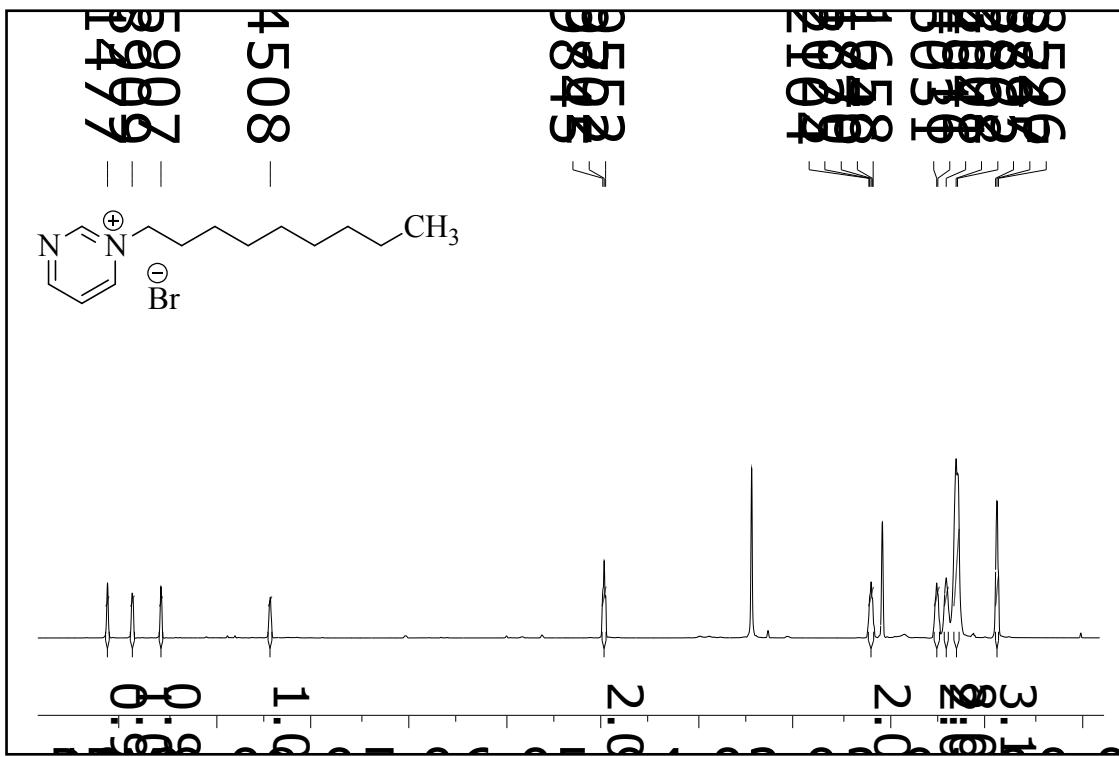
¹H NMR spectrum of 1-hexylpyrimidin-1-iium bromide (**2f**) in D₂O + CD₃OD at 500 MHz



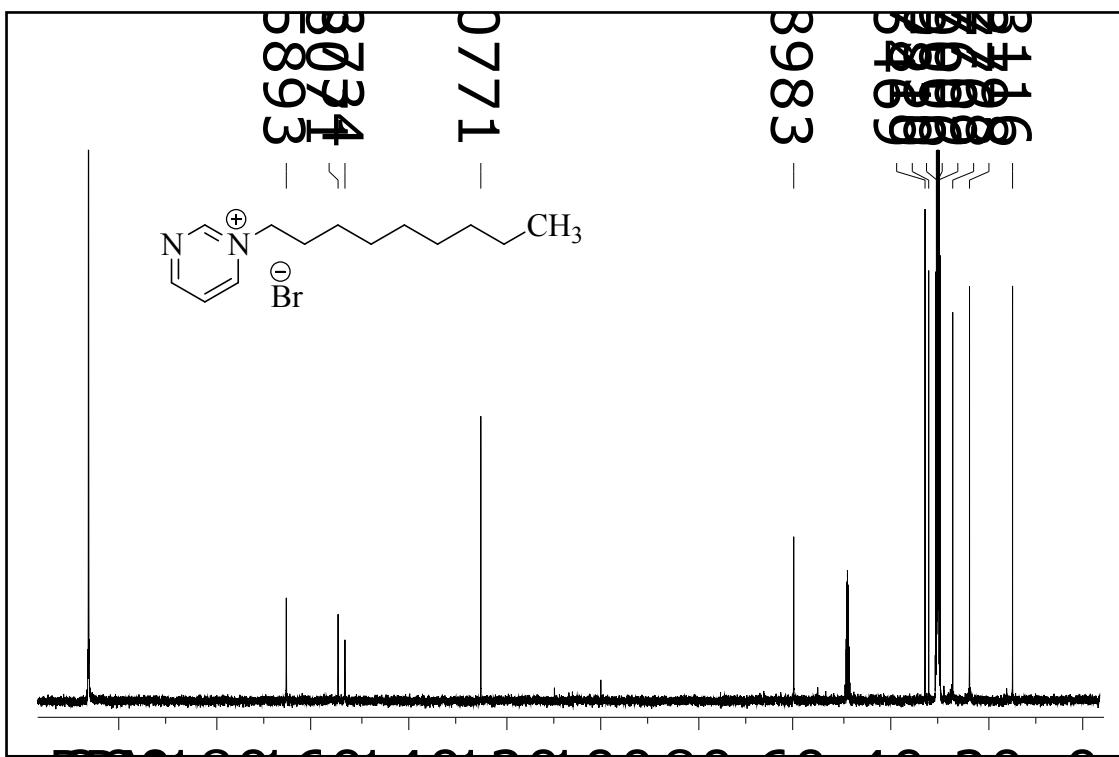
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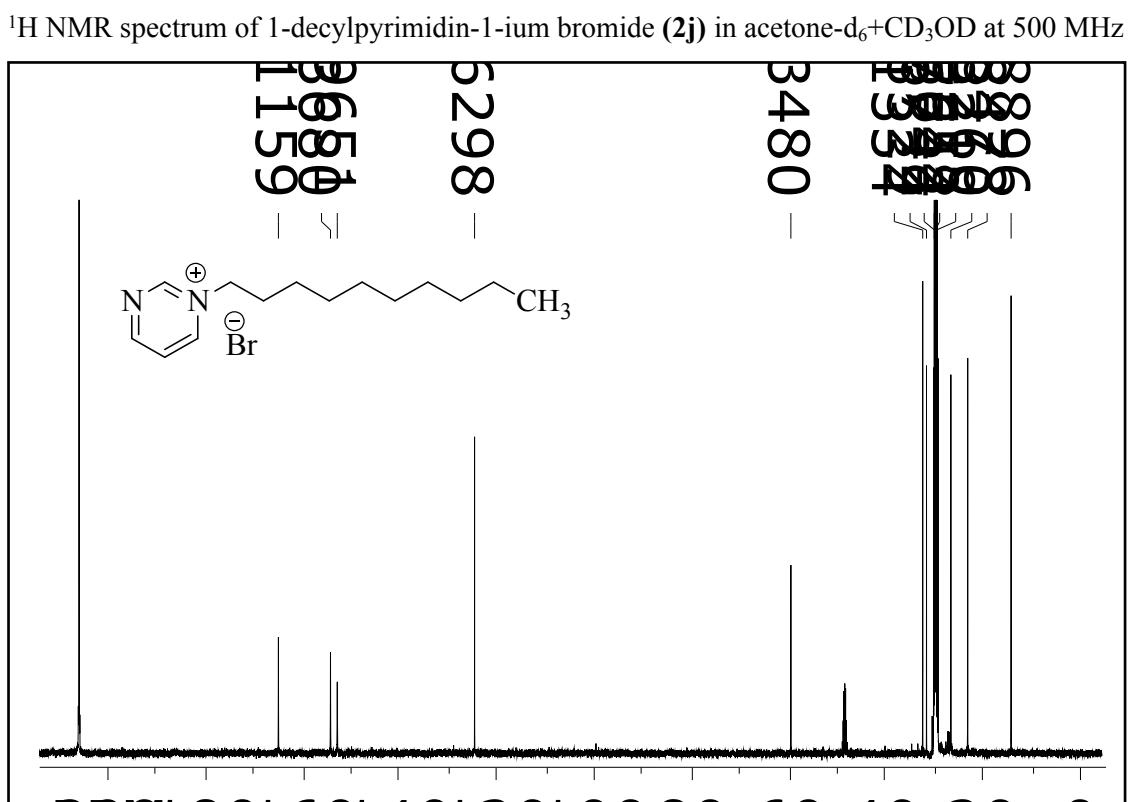
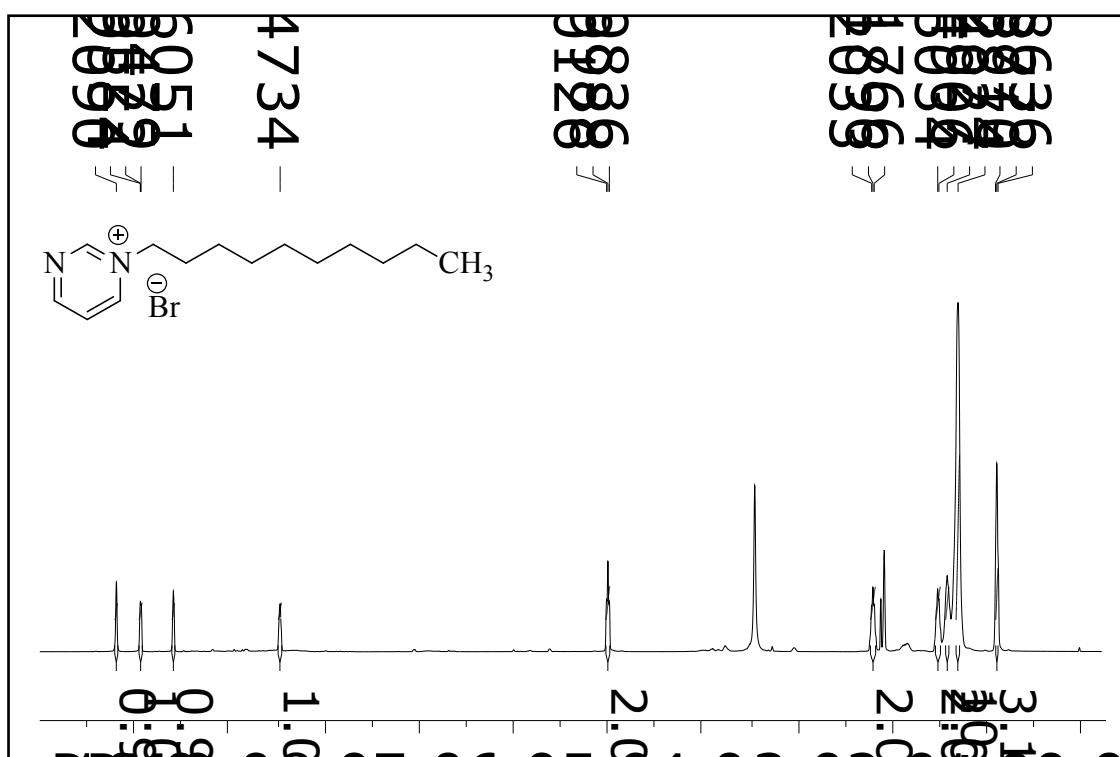


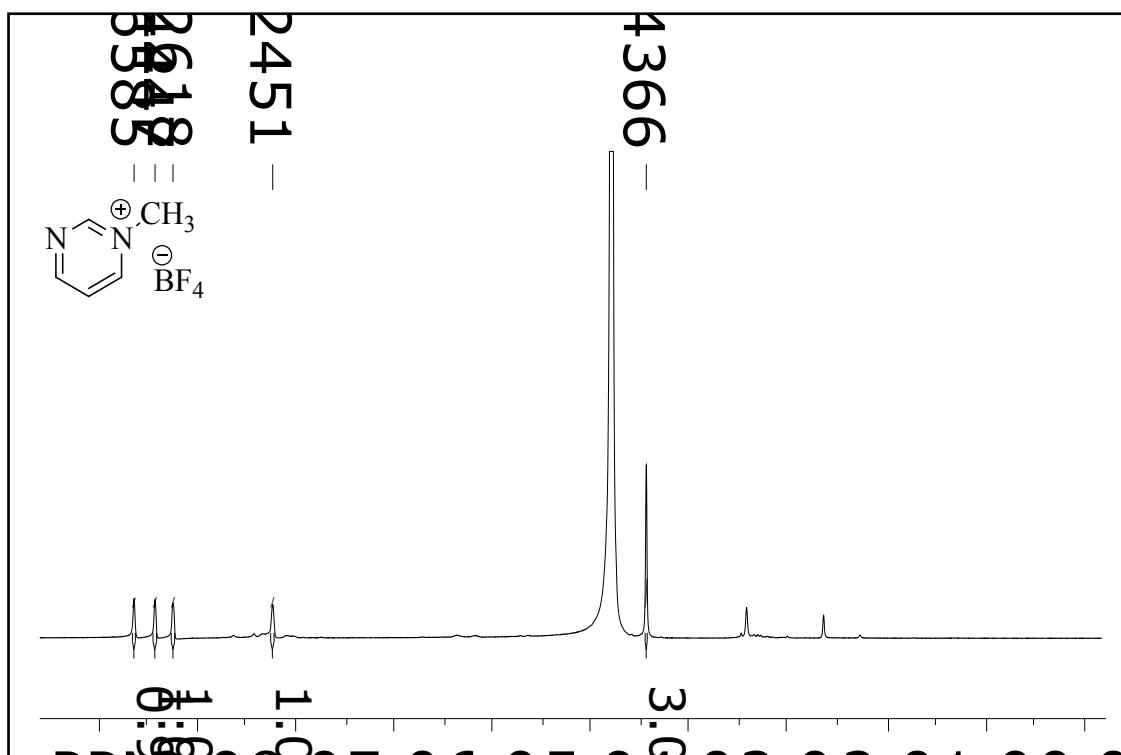


¹H NMR spectrum of 1-nonylpyrimidin-1-ium bromide (**2i**) in acetone-d₆+CD₃OD at 500 MHz

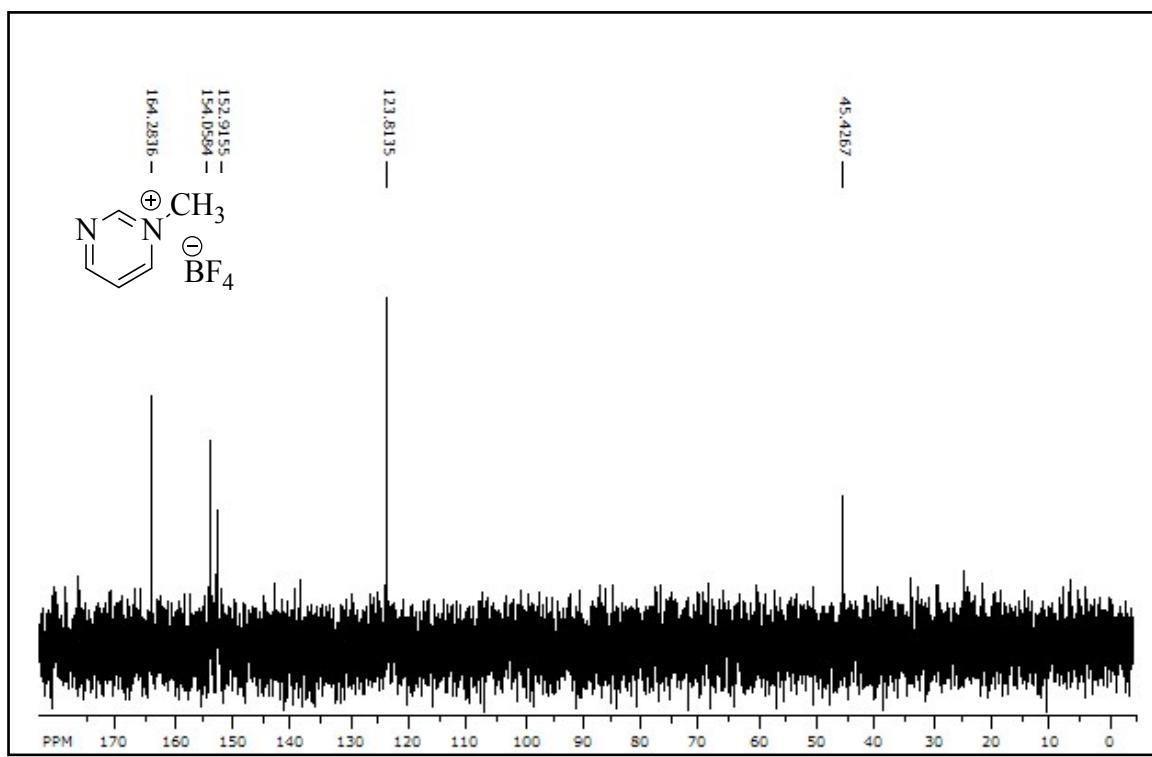


¹³C NMR spectrum of 1-nonylpyrimidin-1-ium bromide (**2i**) in acetone-d₆ + CD₃OD at 500 MHz

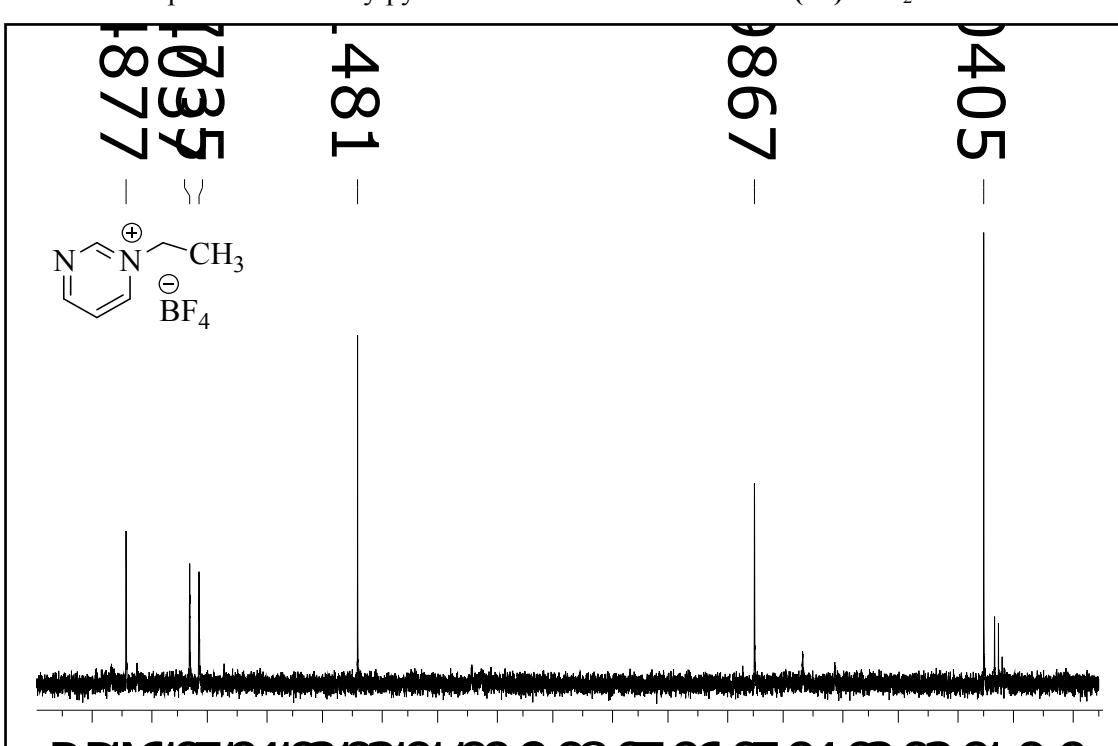
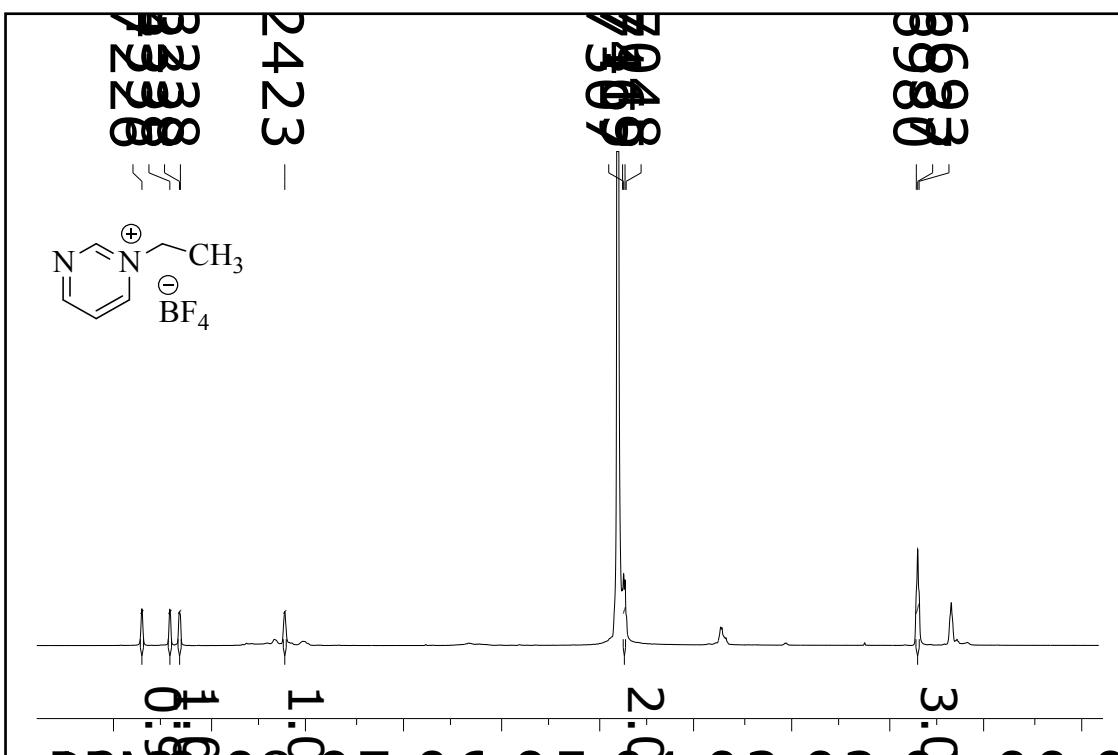


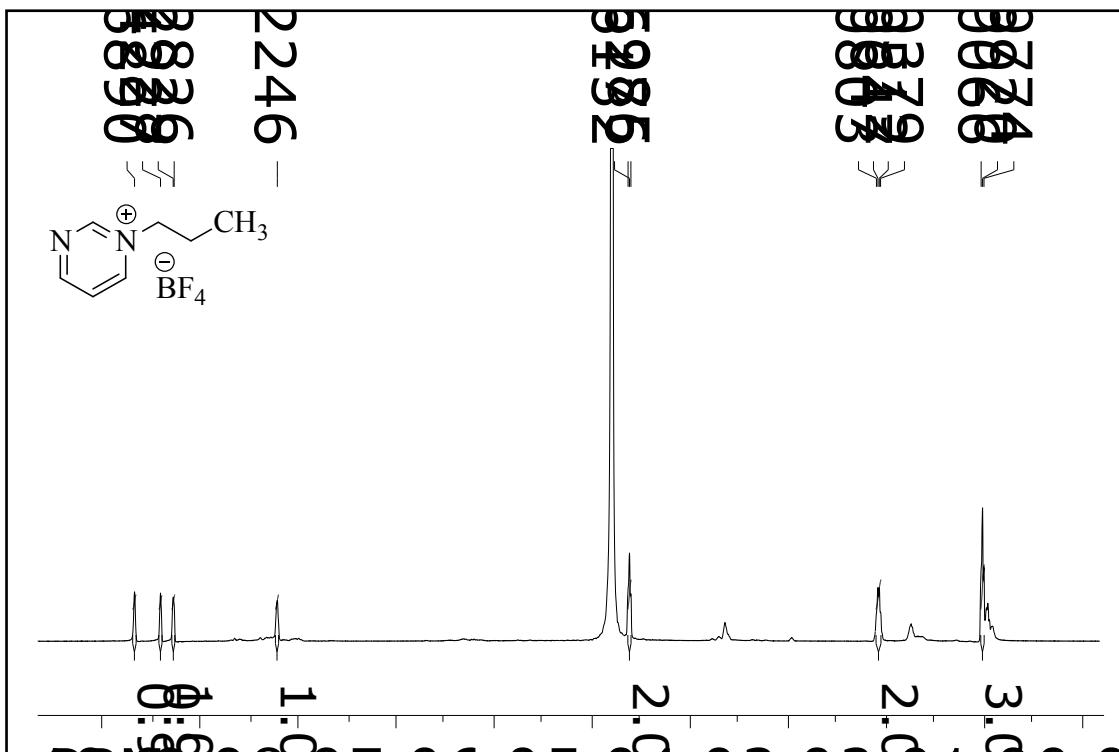


^1H NMR spectrum of 1-methylpyrimidin-1-ium tetrafluoroborate (**3a**) in D_2O at 500 MHz

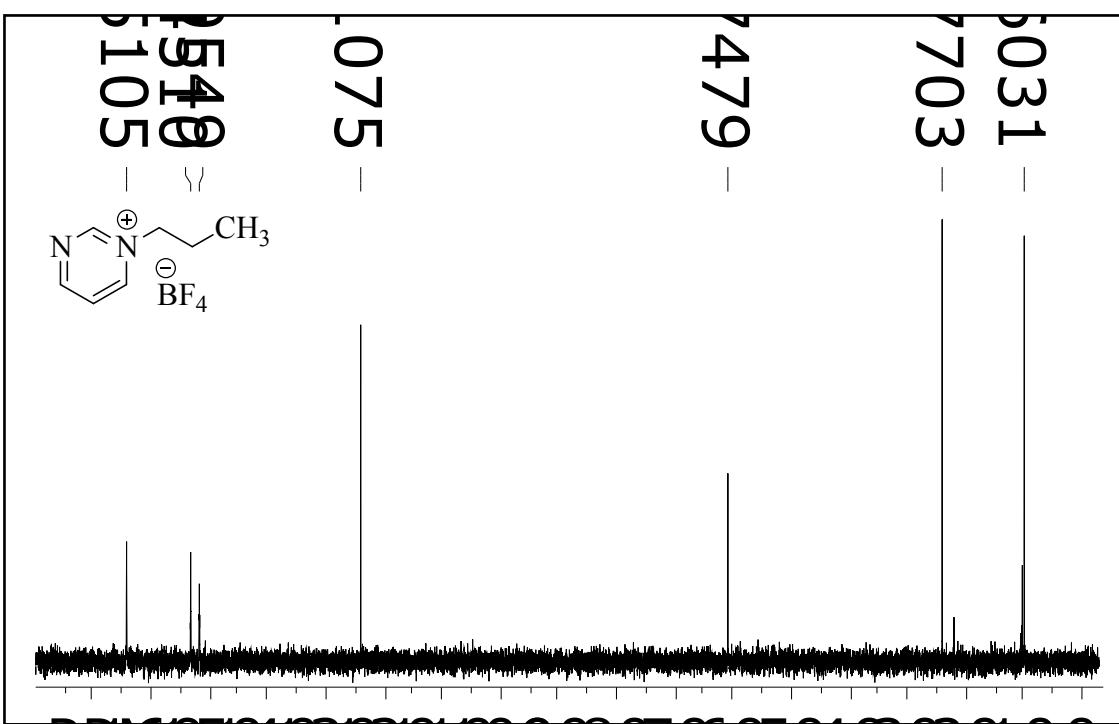


^{13}C NMR spectrum of 1-methylpyrimidin-1-ium tetrafluoroborate (**3a**) in D_2O at 500 MHz

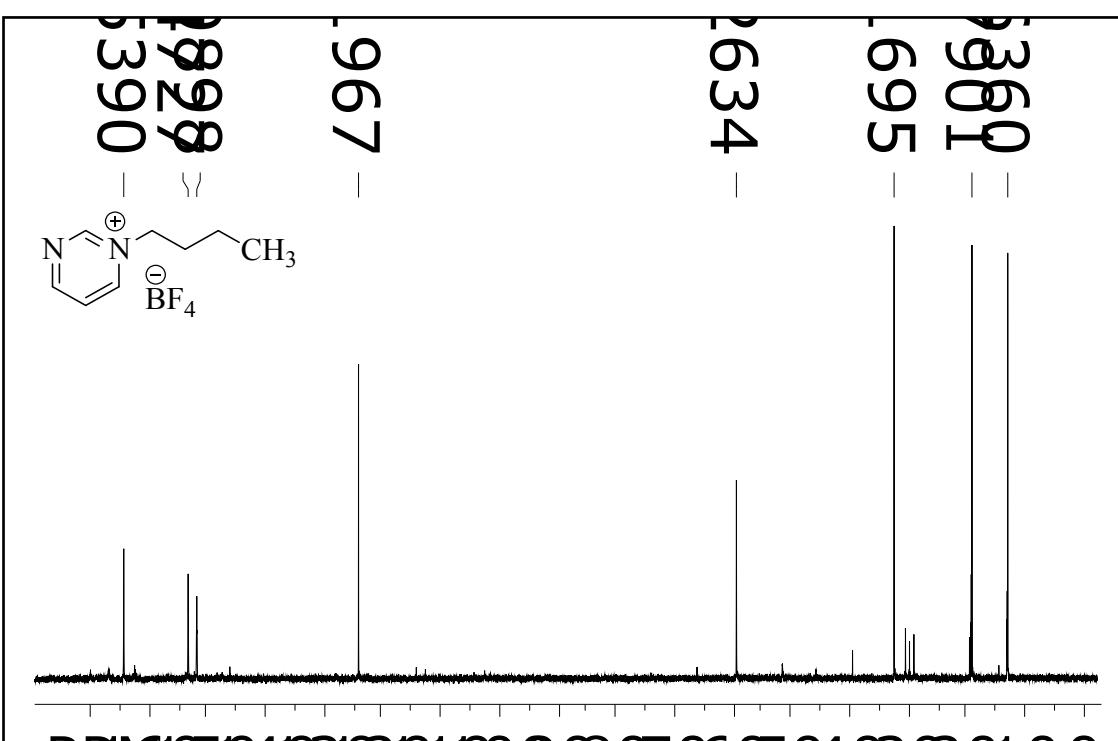
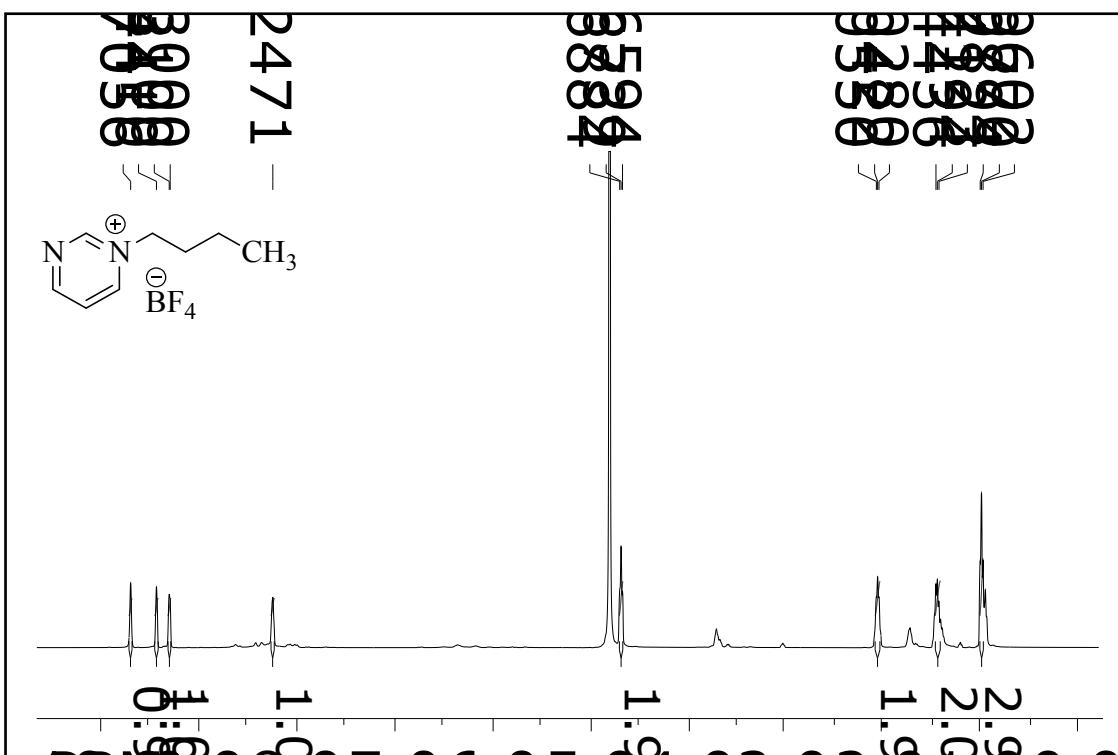


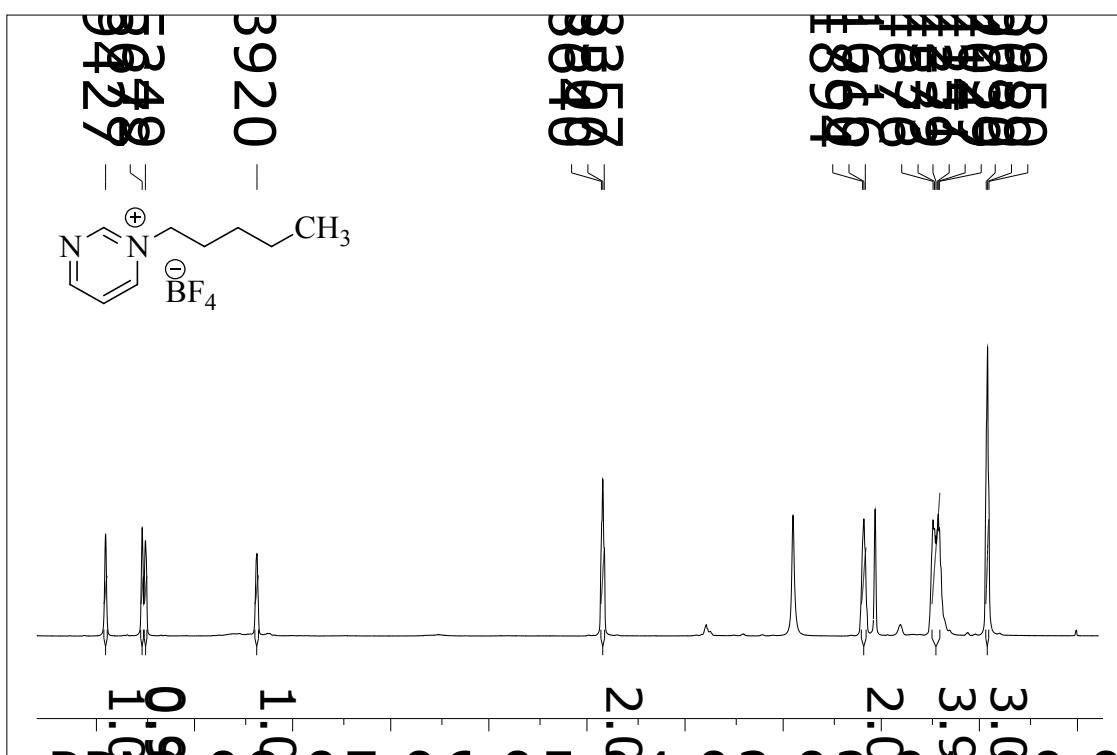


¹H NMR spectrum of 1-propylpyrimidin-1-ium tetrafluoroborate (**3c**) in D₂O at 500 MHz

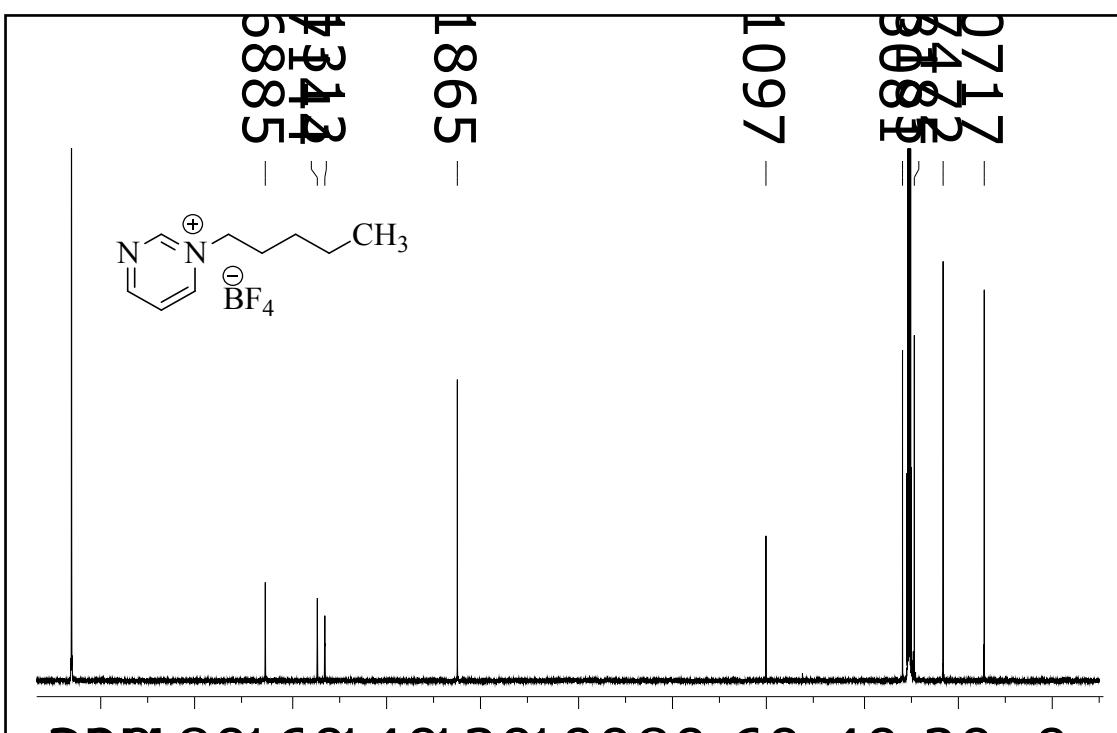


¹³C NMR spectrum of 1-propylpyrimidin-1-ium tetrafluoroborate (**3c**) in D₂O at 500 MHz

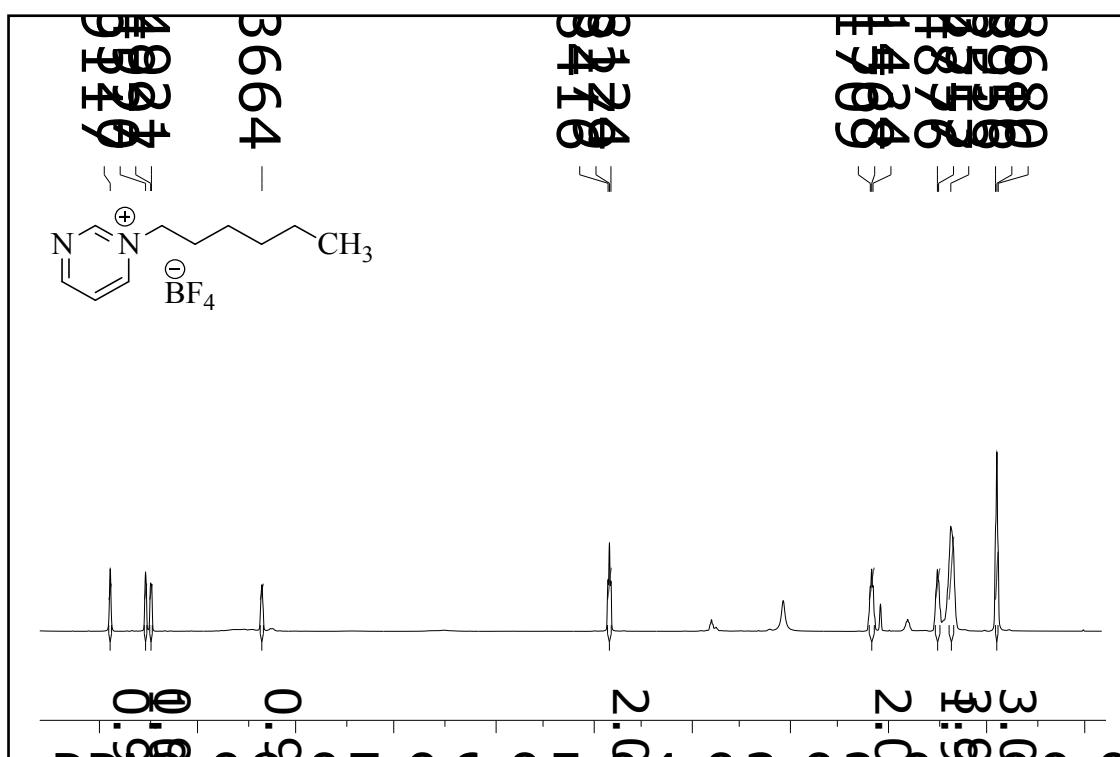




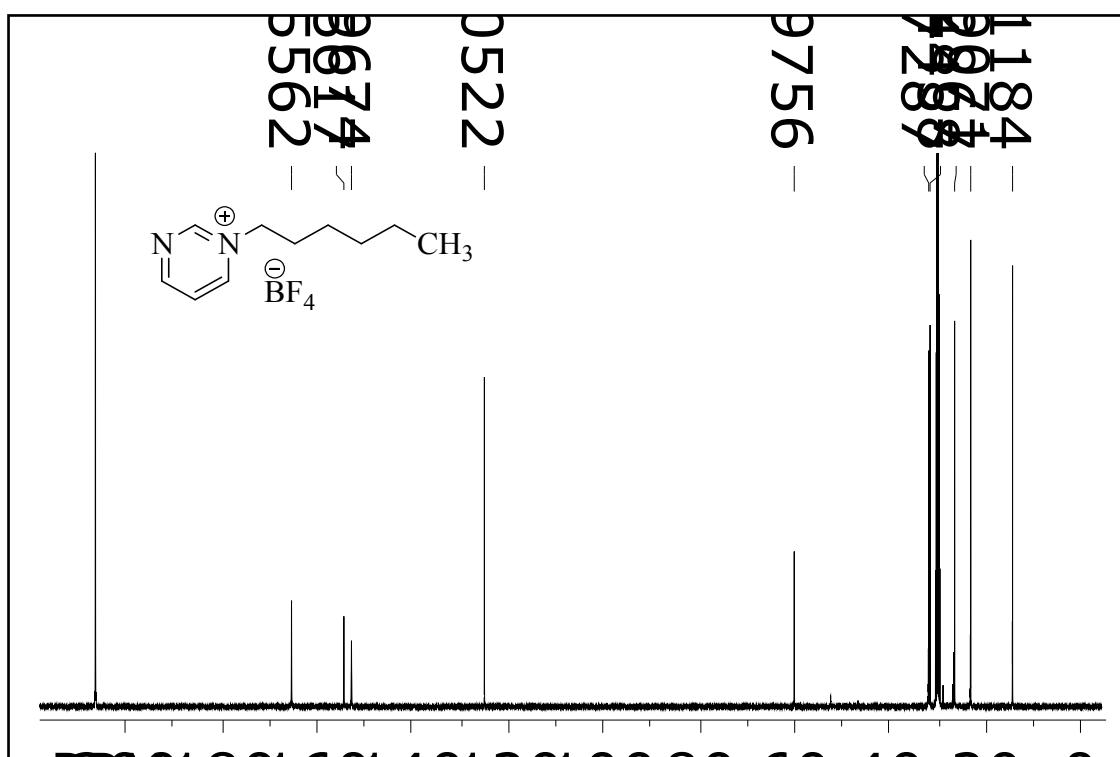
¹H NMR spectrum of 1-pentylpyrimidin-1-ium tetrafluoroborate (**3e**) in acetone-d₆ at 500 MHz



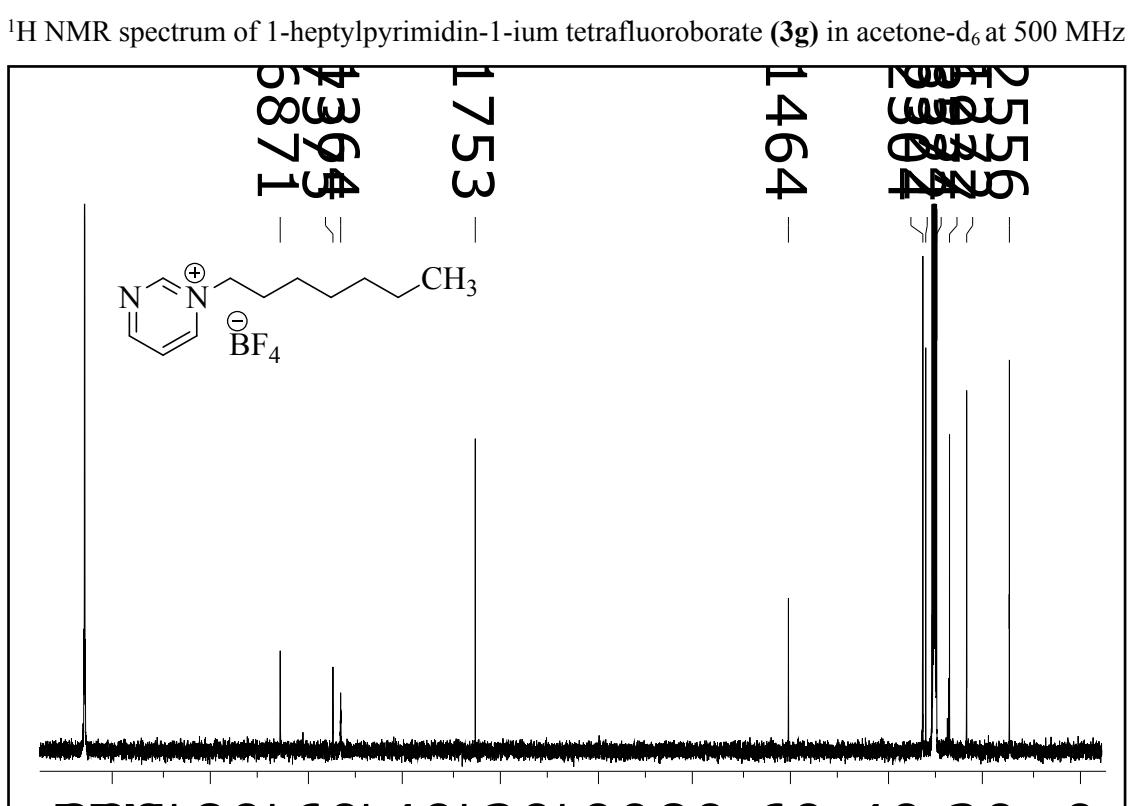
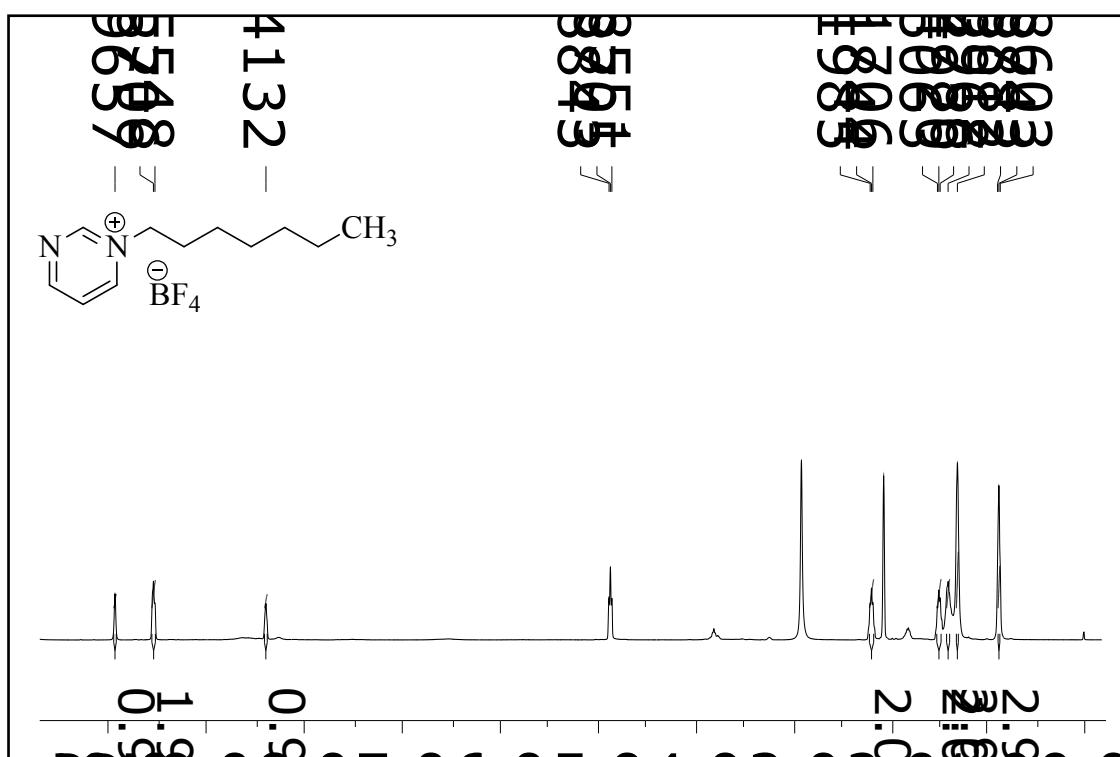
¹³C NMR spectrum of 1-pentylpyrimidin-1-ium tetrafluoroborate (**3e**) in acetone-d₆ at 500 MHz

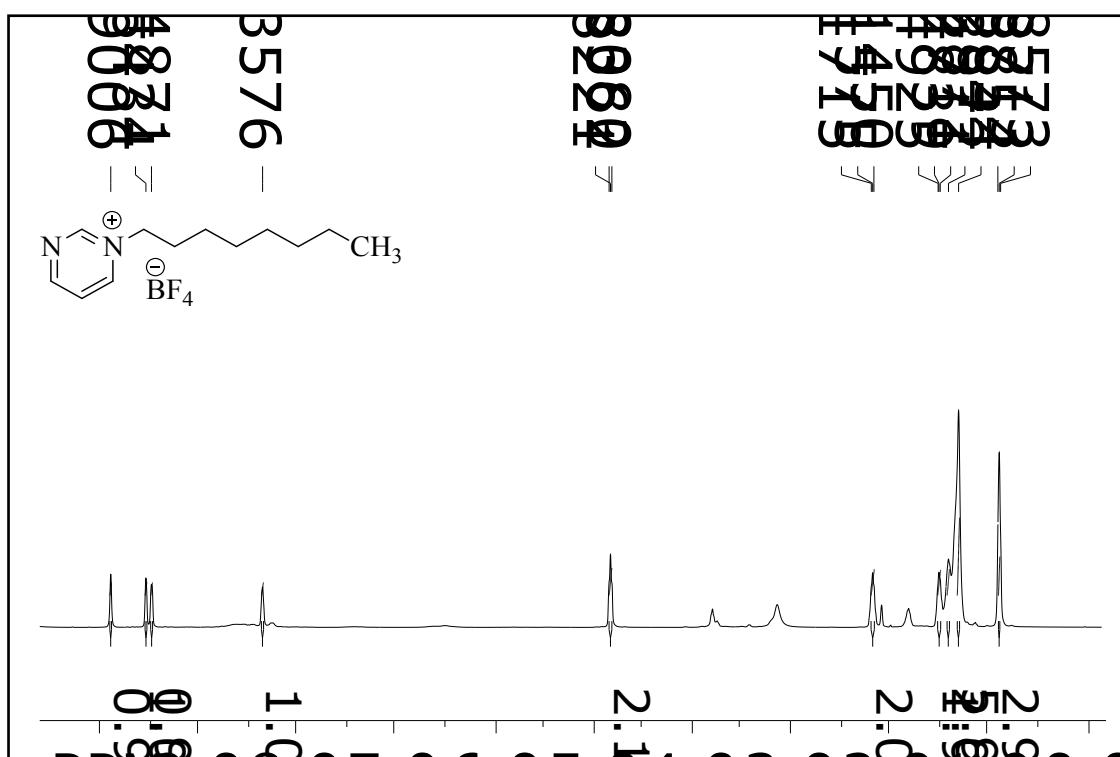


¹H NMR spectrum of 1-hexylpyrimidin-1-ium tetrafluoroborate (**3f**) in acetone-d₆ at 500 MHz

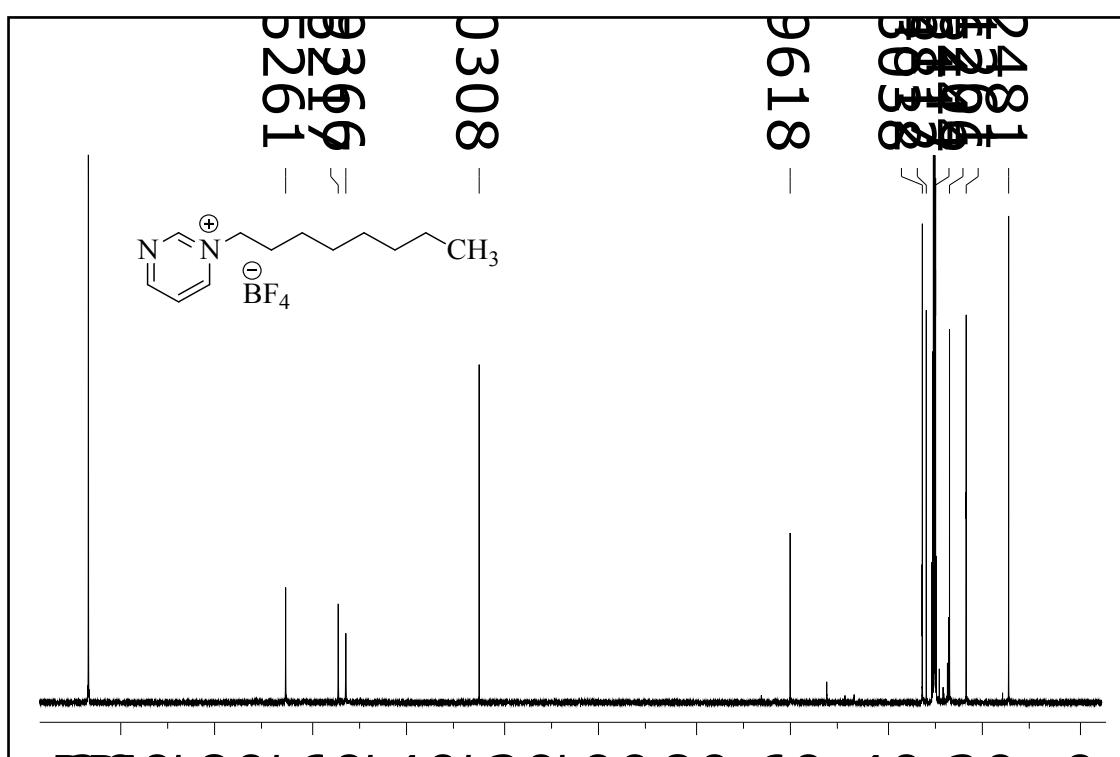


¹³C NMR spectrum of 1-hexylpyrimidin-1-ium tetrafluoroborate (**3f**) in acetone-d₆ at 500 MHz

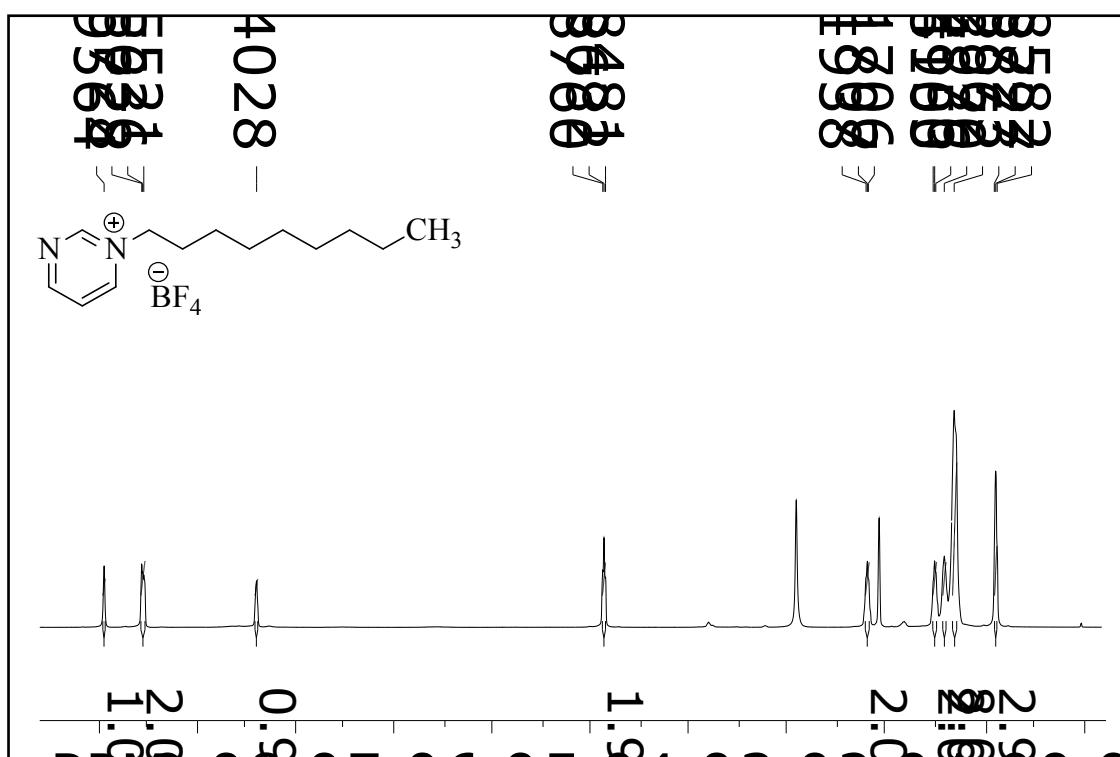




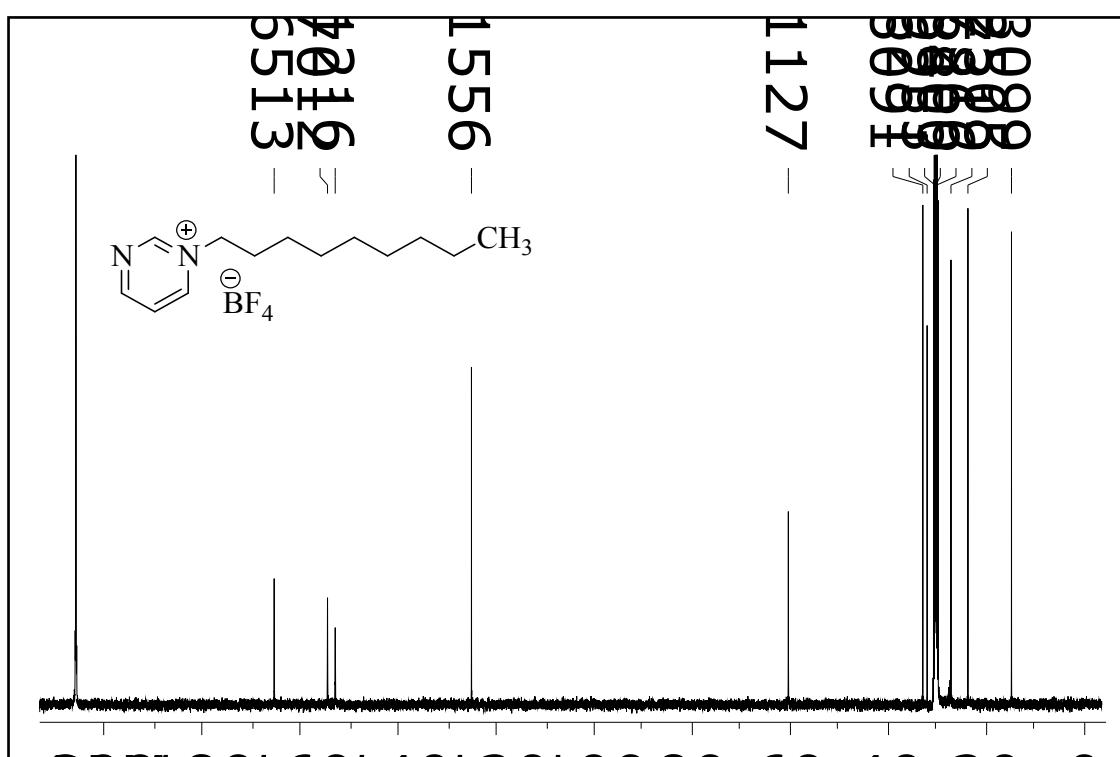
¹H NMR spectrum of 1-octylpyrimidin-1-ium tetrafluoroborate (**3h**) in acetone-d₆ at 500 MHz



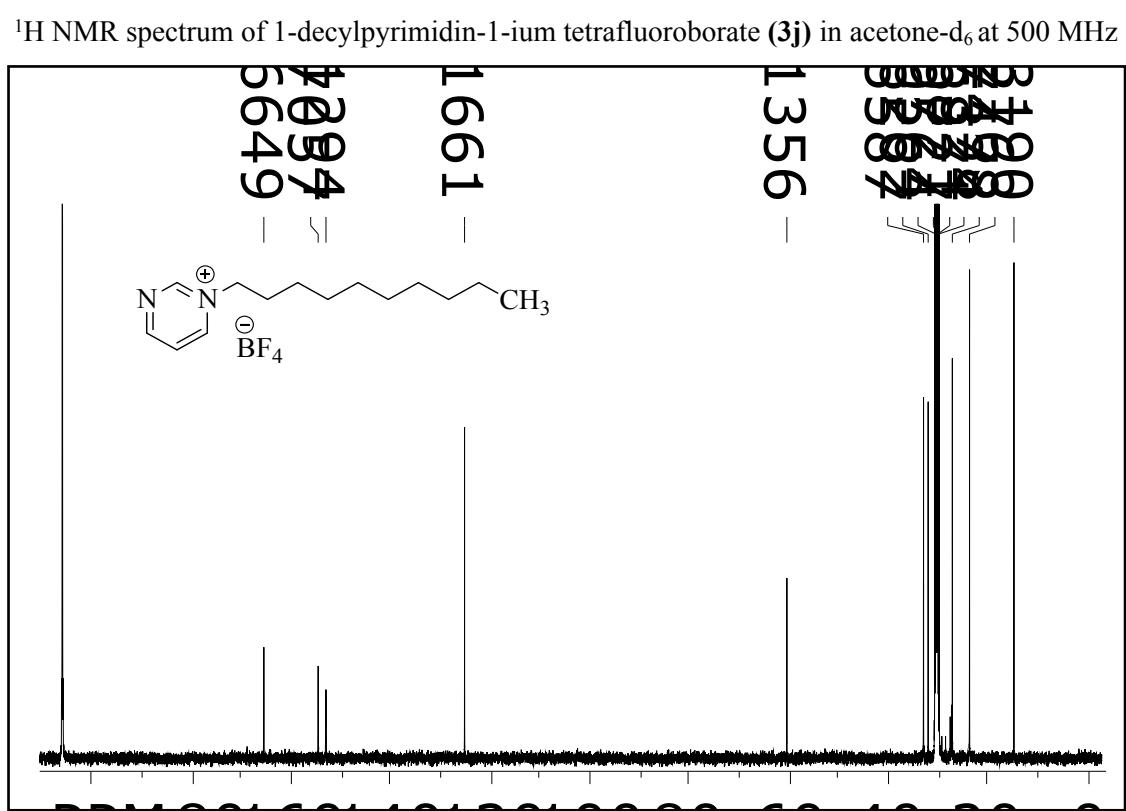
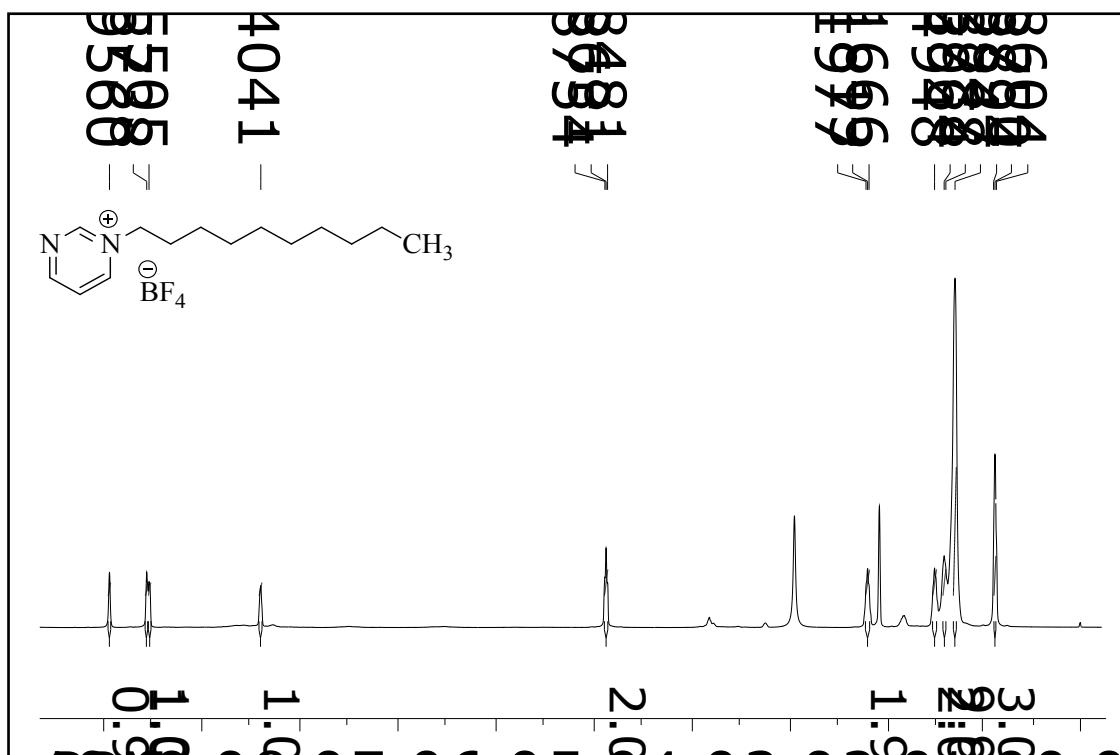
¹³C NMR spectrum of 1-octylpyrimidin-1-ium tetrafluoroborate (**3h**) in acetone-d₆ at 500 MHz

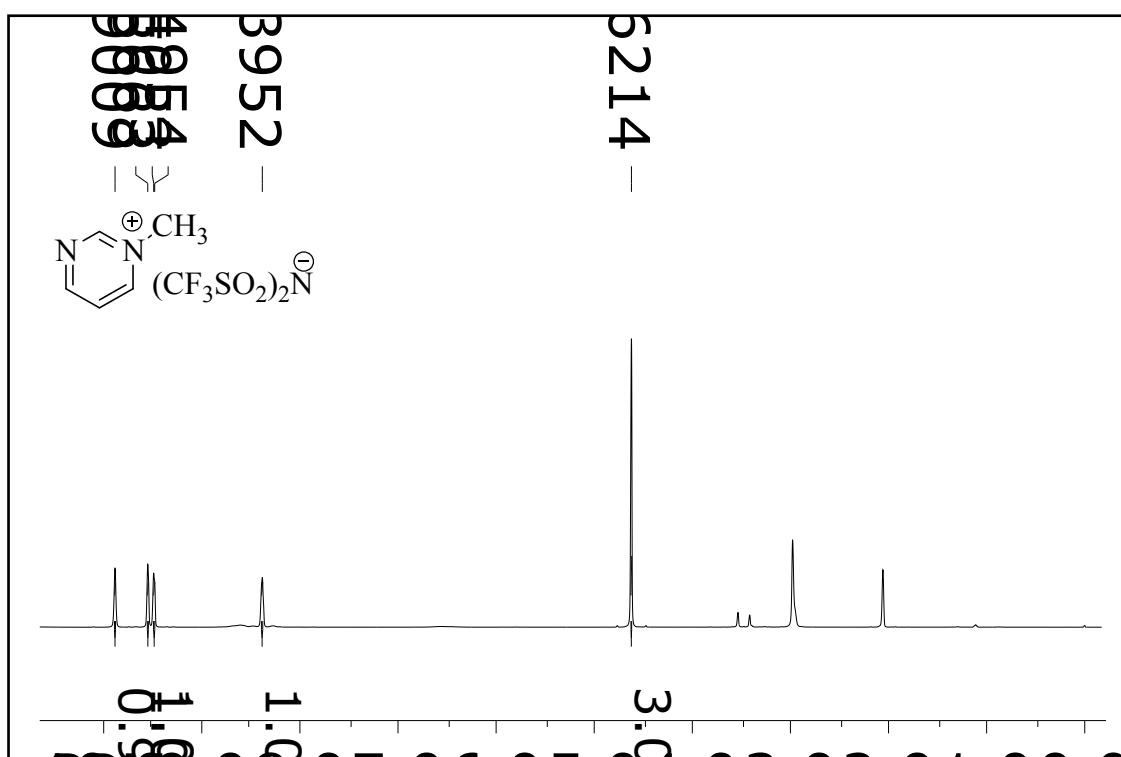


^1H NMR spectrum of 1-nonylpyrimidin-1-ium tetrafluoroborate (**3i**) in acetone- d_6 at 500 MHz

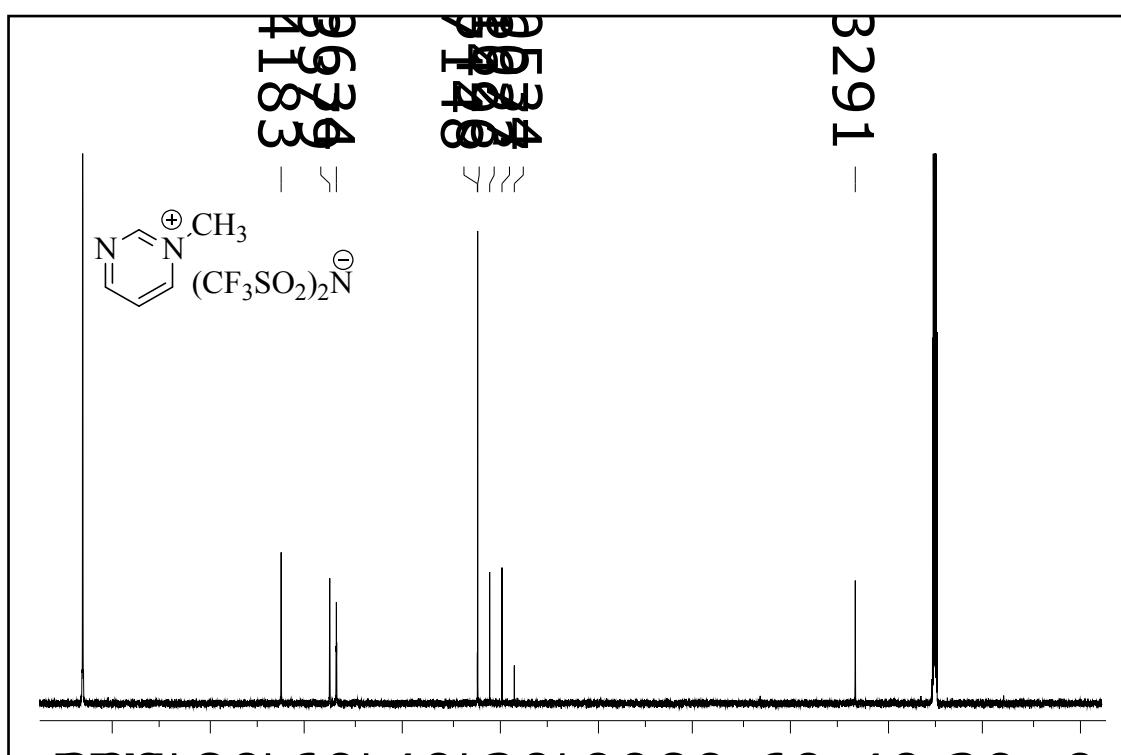


^{13}C NMR spectrum of 1-nonylpyrimidin-1-ium tetrafluoroborate (**3i**) in acetone- d_6 at 500 MHz

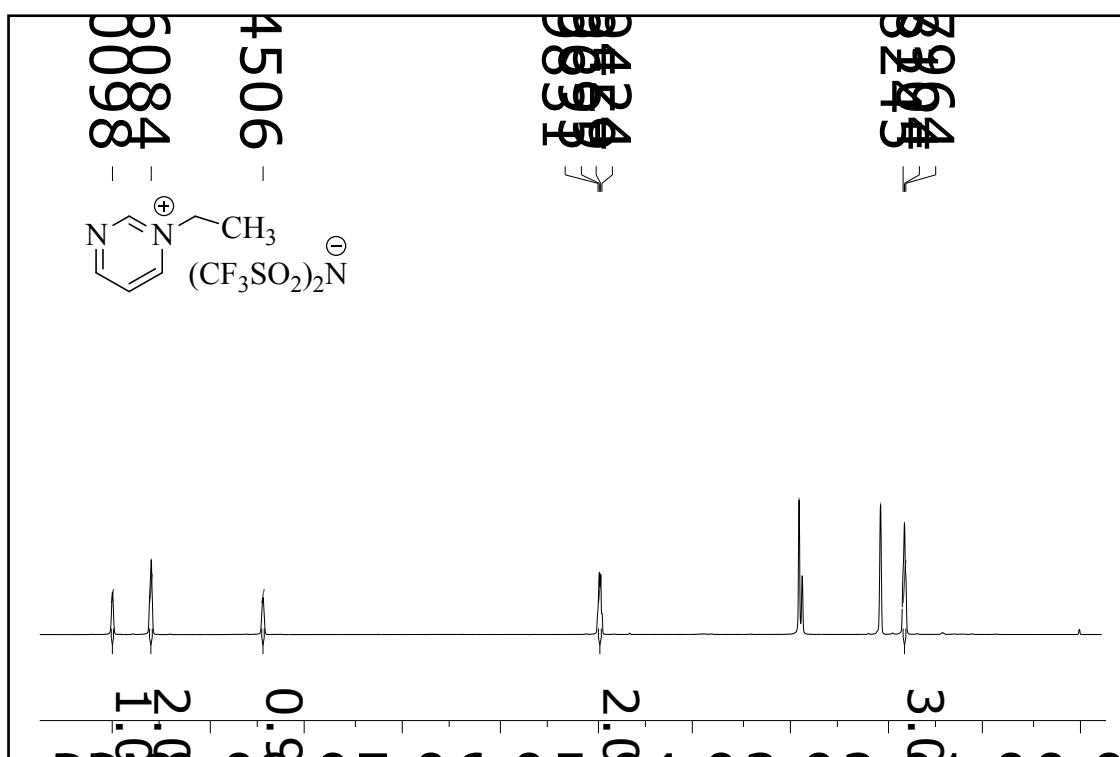




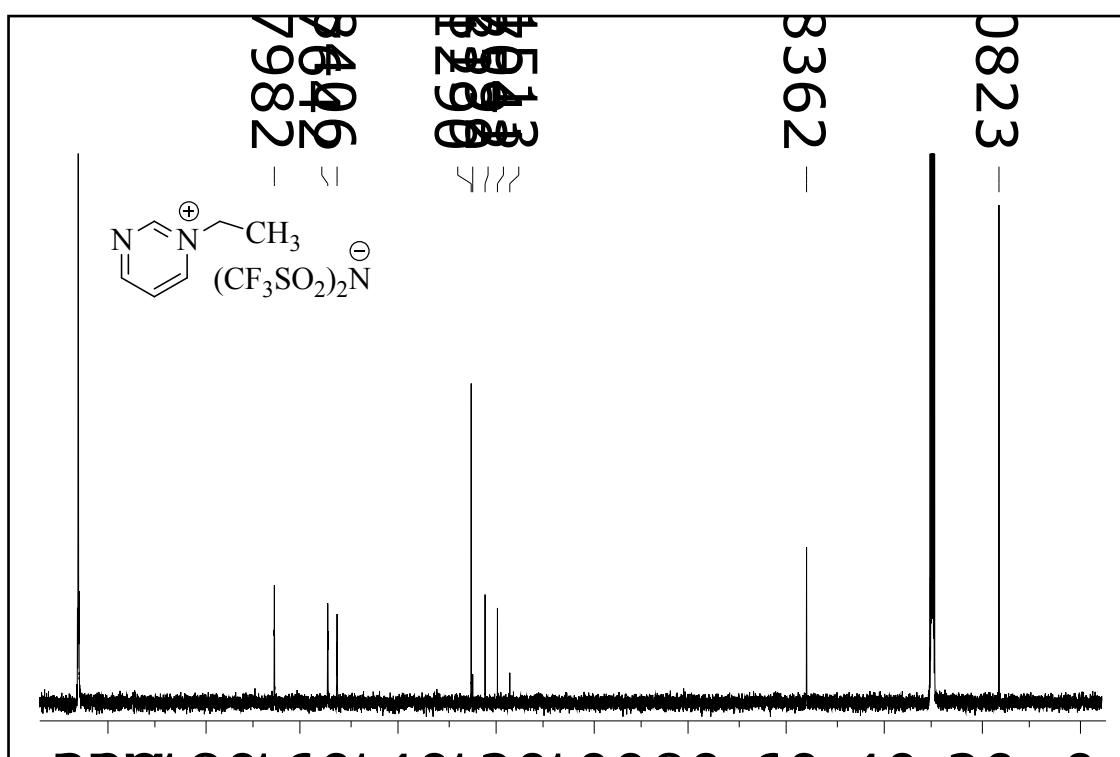
¹H NMR spectrum of 1-methylpyrimidin-1-ium bis(trifluoromethanesulfonyl)amide (**4a**) in acetone- d_6 at 500 MHz



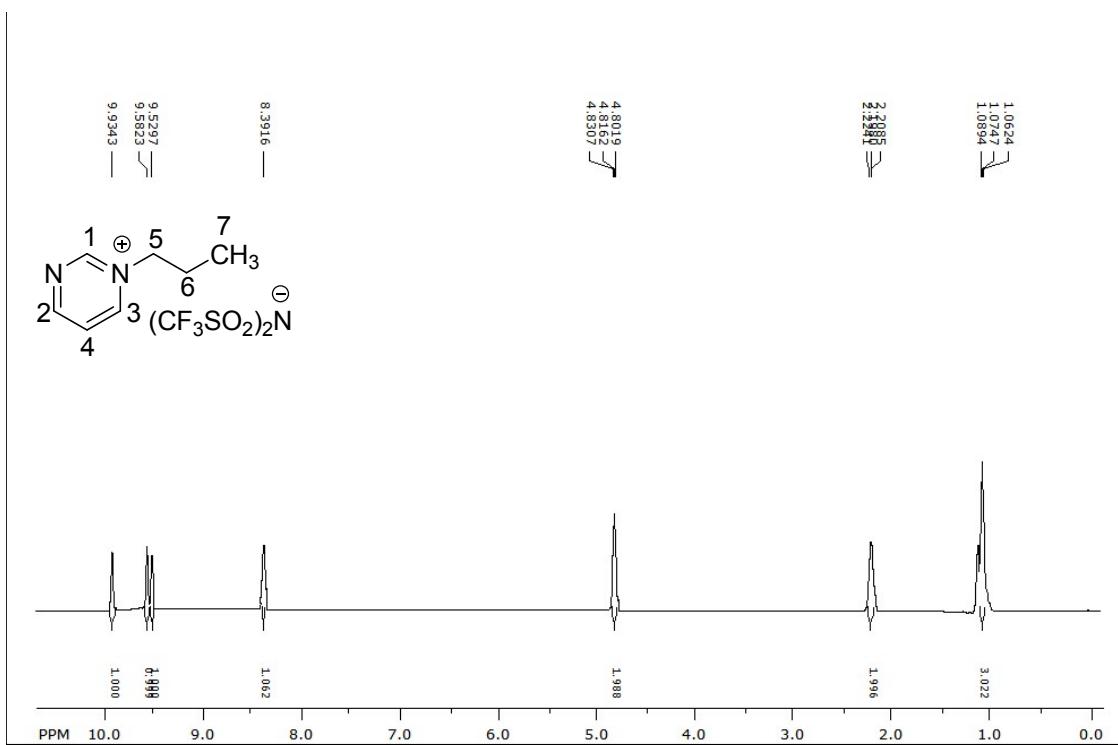
¹³C NMR spectrum of 1-methylpyrimidin-1-ium bis(trifluoromethanesulfonyl)amide (**4a**) in acetone- d_6 at 500 MHz



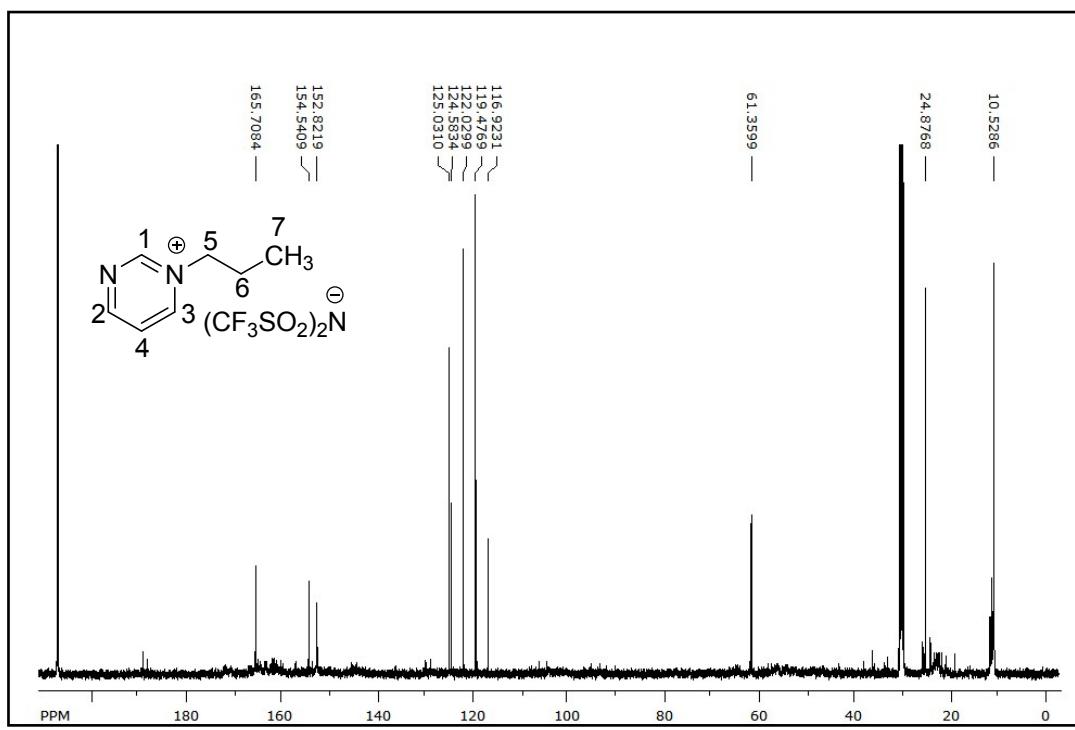
¹H NMR spectra of 1-ethylpyrimidin-1-ium bis(trifluoromethanesulfonyl)amide (**4b**) in acetone-d₆ at 500 MHz



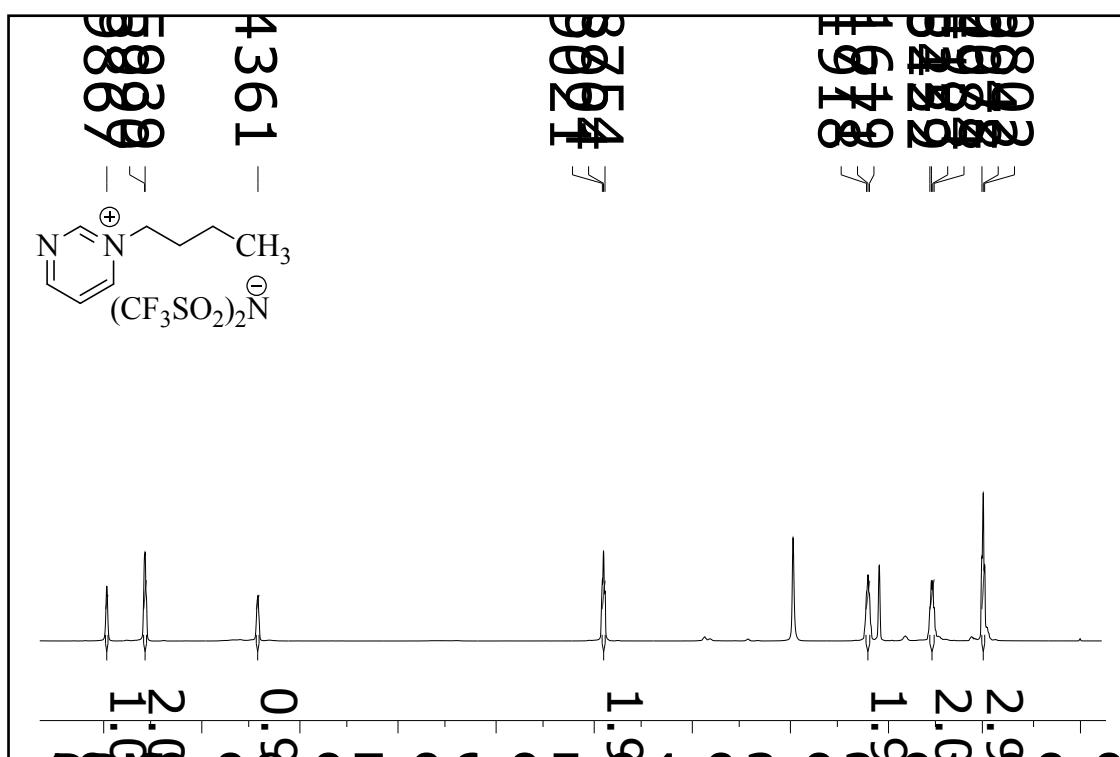
¹³C NMR spectrum of 1-ethylpyrimidin-1-ium bis(trifluoromethanesulfonyl)amide (**4b**) in acetone-d₆ at 500 MHz



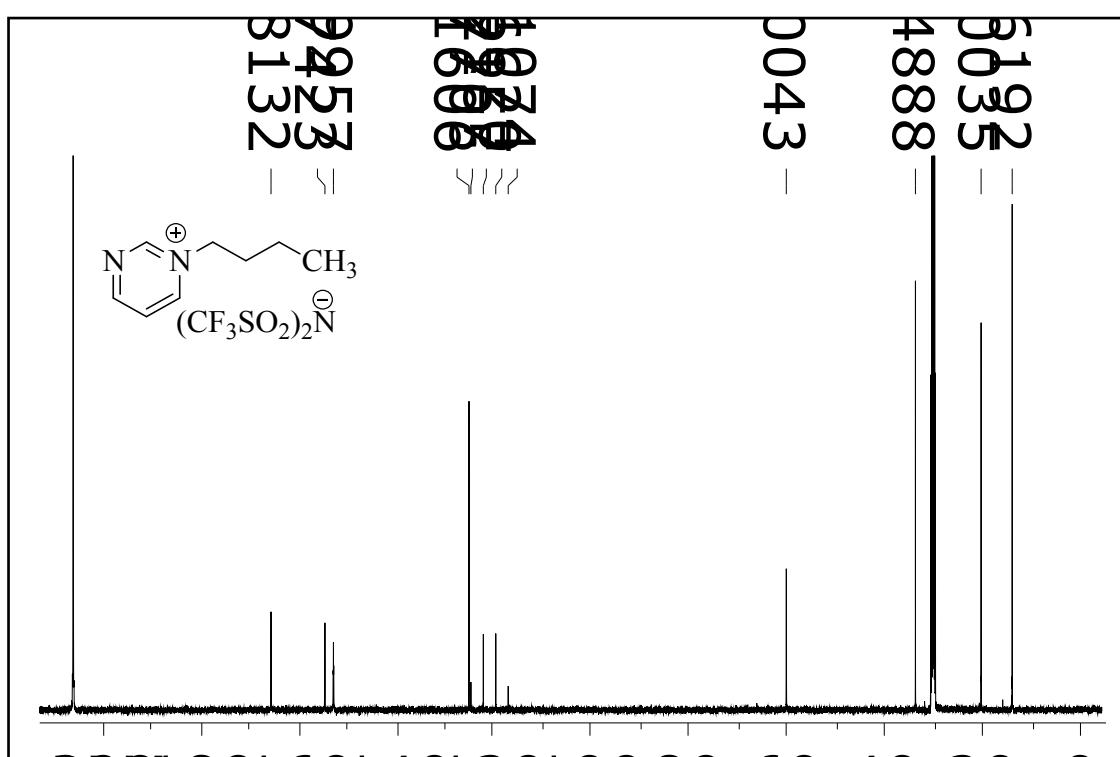
¹H NMR spectrum of 1-propylpyrimidin-1-ium bis(trifluoromethanesulfonyl)amide (**4c**) in acetone-d₆
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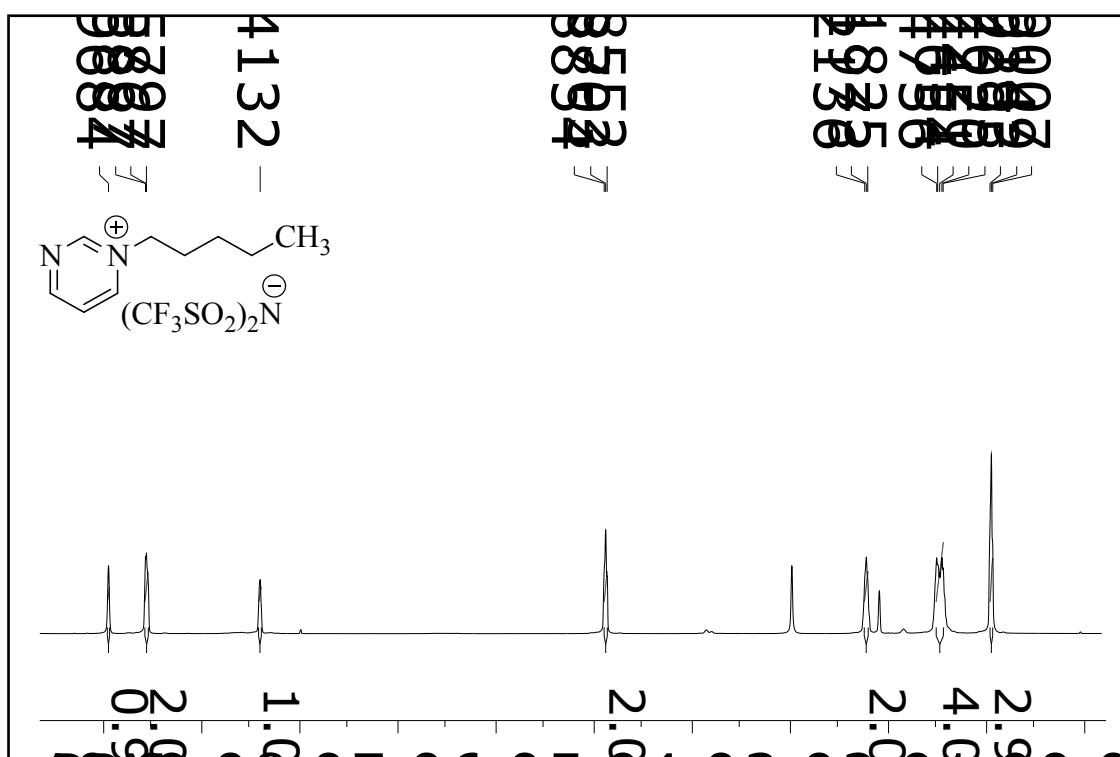
¹³C NMR spectrum of 1-propylpyrimidin-1-ium bis(trifluoromethanesulfonyl)amide (**4c**) in acetone-d₆ at 500 MHz



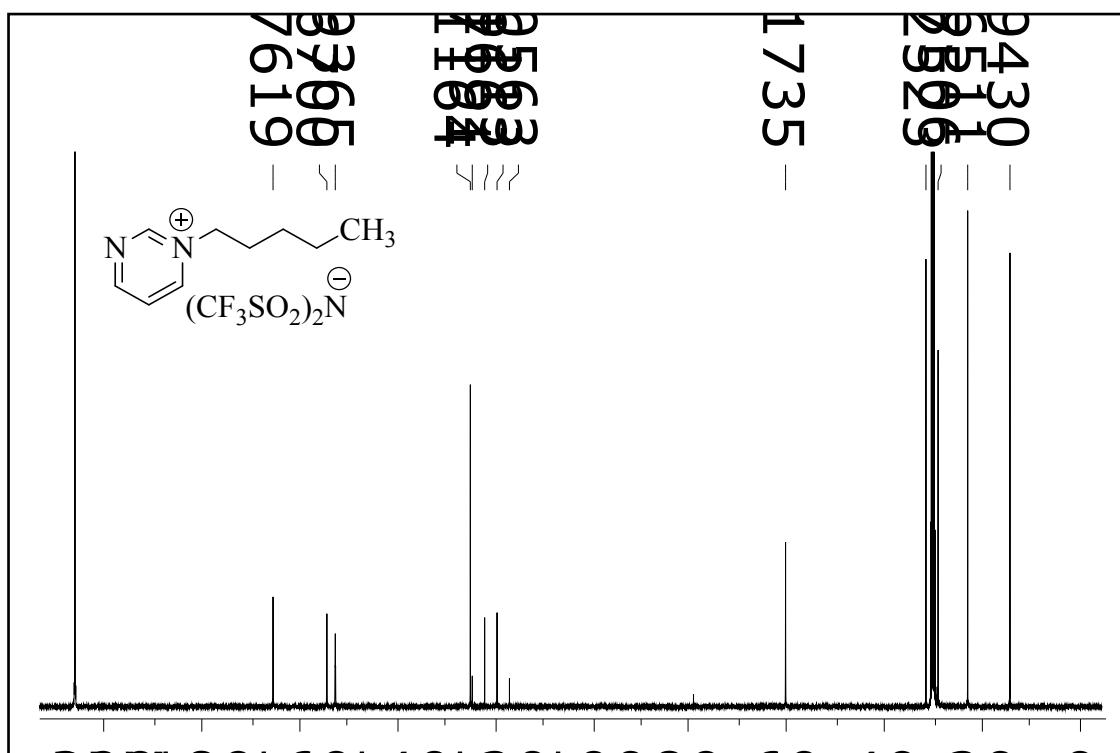
¹H NMR spectrum of 1-butylpyrimidin-1-ium bis(trifluoromethanesulfonyl)amide (**4d**) in acetone-d₆ at 500 MHz



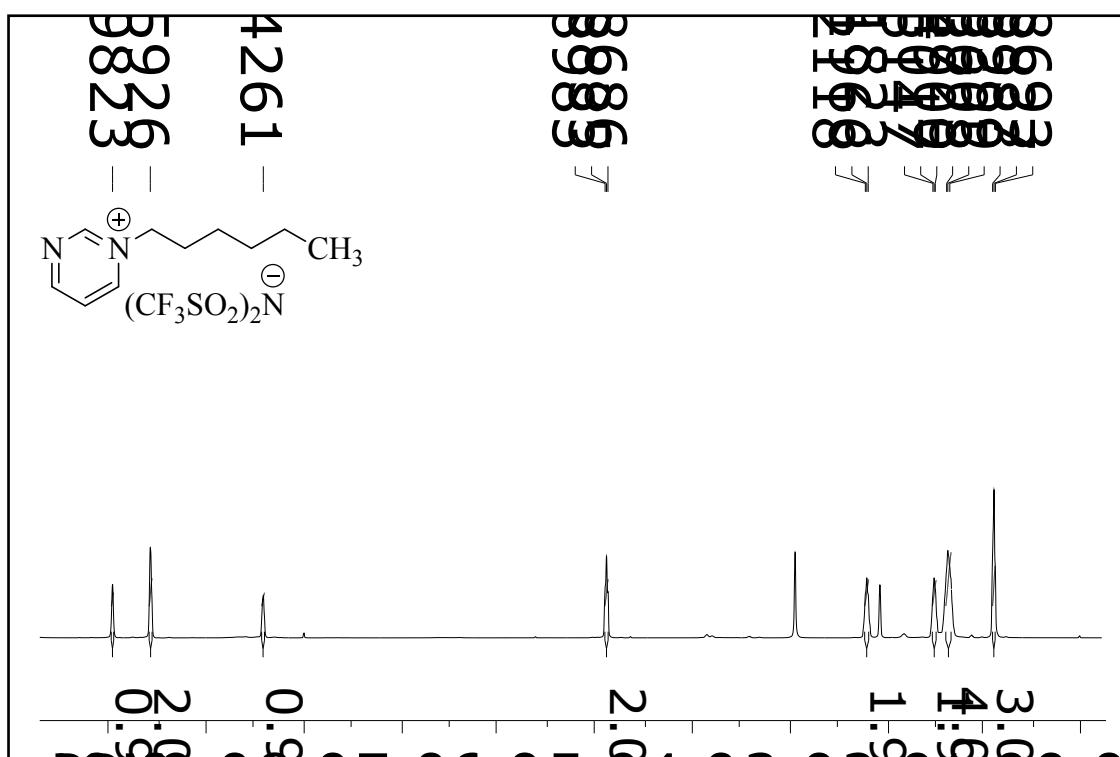
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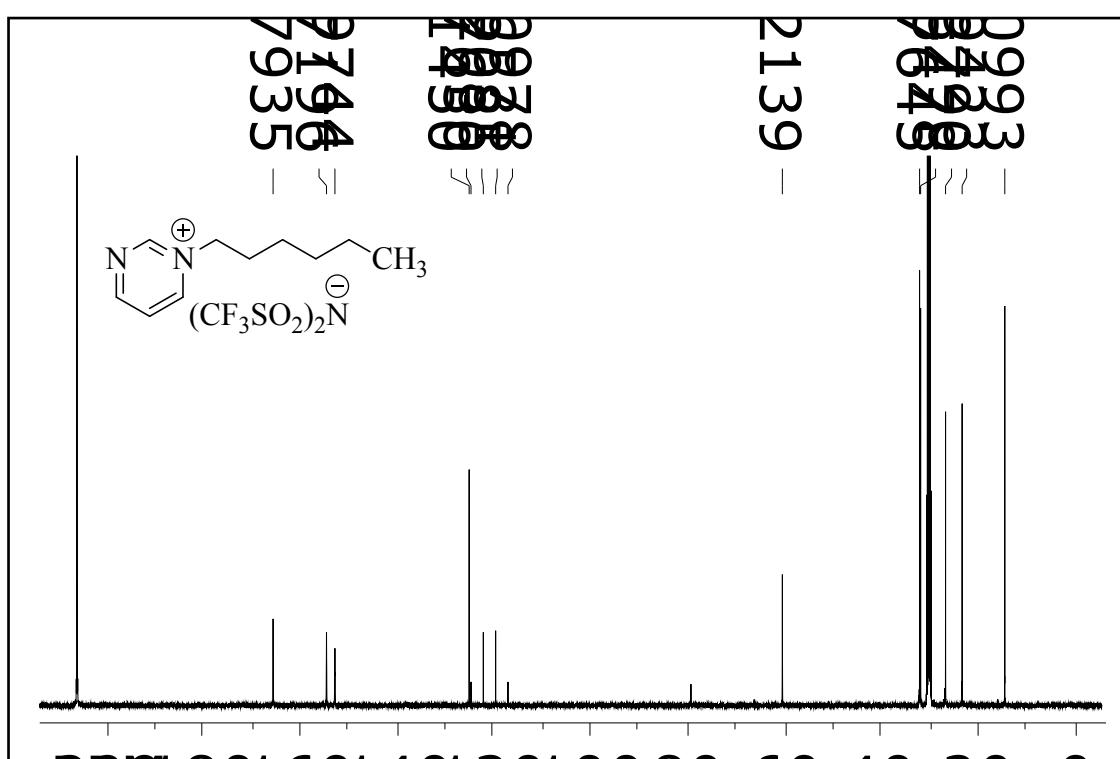
¹H NMR spectrum of 1-pentylpyrimidin-1-ium bis(trifluoromethanesulfonyl)amide (**4e**) in acetone-d₆
at 500 MHz



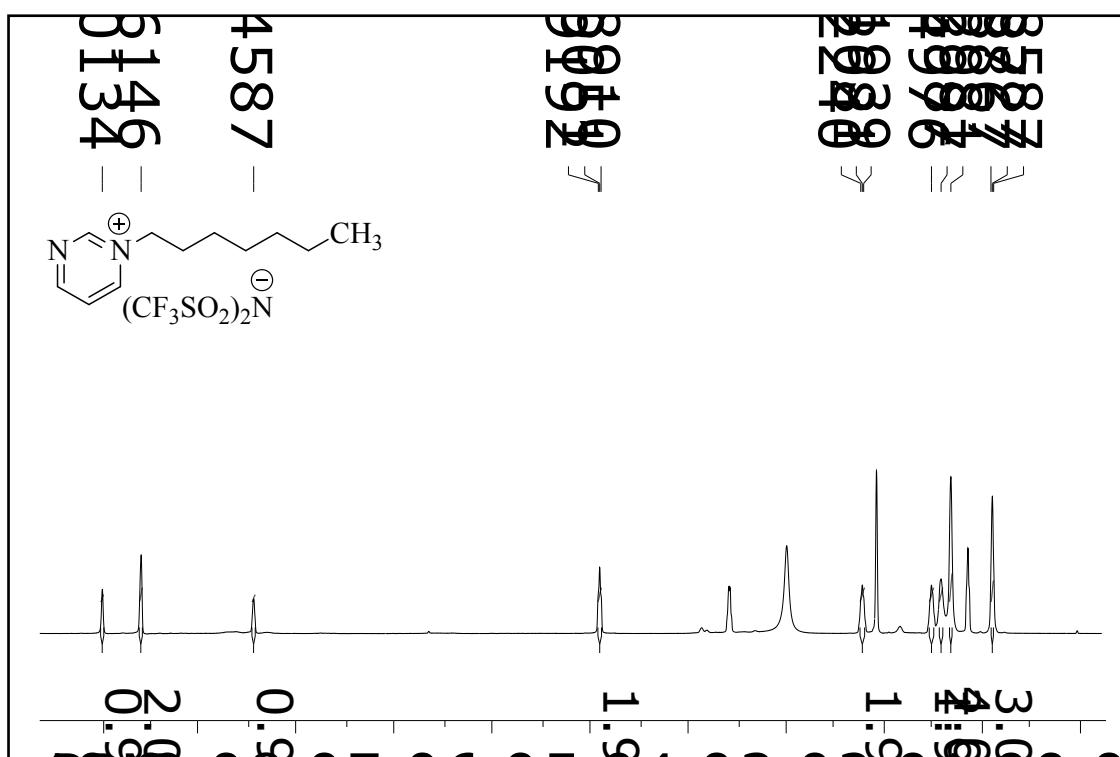
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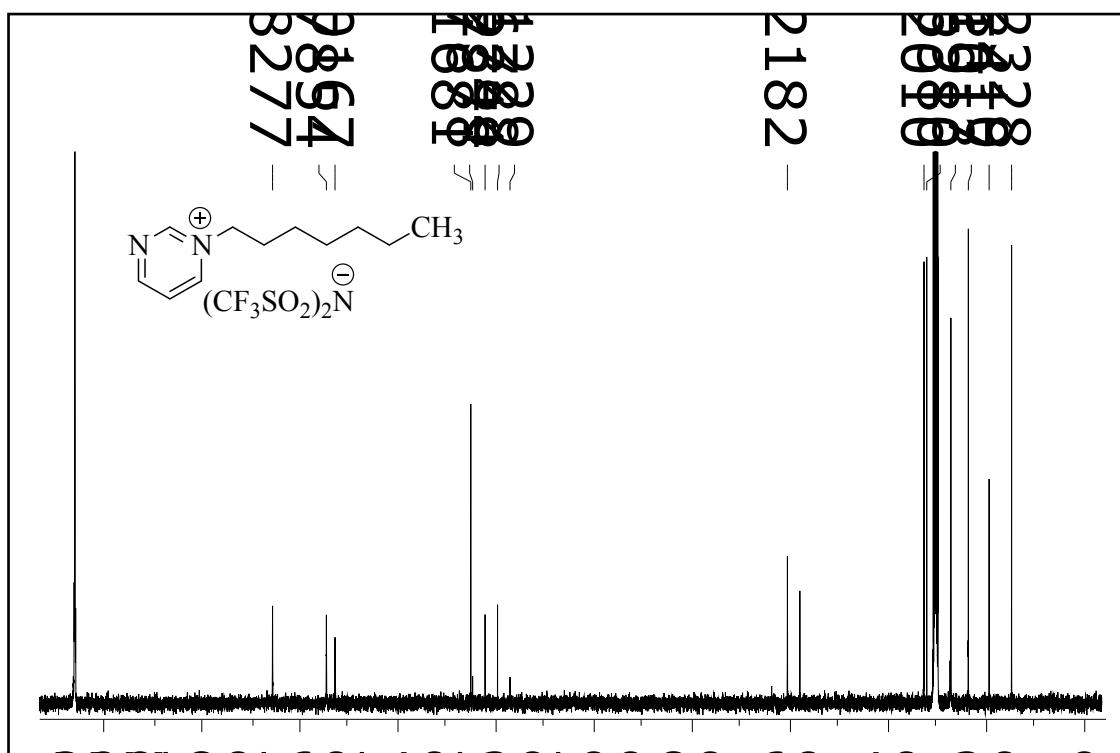
¹H NMR spectrum of 1-hexylpyrimidin-1-i um bis(trifluoromethanesulfonyl)amide (**4f**) in acetone-d₆ at 500 MHz



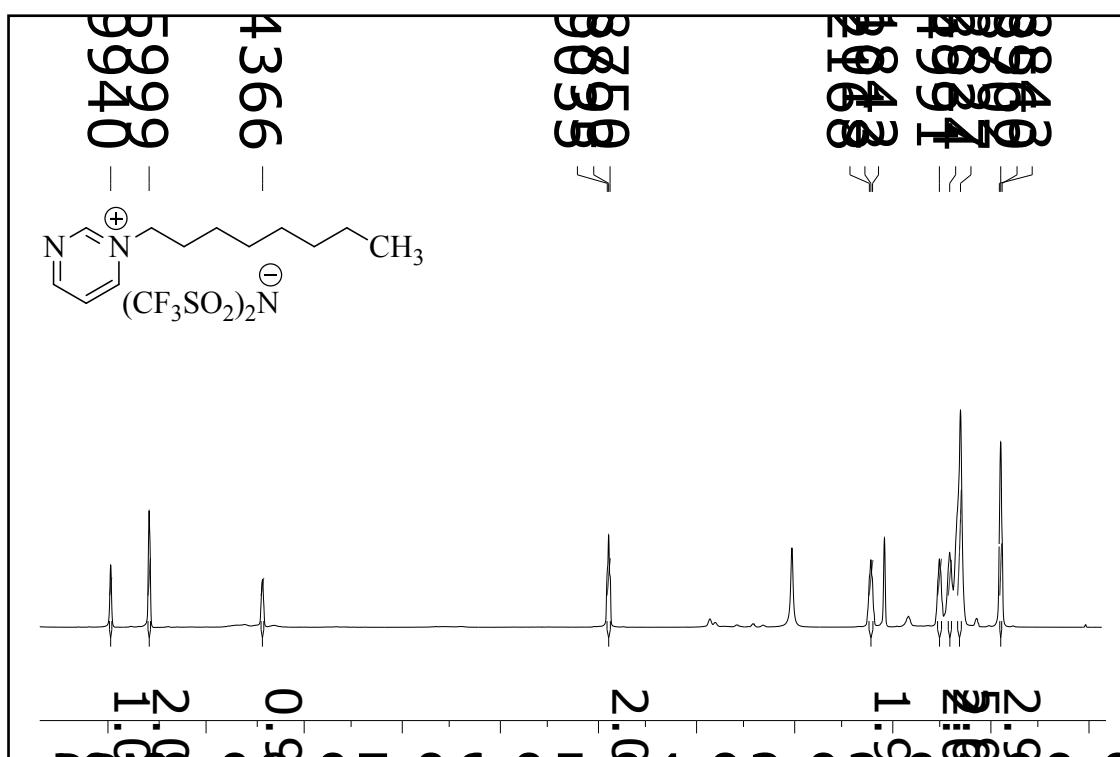
¹³C NMR spectrum of 1-hexylpyrimidin-1-i um bis(trifluoromethanesulfonyl)amide (**4f**) in acetone-d₆ at 500 MHz



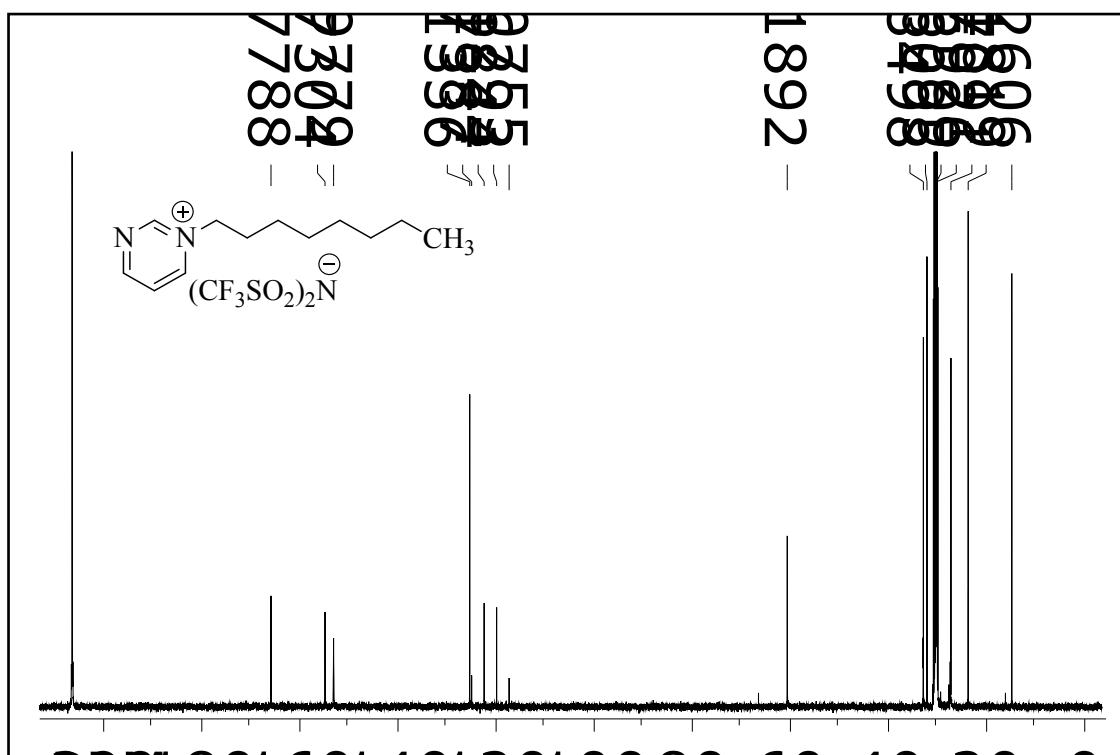
¹H NMR spectrum of 1-heptylpyrimidin-1-ium bis(trifluoromethanesulfonyl)amide (**4g**) in acetone-d₆ at 500 MHz



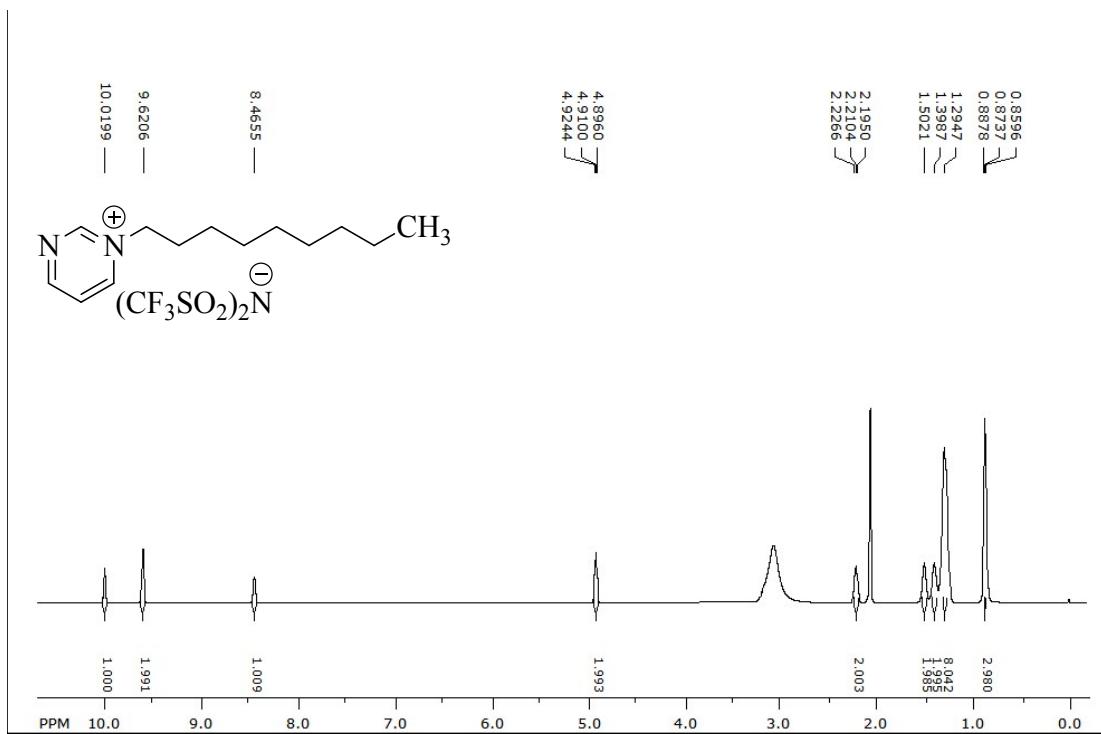
¹³C NMR spectrum of 1-heptylpyrimidin-1-ium bis(trifluoromethanesulfonyl)amide (**4g**) in acetone-d₆ at 500 MHz



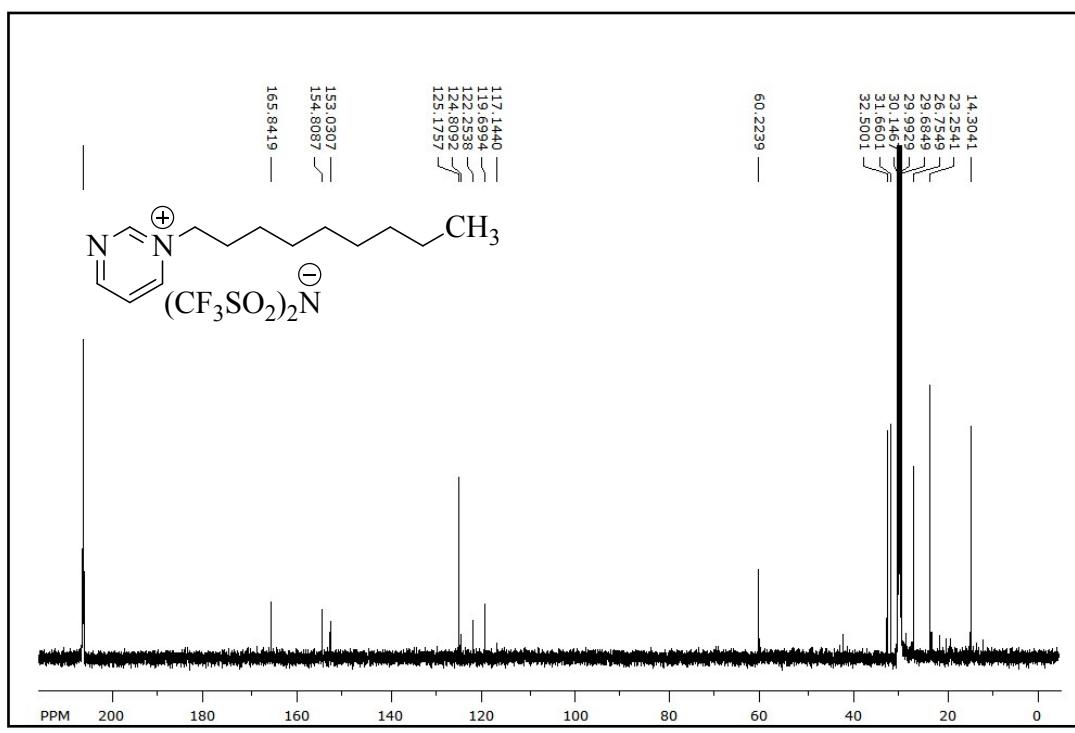
¹H NMR spectrum of 1-octylpyrimidin-1-i um bis(trifluoromethanesulfonyl)amide (**4h**) in acetone-d₆ at 500 MHz



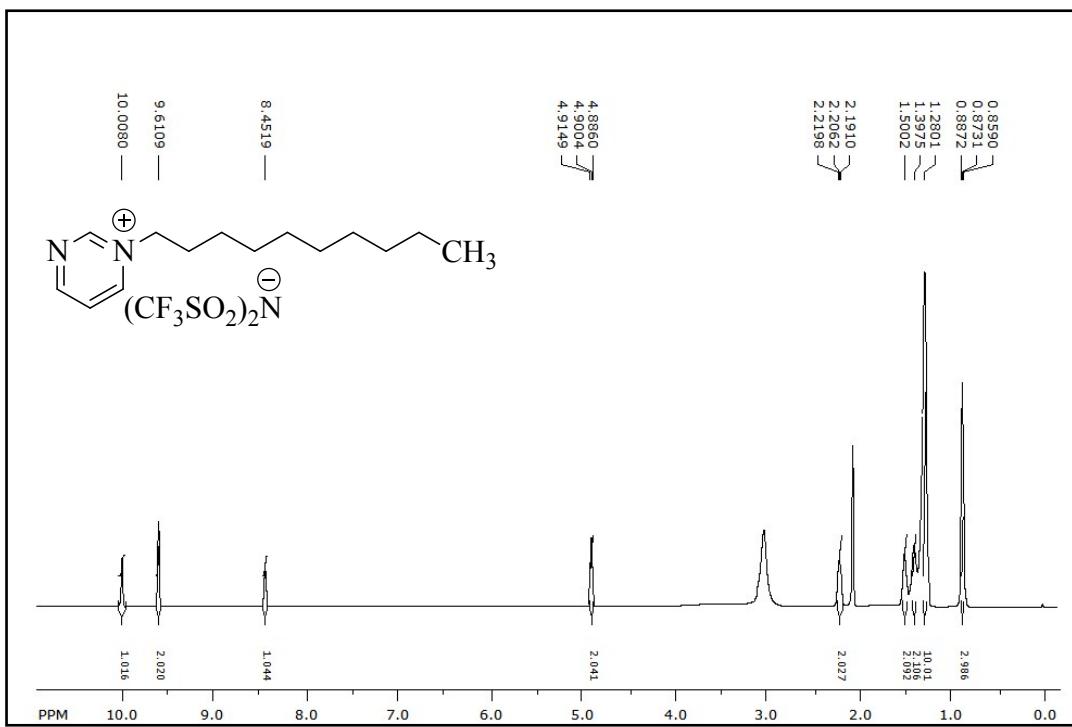
¹³C NMR spectrum of 1-octylpyrimidin-1-i um bis(trifluoromethanesulfonyl)amide (**4h**) in acetone-d₆ at 500 MHz



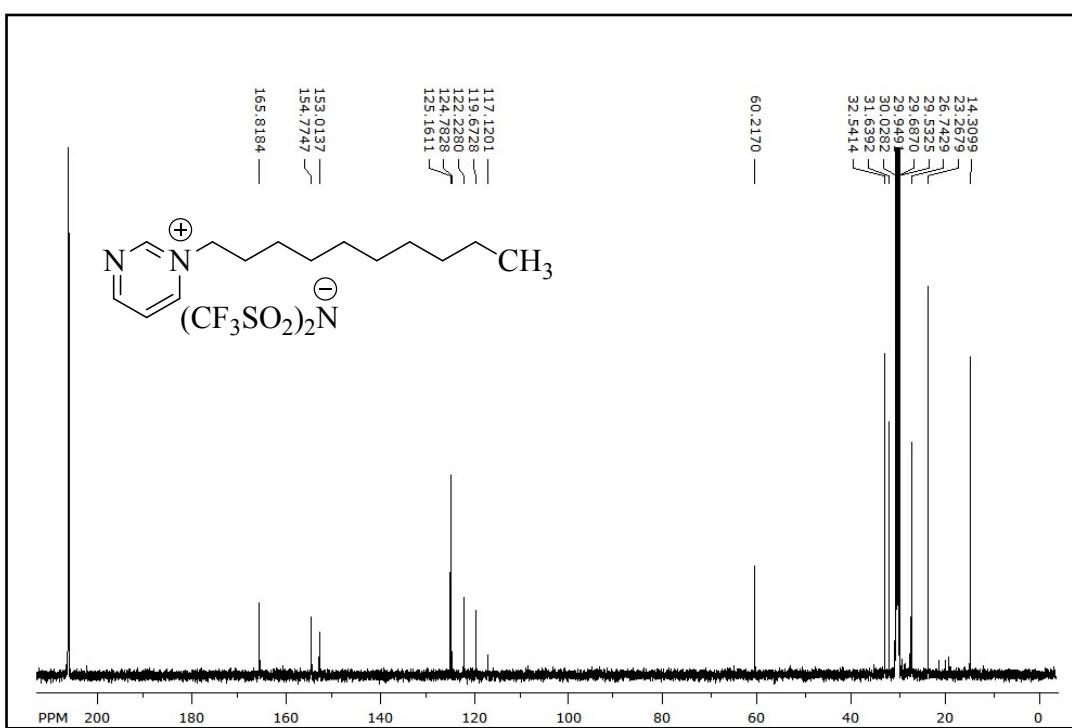
¹H NMR spectrum of 1-nonylpyrimidin-1-ium bis(trifluoromethanesulfonyl)amide (**4i**) in acetone-d₆ at 500 MHz



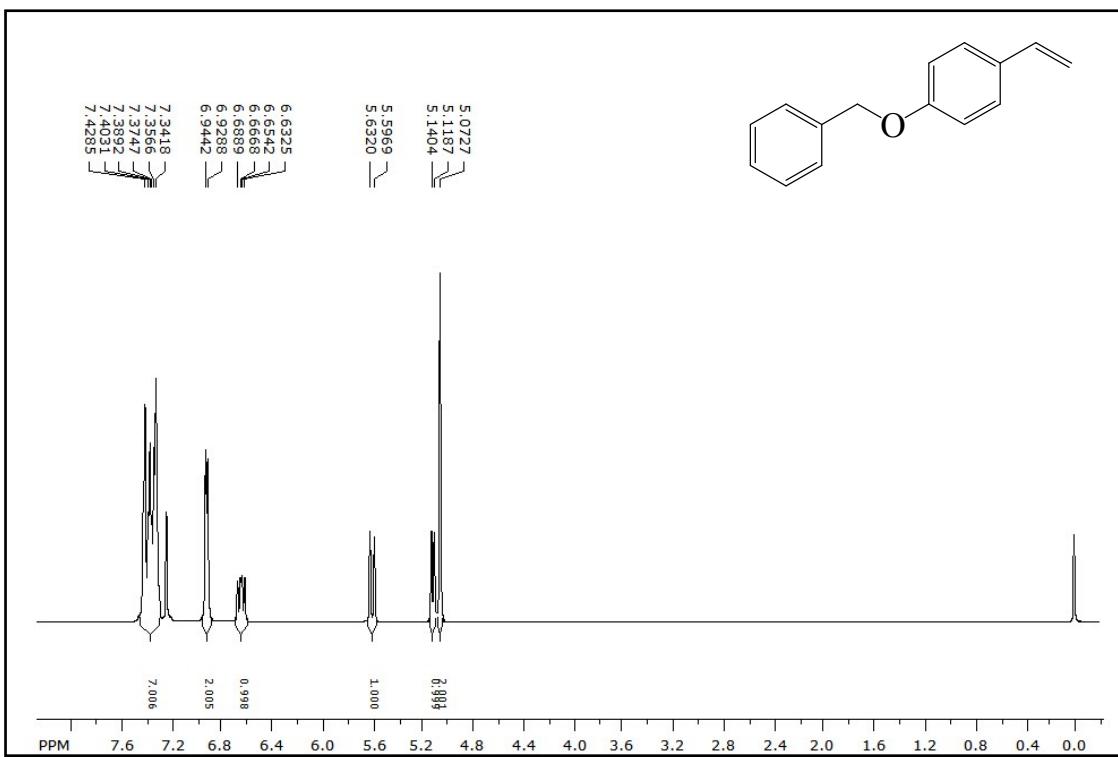
¹³C NMR spectrum of 1-nonylpyrimidin-1-ium bis(trifluoromethanesulfonyl)amide (**4i**) in acetone-d₆ at 500 MHz



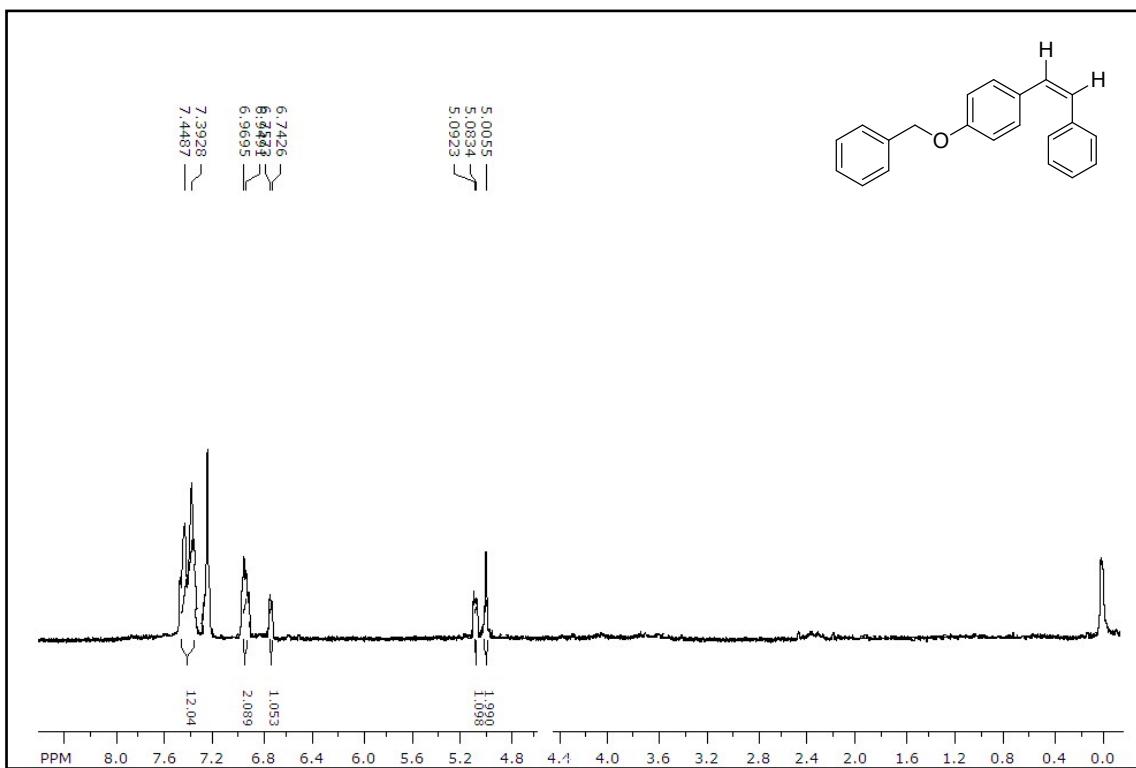
¹H NMR spectrum of 1-decylpyrimidin-1-ium bis(trifluoromethanesulfonyl)amide (**4j**) in acetone-d₆ at 500 MHz



¹³C NMR spectrum of 1-decylpyrimidin-1-ium bis(trifluoromethanesulfonyl)amide (**4j**) in acetone-d₆ at 500 MHz



¹H NMR spectrum of 1-(benzyloxy)-4-vinylbenzene (**5**) in CDCl₃ at 500 MHz



¹H NMR spectrum of (*cis*)-1-(benzyloxy)-4-styrylbenzene (**7**) in CDCl₃ at 500 MHz

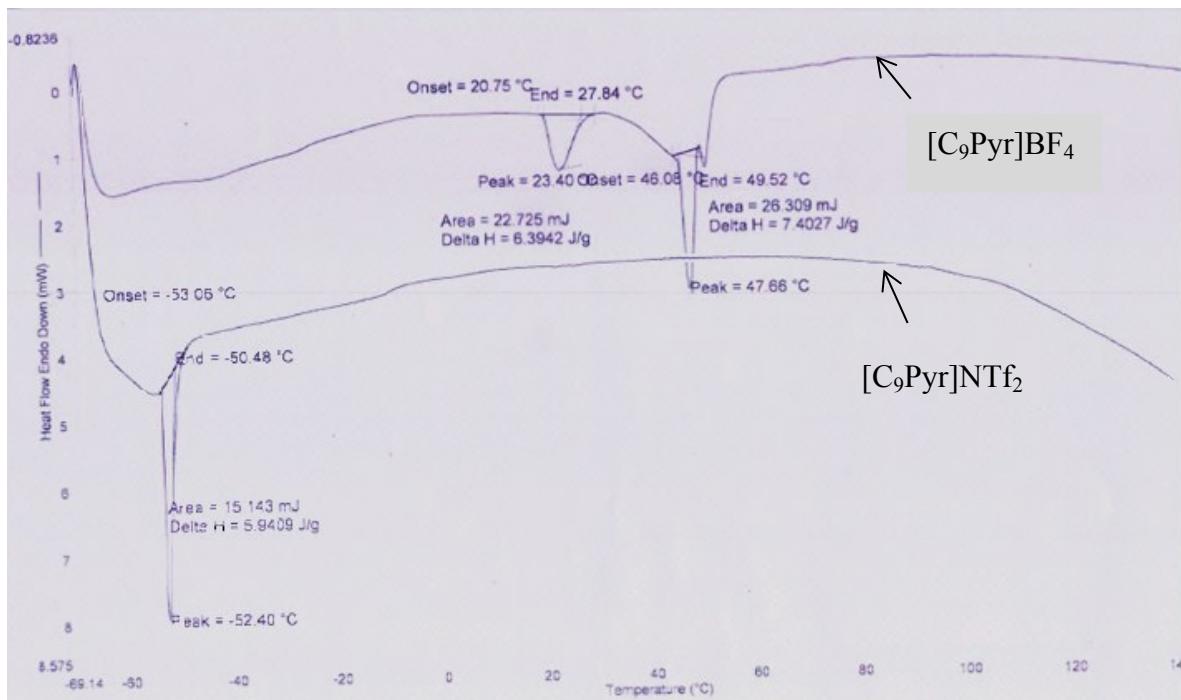


Figure S1. DSC plot of $[C_9\text{Pyr}]BF_4$ and $[C_9\text{Pyr}]NTf_2$ ionic liquid

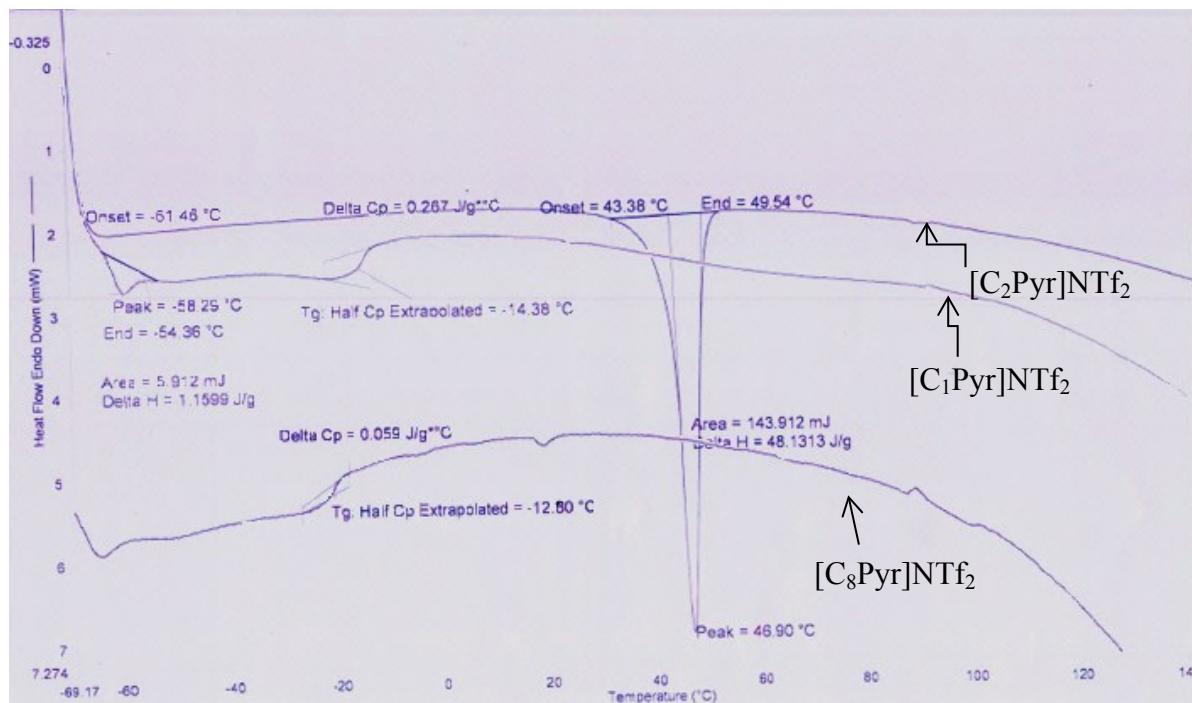


Figure S2. DSC plot of $[C_1\text{Pyr}]NTf_2$, $[C_2\text{Pyr}]NTf_2$ and $[C_8\text{Pyr}]NTf_2$ ionic liquid

Pyrimidinium ionic liquids	$\Delta H_m / \text{J.g}^{-1}$	$T_{\text{onset}} / ^\circ\text{C}$	$T_{\text{peak}} / ^\circ\text{C}$ (T_m)	$T_{\text{endset}} / ^\circ\text{C}$	$\Delta C_p / \text{J.g}^{-1}.^\circ\text{C}$
[C ₉ Pyr]BF ₄	7.4027	46.08	47.66	49.52	-
[C ₁ Pyr]NTf ₂	1.1599	-61.46	-58.29	-54.36	0.267
[C ₂ Pyr] NTf ₂	48.1313	43.38	46.90	49.54	-
[C ₈ Pyr] NTf ₂	-	-	-	-	0.059
[C ₉ Pyr] NTf ₂	5.9409	-53.06	-52.40	-50.48	-

Table 1S. Thermal properties of pyrimidinium ionic liquids