Supporting Information

Experimental and Theoretical Studies on Imidazolium Ionic Liquids-Promoted Conversion of Fructose to 5-Hydroxymethylfurfural

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Contents

1. *General methods*

Materials

D-Fructose was obtained commercially from Aladdin without further purification. Some of the ILs were obtained commercially and dried prior to use. Others were prepared according to the published reports.

Instruments

^{1}H NMR spectra was recorded at Bruck 300 and 400 or Varian Mercury-Plus 400 spectrometer in $CDCl_3$ or D_2O and TMS (0 ppm) was used as internal reference. ^{13}C NMR was recorded at 75 MHz or 100.6 MHz in $CDCl_3$ or D_2O and $CDCl_3$ (77.0 ppm) was used as internal reference. GC-MS were recorded on a Thermo Finnigan Polaris Q GC/MS. ESI-MS were recorded on a Thermo Finnigan LCQ Advantage spectrometer in ESI mode with a spray voltage of 4.8 kV. The products were analyzed on a High Performance Liquid Chromatograph (ComHPLC) equipped with a Comatex^{TM} ODS1 Column (250×4.6 mm) using 6000 PVW UV/VIS detector, 6000 LDI pump and Column Oven Co-IV. The fructose was analyzed on Bio-Rad Aminex HPX-87H column equipped with refractive index detector.

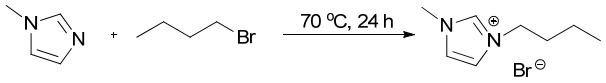
The calculations were carried out by performing DFT by use of the B3PW91 functional with the 6-31++G (d, p) basis set as implemented in Gaussian 03 program package. Vibrational frequency calculations, from which the zero-point energies were derived, have been performed for each optimized structure at the same level to identify the natures of all the stationary points.

Quantification analysis

The product with an injection volume of 20 μL was measured with detector at 282.0 nm, and methanol/water (50/50 v/v) as flowing phase at 0.8 mL/min under the temperature 25 ^{o}C with external standard method. The analysis parameters of fructose performed in the HPLC were as follows: 0.005 mol/L (v/v) H_2SO_4 as mobile phase, injection volume of 20 μL, column temperature of 65 °C, and flow rate of 0.6 mL/min.

2. Synthetic procedure of various ionic liquids

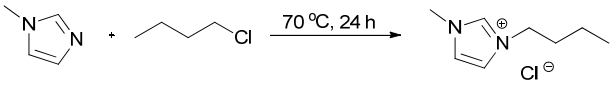
Procedure for the synthesis of BMImBr



Scheme S1. Synthesis of BMImBr

BMImBr was synthesized according to the reported literatures.[1] In a 100 mL round-bottom flask, 1-methylimidazole (8.21 g, 0.1 mol) was mixed with n-butyl bromide (16.44 g, 0.12 mol) and allowed to reflux for 24 h at 70 °C. The excess n-butyl bromide was distilled off under reduced pressure and the residue was finally extracted thoroughly 2-3 times (50 mL each) with diethyl ether to remove the traces of unreacted starting materials. A white solid of 1-n-butyl-3-methylimidazolium bromide was obtained in 87% yield. The IL was dried under vacuum at 70 °C for 24 h.

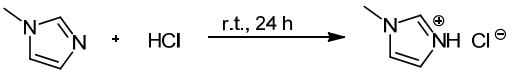
Procedure for the synthesis of BMImCl



Scheme S2. Synthesis of BMImCl

BMImCl was synthesized using the same method for the synthesis of BMImBr. BMImCl was obtained with a 72% yield.

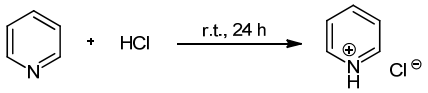
Procedure for the synthesis of HMImCl



Scheme S3. Synthesis of HMImCl

To a 50 mL round bottom flask was added 1-methylimidazole (0.2663 g, 3 mmol) and concentrated hydrochloric acid (0.3 mL, 3 mmol). The reaction mixture was stirred at r.t. for 24 h. The oil residue was dried in vacuo at 65 °C for 24 h to afford 1-hydro-3-methylimidazolium chloride as a colourless, viscous liquid.

Procedure for the synthesis of HPyCl



Scheme S4. Synthesis of HPyCl

According to the synthetic procedure of [HMIm]Cl, pyridinium chloride was yielded as a colourless solid.

Procedure for the synthesis of C_8MImBr

C_8MImBr was synthesized using the same method for the synthesis of BMImBr with, viscous liquid.

Procedure for the synthesis of C_{12}MImBr

C_{12}MImBr was synthesized using the same method for the synthesis of BMImBr.

Procedure for the synthesis of BMImI

BMImI was synthesized using the same method for the synthesis of BMImBr.

Procedure for the synthesis of MMImI

MMImI was synthesized using the same method for the synthesis of BMImI.

Procedure for the synthesis of $HMImHSO_4$[2]

$HMImHSO_4$ was prepared by a dropwise addition of one equivalent of concentrated sulphuric acid to a cooled solution of HMImCl in anhydrous dichloromethane. The mixture was refluxed for 48 h, the by-product HCl formed in the reaction was carried out of the condenser under a stream of dry nitrogen and was dissolved in deionized water at 0 ^oC. When HCl had been completely removed, CH_2Cl_2 was evaporated, evaporated with a rotary evaporator. The IL was dried under vacuum at 60 ^oC for 6 h and stored in a desiccator.

Procedure for the synthesis of $BMImH_2PO_4$[2]

$BMImH_2PO_4$ was prepared by a dropwise addition of one equivalent of concentrated phosphoric acid to a cooled solution of BMImCl in anhydrous dichloromethane. The mixture was refluxed for 48 h, the by-product HCl formed in the reaction was carried out of the condenser under a stream of dry nitrogen and was dissolved in deionized water at 0 ^oC. When HCl had been completely removed, CH_2Cl_2 was evaporated, evaporated with a rotary evaporator. The IL was dried under vacuum at 60 ^oC for 24 h and stored in a desiccator.

Procedure for the synthesis of $(HOOC)CH_2$MImCl.[3]

Under an inert atmosphere of argon, a mixture of 1-methylimidazole (0.020 mol) and $ClCH_2COOCH_3$ (0.020 mol) was stirred at room temperature for 6 h. The resultant mixture turned to a solid during the reaction. The solid was washed with diethyl ether (3×30 mL) and dried under vacuum for 24 h to give 1-ethoxycarbonylmethyl-3-methylimidazolium chloride. In a typical procedure, a mixture of 1-ethoxycarbonylmethyl-3-methylimidazolium chloride (0.020 mol) and 37% HCl aqueous solution (0.022 mol) was refluxed for 4 h. The solvent was

removed and the residue was washed with acetone and diethyl ether to give the product as a white powder. The IL was dried under vacuum at 60 ^{o}C for 24 h and stored in a desiccator.

Procedure for the synthesis of $(CH_2)_4SO_3HMImHSO_4$

$(CH_2)_4SO_3HMImHSO_4$ was synthesized according to the reported literatures.[4] A mixture of 1-Methylimidazole (0.1 mol, 8.21 g) and 1, 4-butane sultone (0.1 mol, 13.62 g) was charged into a 100 mL conical flask. The mixture was stirred at room temperature for 4 days until it turned into solid. Thus, the white solid zwitterion formed was washed repeatedly with ether, filtrated to remove non-ionic residues and dried in vacuum. Then, to a stoichiometric amount of concentrated sulfuric acid (98%, 5.5 mL) in a 100 mL conical flask was added dropwise the white solid zwitterion slowly at 0 ^{o}C. The mixture was stirred at 80 ^{o}C for 6 h. Product was washed with diethyl ether and dried in vacuo at 60 ^{o}C for 24 h to get the viscous clear $[(CH_2)_4SO_3HMIm][HSO_4]$.

3. Characterization of various ionic liquids

1-n-butyl-3-methylimidazolium bromide (BMImBr)

^{1}H NMR (300 MHz, D_2O)： δ = 0.82(t, $^{3}J_{HH}$ = 7.4 Hz, 3H, CH_3); 1.23(m, 2H, CH_2); 1.75(m, 2H, CH_2); 3.79(s, 3H, N CH_3); 4.10(t, $^{3}J_{HH}$ = 7.2 Hz, 2H, NCH_2); 7.33(s, 1H, CH); 7.38(s, 1H, CH); 8.61(s, 1H, CH); ^{13}C {^{1}H} NMR (100.6 MHz, D_2O): δ = 12.64; 18.74; 31.25; 35.67; 49.27; 122.20; 123.45; 135.82; ESI-MS (4.8 kV): *m/z* (%) =139.0 (100) $[M\text{-}Br]^{+}$, 78.9 (100) $[M\text{-}C_8H_{15}N_2]^{-}$.

1-n-butyl-3-methylimidazolium chloride (BMImCl)

^{1}H NMR (400MHz, $CDCl_3$): δ = 0.93 (t, $^{3}J_{HH}$ = 7.6 Hz, 3H, CH_3); 1.30-1.40 (m, 2H, CH_2); 1.83-1.90 (m, 2H, CH_2); 4.09 (s, 3H, NCH_3); 4.30 (t, $^{3}J_{HH}$ = 7.4 Hz, 2H, NCH_2); 7.37 (s, 1H, CH); 7.50 (s, 1H, CH); 10.73 (s, 1H, CH); ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ = 13.36; 19.40; 32.09; 36.51; 49.76; 121.64; 123.29; 138.24; ESI-MS (4.8 kV): *m/z* (%) =139.0 (100) $[M\text{-}Cl]^{+}$.

1-hydrogen-3-methylimidazolium chloride (HMImCl)

^{1}H NMR (400 MHz, D_2O): δ = 8.70 (s, 1 H), 7.47 (s, 2 H), 3.95 (s, 3 H); ^{13}C {^{1}H} NMR (100.6 MHz, D_2O): δ = 135.0, 123.0, 119.5, 35.5; ESI-MS (4.8 kV): m/z (%) = 83.16 (100) $[M\text{-}Cl]^{+}$.

Pyridine hydrochloride (HPyCl)

^{1}H NMR (400 MHz, D_2O): δ = 8.78 (d, $^{3}J_{H\,H}$ = 5.6 Hz, 2 H), 8.62 (t, $^{3}J_{H\,H}$ = 8 Hz, 1 H), 8.07 (t, $^{3}J_{H\,H}$ = 6.4 Hz, 2 H); ^{13}C {^{1}H} NMR (100.6 MHz, D_2O): δ = 147.2, 141.0, 127.4; ESI-MS (4.8 kV): m/z (%) = 80.11 (100) $[M\text{-}Cl]^{+}$.

1-n-octyl-3-methylimidazolium bromide (C_8MImBr)

^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.686 (t, $^{3}J_{HH}$ = 10.4 Hz, 3H, CH_3), 1.093-1.166 (m, 10H, $(CH_2)_5$), 1.762 (d, $^{3}J_{HH}$ = 2.8 Hz, 2H, CH_2), 3.980 (d, $^{3}J_{HH}$ = 3.2 Hz, 3H, CH_3), 4.170 (t, $^{3}J_{HH}$ = 7.0 Hz, 2H, CH_2), 7.403 (s, 1H, NCH), 7.587 (s, 1H, NCH), 10.059 (s, 1H, NCHN). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ = 13.180; 21.643; 25.300; 28.030; 28.095; 29.440; 30.740; 35.855; 49.159; 121.446; 123.129; 136.005; ESI-MS (4.8 kV): *m/z* (%) =195.3 (100) $[M\text{-}Br]^{+}$, 78.9 (100) $[M\text{-}C_{12}H_{23}N_2]^{-}$

1-n-dodecyl -3-methylimidazolium bromide (C_{12}MImBr)

^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.848 (s, 3H, CH_3), 1.217 (m, 18H, $(CH_2)_9$), 1.889 (t, $^{3}J_{HH}$ = 6.8 Hz, 2H, CH_2), 4.114 (s, 3H, CH_3), 4.292 (t, $^{3}J_{HH}$ = 7.2 Hz, 2H, CH_2), 7.355 (s, 1H, NCH), 7.511 (s, 1H, NCH), 10.492 (s, 1H, NCHN). ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ = 13.772; 22.307; 25.900; 28.653; 28.954; 29.024; 29.221; 29.142; 29.997; 31.523; 36.381; 49.753; 121.781; 123.565; 136.771; ESI-MS (4.8 kV): *m/z* (%) =251.4 (100) $[M\text{-}Br]^{+}$, 78.9 (100) $[M\text{-}C_{16}H_{31}N_2]^{-}$

1-n-butyl-3-methylimidazolium iodide (BMImI)

^{1}H NMR (400 MHz, $CDCl_3$)：δ = 0.803-0.852(m, 3H, CH_3); 1.220-1.276(m, 2H, CH_2); 1.760-1.797(m, 2H, CH_2); 4.000-4.015(m, 3H, NCH_3); 4.217(t, $^{3}J_{HH}$ = 7.2 Hz, 2H, NCH_2); 7.473(d, $^{3}J_{HH}$ = 0.6 Hz, 1H, NCH); 7.601(d, $^{3}J_{HH}$ = 0.6 Hz, 1H, NCH); 8.61(s, 1H, NCHN); ^{13}C {^{1}H} NMR (100.6 MHz, $CDCl_3$): δ = 18.477; 28.420; 36.145; 55.632; 121.932; 122.798; 135.361; ESI-MS (4.8 kV): *m/z* (%) =139.0 (100) $[M\text{-}I]^{+}$, 126.9 (100) $[M\text{-}C_8H_{15}N_2]^{-}$

1-methyl-3-methylimidazolium iodide (MMImI)

^{1}H NMR (400 MHz, D_2O): δ = 3.877-3.964 (m, 6H, $2CH_3$), 7.402-7.493 (m, 2H, 2NCH), 8.636-8.740 (m, 1H, NCHN). ^{13}C {^{1}H} NMR (100.6 MHz, D_2O): δ = 35.973; 123.470; 136.609; ESI-MS (4.8 kV): *m/z* (%) =97.1 (100) $[M\text{-}I]^{+}$, 126.9 (100) $[M\text{-}C_5H_9N_2]^{-}$

1-hydrogen-3-methyl imidazolium hydrosulfate ($HMImHSO_4$)

^{1}H NMR (400 MHz, D_2O): δ = 3.788 (s, 3H, CH_3), 7.303 (s, 2H, 2NCH), 8.527 (s, 1H,

NCHN). ^{13}C {^{1}H} NMR (100.6 MHz, D_2O): δ = 35.411; 119.410; 122.908; 134.917; ESI-MS (4.8 kV): *m/z* (%) =83.1 (100) $[M\text{-}HSO_4]^+$, 97.1 (100) $[M\text{-}C_4H_7N_2]^-$

1-butyl-3-methyl imidazolium phosphate ($BMImH_2PO_4$)

^{1}H NMR (400 MHz, D_2O): δ = 0.681 (s, 3H, CH_3), 1.100 (d, $^{3}J_{HH}$ = 7.2 Hz, 2H, CH_2), 1.634 (t, $^{3}J_{HH}$ = 7.2 Hz, 2H, CH_2), 3.689 (s, 3H, CH_3), 3.989 (t, $^{3}J_{HH}$ = 7.2 Hz, 2H, CH_2), 7.256 (d, $^{3}J_{HH}$ = 9.8 Hz, 2H, 2NCH), 8.516 (s, 1H, NCHN).

^{13}C {^{1}H} NMR (100.6 MHz, D_2O): δ = 12.566; 18.626; 31.131; 35.577; 49.144; 122.096; 123.359; 135.642; ESI-MS (4.8 kV): *m/z* (%) =139.0 (100) $[M\text{-}H_2PO_4]^+$, 96.9 (100) $[M\text{-}C_8H_{15}N_2]^-$

1-(carboxymethyl)-3-methylimidazolium chloride ($(HOOC)CH_2MimCl$)

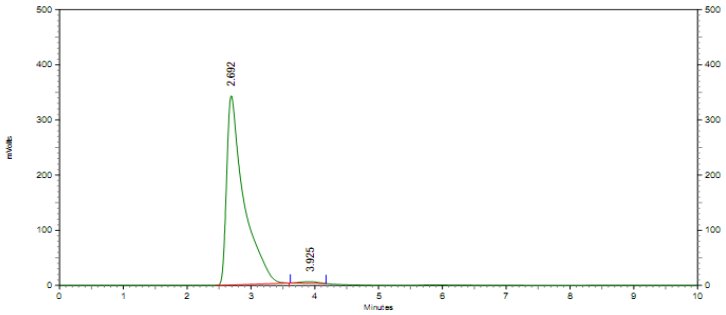
1-ethoxycarbonylmethyl-3-methylimidazolium chloride: ^{1}H NMR (300 MHz, D_2O): δ = 1.22 (t, $^{3}J_{H,H}$ =7.2 Hz, 3H), 3.88 (s, 3 H), 4.23 (q, 2H), 5.10 (s, 2 H), 7.45 (s, 2 H), 8.76 (s, ^{1}H); ^{13}C NMR (75 MHz, D_2O): δ =13.3, 36.1, 50.0, 63.7, 123.6, 137.5, 168.3.

HOOCMImCl: ^{1}H NMR (300 MHz, D_2O): δ = 3.82 (s, 3 H), 5.03 (s, 2 H), 7.40 (d, $^{3}J_{H,H}$ =2.7 Hz), 8.70 (s, 1H); ^{13}C {^{1}H} NMR (75 MHz, D_2O): δ = 36.09, 50.0, 123.6, 137.4, 169.9; ESI-MS (4.8 kV): m/z (%) = 141 (100) $[M\text{-}Cl]^+$.

1-(butyl-4-sulfonate)-3-methyl imidazolium hydrosulfate ($(CH_2)_4SO_3HMImHSO_4$)

^{1}H NMR(400 MHz, D_2O)： δ = 1.630-1.707(m, 2H, CH_2) 1.912-1.987(m, 2H, CH_2); 2.871(t, $^{3}J_{HH}$ = 7.6 Hz, 2H); 3.818(s, 3H, CH_3); 4.173(t, 2H, $^{3}J_{HH}$ = 7.2 Hz, CH_2); 7.365(s, 1H, NCH); 7.422(s, 1H, NCH); 8.666(s, 1H, NCHN); ^{13}C {^{1}H} NMR (100.6 MHz, D_2O): δ = 20.854; 28.024; 35.603; 48.844; 49.996; 122.099; 123.598; 135.896; ESI-MS (4.8 kV): *m/z* (%) =205.3 (100) $[M\text{-}HSO_4]^+$, 97.1 (100) $[M\text{-}C_7H_{13}N_2O_3S]^-$.

4. Characterization of 5-hydroxymethylfurfural



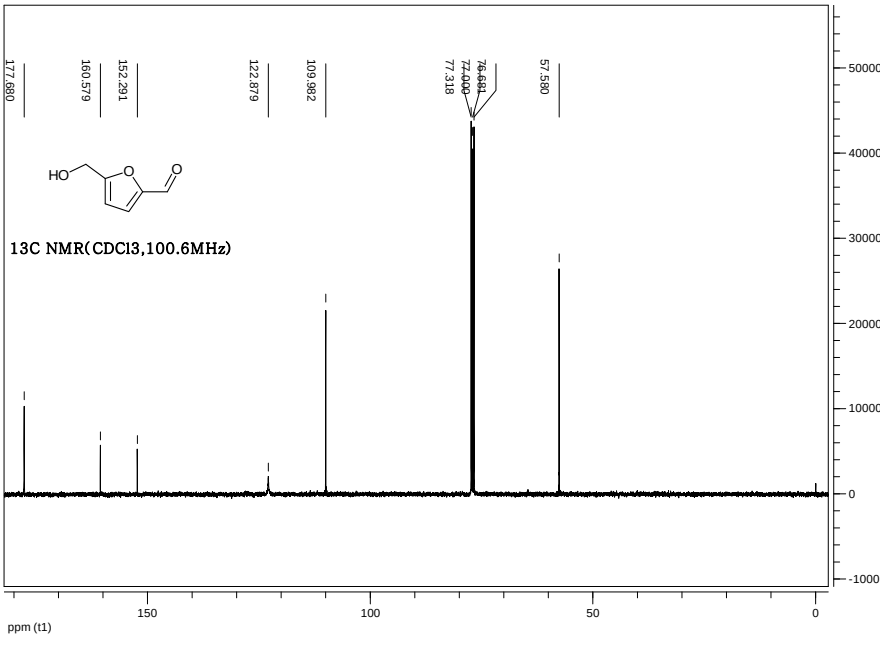
Channel A Results

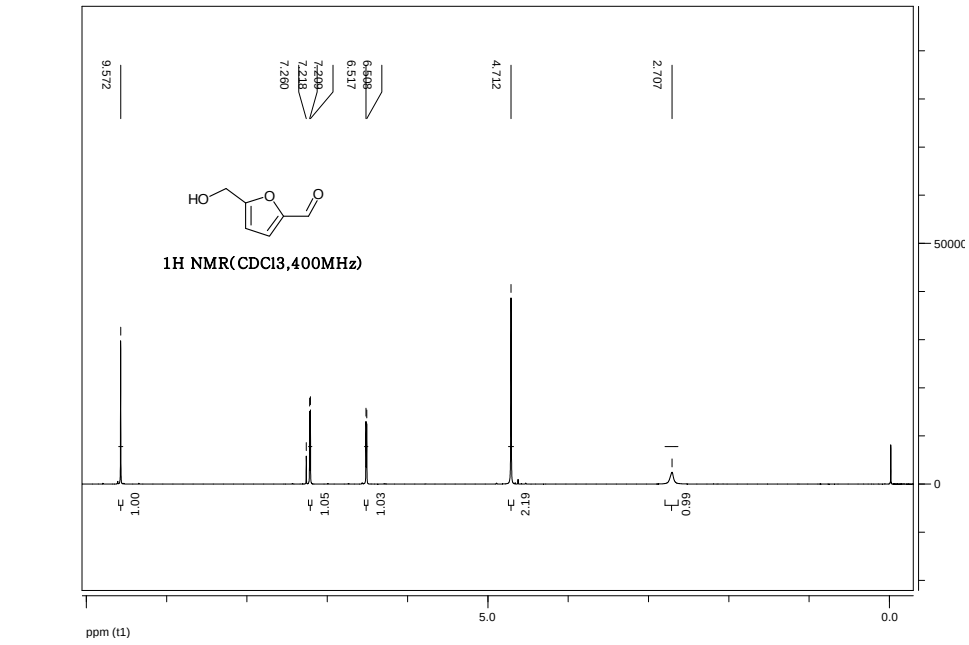
Pk #	Name	Retention Time	Area	Area Percent	Height	Height Percent
1		2.692	6423832	99.119	342497	99.133
2		3.925	57086	0.881	2995	0.867
Totals			6480918	100.000	345492	100.000

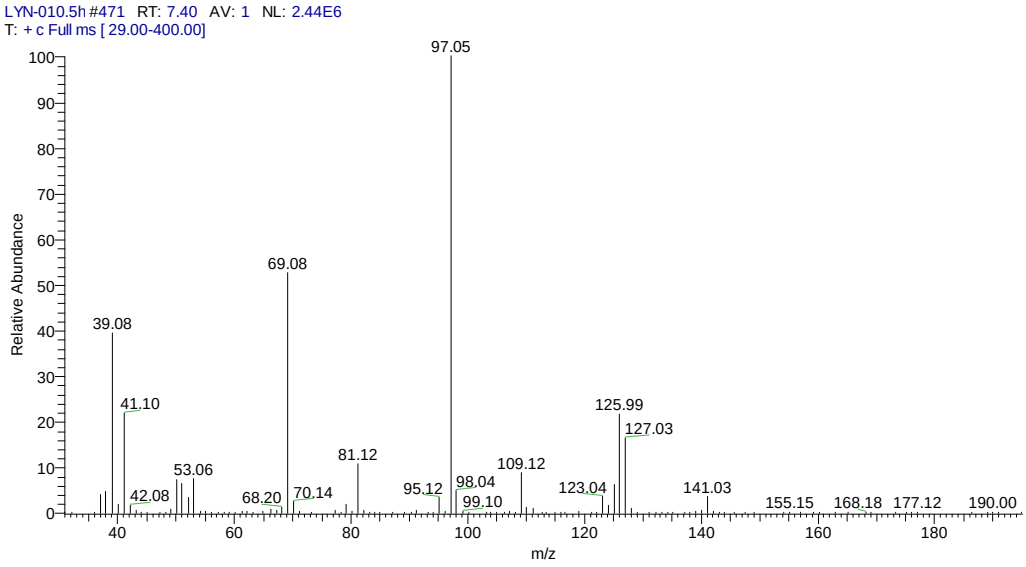
HPLC Analysis with the retention time 2.692.

NMR and EI-MS Analysis:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.707 (s, 1H, OH), 4.712 (s, 1H, CH_2), 6.513 (d, $^{3}J_{HH}$ = 1.8 Hz, 1H, CH), 7.209 (d, $^{3}J_{HH}$ = 3.6 Hz, 1H, CH), 9.572 (s, 1H, CHO). ^{13}C {^{1}H} NMR(100.6 MHz, $CDCl_3$): δ 57,580, 109.982, 122.879; 152.291, 160.579, 177.680. EI-MS calcd for $C_6H_6O_3$ 125.99.







5. References

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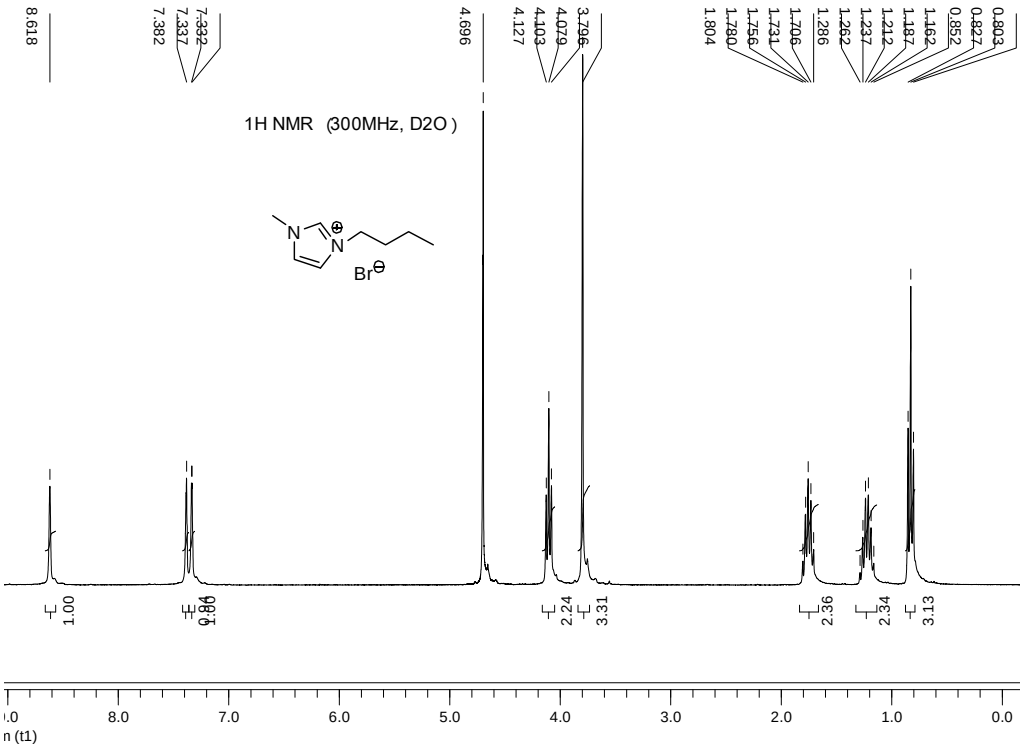
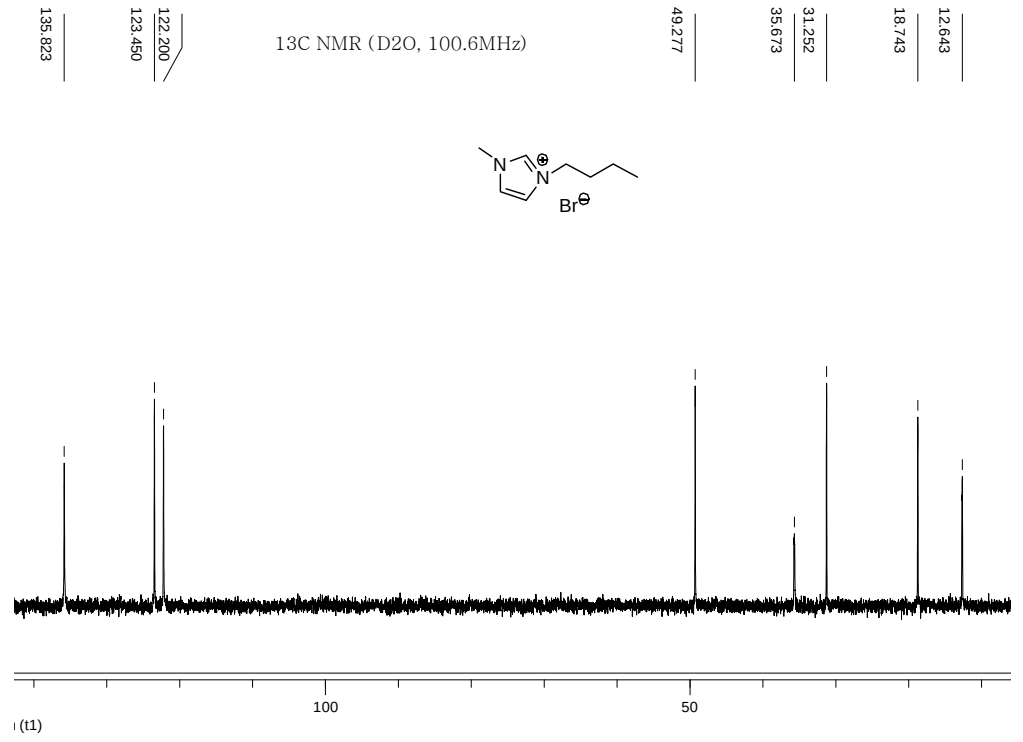
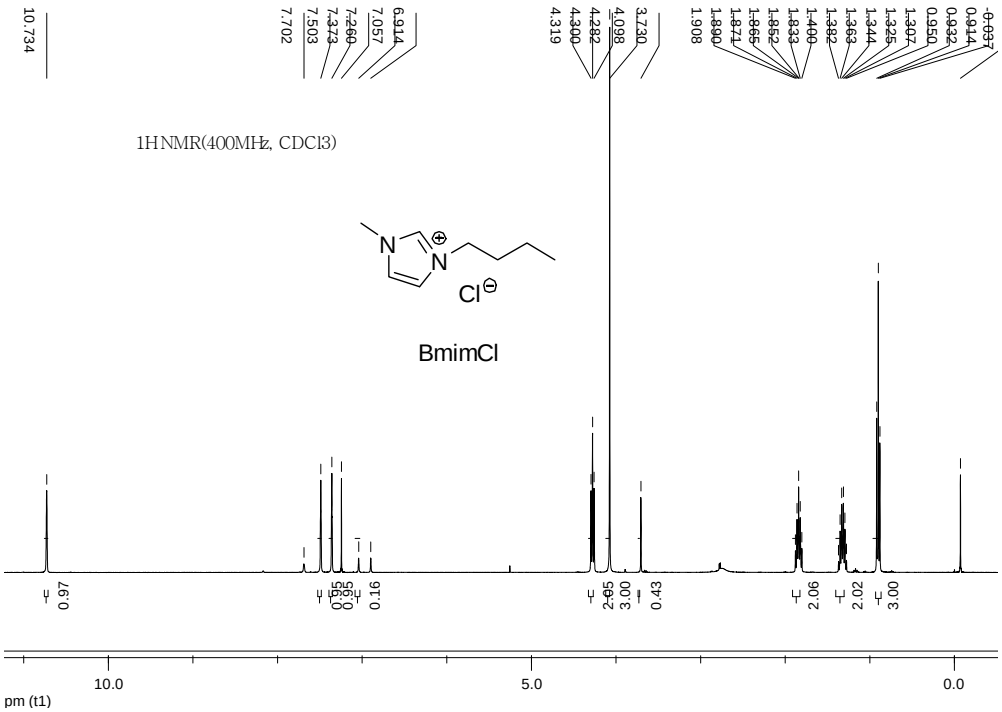
6. The ^{1}H NMR and ^{13}C NMR charts of various ionic liquids

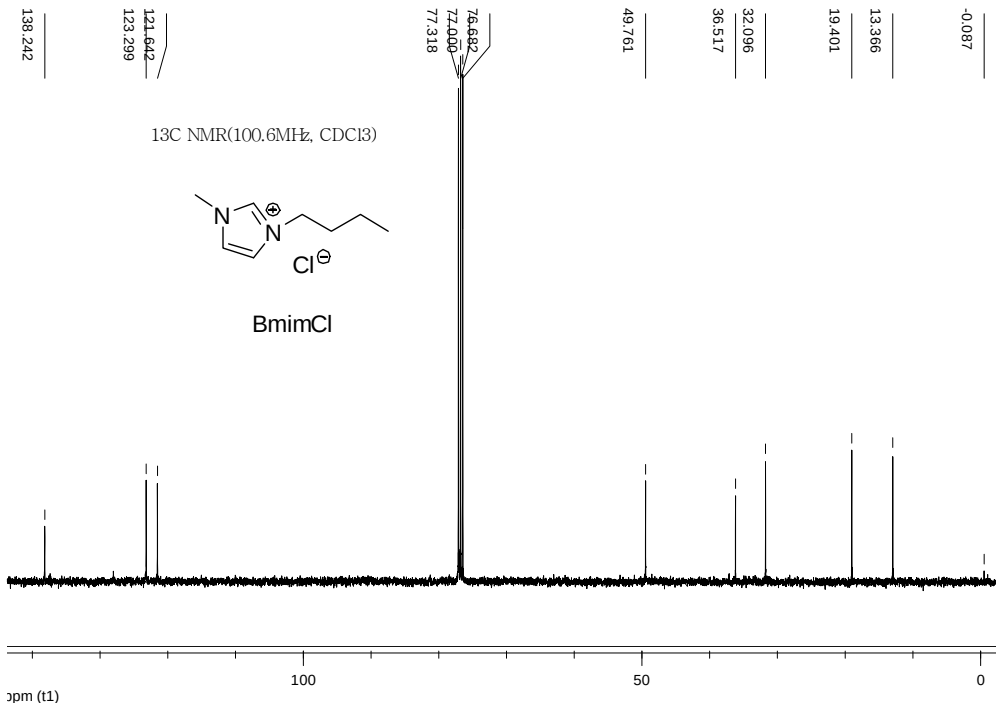
1-n-butyl-3-methylimidazolium bromide (BMImBr)



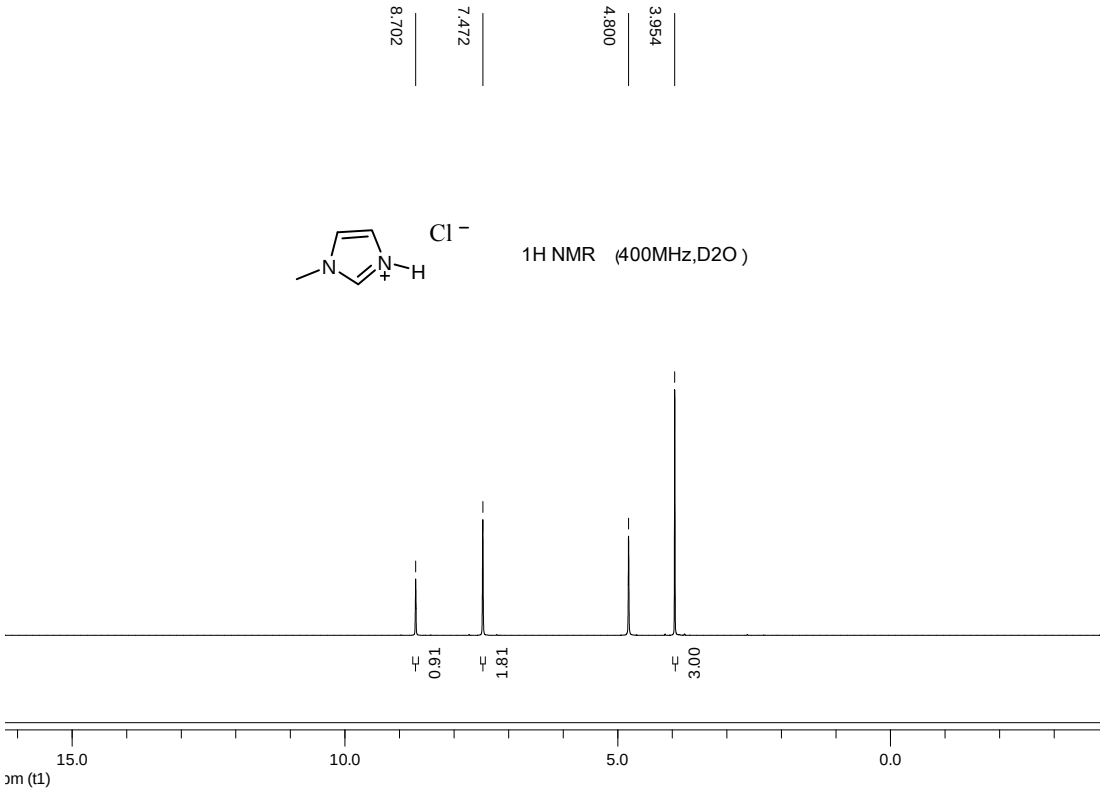


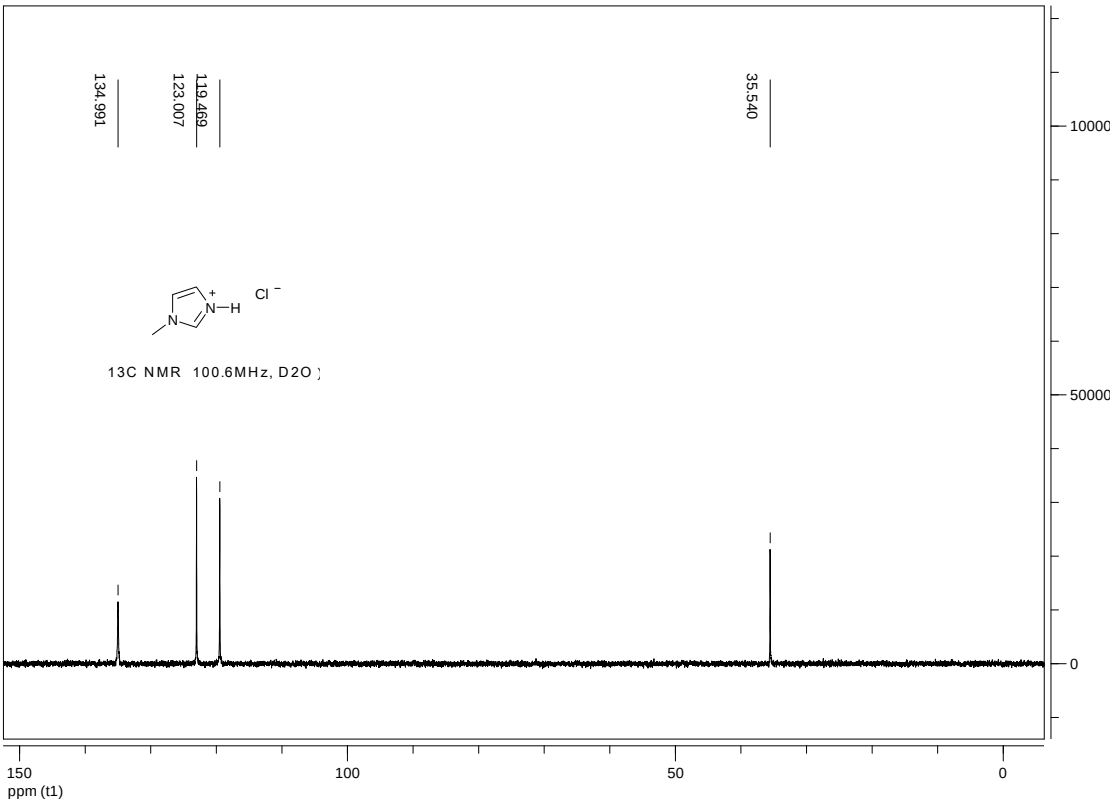
1-n-butyl-3-methylimidazolium chloride (BMImCl)



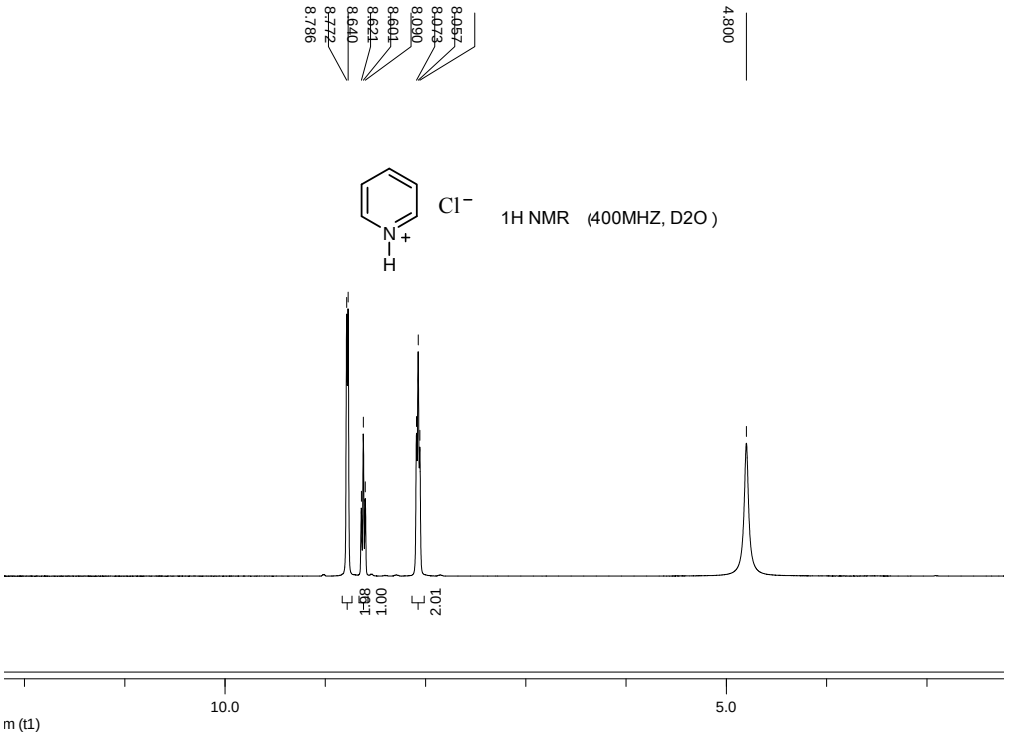


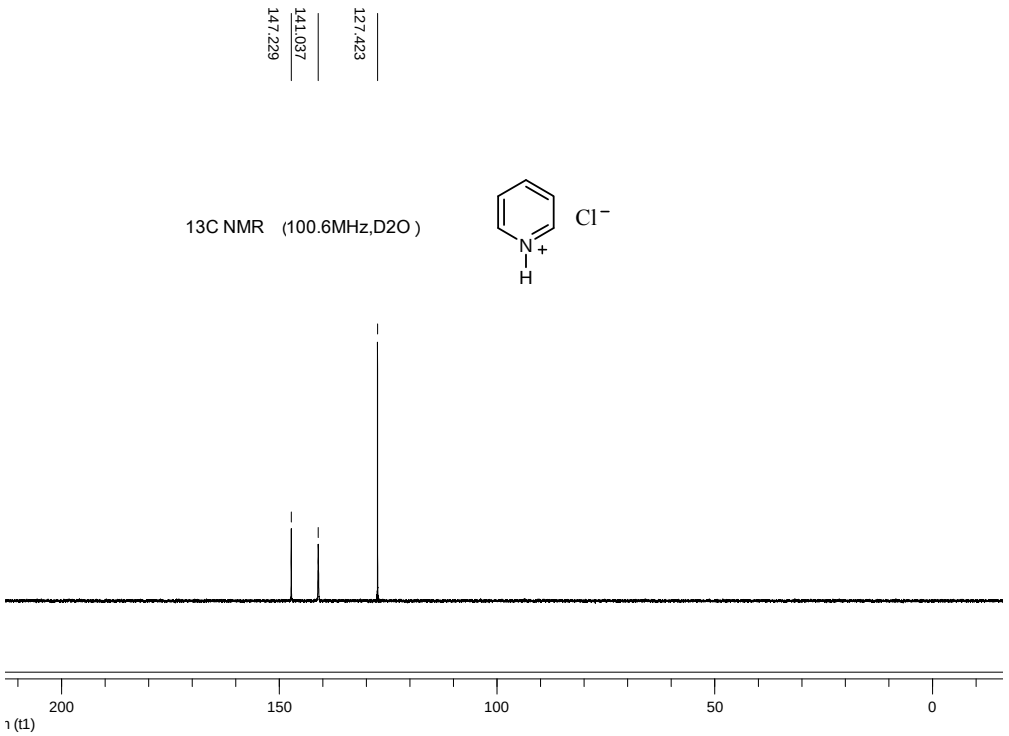
1-hydrogen-3-methylimidazolium chloride (HMImCl)



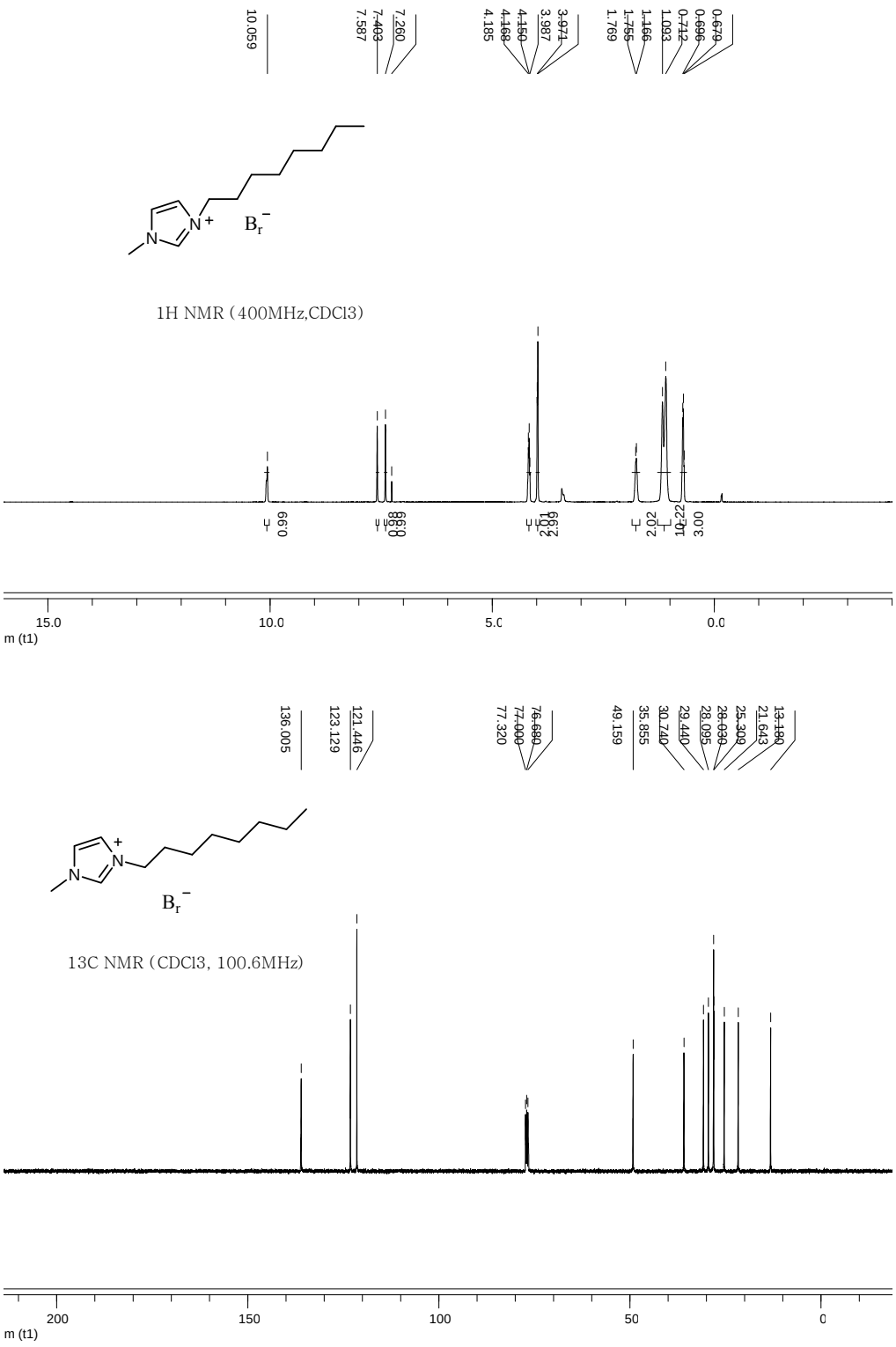


Pyridine hydrochloride (HPyCl)

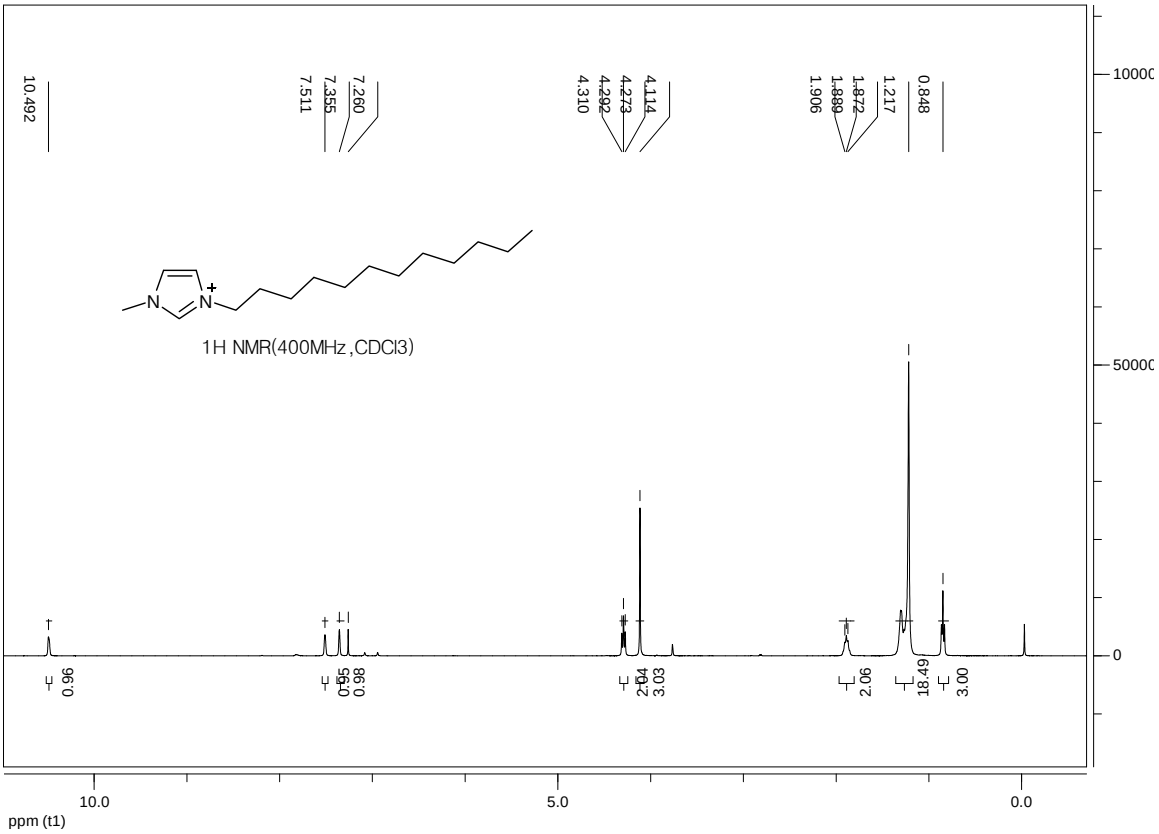


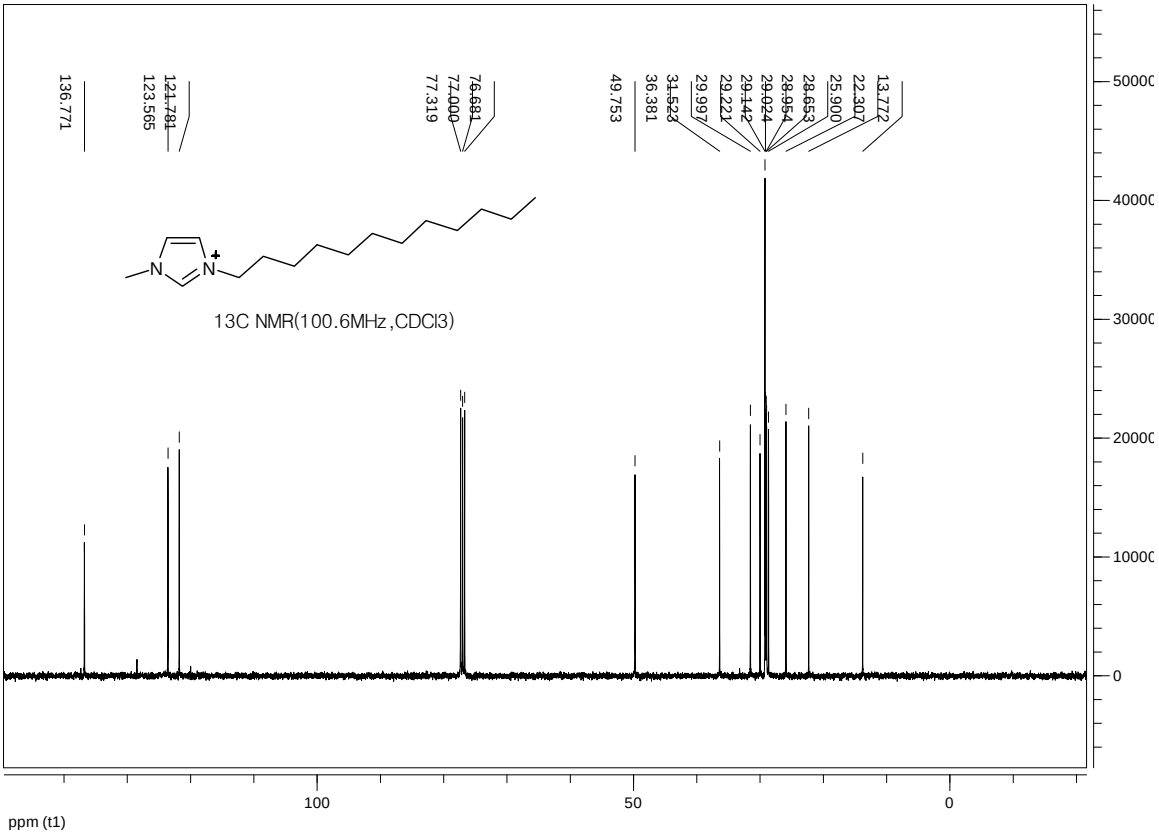


1-n-octyl-3-methylimidazolium bromide (C_8MImBr)

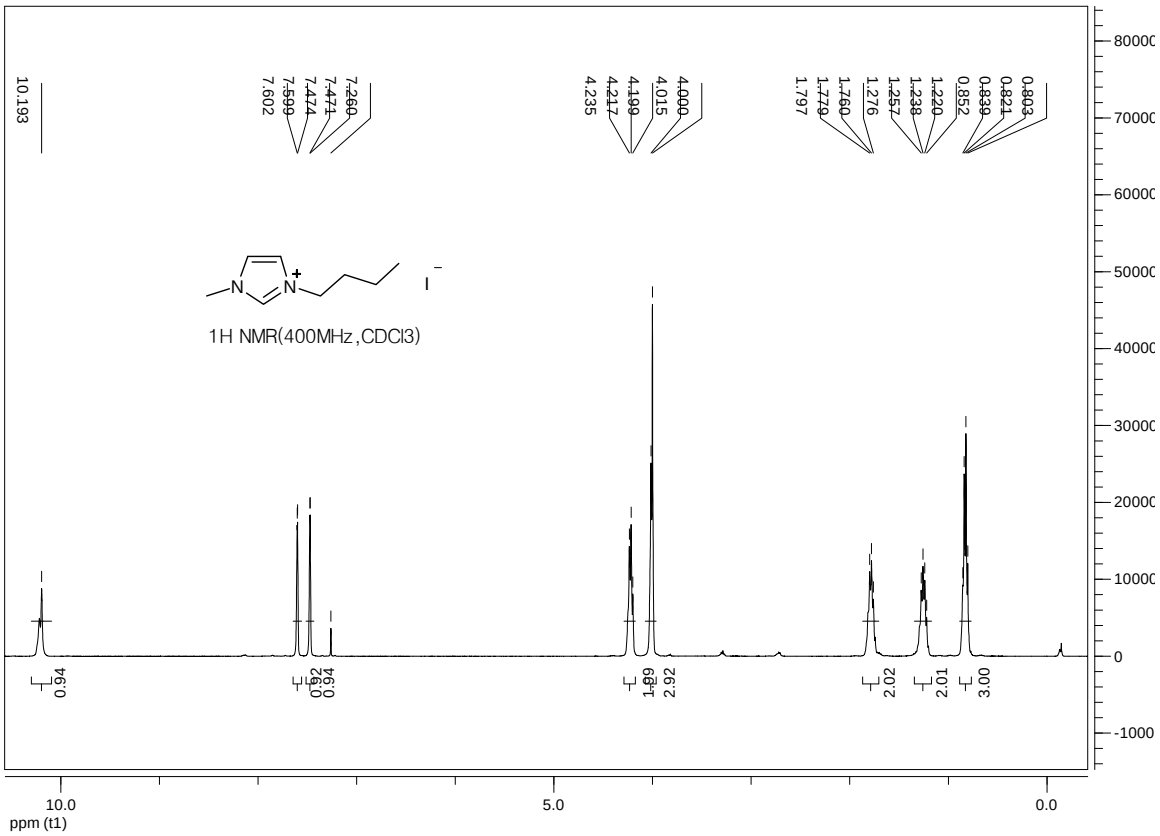


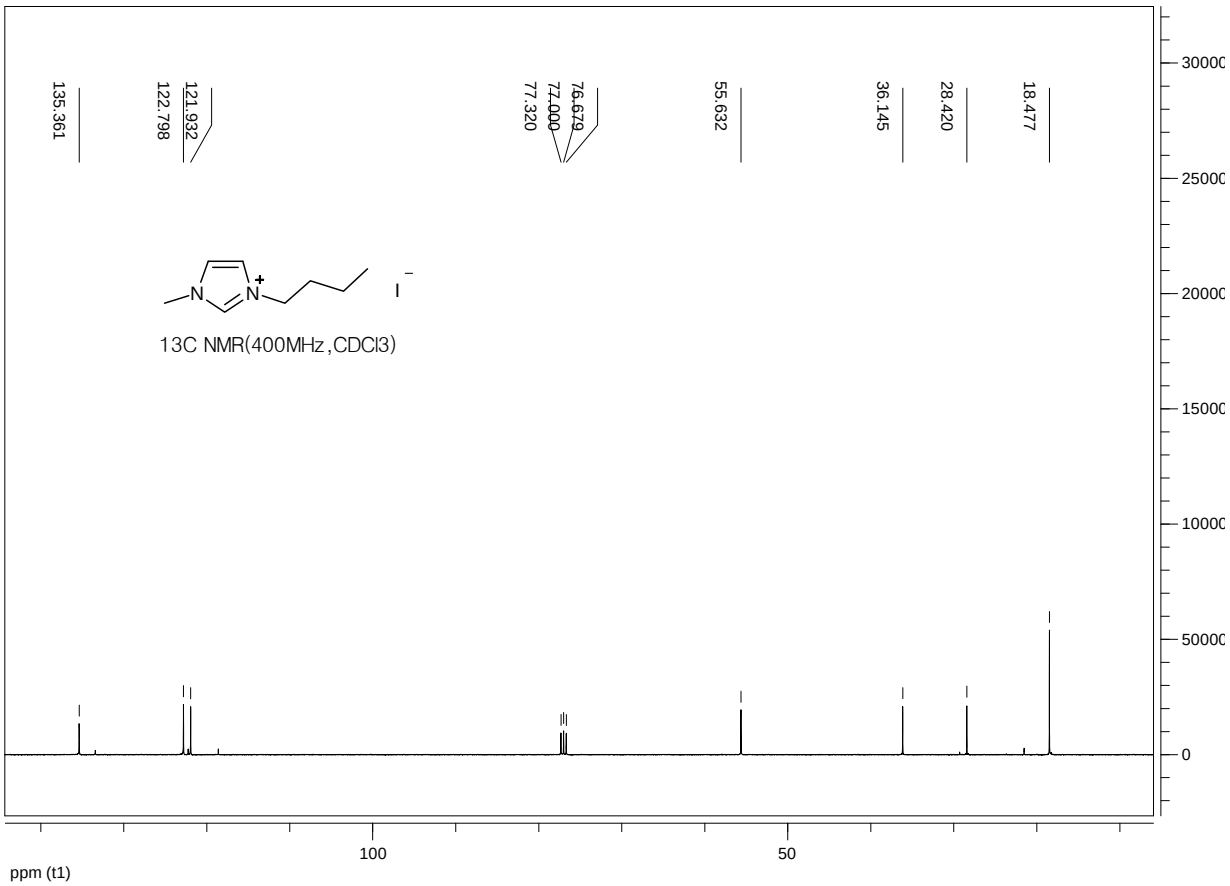
1-n-dodecyl-3-methylimidazolium bromide (C_{12}MImBr)



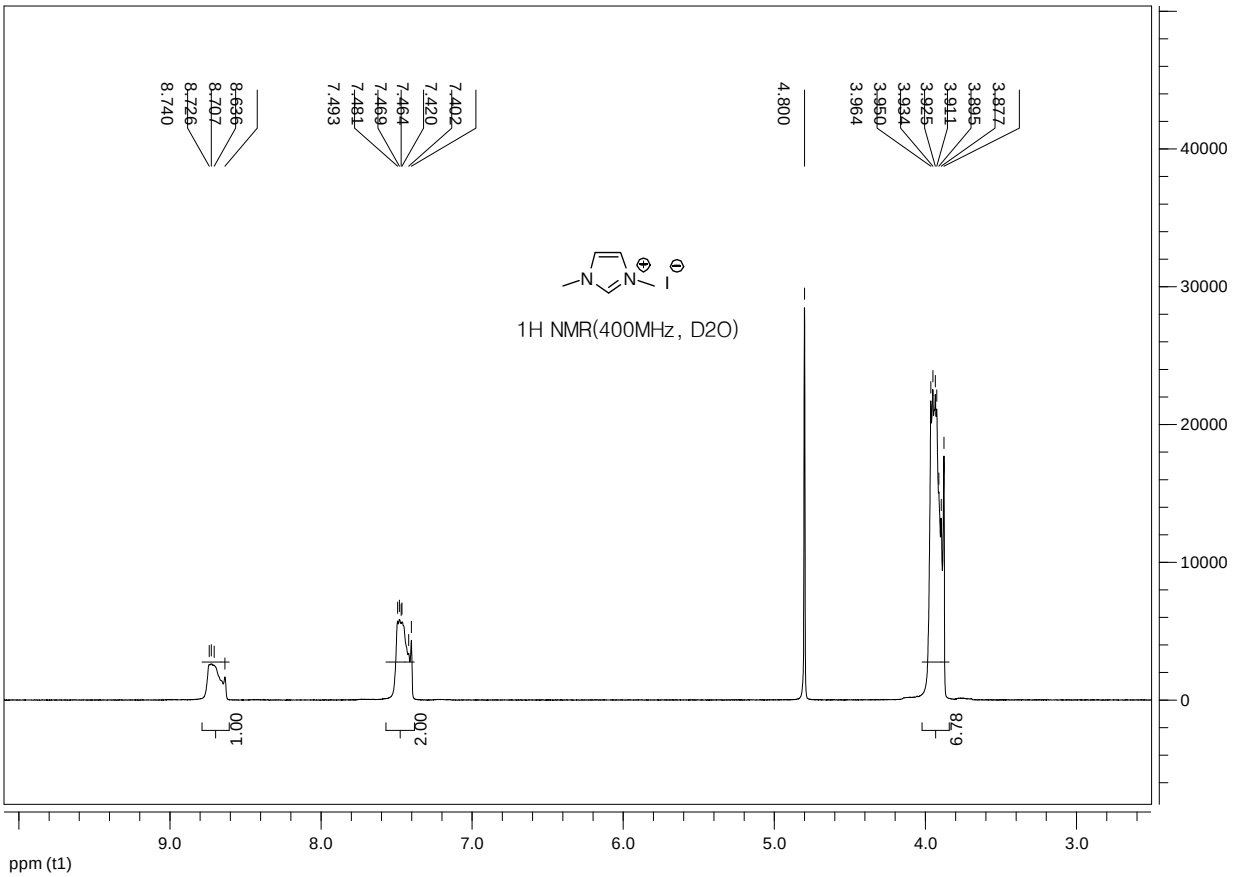


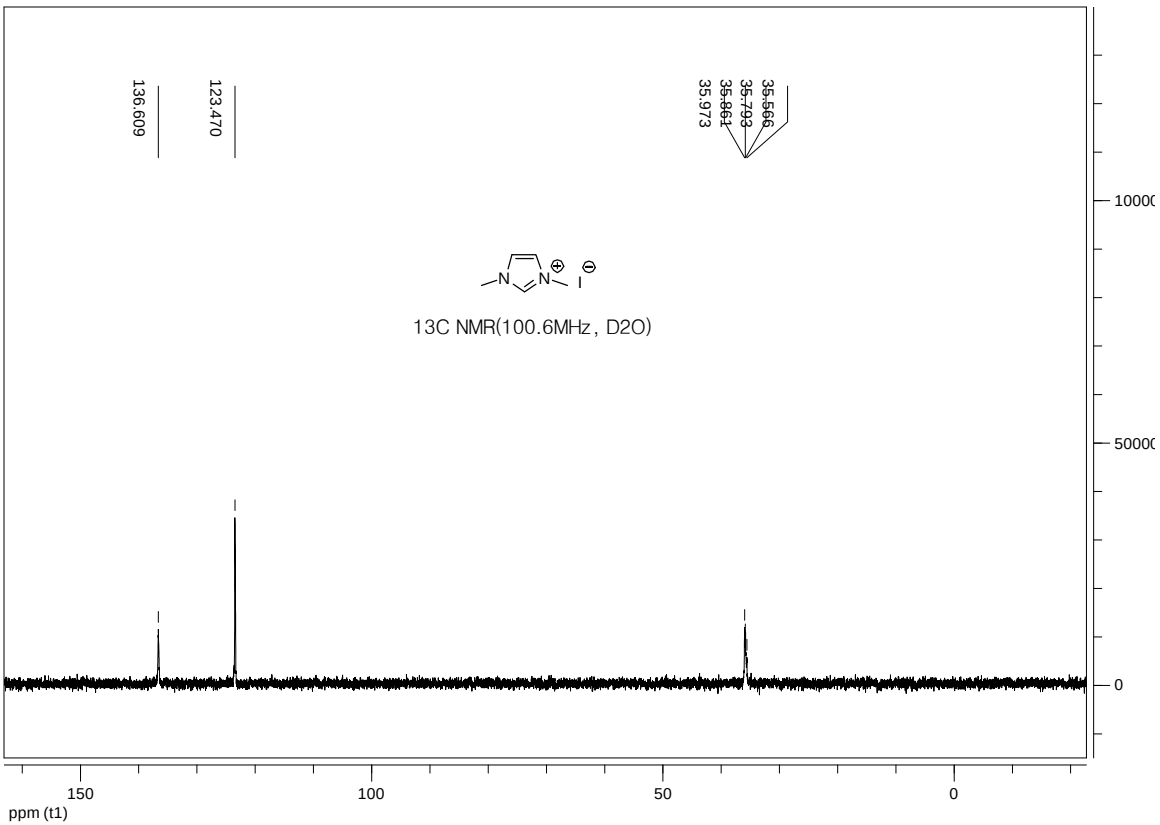
1-n-butyl-3-methylimidazolium iodide (BMImI)



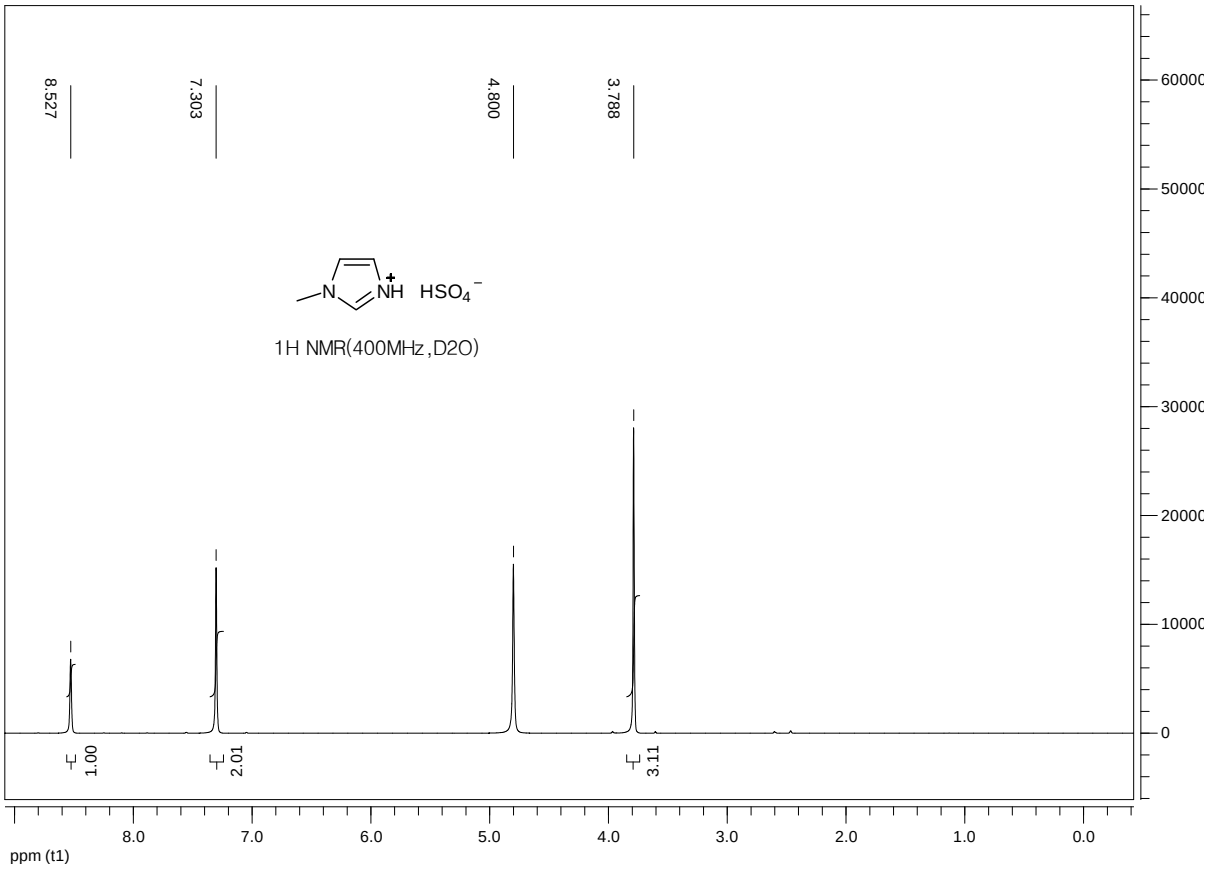


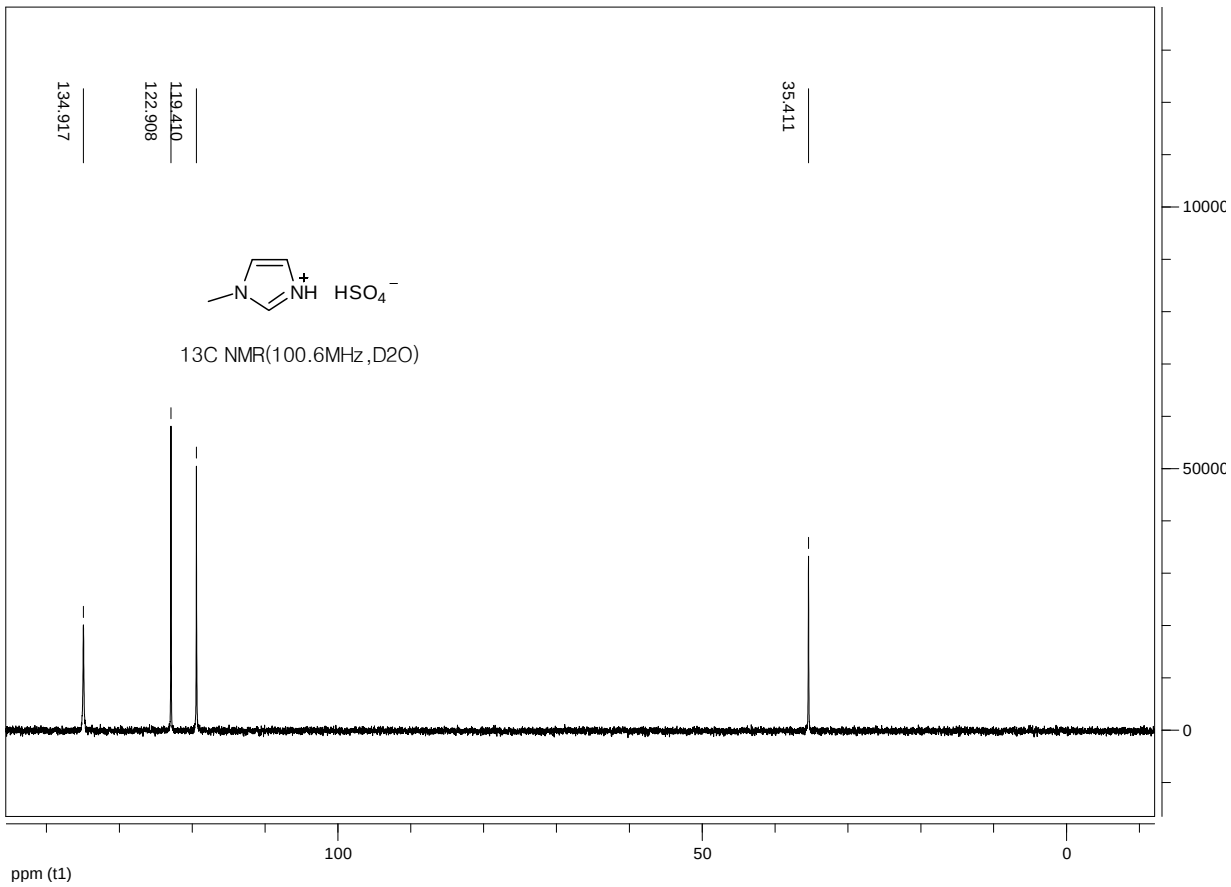
1-methyl-3-methylimidazolium iodide (MMImI)



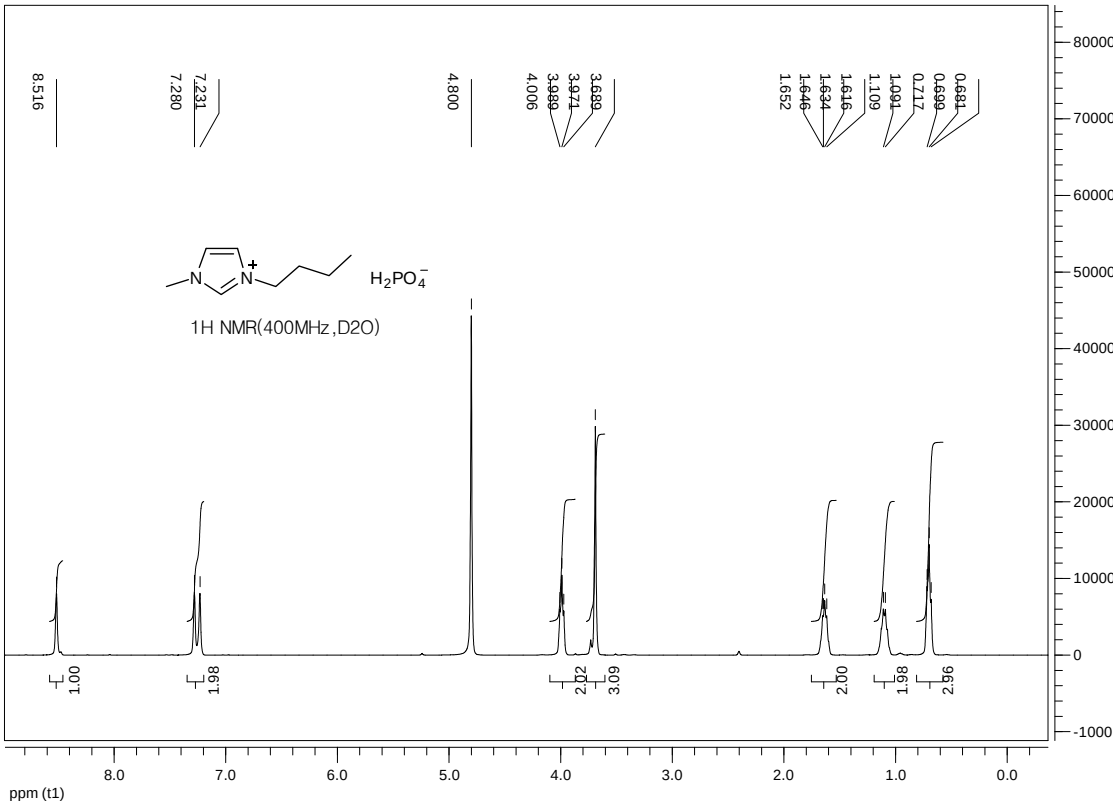


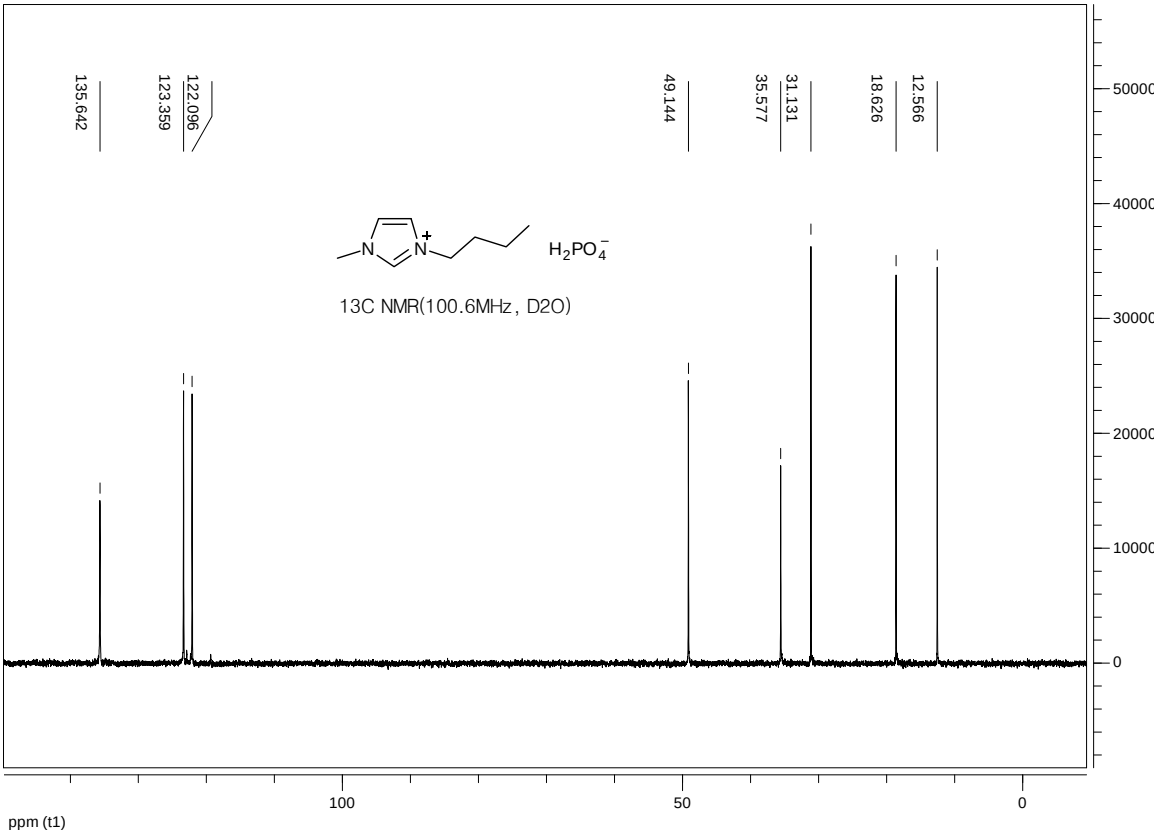
1-hydrogen-3-methyl imidazolium hydrosulfate ($HMImHSO_4$)



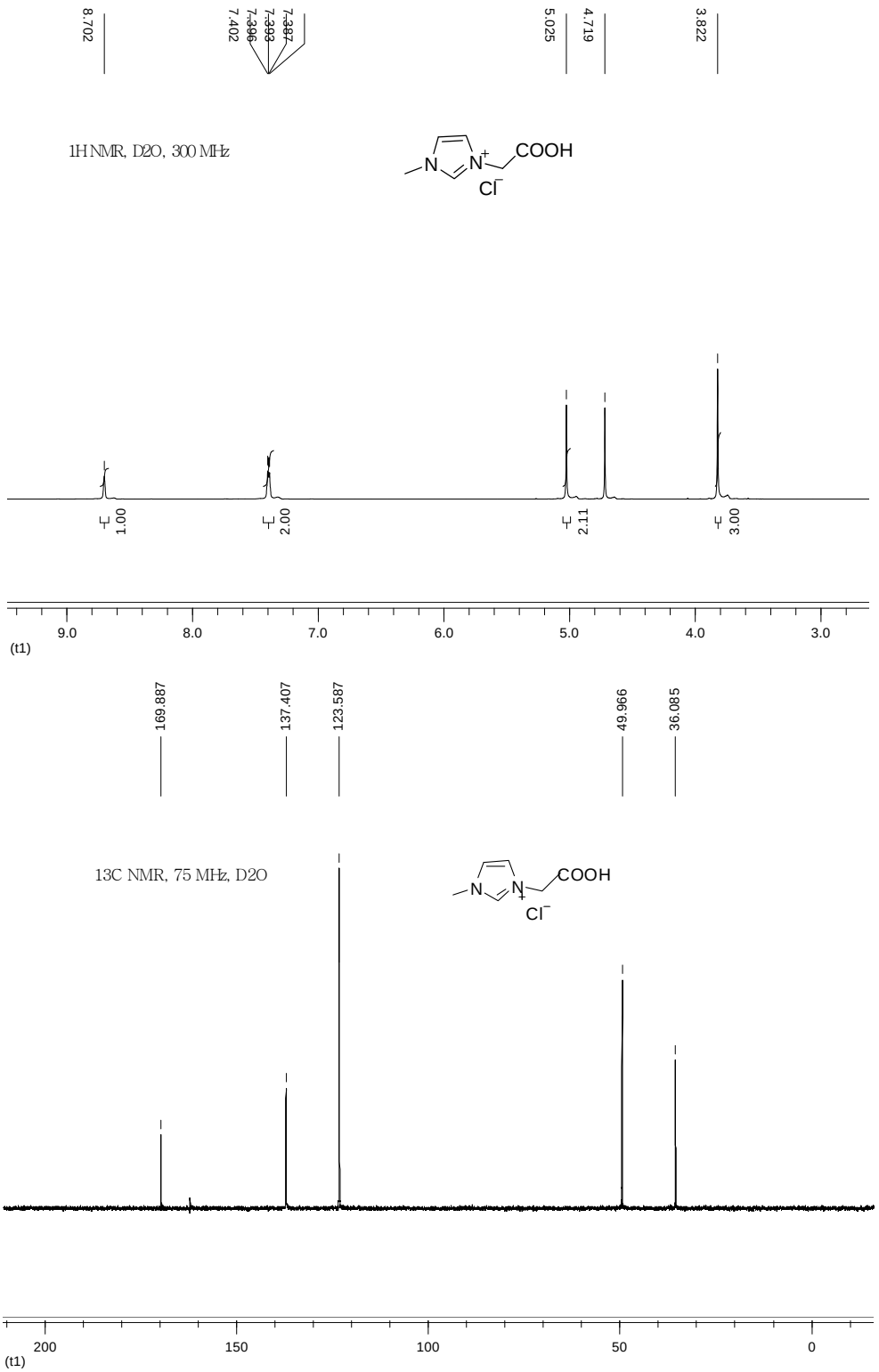


1-butyl-3-methyl imidazolium phosphate ($BMImH_2PO_4$)

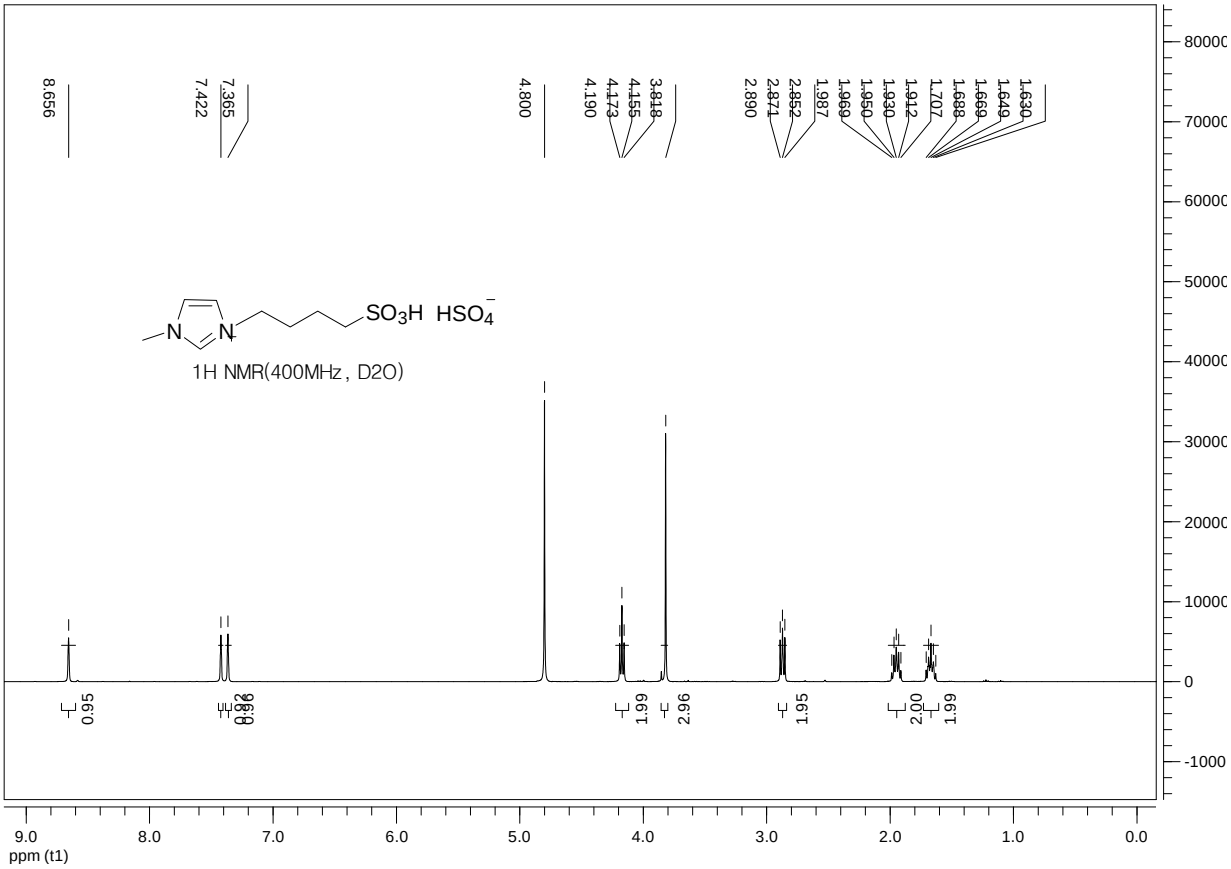


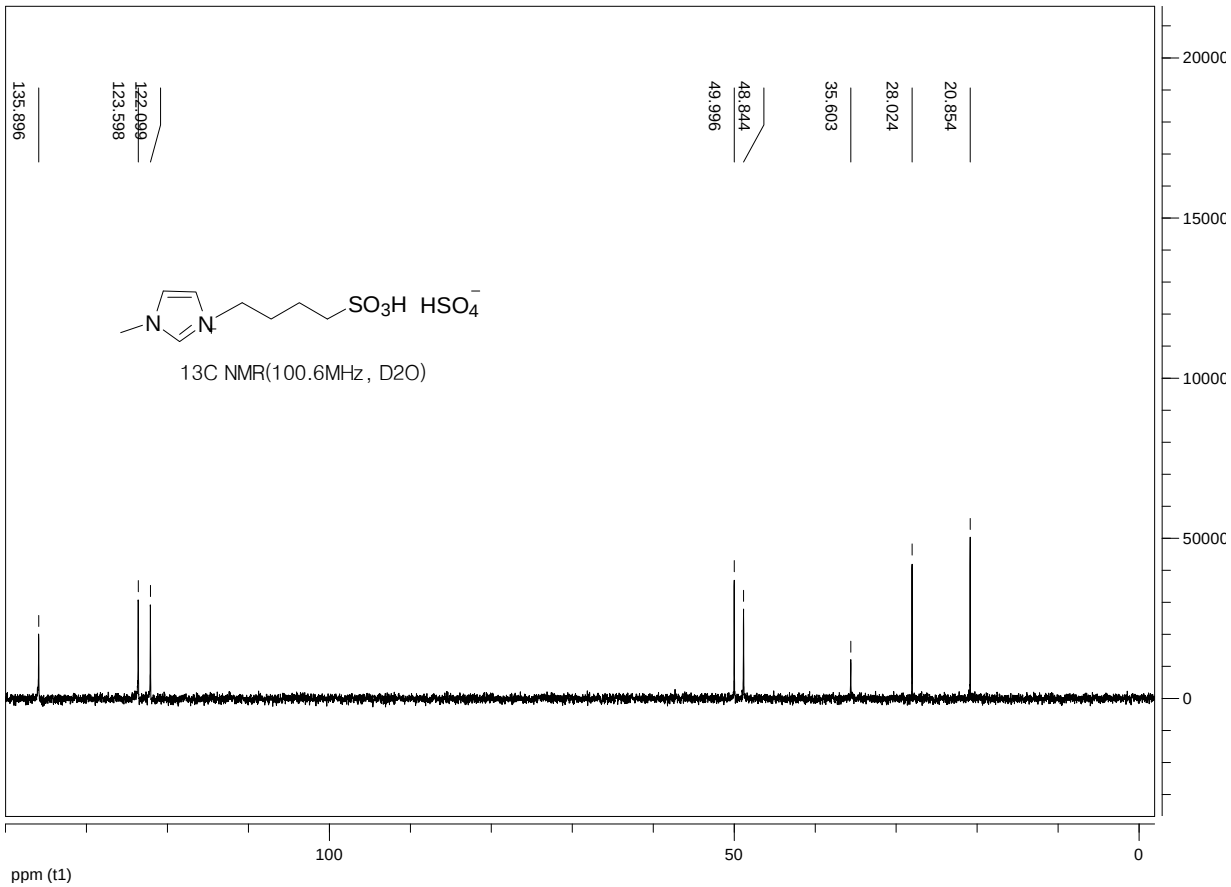


1-(carboxymethyl)-3-methylimidazolium chloride ((HOOC)CH_2MImCl)

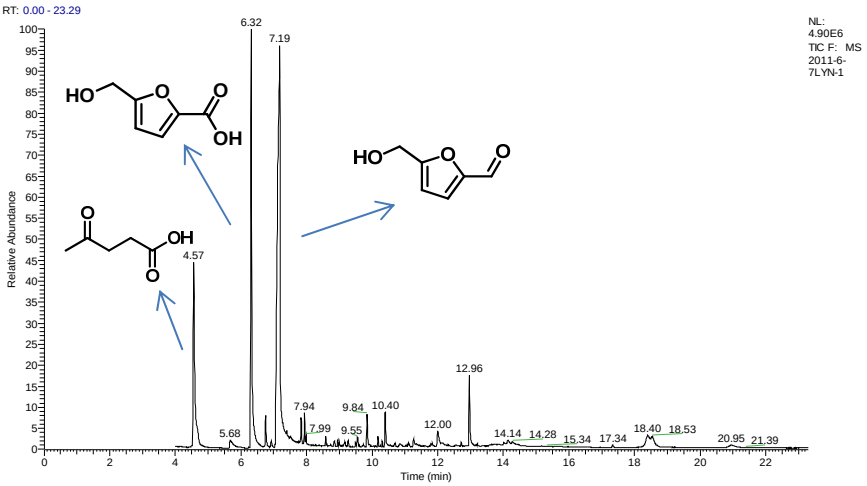


1-(butyl-4-sulfonate)-3-methyl imidazolium hydrosulfate ($(CH_2)_4SO_3HMImHSO_4$)

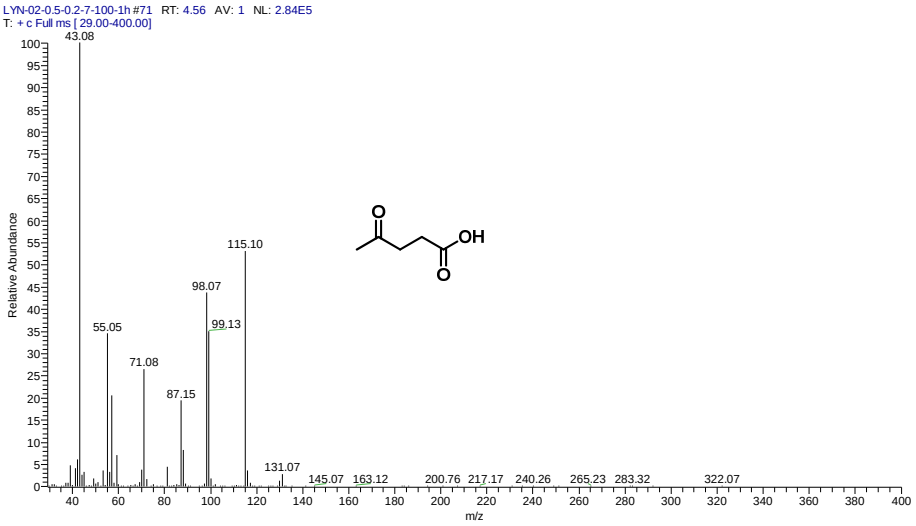


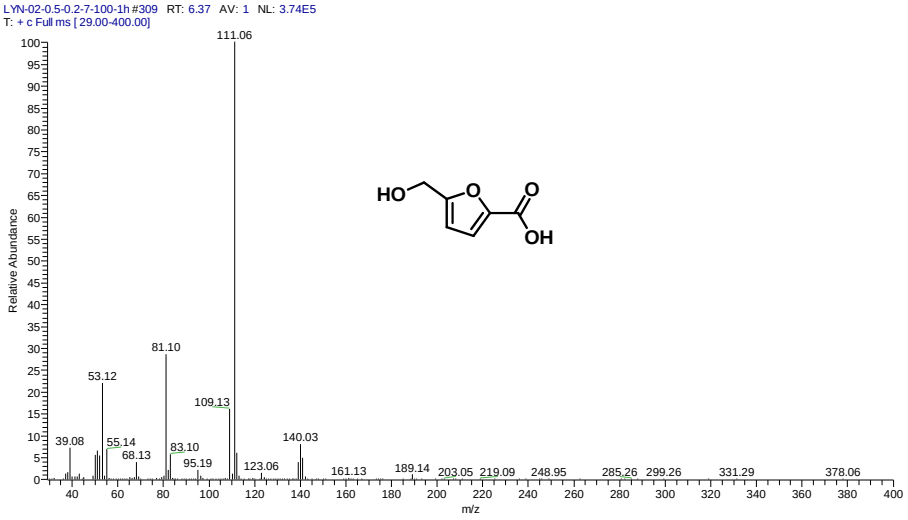


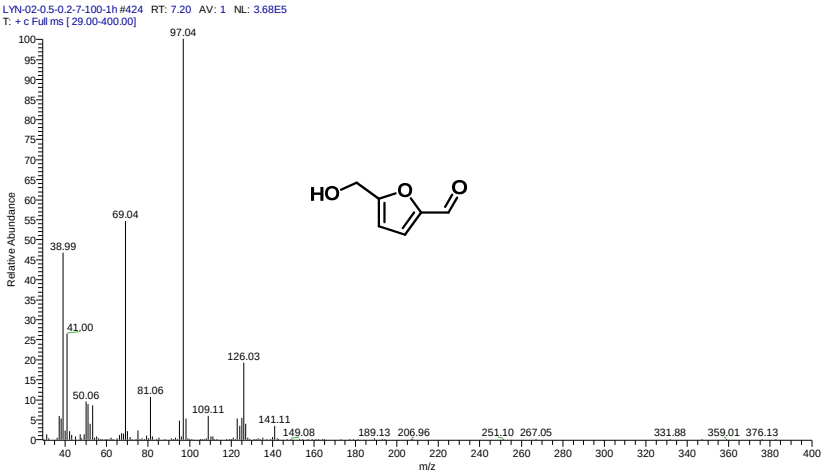
7. Supporting Figures



(a)







(b)

Fig. S1 GC-MS spectroscopy of probable byproducts with reaction time prolongation. Reaction conditions: fructose (0.5 mmol, 0.09 g), BMImBr (0.3 g), 100 ^{o}C, 2h. (a) GC spectroscopy; (b) MS spectroscopy.

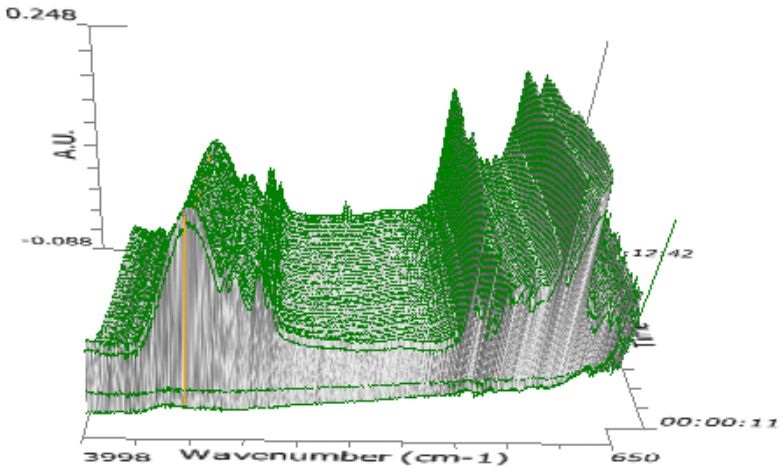


Fig. **S2** Stacked FT-IR spectra monitoring at various reaction time (min). Reaction conditions: fructose (10 mmol, 1.8 g), BMImBr (6 g), 100 ^{o}C.

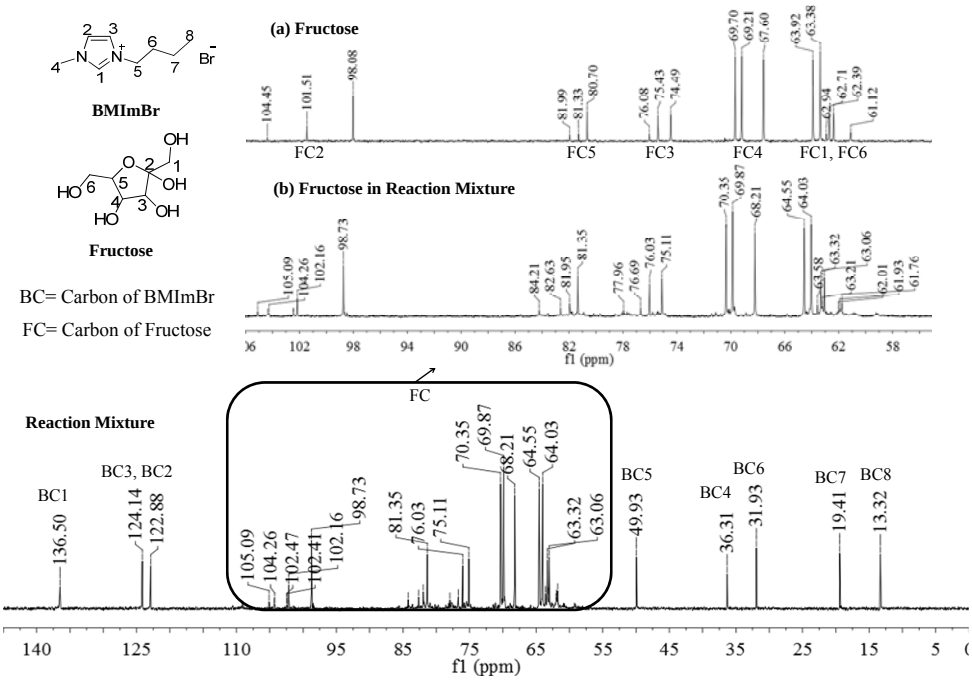


Fig. S3 ^{13}C NMR spectrum of the reaction mixture in D_2O (100.6 MHz). (a) ^{13}C NMR spectrum of fructose for comparison; (b) Signals of fructose in reaction mixture. Reaction conditions: 100 ^{o}C, 3 min.

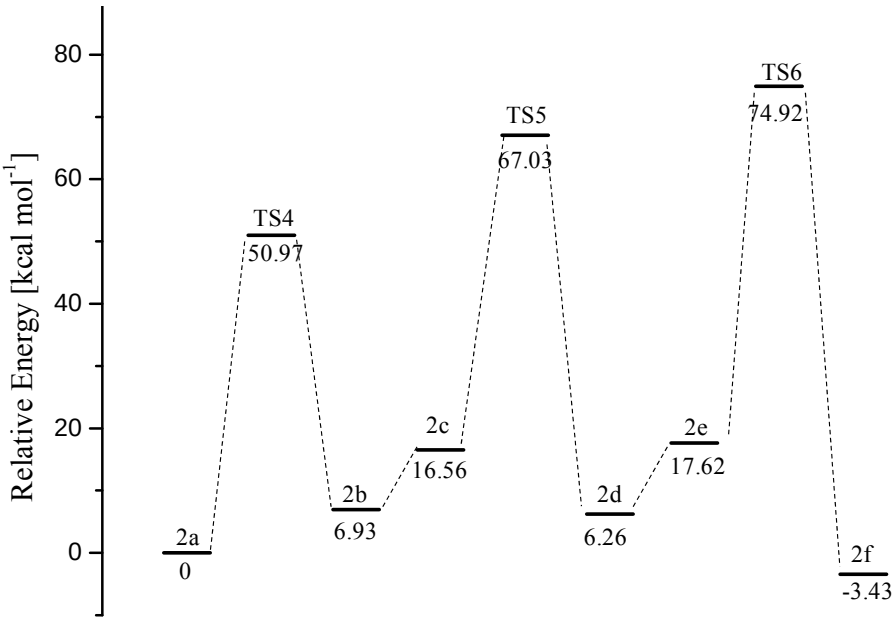


Fig. S4 Overview of the reaction pathway for dehydration of fructose into 5-hydroxymethylfurfural in the presence of EMImBr.

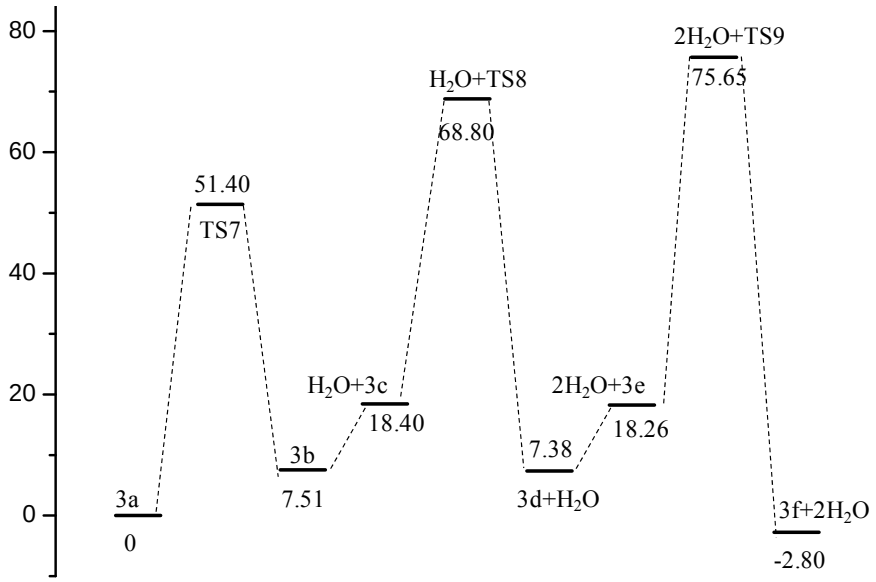
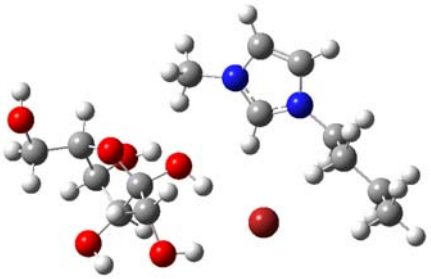


Fig. S5 Overview of the reaction pathway for dehydration of fructose into 5-hydroxymethylfurfural in the absence of HMImBr.

8. The optimized geometries and their Cartesian coordinates for the intermediates and transition states



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C	-1.52442800	-1.02499300	1.48748000
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O	-3.71372000	-0.06558900	-2.39256800
H	-2.75797400	0.07631900	-2.32332300
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H	-5.41171300	2.78234100	1.13764300
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H	4.44077600	3.40049200	-0.32896600
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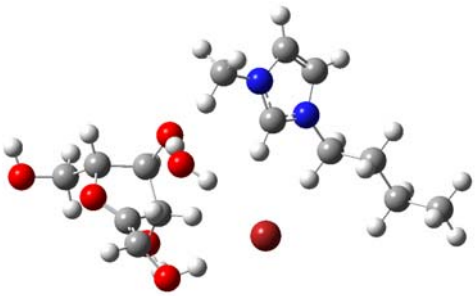

TS1 (523i)

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H	-0.03390300	2.19281200	2.18757400
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C	4.61728200	-0.06643800	-0.60937700
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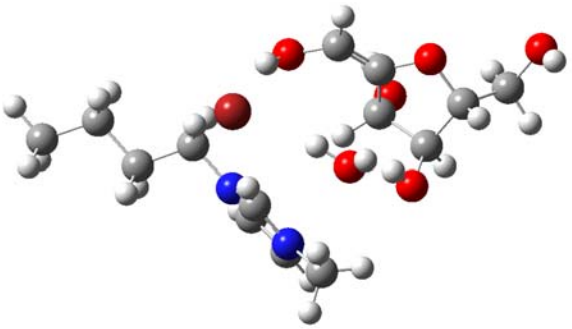

1b

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C	-6.63403600	-0.59329200	-1.82825500
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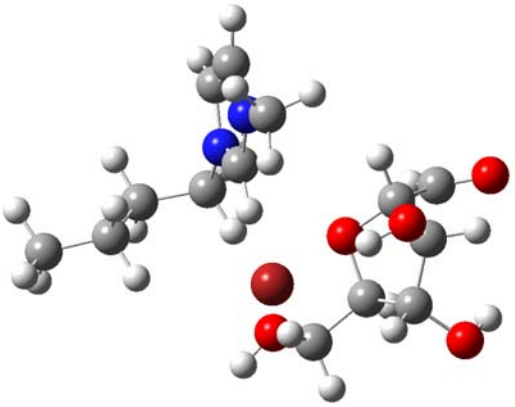

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C	-1.94987400	-1.52605300	-0.54396800
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O	-1.15267600	-1.00198300	0.53983500
O	-4.30460700	-1.00843600	-1.10718900
H	-4.65590100	-1.39838200	-0.29859000
C	-1.07526400	-1.85445000	-1.73041600
H	-1.73035900	-2.21376000	-2.53326000
H	-0.56242100	-0.94672200	-2.06590800
O	-0.13210400	-2.87295300	-1.35404200
H	0.31604800	-3.16916100	-2.15209600
C	-2.04986300	-0.24265200	1.34923300
C	-2.96372200	0.52021700	0.36977000
H	-3.95851300	0.65341400	0.79907200
C	-2.77685400	-1.17116900	2.32146400
O	-3.86480000	-0.95952500	2.79578400
H	-2.20054400	-2.08718800	2.57908800
H	-1.46262500	0.45861000	1.95206000
O	-2.47298500	1.80900200	0.07596600
H	-1.77284100	1.77599300	-0.61219300
C	1.44610100	0.80256600	0.79069400
C	2.20950800	1.60961100	2.70459700
C	2.46892600	0.27447900	2.67873300
N	1.98208600	-0.21167500	1.47815500
H	0.98154800	0.77477800	-0.19937500
H	2.41357900	2.35247400	3.45624100
H	2.94510200	-0.36259000	3.40380300
N	1.57450900	1.91996900	1.51578100
C	1.08764600	3.24721300	1.10706100
H	1.90053400	3.96731300	1.20118200
H	0.75774900	3.18192400	0.06802100
H	0.24917800	3.53812100	1.74022100
C	2.07045900	-1.61120000	1.00914900
C	3.44694500	-1.95987100	0.43558100
H	1.27712100	-1.75656500	0.27571900
H	1.83566500	-2.24267000	1.86821500
H	4.21771700	-1.82344900	1.20455000
Br	0.02885700	1.78987000	-2.14296700
H	3.42498700	-3.03280300	0.21327400
C	3.82622100	-1.18283400	-0.82979600
C	5.16879700	-1.63012000	-1.41481300
H	3.86983900	-0.11033700	-0.61113000
H	3.03656700	-1.30433300	-1.57896300
H	5.41463700	-1.05927100	-2.31331500
H	5.98322700	-1.48808800	-0.69725400

H 5.14958700 -2.68958000 -1.68858700

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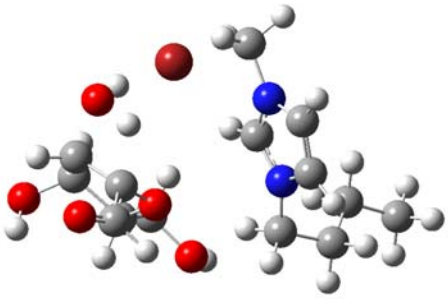

TS2 (1565i)

C	-1.75147300	-1.83986900	0.12509600
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H	-2.86326700	-0.74744700	-1.42289500
O	-0.95780100	-0.88701800	0.84004200
O	-4.18550500	-1.82952500	-0.36916900
H	-4.32937900	-2.17102000	0.52149500
C	-0.95913800	-2.47125800	-0.99721000
H	-1.63368000	-3.13270600	-1.55380300
H	-0.59770600	-1.68464500	-1.66842800
O	0.13590600	-3.21761700	-0.44180400
H	0.51470500	-3.75806500	-1.14148400
C	-1.87217400	0.02263800	1.48320500
C	-3.03465500	0.15947200	0.55544700
H	-4.00516600	0.35417900	1.00221400
C	-2.00634200	-0.08288800	2.91601000
O	-2.90767000	0.40106400	3.59234000
H	-1.14864700	-0.60056200	3.40442800
H	-1.81578200	1.38123200	0.75879600
O	-2.62244400	1.48965900	-0.09288000
H	-2.13553800	1.37011300	-0.98052600
C	1.42167300	1.08244700	0.31140700
C	2.45786200	2.51205600	1.64357500
C	2.77938900	1.25384700	2.04551700
N	2.12468100	0.37540600	1.20212800
H	0.78856700	0.69839500	-0.48348500
H	2.74365800	3.47239900	2.03635700
H	3.40201400	0.91329500	2.85436200
N	1.61417500	2.38464200	0.55619000

C	1.00419400	3.49138300	-0.19487600
H	1.79039000	4.16282700	-0.54048600
H	0.46734800	3.07387900	-1.04914400
H	0.31144400	4.02938900	0.45309800
C	2.21215200	-1.09991900	1.26543700
C	3.56330300	-1.63197700	0.78178600
H	1.38669600	-1.49767900	0.67794600
H	2.03053500	-1.37946100	2.30482400
H	4.37138800	-1.23771100	1.41072000
Br	-0.72546500	1.18458100	-2.54636500
H	3.54588900	-2.71399200	0.95325900
C	3.86730400	-1.35193600	-0.69383600
C	5.18898000	-1.97422800	-1.15318200
H	3.90022000	-0.27048100	-0.86788500
H	3.04495600	-1.73458100	-1.30823800
H	5.38182300	-1.75591200	-2.20631200
H	6.03333900	-1.58783900	-0.57371500
H	5.17725000	-3.06211200	-1.03578700

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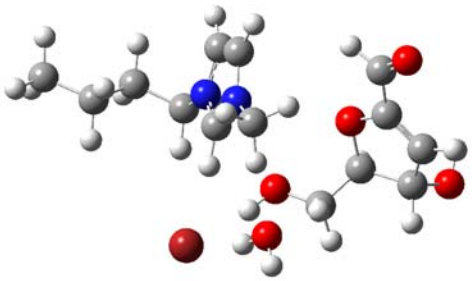

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C	2.74325200	-0.80296400	-1.39283400
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C	4.17658300	-1.06429700	-0.84992400
H	4.21210300	-1.99348800	-0.27618100
O	2.42445100	0.58334900	-1.03879000
O	5.16414100	-1.24780000	-1.86864200
H	5.31300200	-0.40153000	-2.30664500
C	1.70605300	-1.73818400	-0.80064500
H	2.03509300	-2.76569600	-1.01756000
H	1.67889000	-1.61928700	0.29151500
O	0.44761000	-1.46936200	-1.38294800
H	-0.23235000	-1.97079500	-0.88512500

C	3.41054500	1.01876200	-0.20534700
C	4.41791600	0.15584000	-0.00472300
H	5.28137400	0.32652400	0.61939300
C	3.22094300	2.38562100	0.32231100
O	3.92021300	2.90047600	1.16501700
H	2.35982700	2.92153000	-0.12486600
H	0.48632500	-2.40920400	3.52635400
O	0.31798800	-1.73922800	2.85684800
H	-0.32912800	-2.15296700	2.24231600
C	-1.19674800	0.74926500	0.77706100
C	-0.66726400	2.89016900	0.92437900
C	-1.20473000	2.67334300	-0.30654600
N	-1.53143400	1.33294400	-0.37623800
H	-1.34504500	-0.31097400	0.98819400
H	-0.28366400	3.78756500	1.37842600
H	-1.36984500	3.34875400	-1.12749200
N	-0.66893100	1.67510500	1.58641300
C	-0.19262500	1.43470300	2.95568500
H	-0.92040400	1.82360100	3.66955400
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H	0.76214600	1.94299500	3.08983300
C	-2.11693100	0.62574200	-1.53836800
C	-3.50157000	1.15328000	-1.91542600
H	-2.16178700	-0.42689400	-1.25631700
H	-1.40612500	0.71959700	-2.36063000
H	-3.44411200	2.21447800	-2.18944900
Br	-1.88562300	-2.66449400	0.61102600
H	-3.79300700	0.62351800	-2.82915100
C	-4.57289400	0.94289300	-0.83912800
C	-5.96244700	1.39542400	-1.29608900
H	-4.29611700	1.48919200	0.07017000
H	-4.59785500	-0.11646200	-0.56309000
H	-6.70620500	1.23574300	-0.51158000
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H	-6.28818500	0.83805200	-2.17947800

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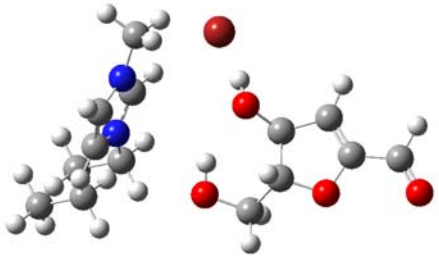

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C	2.55942600	-1.34811300	0.67956800
C	2.33512900	-0.07672500	-0.16542800
C	3.76607300	0.33166400	-0.42226200
C	4.54882400	-0.72586000	-0.15300800
H	1.85628700	-0.31052300	-1.12959800
H	4.08355300	1.27367400	-0.84443700
H	2.57330200	-1.04073500	1.73379800
O	3.88324000	-1.81808000	0.34242600
C	6.00263300	-0.81215800	-0.35465000
O	6.68210700	-1.78439600	-0.11919900
H	6.44177200	0.12288500	-0.75696900
C	1.50618500	-2.42099400	0.47759000
H	1.71792600	-3.29928100	1.09156400
H	1.48273000	-2.72990300	-0.57447100
O	0.22887100	-1.89874400	0.87231000
H	0.29524400	-0.93141200	0.85782700
O	1.49300300	0.80235900	0.56215600
H	1.09018600	1.44289100	-0.07759300
Br	-0.06181100	2.60036400	-1.59955200
C	-2.37379800	0.86067900	2.78005000
C	-2.73709300	-0.30678700	2.18440500
H	-2.35553300	1.14386700	3.81817800
H	-3.08345100	-1.23254500	2.60880000
C	-1.44149300	3.08096000	1.94010900
H	-0.66716300	3.06997400	2.70651100
H	-1.00612300	3.39133400	0.98848100
H	-2.24818700	3.75569800	2.22895800
C	-2.77450000	-1.16026600	-0.22227000
C	-4.25333700	-1.50444300	-0.40139000
H	-2.17467800	-2.03090200	0.04944500
H	-2.35470700	-0.74918000	-1.14160100
H	-4.66359000	-1.88278700	0.54222000
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N	-2.55028700	-0.14186200	0.82324200

C	-2.08517700	1.09181100	0.59995600
H	-1.74235500	1.51055200	-0.35219000
C	-4.46131000	-2.55044300	-1.50372300
C	-5.93495400	-2.91365400	-1.70439100
H	-3.89038100	-3.45355600	-1.25911000
H	-4.04658800	-2.17060200	-2.44427900
H	-6.05179100	-3.65637000	-2.49717400
H	-6.36924700	-3.33168800	-0.79106900
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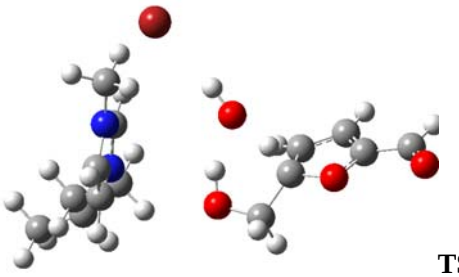

TS3 (445i)

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C	2.85605300	-0.77357700	-1.18463700
C	4.15647000	-0.44217900	-1.56560900
C	4.94216200	-0.54778300	-0.42604700
H	2.00826600	-0.95532000	-1.81991800
H	4.51164200	-0.18851600	-2.55253200
H	2.37668600	0.03738200	0.57104400
O	4.25935700	-0.90164100	0.65053400
C	6.40415700	-0.32351700	-0.31045500
O	7.02255800	-0.44140400	0.71767700
H	6.88709500	-0.03541100	-1.26306000
C	2.03207200	-2.04085800	0.93372900
H	2.18682600	-1.98328200	2.01878300
H	2.34413000	-3.03434700	0.59470400
O	0.68300600	-1.82427400	0.58024300
H	0.60517300	-0.88176500	0.23651900
O	1.10565800	0.59617000	-0.41363600
H	0.52690000	1.34985100	-0.64351100
Br	-1.19964400	3.09774900	-1.37349500
C	-2.20157300	0.32651300	2.98217300
C	-2.35486300	-0.83780400	2.29658300
H	-2.15894100	0.51936900	4.04012200
H	-2.45733200	-1.85011600	2.64573900
C	-1.86205100	2.76459800	2.30486000
H	-1.01729600	2.87832400	2.98427700

H	-1.63771800	3.24835300	1.35046200
H	-2.76021800	3.19714300	2.74761500
C	-2.42426700	-1.46713000	-0.17524100
C	-3.83440300	-2.03413800	-0.34538600
H	-1.68295100	-2.24884200	0.00062900
H	-2.11358700	-0.91600400	-1.06403500
H	-4.14102500	-2.54619100	0.57452100
H	-4.53882500	-1.20890200	-0.49713400
N	-2.07842600	1.33522800	2.04290500
N	-2.32654700	-0.52019000	0.95024100
C	-2.15622000	0.79920600	0.82082900
H	-2.02742300	1.38043900	-0.10543500
C	-3.91537600	-3.01015900	-1.52530600
C	-5.31767600	-3.59390000	-1.71745200
H	-3.19659300	-3.82378000	-1.37260600
H	-3.60521900	-2.49444900	-2.44116800
H	-5.34412700	-4.28428300	-2.56416700
H	-5.64407900	-4.14427000	-0.82955600
H	-6.05164500	-2.80555700	-1.90894400

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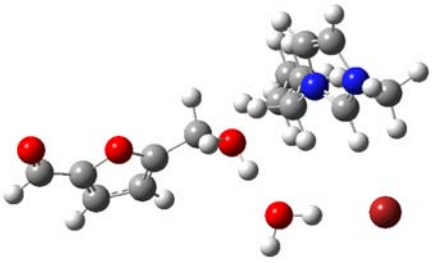

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C	-4.94160000	0.42736600	-1.46232200
C	-5.52652800	-0.01996200	-0.30365000
H	-2.75205800	0.64226600	-1.94929000
H	-5.46638200	0.75700700	-2.34612500
H	-0.47471800	-2.59026600	-2.02566800
O	-4.54794700	-0.35210100	0.59854600
C	-6.92256900	-0.16666600	0.05729900
O	-7.34656600	-0.56391200	1.12351400
H	-7.60894100	0.13041000	-0.76272400
C	-2.13045600	-0.41119500	0.81863800
H	-2.13533900	-1.47371400	1.09664700
H	-2.18172500	0.16077500	1.75247100
O	-0.94497900	-0.05754600	0.14307500
H	-0.65724900	-0.82356500	-0.40570600

O	-0.12352500	-2.25818200	-1.19383900
H	0.85572900	-2.39853700	-1.25401400
Br	3.09091400	-2.51931600	-1.40575700
C	2.11789200	0.21789200	3.02992600
C	1.67786400	1.30447700	2.33986000
H	2.10038400	-0.00044500	4.08369400
H	1.19662900	2.20331100	2.68275000
C	3.21538400	-1.98990600	2.37123000
H	2.52341800	-2.56306000	2.98806600
H	3.36130600	-2.49455200	1.41377300
H	4.16960400	-1.87565600	2.88689400
C	1.56895100	1.93513100	-0.13135300
C	2.28431800	3.28554900	-0.10322800
H	0.48258900	2.03629700	-0.11032400
H	1.82380500	1.37763800	-1.03380500
H	2.04258600	3.81731600	0.82468100
H	3.36762400	3.12152600	-0.09940900
N	2.63612700	-0.66671900	2.10170900
N	1.94080700	1.06899100	1.00305100
C	2.51625300	-0.12956800	0.88307700
H	2.79575000	-0.65121600	-0.04073700
C	1.89474900	4.15719900	-1.30358600
C	2.59644500	5.51781700	-1.30053800
H	0.80843800	4.30399000	-1.30754800
H	2.13556100	3.62337300	-2.22991600
H	2.30136200	6.11438900	-2.16712800
H	2.34768200	6.09144800	-0.40235200
H	3.68398900	5.40275700	-1.33169300

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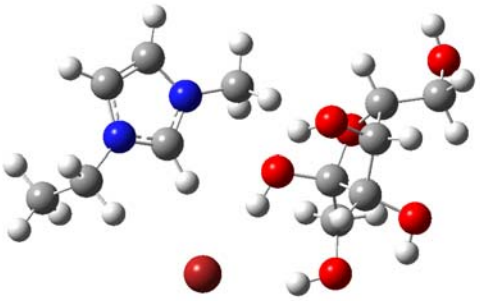

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C	3.25293600	1.17496100	0.43255900
H	2.96169400	2.17020800	0.78891000
C	3.14112200	0.17305800	1.60024200
H	4.09938900	-0.00987000	2.08664200
C	2.61941100	-1.09393900	0.90947400

C	1.50829300	-1.35314500	-1.41393800
H	2.41889400	-1.26476800	-2.00670200
C	1.68052000	-0.48510700	-0.15990000
O	2.26649800	0.74687700	-0.53950400
O	1.34296300	-2.72545000	-1.09380300
H	0.40856400	-2.88272200	-0.85771800
O	2.24419800	0.62963100	2.60684700
H	1.34942700	0.55594100	2.24235400
C	4.63548300	1.25449100	-0.20984600
H	5.37625500	1.45132500	0.57782000
H	4.88242500	0.30309800	-0.67987600
O	4.71555300	2.24242200	-1.23568700
H	4.60998000	3.11084600	-0.83408700
O	3.71444700	-1.79897400	0.34718900
H	3.34548400	-2.57948200	-0.08947600
H	2.05825500	-1.72029700	1.60679400
O	0.43538000	-0.15250900	0.46977500
H	-0.17577800	-0.92586100	0.44853300
H	0.67019100	-0.97397900	-2.00842400
C	-2.53350600	3.22727800	-0.13120700
C	-3.55618700	2.64734000	0.55422500
C	-2.36421200	1.03951600	-0.38361700
N	-1.80209700	2.20841300	-0.71156000
H	-2.26247700	4.26205200	-0.24783000
H	-4.34343700	3.08367000	1.14395300
H	-2.02197400	0.03814100	-0.64175800
C	-0.57885100	2.36581400	-1.51394500
H	-0.73846500	1.94801300	-2.50774100
H	-0.36764400	3.42970700	-1.60354100
H	0.25177700	1.85659200	-1.02409700
N	-3.43129100	1.28198900	0.38537700
C	-4.32580700	0.23896600	0.93740200
C	-5.59363500	0.06697200	0.10750500
H	-4.55166900	0.53116800	1.96461400
H	-3.74312100	-0.68473500	0.95693700
H	-6.17844800	0.98907700	0.05400200
H	-5.35105300	-0.25834900	-0.90609600
Br	-1.85468900	-2.37803500	-0.15879500
H	-6.21614700	-0.70456800	0.56564500

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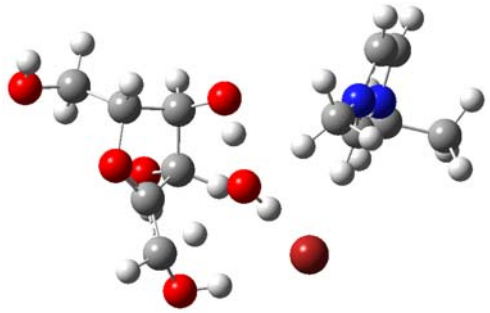

TS4 (544i)

C	-3.06778300	1.47369800	-0.25105600
H	-2.93137800	2.31127500	0.43435900
C	-1.71203900	1.06951100	-0.88003100
H	-1.65087200	1.39382400	-1.92286100
C	-1.78586400	-0.47457100	-0.83145400
C	-2.43730000	-1.73135800	1.37077400
H	-3.27128000	-1.87347200	2.05934000
C	-2.62447300	-0.68088600	0.40608800
O	-3.39107200	0.32087200	0.65093200
O	-1.94454500	-2.93932900	0.86982900
H	-0.96702400	-2.90279900	0.77740900
O	-0.63078200	1.57375100	-0.16030500
H	-0.49235300	0.97983000	0.69931100
C	-4.22714500	1.70756600	-1.20623900
H	-3.92964900	2.51750800	-1.88625500
H	-4.40453900	0.81470000	-1.80640900
O	-5.45173500	2.00142800	-0.55093500
H	-5.37504700	2.84543400	-0.09381100
O	-2.54181600	-0.96358100	-1.94365500
H	-2.40895200	-1.91872500	-1.99350600
H	-0.80253500	-0.94211700	-0.76145400
O	-0.36340100	0.06605700	1.85413300
H	0.24050100	-0.65182300	1.61152900
H	-1.60493200	-1.07579300	1.91081500
C	3.17629300	2.89007000	0.56115300
C	3.56700700	2.37403200	-0.63545700
C	2.54601900	0.77660300	0.49918200
N	2.54271400	1.87780200	1.25615000
H	3.28079700	3.88098700	0.96722900
H	4.07540400	2.83177000	-1.46592300
H	2.11313400	-0.19204300	0.73272800
C	1.93363900	1.98305100	2.59209600
H	2.66844900	1.71229100	3.35202400
H	1.61505100	3.01431300	2.73833900

H	1.06107400	1.31406200	2.61899900
N	3.16528400	1.05175100	-0.65334900
C	3.36560900	0.08169600	-1.75052300
C	4.80856900	-0.40519200	-1.83453300
H	3.05248300	0.57565400	-2.67272100
H	2.68402500	-0.74886700	-1.55251400
H	5.50984300	0.41517100	-2.00947100
H	5.09517600	-0.92485400	-0.91803100
Br	1.28339100	-2.50372800	0.10353600
H	4.89956600	-1.11165400	-2.66247600

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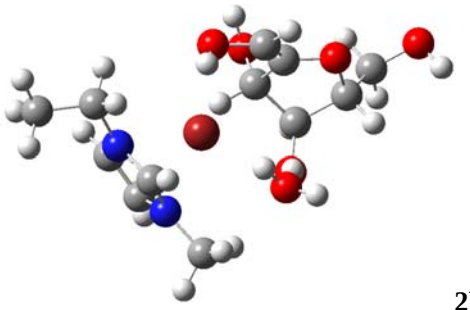

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C	3.62223000	0.06166500	0.33423600
H	3.77704700	0.51665100	1.32070900
C	2.50459200	-1.00719000	0.44267700
H	2.90916900	-2.01948600	0.40829900
C	1.65337900	-0.72779100	-0.80930600
C	0.96127900	1.64964600	-1.38250500
H	1.18867400	2.71165300	-1.36917500
C	1.85050000	0.74425900	-0.97165000
O	3.11852900	1.09390300	-0.54438500
O	-0.26413100	1.26919500	-1.87192600
H	-0.94887000	1.77532200	-1.37875000
O	1.75115300	-0.91918600	1.64184900
H	1.31117300	-0.04914100	1.72231700
C	4.94564800	-0.48739300	-0.18796500
H	5.25821800	-1.30824000	0.47484300
H	4.80640600	-0.89268900	-1.19097100
O	5.96854100	0.49352800	-0.29531900
H	6.08014800	0.92429500	0.55865500
O	2.20552200	-1.49923300	-1.89345900
H	2.02895500	-1.02097600	-2.71108500
H	0.60681300	-0.99353600	-0.65279900
O	0.11867400	1.30507300	2.28256600
H	-0.53543400	1.73019500	1.68000600

H	0.45681000	2.02602600	2.82344600
C	-1.48059900	-3.07055800	0.68959400
C	-1.99948800	-2.81015500	-0.54061200
C	-2.18631200	-0.97740000	0.67893700
N	-1.60878500	-1.91487800	1.43704000
H	-1.02142100	-3.95920700	1.08634300
H	-2.07784900	-3.43342400	-1.41409300
H	-2.37174100	0.06438000	0.94078300
C	-1.14544600	-1.72985800	2.81859000
H	-1.74920300	-2.34170200	3.48989100
H	-0.09265100	-2.00385700	2.87004100
H	-1.23425800	-0.67612700	3.07368200
N	-2.43455400	-1.49830700	-0.52730600
C	-3.04070000	-0.75644500	-1.65581300
C	-4.41900700	-1.29317200	-2.02483800
H	-2.34025800	-0.81495500	-2.49035800
H	-3.08760400	0.28642500	-1.33831400
H	-4.38336000	-2.33830800	-2.34325900
H	-5.11300800	-1.20763000	-1.18575300
Br	-2.31797500	2.46004800	0.37739000
H	-4.81801400	-0.70491800	-2.85393100

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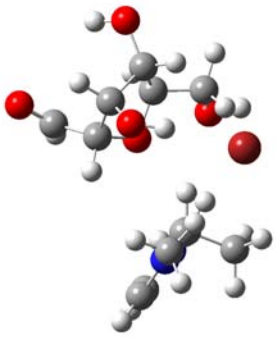

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C	-2.02857100	-0.44102700	-1.09426900
H	-2.72319900	-1.23067900	-1.42035000
C	-2.75911600	0.48151200	-0.07822500
H	-2.50826900	1.52807100	-0.25351600
O	-0.94113400	-1.05464700	-0.36825300
O	-4.17371200	0.41097600	-0.19807700
H	-4.48005000	-0.46157000	0.07429500
C	-1.50350400	0.29221400	-2.30563500
H	-2.35968200	0.76427000	-2.80274200
H	-0.80347400	1.07116400	-1.98537000
O	-0.86447400	-0.65005000	-3.18352400
H	-0.64300400	-0.18991700	-3.99884300

C	-1.41723200	-1.23197500	0.96529000
C	-2.19580700	0.05336900	1.30840500
H	-3.01207000	-0.16266900	2.00034100
C	-2.22652800	-2.52474800	1.05815400
O	-3.09282100	-2.73881200	1.86881300
H	-1.93663900	-3.28865700	0.30329400
H	-0.55349900	-1.34610100	1.62914600
O	-1.37319900	1.01615000	1.93106300
H	-0.88311600	1.55050100	1.26835400
C	2.06110900	-0.17462600	0.28553800
C	3.25776900	-1.30585200	1.76383700
C	3.14074700	-2.07064600	0.64459700
N	2.38812400	-1.34925200	-0.26466200
H	1.47685300	0.63993800	-0.15554000
H	3.75169400	-1.49863100	2.70042500
H	3.51830900	-3.05373100	0.42239100
N	2.58006900	-0.12590100	1.51748100
C	2.41255500	0.99757500	2.45328300
H	3.39144900	1.29271200	2.83104200
H	1.94923100	1.82373800	1.91053800
H	1.76366500	0.69321000	3.27463800
C	2.03063000	-1.77335200	-1.63585600
C	3.03231000	-1.27223300	-2.67212200
H	1.02355800	-1.40885900	-1.83734900
H	1.98910500	-2.86373900	-1.61799400
H	3.05516600	-0.18060200	-2.69821600
H	4.04261300	-1.63826500	-2.47166800
Br	0.49054900	2.79608200	-0.19544000
H	2.73135200	-1.62718000	-3.66035700

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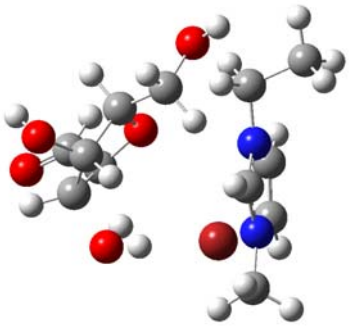

TS5 (1570i)

C	-1.93774000	1.13933900	0.81451800
H	-2.41218400	2.13430300	0.77548900
C	-2.89285900	0.11162800	0.14219400
H	-2.83116600	-0.86065100	0.63334100
O	-0.75335500	1.15772600	0.00967100
O	-4.25754800	0.48799000	0.21331000

H	-4.36372000	1.36894000	-0.16523200
C	-1.61215100	0.78788400	2.24839400
H	-2.55699700	0.71690300	2.80061100
H	-1.10905300	-0.18473400	2.27611100
O	-0.77748200	1.81612900	2.80509100
H	-0.68970400	1.65115300	3.74866000
C	-1.17215100	0.96115000	-1.35625900
C	-2.34535200	0.03886300	-1.29480700
H	-3.09855500	0.14321200	-2.07018500
C	-1.10466000	2.10296700	-2.23628800
O	-1.65876400	2.20553800	-3.32542200
H	-0.41748700	2.90227900	-1.87451700
H	-0.75967300	-0.45289400	-1.80507300
O	-1.60142800	-1.26036500	-1.63738900
H	-1.33328800	-1.79731800	-0.81342500
C	2.06094800	-0.19443500	-0.09036700
C	3.76620500	0.00539000	-1.48502400
C	3.66878500	1.15895700	-0.77239700
N	2.59968900	1.01592100	0.09218900
H	1.20266300	-0.61692600	0.42452800
H	4.44854100	-0.28656100	-2.26434800
H	4.25524000	2.06043600	-0.81164800
N	2.75755300	-0.82899200	-1.04102200
C	2.47287200	-2.17965400	-1.54713700
H	3.37576000	-2.78562600	-1.47040600
H	1.67806800	-2.61523400	-0.93817300
H	2.15291300	-2.11559900	-2.58766100
C	2.15682600	2.01605500	1.08794700
C	2.99151100	1.96206400	2.36375500
H	1.10321000	1.82920400	1.28552900
H	2.23262900	2.99055600	0.60232900
H	2.89967700	0.98880800	2.85122500
H	4.05001500	2.15646800	2.17152600
Br	-0.33942200	-2.68501200	0.82989600
H	2.62739900	2.72281200	3.05755200

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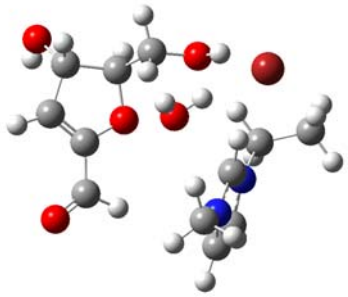

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C	-2.25458800	1.39026300	-0.85115600

H	-2.42685400	1.66652500	-1.89363200
C	-3.50685000	1.69549100	0.01942800
H	-3.28612700	2.46721300	0.76100700
O	-2.08681700	-0.06631500	-0.82457700
O	-4.61272000	2.22704800	-0.71573500
H	-4.98181600	1.52469100	-1.26407500
C	-0.99528100	2.06264600	-0.33884600
H	-1.20202800	3.14168100	-0.28048200
H	-0.77114600	1.70620300	0.67523600
O	0.07402700	1.79928200	-1.22664700
H	0.91670400	2.00818500	-0.76674000
C	-2.97799100	-0.55458700	0.08520600
C	-3.79282300	0.35571600	0.63794000
H	-4.55516800	0.15454900	1.37455800
C	-2.91535700	-2.01494500	0.30374600
O	-3.57779800	-2.61443000	1.11918000
H	-2.19393200	-2.53830100	-0.35542800
H	0.80265200	1.46659800	3.67693100
O	0.79321100	0.91670400	2.88765700
H	1.42944300	1.34390300	2.27052800
C	1.46860200	-1.28112600	0.04212100
C	0.95565500	-3.42920600	0.17484900
C	0.96895900	-3.07921100	-1.14032700
N	1.28976300	-1.73766500	-1.20198800
H	1.77440800	-0.26355200	0.30122700
H	0.74309900	-4.36987000	0.65253300
H	0.76910200	-3.65988300	-2.02407300
N	1.26858700	-2.29224900	0.89649400
C	1.39330700	-2.20511800	2.35878900
H	2.37204500	-2.57747400	2.66467400
H	1.26806600	-1.16504800	2.66505400
H	0.60891500	-2.81248700	2.80946500
C	1.41253300	-0.91998500	-2.43353800
C	2.86571200	-0.60249800	-2.77145600
H	0.83021800	-0.01221800	-2.26574400
H	0.93197200	-1.49896300	-3.22373000
H	3.32275600	0.00647100	-1.98831800
H	3.45490100	-1.51257900	-2.91321000
Br	2.82682700	1.90166600	0.52923300
H	2.89490700	-0.02753200	-3.70001700

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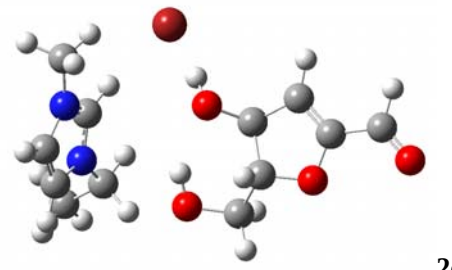

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C	2.35894500	-1.25642900	0.37691000
C	1.91339100	0.16712000	-0.01614500
C	3.22613700	0.90341900	0.10633700
C	4.20885100	-0.01186200	0.12187200
H	1.58017300	0.21247600	-1.06516400
H	3.34860400	1.97614900	0.08092600
H	2.21910100	-1.35405400	1.46183100
O	3.77730100	-1.31404900	0.11050100
C	5.65444500	0.25581500	0.13007200
O	6.51939100	-0.58931100	0.12431300
H	5.89615900	1.33768600	0.14058400
C	1.60007100	-2.36047900	-0.33438500
H	1.95418200	-3.34542200	-0.02152600
H	1.73696800	-2.27036100	-1.41871700
O	0.20763100	-2.25810100	0.00063200
H	0.05624600	-1.36299900	0.34296700
O	0.83458800	0.54517600	0.82310200
H	0.34658900	1.28405900	0.38044400
Br	-0.88990800	2.66833000	-0.87679900
C	-3.35736600	-0.93675500	2.00474700
C	-3.28363800	-1.86420200	1.01274900
H	-3.59507600	-1.04239600	3.04906600
H	-3.43348600	-2.92913400	1.03647100
C	-2.94588700	1.57695700	2.13678700
H	-2.36379000	1.44764700	3.04862300
H	-2.43552800	2.27973900	1.47524400
H	-3.94690200	1.93699300	2.37729800
C	-2.66908200	-1.79917400	-1.46644200
C	-3.92133000	-2.42718700	-2.06820300
H	-1.86080900	-2.51972200	-1.33231100
H	-2.28935900	-0.99516000	-2.09740100
H	-4.30593000	-3.24132300	-1.44924800
H	-4.71360400	-1.68711700	-2.20130900
H	-3.67633300	-2.84390900	-3.04755900
N	-3.03596200	0.28500900	1.44212900

N	-2.92289600	-1.19291700	-0.14230600
C	-2.77864600	0.10556400	0.14235000
H	-2.40506000	0.89420400	-0.51926500

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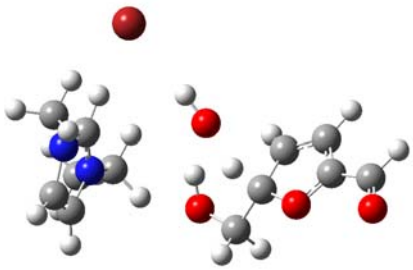

TS6 (439i)

C	2.64096000	-0.73048400	-0.06311900
C	2.71636900	0.11862600	-1.25261200
C	3.93613000	0.79197000	-1.19011500
C	4.61886800	0.27394100	-0.09766300
H	1.99043400	0.13842900	-2.04513900
H	4.31225700	1.54270200	-1.86795000
H	1.90716500	-0.10998700	0.55558600
O	3.93968200	-0.65735100	0.55116300
C	5.97478600	0.64073700	0.38050500
O	6.50666200	0.13953100	1.33924400
H	6.46455800	1.42472900	-0.22700200
C	2.01720200	-2.12805100	-0.14073400
H	2.06194300	-2.58130900	0.85788800
H	2.57640500	-2.76645700	-0.83295700
O	0.68972900	-1.98570600	-0.59690300
H	0.43082000	-1.01797900	-0.48814000
O	0.62730300	0.63913100	-0.28672900
H	-0.09484800	1.29736100	-0.26427800
Br	-2.13991700	2.84363800	-0.46945000
C	-2.71527900	-1.71128100	2.08884300
C	-2.57603200	-2.45186600	0.95691300
H	-2.76749100	-2.00891100	3.12180000
H	-2.47151700	-3.51393400	0.82151600
C	-2.88541600	0.78889700	2.57626900
H	-2.11484400	0.73513300	3.34531500
H	-2.73370300	1.68039700	1.96186800
H	-3.87428700	0.80847400	3.03617500
C	-2.38088500	-1.90785900	-1.52969000
C	-3.60933300	-2.59827300	-2.11404600
H	-1.48309800	-2.52336200	-1.60049900
H	-2.17459900	-0.96835800	-2.04300700
H	-3.82406200	-3.54219600	-1.60654000
H	-4.49220100	-1.95885700	-2.04573900
H	-3.43021500	-2.81988700	-3.16861400
N	-2.77101000	-0.38461700	1.69953500

N	-2.55356900	-1.56522400	-0.10506000
C	-2.66972100	-0.32069900	0.36820400
H	-2.62647600	0.62677900	-0.19158500

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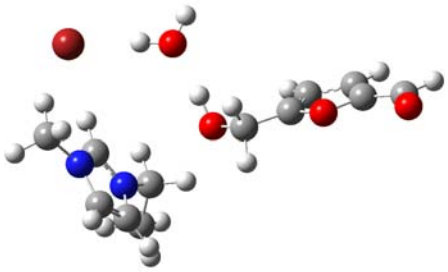

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C	3.16532000	0.01861000	-0.06125500
C	3.43172800	0.46926900	-1.32614400
C	4.83744400	0.67493600	-1.38027600
C	5.33659600	0.33376300	-0.14780700
H	2.70463100	0.62695500	-2.10513000
H	5.41766500	1.02916300	-2.21873000
H	0.11040000	2.98555700	-0.34940000
O	4.30564500	-0.06979600	0.66231700
C	6.69447100	0.33936900	0.35920300
O	7.04191400	0.00444500	1.47341000
H	7.42983700	0.69186000	-0.39361100
C	1.89806700	-0.37738000	0.63509500
H	1.76698400	0.25363800	1.52443800
H	2.00182600	-1.40908200	0.99083900
O	0.77758900	-0.31120100	-0.21757100
H	0.42205900	0.60750900	-0.19624700
O	-0.24199500	2.17948600	0.04006800
H	-1.22622200	2.26538000	-0.03802400
Br	-3.45096400	2.31657200	-0.32448700
C	-2.31617800	-2.41762700	1.75574900
C	-1.75557900	-2.86570000	0.60011400
H	-2.34032600	-2.85217600	2.74013000
H	-1.19190200	-3.75915500	0.39736000
C	-3.61991700	-0.32407500	2.41259300
H	-3.00695500	-0.18121200	3.30225300
H	-3.78435100	0.63621700	1.91893600
H	-4.57399000	-0.77746700	2.68399300
C	-1.53042900	-1.92678700	-1.76498600
C	-2.04978600	-3.12230300	-2.55560300
H	-0.44127100	-1.89252800	-1.71806800
H	-1.86559200	-0.98793100	-2.20638200
H	-1.71168700	-4.07108100	-2.13174000
H	-3.14130000	-3.12915800	-2.59540700
H	-1.67193000	-3.06543000	-3.57874200
N	-2.90461500	-1.19859300	1.47284700

N	-2.01724400	-1.91682300	-0.37111300
C	-2.70920400	-0.91707500	0.18046900
H	-3.02153400	0.02334500	-0.29026100

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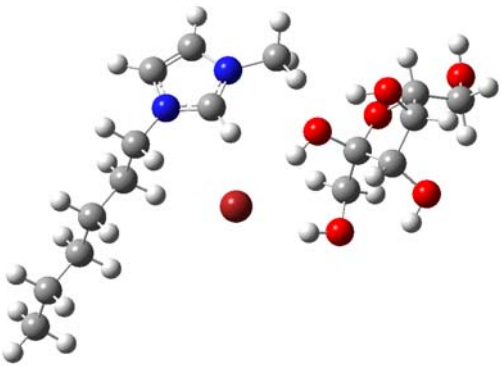

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C	4.79873700	0.38900500	-0.18213700
H	4.95634800	1.38209500	0.25538200
C	4.76599400	-0.65784500	0.95133200
H	5.72114200	-1.16883200	1.07420400
C	3.67714900	-1.63209600	0.48091500
C	1.85398300	-1.30282800	-1.32849900
H	2.50106900	-1.42067400	-2.19768100
C	2.68794900	-0.66309900	-0.21004300
O	3.47498900	0.36855800	-0.77007200
O	1.38278900	-2.59419300	-0.97660000
H	0.59672900	-2.49905800	-0.40440400
O	4.44484800	-0.07357800	2.20831000
H	3.50663000	0.16602900	2.18014000
C	5.86069100	0.13250300	-1.24798600
H	6.83595900	0.03273900	-0.75106500
H	5.64654800	-0.80014800	-1.76927800
O	5.90629800	1.14930800	-2.24728200
H	6.18106800	1.97370800	-1.83310200
O	4.24994800	-2.56798600	-0.41848700
H	3.53184200	-3.15020300	-0.70387500
H	3.20494400	-2.13279400	1.32958500
O	1.88362700	-0.04038200	0.80460600
H	1.11158300	-0.61006100	1.03185200
H	1.03173000	-0.63094700	-1.59874600
C	-1.12818000	4.05141000	-0.15448500
C	-2.36583400	3.62689800	0.21861800
C	-0.98327500	1.90988300	0.37370900
N	-0.27843400	2.96516000	-0.05081400
H	-0.78191300	5.01909700	-0.47389300
H	-3.30011800	4.15690200	0.28492000
H	-0.62627200	0.89636800	0.55074000
C	1.15798600	2.95932800	-0.36778000
H	1.29494500	3.09185100	-1.44122400

H	1.64230300	3.77335300	0.17175500
H	1.58337400	2.00552400	-0.05838000
N	-2.25415100	2.28937400	0.54689400
C	-3.35422900	1.39284500	0.96890600
C	-4.18089500	0.89395400	-0.21648200
H	-3.96541700	1.95335800	1.68008800
H	-2.88818400	0.55173800	1.48534600
H	-4.59445400	1.74553400	-0.77057500
H	-3.51761200	0.35098700	-0.89717500
Br	-1.00336700	-1.50346600	1.10078600
C	-5.31333900	-0.03214800	0.24223000
C	-6.16018900	-0.55889100	-0.92158700
H	-5.96118900	0.50190900	0.94975300
H	-4.88073700	-0.87680500	0.78999100
C	-7.29826900	-1.48387300	-0.47517700
H	-6.58107700	0.28786100	-1.48001500
H	-5.51173800	-1.09739600	-1.62354300
C	-8.14102800	-2.00708200	-1.64168500
H	-6.87625200	-2.32994500	0.07945900
H	-7.94381400	-0.94739100	0.23098000
H	-8.94021600	-2.66580700	-1.29145300
H	-8.60670600	-1.18521500	-2.19500200
H	-7.52806900	-2.57578800	-2.34775800

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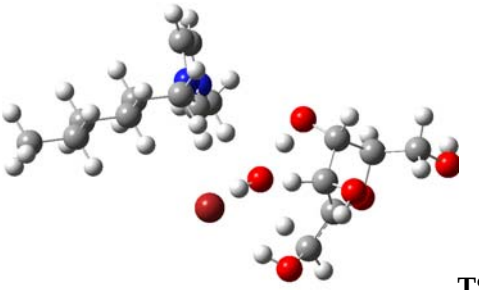

TS7(555i)

C	4.43723100	0.41459200	0.90003100
H	4.70258000	1.38303300	0.47397800
C	2.92839300	0.37391100	1.24262800
H	2.76819800	0.44885300	2.32187300
C	2.53033600	-1.04165900	0.76406900
C	3.17678100	-1.89928200	-1.62253300
H	4.04262900	-2.15768900	-2.23357400
C	3.48794300	-1.23245300	-0.38691200
O	4.55690600	-0.53160800	-0.25663200
O	2.25132600	-2.94304100	-1.53541700
H	1.33290100	-2.59366800	-1.54103800
O	2.21704800	1.37596600	0.58499700
H	2.06606400	1.08051900	-0.41241100
C	5.40332200	-0.00411000	1.99677100
H	5.24205100	0.67194600	2.84758900
H	5.17816300	-1.01822800	2.32794000
O	6.76199000	-0.00769600	1.58498500
H	7.03857700	0.89344700	1.38846900
O	2.86639000	-2.00981400	1.76237500
H	2.43500900	-2.84032200	1.52449800
H	1.48416600	-1.10435400	0.46070600
O	1.88602100	0.56517300	-1.79327800
H	1.05714500	0.06646900	-1.84616700
H	2.70483800	-0.88991200	-2.03824400
C	-1.09007300	4.08782500	-0.22117600
C	-1.95368200	3.44334200	0.60956000
C	-0.91323800	1.92277700	-0.60920800
N	-0.45117600	3.12182900	-0.97571300
H	-0.86932900	5.13523000	-0.33143300
H	-2.62726600	3.82423900	1.35727800
H	-0.61807600	0.95296300	-0.99619400
C	0.57156400	3.35909100	-2.00725200
H	0.08798500	3.69622100	-2.92563500
H	1.25426400	4.12634800	-1.64304700
H	1.12196400	2.42094500	-2.16732600
N	-1.82760000	2.09130900	0.35186500
C	-2.58946900	0.99487800	0.98553500
C	-3.99402100	0.85051800	0.39826400
H	-2.62043800	1.20321700	2.05765000
H	-2.01314400	0.08212300	0.81892700
H	-4.55429600	1.78435700	0.53007600
H	-3.90274500	0.67624200	-0.67877500
Br	-0.77392800	-1.61261900	-1.02706000

C	-4.75652300	-0.31342400	1.04168000
C	-6.16608700	-0.49224900	0.46697300
H	-4.82435600	-0.15378300	2.12589600
H	-4.18317500	-1.23575900	0.89681900
C	-6.93700700	-1.65935100	1.09415700
H	-6.73816000	0.43478100	0.60610000
H	-6.09517100	-0.64882300	-0.61658200
C	-8.34428000	-1.83154900	0.51543600
H	-6.36666300	-2.58431900	0.95044900
H	-7.00387600	-1.50738000	2.17851100
H	-8.86690900	-2.67102100	0.98196300
H	-8.95061300	-0.93378000	0.67320300
H	-8.30800700	-2.02118000	-0.56182700

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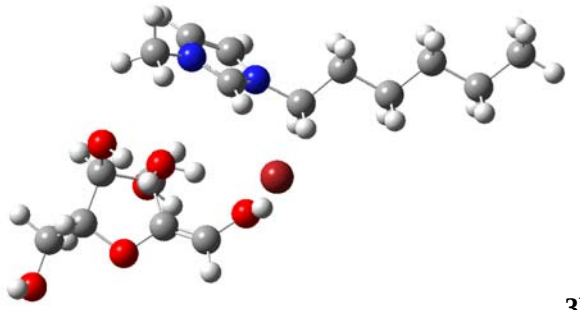

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H	-3.96786000	2.10671600	0.25290500
C	-2.42492200	1.02409200	-0.83202800
C	-1.65843500	-1.19689900	-1.80261300
H	-1.91139400	-2.19349900	-2.15283100

C	-2.60405200	-0.32517600	-1.44874800
O	-3.95253300	-0.61878400	-1.54458200
O	-0.32970600	-0.85342300	-1.77169500
H	0.14278300	-1.54734400	-1.25836100
O	-3.31889400	0.59288200	1.41898300
H	-2.95456300	-0.31395300	1.38210700
C	-5.73360900	1.04375000	-1.36140900
H	-6.22029100	1.70824800	-0.63174100
H	-5.24857800	1.66323000	-2.11665600
O	-6.69668600	0.25803300	-2.05089100
H	-7.10653000	-0.35165100	-1.42833400
O	-2.56680200	2.10541200	-1.77363600
H	-2.14270800	1.83425800	-2.59524000
H	-1.47982600	1.11513800	-0.29413100
O	-2.03600400	-1.89756900	1.88817000
H	-1.23958300	-2.23307500	1.41445900
H	-2.55076900	-2.68595100	2.08858000
C	0.17933400	2.53405900	2.16413300
C	1.07209800	2.52824000	1.13745400
C	0.72936400	0.43460100	1.75292800
N	-0.01963000	1.21766000	2.53617000
H	-0.33716100	3.34743700	2.64335000
H	1.47934600	3.33809000	0.55782600
H	0.76257100	-0.65491500	1.74194300
C	-0.93290600	0.74959300	3.58714000
H	-0.55912300	1.06685000	4.56140700
H	-1.92489900	1.15416600	3.39130500
H	-0.99359400	-0.33527600	3.53197500
N	1.40225100	1.20839700	0.89495900
C	2.32302800	0.70333100	-0.14636500
C	3.78543100	1.02932900	0.15740700
H	1.99938100	1.13163100	-1.09705000
H	2.16066500	-0.37496800	-0.19474700
H	3.92028400	2.11433200	0.24300900
H	4.05199000	0.59827500	1.12868200
Br	0.84819300	-2.81324000	0.56015100
C	4.71772900	0.47702200	-0.92784300
C	6.19753600	0.76738200	-0.65396800
H	4.43788100	0.90275000	-1.89960400
H	4.56807900	-0.60543900	-1.01265700
C	7.13481400	0.21753500	-1.73527000
H	6.34651000	1.85150800	-0.56402900
H	6.47668700	0.33899800	0.31708100
C	8.61250300	0.50578800	-1.45580400

H	6.98403300	-0.86456000	-1.82546600
H	6.85611800	0.64541600	-2.70579000
H	9.25256600	0.10174800	-2.24463900
H	8.80192400	1.58217300	-1.39348300
H	8.93095600	0.05841400	-0.50902600

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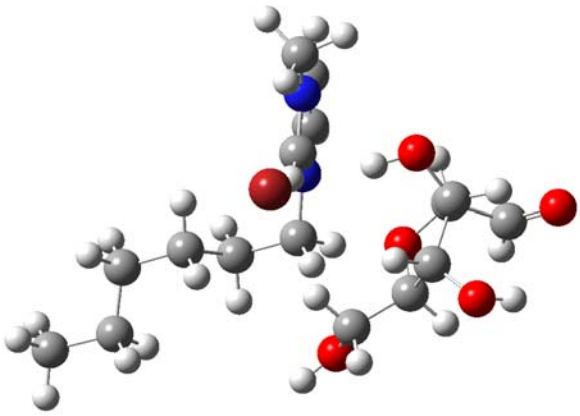

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C	1.92290800	-1.91637500	-0.48704400
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H	2.78948000	-1.57896100	1.49802800
O	1.49179200	-0.66085500	-1.05291300
O	4.15484500	-2.53908000	0.38477100
H	4.57139700	-2.50293100	-0.48379600
C	0.77488300	-2.60162700	0.21520000
H	1.16431700	-3.52701600	0.65639500
H	0.40015500	-1.95528500	1.01585700
O	-0.25758400	-2.89244700	-0.74244700
H	-0.90645200	-3.45942900	-0.31477300
C	2.67734000	0.11830300	-1.20972700

C	3.51932300	-0.12844500	0.05907700
H	4.58490200	-0.08378600	-0.17434200
C	3.36632800	-0.24709500	-2.52363000
O	4.54149900	-0.10056200	-2.74904200
H	2.67500200	-0.65923000	-3.29161700
H	2.39175500	1.17337400	-1.27973400
O	3.27881900	0.84313200	1.05295000
H	2.48029600	0.62141500	1.58010500
C	-0.50919600	1.63881600	-0.16108200
C	-0.66224900	3.58277100	-1.20727400
C	-1.23411600	2.63438700	-1.99735200
N	-1.12613900	1.42770300	-1.32879700
H	-0.27112900	0.90901100	0.61865600
H	-0.52901000	4.63990200	-1.35939600
H	-1.69627600	2.71262900	-2.96613700
N	-0.21972300	2.94170400	-0.06455300
C	0.47868400	3.56351500	1.07170400
H	-0.09558700	4.42555600	1.41115900
H	0.55538400	2.82130100	1.86891100
H	1.47737500	3.87168600	0.76168500
C	-1.64207600	0.12495400	-1.80131600
C	-3.14320100	-0.04834200	-1.54760700
H	-1.05501900	-0.65183500	-1.31120100
H	-1.41892700	0.07156000	-2.86861200
H	-3.70270300	0.73323700	-2.07734100
Br	0.48093600	0.24918000	2.78408300
H	-3.42161300	-0.99658400	-2.01760600
C	-3.53428500	-0.05466000	-0.06481600
C	-5.03805500	-0.24393200	0.18825200
H	-3.22452800	0.88928200	0.39634000
H	-2.97336100	-0.83941800	0.45636100
H	-5.22913200	-0.07780600	1.25451800
H	-5.59859900	0.53640900	-0.34403900
C	-5.59368200	-1.62064600	-0.19910000
C	-7.07549700	-1.78369900	0.15282400
H	-5.01030500	-2.39735900	0.31060500
H	-5.46127800	-1.79318700	-1.27310500
H	-7.44681600	-2.77181300	-0.13195400
H	-7.24153800	-1.66311700	1.22763700
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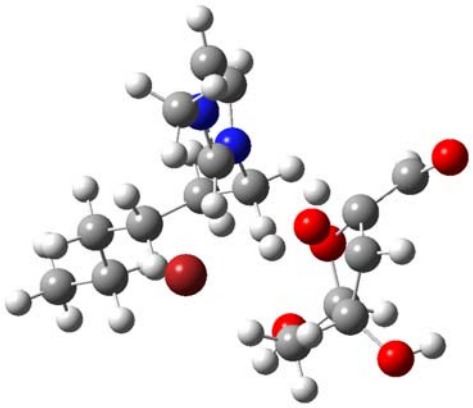

TS8 (1562i)

C	1.67427700	-2.03140200	-0.71285200
H	1.88761100	-2.61251400	-1.62591800
C	2.99022400	-1.90104900	0.10665200
H	2.78706000	-1.91413900	1.17848000
O	1.30903300	-0.69776300	-1.08333200
O	3.89785200	-2.96568700	-0.12126700
H	4.07626700	-3.03306600	-1.06691100
C	0.56535300	-2.69986300	0.06753500
H	0.92736200	-3.68310000	0.39081400
H	0.33484700	-2.09664300	0.95254300
O	-0.58927300	-2.83868100	-0.77629300
H	-1.21508300	-3.41990500	-0.33392000
C	2.53474300	0.02618200	-1.30884700
C	3.52383800	-0.52663500	-0.33631800
H	4.56802000	-0.52252900	-0.63479100
C	2.86261900	0.35779100	-2.67429300
O	3.96046800	0.72132200	-3.08269600
H	1.98474300	0.33144600	-3.36012200
H	2.75264100	1.01860100	-0.15025800
O	3.41103000	0.58168300	0.72264300
H	2.77640200	0.34727600	1.48516300
C	-0.44419700	1.64749400	-0.01927600
C	-0.79357500	3.67234700	-0.83794200
C	-1.41957200	2.77740200	-1.64747500
N	-1.19100700	1.51978800	-1.12044400

H	-0.08253500	0.85255800	0.62689400
H	-0.71442400	4.74387200	-0.89937000
H	-1.99339400	2.92503700	-2.54569400
N	-0.19572800	2.94832600	0.17670400
C	0.60781800	3.50431400	1.27469000
H	0.02963900	4.27589800	1.78336200
H	0.84582100	2.69746100	1.97065900
H	1.52654800	3.93131400	0.87106700
C	-1.72378500	0.25167800	-1.66387200
C	-3.21962300	0.07469100	-1.38580000
H	-1.13366000	-0.55700600	-1.23585000
H	-1.52316000	0.26308700	-2.73673300
H	-3.78687300	0.88965800	-1.85326400
Br	1.13170800	0.13433600	2.80339200
H	-3.51666100	-0.84149500	-1.90476600
C	-3.57530200	-0.01775700	0.10293900
C	-5.07664900	-0.18785300	0.38279700
H	-3.23075100	0.88794400	0.61445900
H	-3.02185200	-0.84921700	0.55554300
H	-5.23891300	-0.08880000	1.46229600
H	-5.62923200	0.63960800	-0.08213000
C	-5.67662000	-1.52159600	-0.08124900
C	-7.15347500	-1.67162800	0.29612400
H	-5.10175800	-2.34502500	0.36052400
H	-5.57341300	-1.62443300	-1.16715900
H	-7.55671500	-2.62927800	-0.04375700
H	-7.29152100	-1.61858600	1.38038800
H	-7.75894600	-0.87827300	-0.15342300

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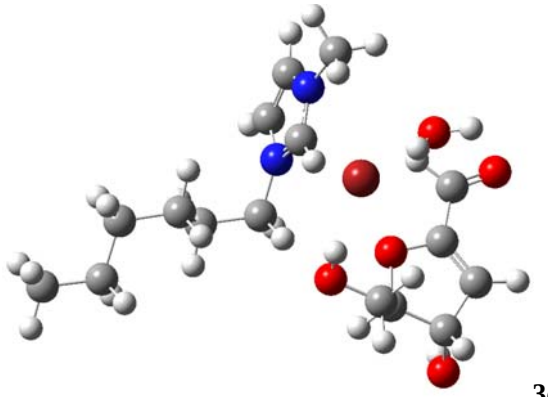

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C	1.83040800	-2.38325800	0.35039800
H	1.12077700	-3.12940600	-0.01315000
C	3.26772000	-2.96674300	0.41229500
H	3.58852000	-3.09665600	1.44872400
O	1.87329400	-1.31233700	-0.64488000
O	3.39270900	-4.27535700	-0.15964600
H	3.38582100	-4.18646600	-1.11985800
C	1.36823300	-1.81928900	1.68597200
H	1.40684300	-2.63696100	2.41974800
H	2.06072500	-1.03589300	2.01449000
O	0.05062600	-1.30808300	1.59189500
H	0.04200900	-0.43454300	2.03878200
C	3.19116000	-1.06793400	-0.90521600
C	4.05112500	-1.92132400	-0.33018500
H	5.12539900	-1.88954300	-0.42500500
C	3.46887800	0.08441900	-1.79649600
O	4.58161100	0.39293300	-2.15659700
H	2.57184200	0.63771600	-2.12303900
H	3.47422700	2.42924600	0.42820800
O	2.59383800	2.17896400	0.13082400
H	2.08065400	2.03232100	0.95462900
C	-0.66346200	1.59448100	-0.64660900
C	-0.81850600	2.67662200	-2.56672500
C	-1.19468700	1.38651300	-2.78033200
N	-1.09049000	0.72686600	-1.56912400
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C	0.01504500	3.98564500	-0.54887800
H	-0.59386900	4.84197200	-0.83827200
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H	1.05941400	4.13143500	-0.82125400

C	-1.41918900	-0.69260100	-1.31627700
C	-2.92685800	-0.95975600	-1.29262200
H	-0.95022500	-0.95573400	-0.36585900
H	-0.92915200	-1.27114700	-2.10154000
H	-3.37343700	-0.67969700	-2.25538400
Br	0.43842800	1.76776000	2.63644000
H	-3.03932500	-2.04496000	-1.20801800
C	-3.66969200	-0.26133700	-0.14696200
C	-5.17946100	-0.54606400	-0.11118500
H	-3.52382900	0.82185700	-0.22840300
H	-3.21896300	-0.55901000	0.80699000
H	-5.63509600	0.11076700	0.63877500
H	-5.62834800	-0.26277400	-1.07282800
C	-5.55499600	-1.99708700	0.21733800
C	-7.06785200	-2.20817500	0.33031000
H	-5.07341200	-2.28579800	1.15920400
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H	-7.30885700	-3.24843700	0.56486000
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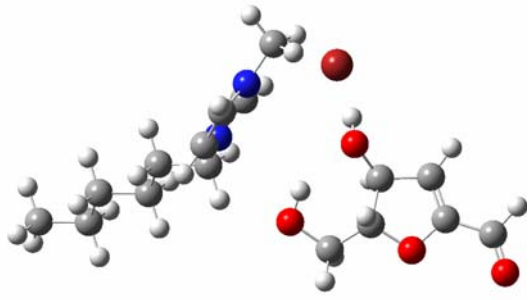

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C	2.83769100	-1.63649200	0.83261000
C	2.81887100	-0.51854500	-0.23026500
C	4.26695000	-0.53061300	-0.65839100
C	4.80775500	-1.68697400	-0.24110300

H	2.19347500	-0.79205600	-1.09502800
H	4.74424900	0.21419700	-1.27790100
H	3.04582800	-1.16213400	1.80108200
O	3.96723800	-2.47468900	0.50376800
C	6.16848700	-2.16856500	-0.52053800
O	6.62443100	-3.22389600	-0.14531800
H	6.76493200	-1.45837000	-1.12784300
C	1.54715200	-2.42858200	0.92318900
H	1.61850300	-3.20952700	1.68357300
H	1.32853800	-2.90184500	-0.04161900
O	0.48295100	-1.54013100	1.29491900
H	0.77148800	-0.63910200	1.08161300
O	2.28982500	0.65618200	0.36310300
H	1.98771400	1.25813700	-0.36389800
Br	1.02096700	2.40655000	-2.01638000
C	-0.96488200	2.12866200	2.77807100
C	-1.67505900	1.00875400	2.47685400
H	-0.69840700	2.55729300	3.72856300
H	-2.13232900	0.27449400	3.11623000
C	0.26285500	3.89094400	1.40463100
H	1.11432900	3.82979500	2.08142500
H	0.62065300	3.90564400	0.37340300
H	-0.32545100	4.78400200	1.61918300
C	-2.33523700	-0.17386900	0.31292200
C	-3.86089200	-0.15884600	0.41416500
H	-1.90565100	-1.11278900	0.66731600
H	-2.00903600	-0.03249600	-0.71866100
H	-4.16204200	-0.26567600	1.46269300
H	-4.23616800	0.81325400	0.07552600
N	-0.56902500	2.69259300	1.57907800
N	-1.70486900	0.90757600	1.09695700
C	-1.02941900	1.93763900	0.57626200
H	-0.76941400	2.09417400	-0.47395400
C	-4.49471400	-1.28148600	-0.41614700
C	-6.02480300	-1.30341200	-0.32622500
H	-4.09725700	-2.24835000	-0.08361200
H	-4.19418000	-1.17108200	-1.46514700
H	-6.32489900	-1.41135900	0.72414300
H	-6.42176000	-0.33582400	-0.65892200
C	-6.66773400	-2.42342700	-1.15210800
C	-8.19576400	-2.44174000	-1.05521200
H	-6.26898700	-3.38993100	-0.82126600
H	-6.36914100	-2.31427800	-2.20148100
H	-8.62221600	-3.25090500	-1.65379900

H	-8.52554800	-2.58448600	-0.02134200
H	-8.62692500	-1.50165200	-1.41330600

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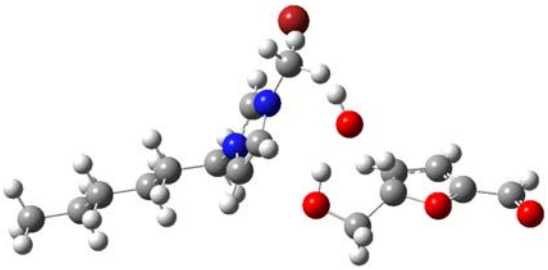

TS9 (454i)

C	3.08940500	-1.48890500	0.23125500
C	3.04513500	-1.51293000	-1.23122000
C	4.36547800	-1.60882200	-1.67185200
C	5.15017800	-1.77378800	-0.53882500
H	2.14818400	-1.53667500	-1.82322300
H	4.72508100	-1.59852300	-2.68927300
H	2.89447100	-0.37403200	0.39722300
O	4.45303800	-1.77712500	0.58576700
C	6.62199000	-1.94856700	-0.47387800
O	7.23660700	-2.09056800	0.55349700
H	7.11600200	-1.93830300	-1.46358500
C	2.01767100	-2.20862400	1.05595000
H	2.24160900	-2.05646600	2.11969300
H	2.02708100	-3.28501000	0.85382700
O	0.76246000	-1.67144900	0.69940400
H	0.92706200	-0.80605200	0.21162600
O	1.77945500	0.37874300	-0.63806200
H	1.39345400	1.21779800	-0.95925500
Br	0.12562000	3.29466400	-1.77846800
C	-0.75008000	1.54893100	3.09670500
C	-1.39963800	0.43767800	2.65797800
H	-0.41964900	1.82725000	4.08243900
H	-1.72845200	-0.43849800	3.18826400
C	0.16509500	3.64507700	1.96233000
H	1.13046800	3.53896800	2.45725000

H	0.31555200	3.91947100	0.91489200
H	-0.43628800	4.39997400	2.47063400
C	-2.19141000	-0.39291700	0.37796800
C	-3.70084600	-0.52093900	0.58775300
H	-1.67237100	-1.34175000	0.52620700
H	-1.96423800	-0.04805200	-0.63187100
H	-3.90523900	-0.84239600	1.61590100
H	-4.16604900	0.46345000	0.46626000
N	-0.53345800	2.35311500	1.99167800
N	-1.57327100	0.58383500	1.29322800
C	-1.03902500	1.74820200	0.91211100
H	-0.93911200	2.14700000	-0.10931700
C	-4.32709500	-1.51798900	-0.39430900
C	-5.83784500	-1.68689700	-0.19854700
H	-3.83549300	-2.49299800	-0.28657400
H	-4.12881000	-1.18659700	-1.42079400
H	-6.03576300	-2.02332100	0.82759100
H	-6.32799900	-0.71014400	-0.29897300
C	-6.47411200	-2.67367000	-1.18404400
C	-7.98198900	-2.84306100	-0.97823100
H	-5.98036800	-3.64836200	-1.08838300
H	-6.28083100	-2.33405800	-2.20852600
H	-8.40486700	-3.55082100	-1.69621100
H	-8.20521800	-3.21606200	0.02639300
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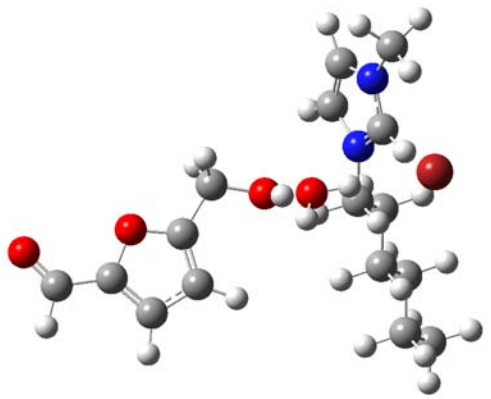

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C	-3.55169800	0.60241900	0.08310900
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C	-5.49432600	1.52536900	-0.35966600
H	-2.53610000	1.17085300	-1.76241900
H	-4.96324700	2.32294500	-2.32458300
H	-1.81957000	-2.53601200	-2.05601400
O	-4.79664800	0.80290600	0.57484500
C	-6.87096900	1.89993400	-0.10375200
O	-7.50790200	1.63876800	0.89646800
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O	-1.31978200	-2.45136500	-1.23816100
H	-0.43246600	-2.84409300	-1.44018000
Br	1.64959000	-3.57038000	-1.86133100
C	1.55528900	-1.69319300	3.09813900
C	1.54588400	-0.39883200	2.67987700
H	1.43050200	-2.11598900	4.07999500
H	1.40114200	0.51355700	3.23088400
C	1.82223400	-3.94498900	1.92716400
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H	2.73402100	-4.28934400	2.41657700
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H	4.96472300	3.37880600	-0.15529300

C	3.98020300	5.10387600	-1.00217600
C	5.13067600	6.08648000	-0.76647600
H	3.02332100	5.62874200	-0.89451200
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H	5.08329500	6.92846300	-1.46202600
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H	6.10132200	5.59915900	-0.90115900

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