Electronic Supplementary Material (ESI) for RSC Advances

Electronic Supplementary Information for the article

Tartrate-based ionic liquids: unified synthesis and characterisation

Anne Rouch,[a] Tessa Castellan,[a] Isabelle Fabing,[a] Nathalie Saffon,[b] Jean Rodriguez,[c]

Thierry Constantieux,[c] Jean-Christophe Plaquevent[a] and Yves Génisson*[a]

[a] *LSPCMIB, UMR CNRS 5068, Université Paul Sabatier - Toulouse III, Toulouse, France.*
Fax: 33 (0)5 61 55 60 11; Tel: 33 (0)5 61 55 62 99; E-mail: genisson@chimie.ups-tlse.fr
[b] *Institut de Chimie de Toulouse, ICT FR 2599, Université Paul Sabatier - Toulouse III, Toulouse, France.*
[c] *Aix Marseille Université, CNRS, iSm2 UMR 7313, 13397 Marseille cedex 20, France.*

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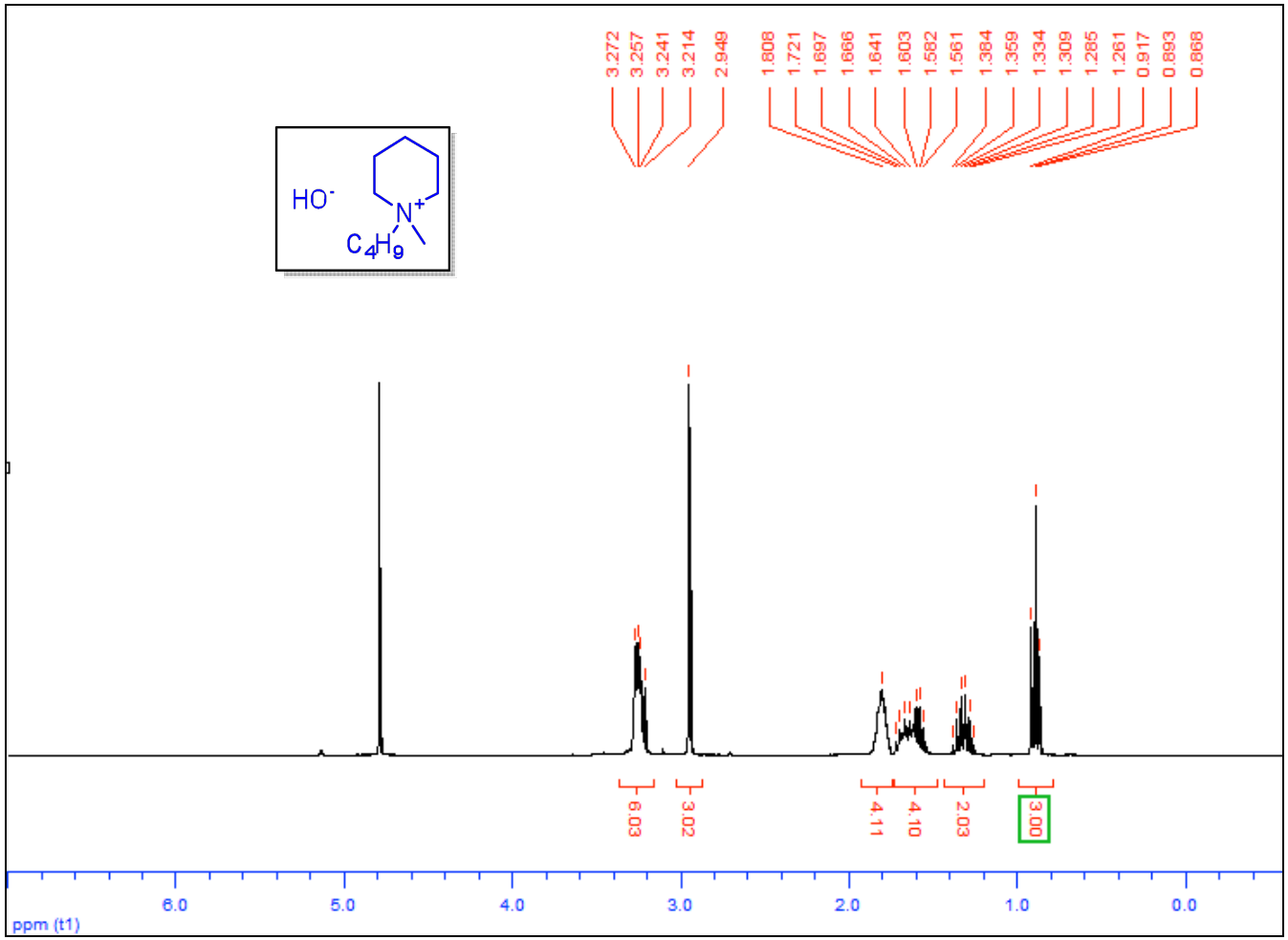
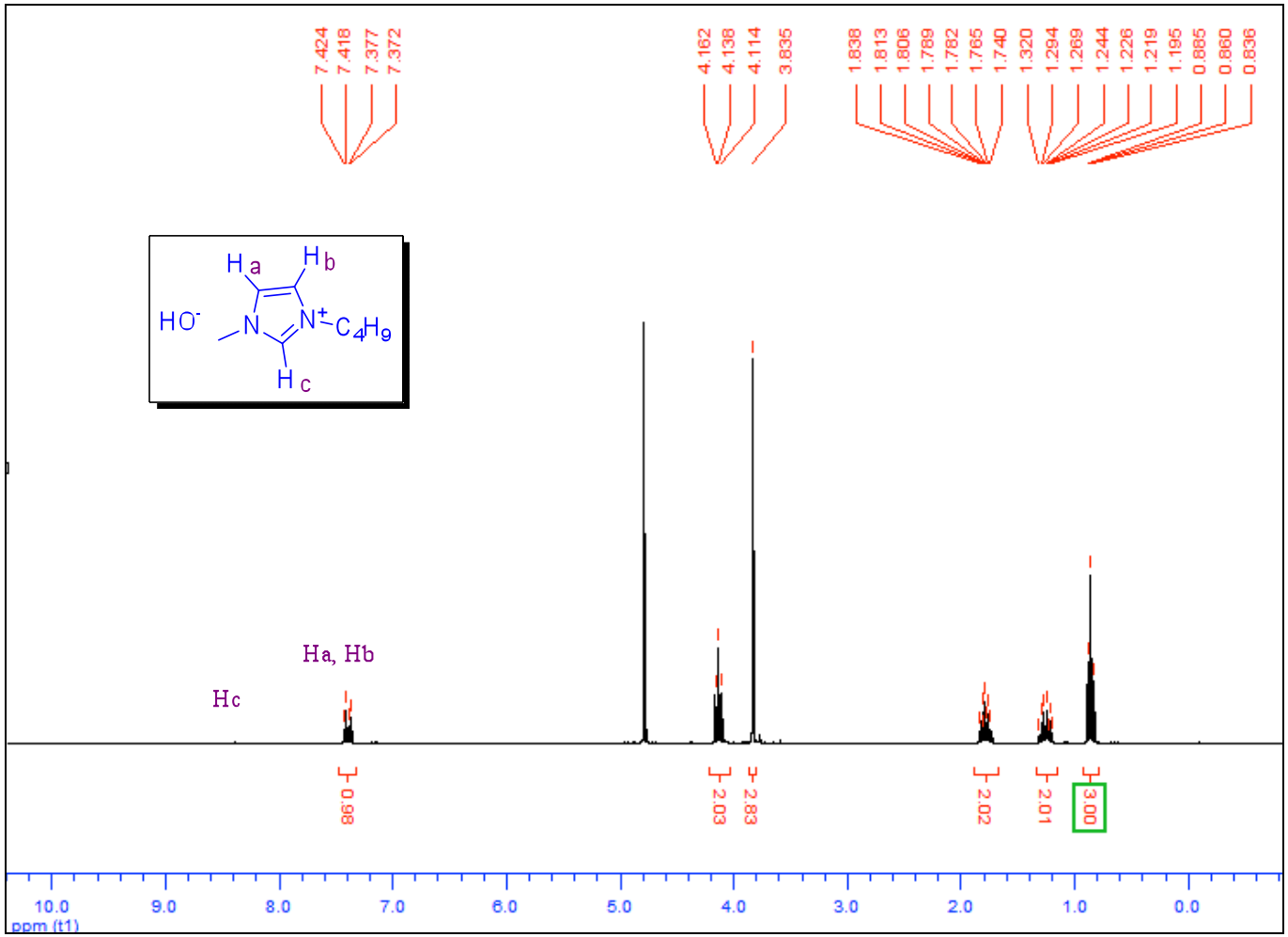
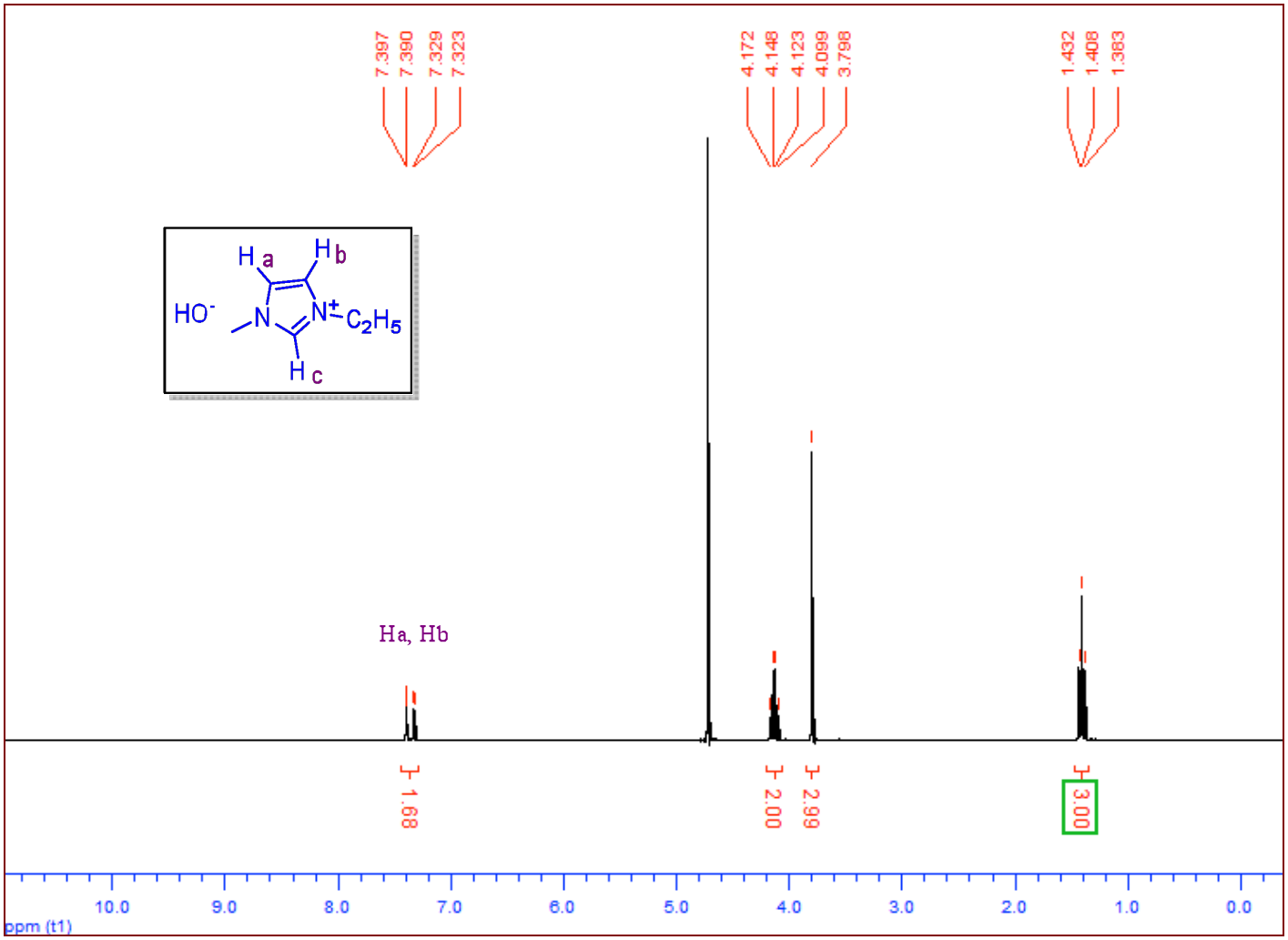


^{1}H-NMR (300 MHz, D_2O) spectrum of [Bmpip]OH



^{1}H-NMR (300 MHz, D_2O) spectrum of [Bmim]OH



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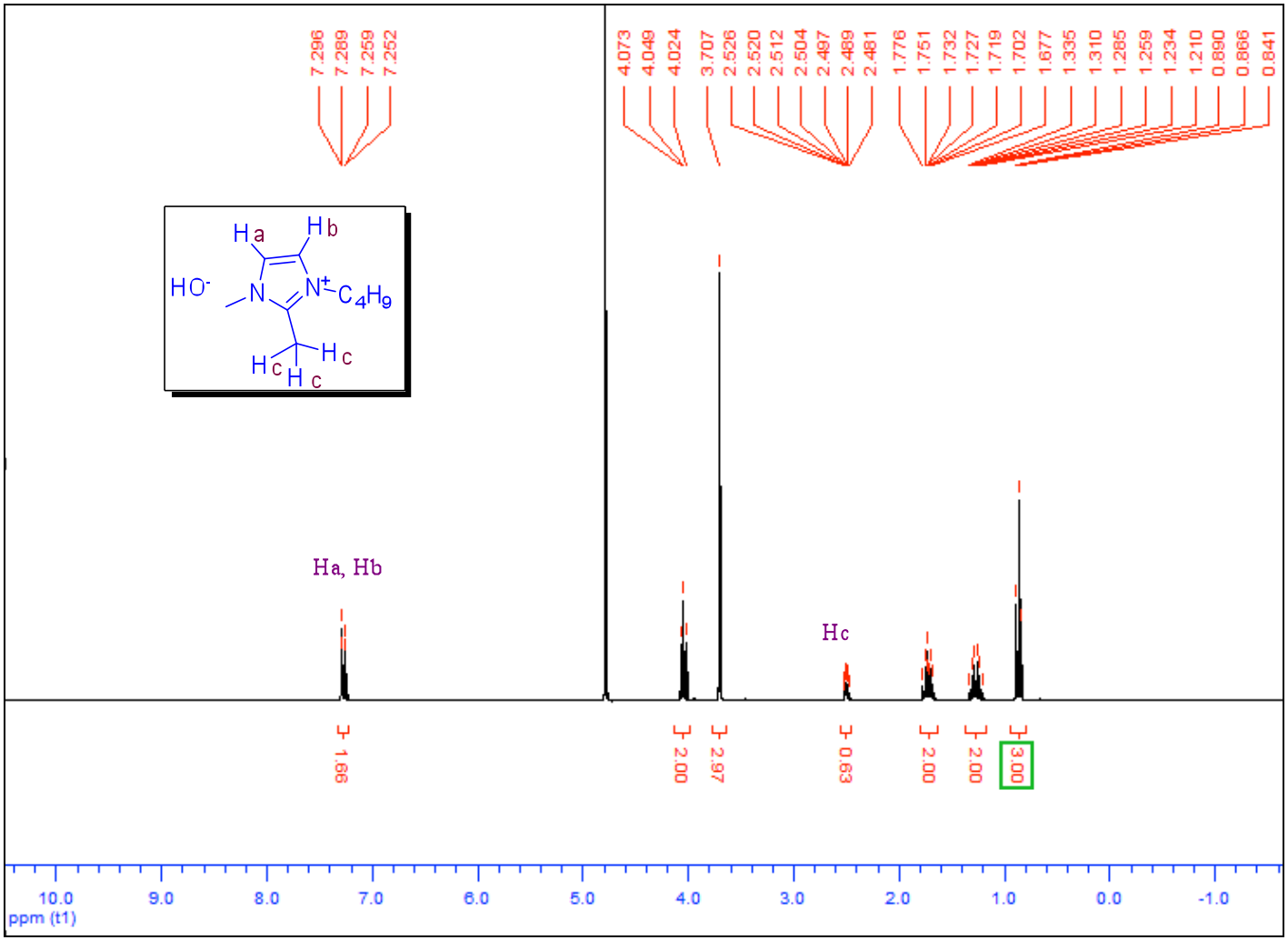

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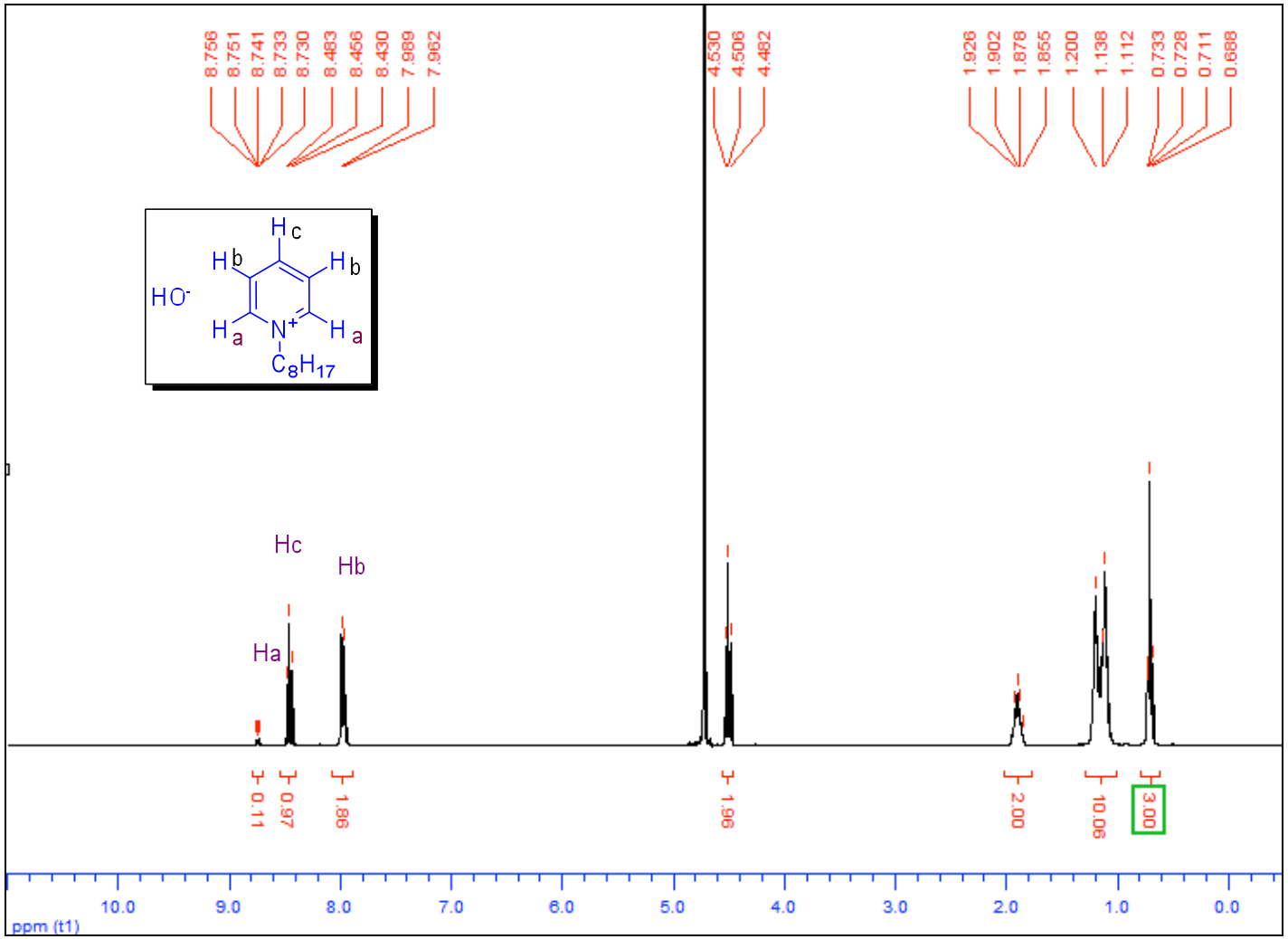

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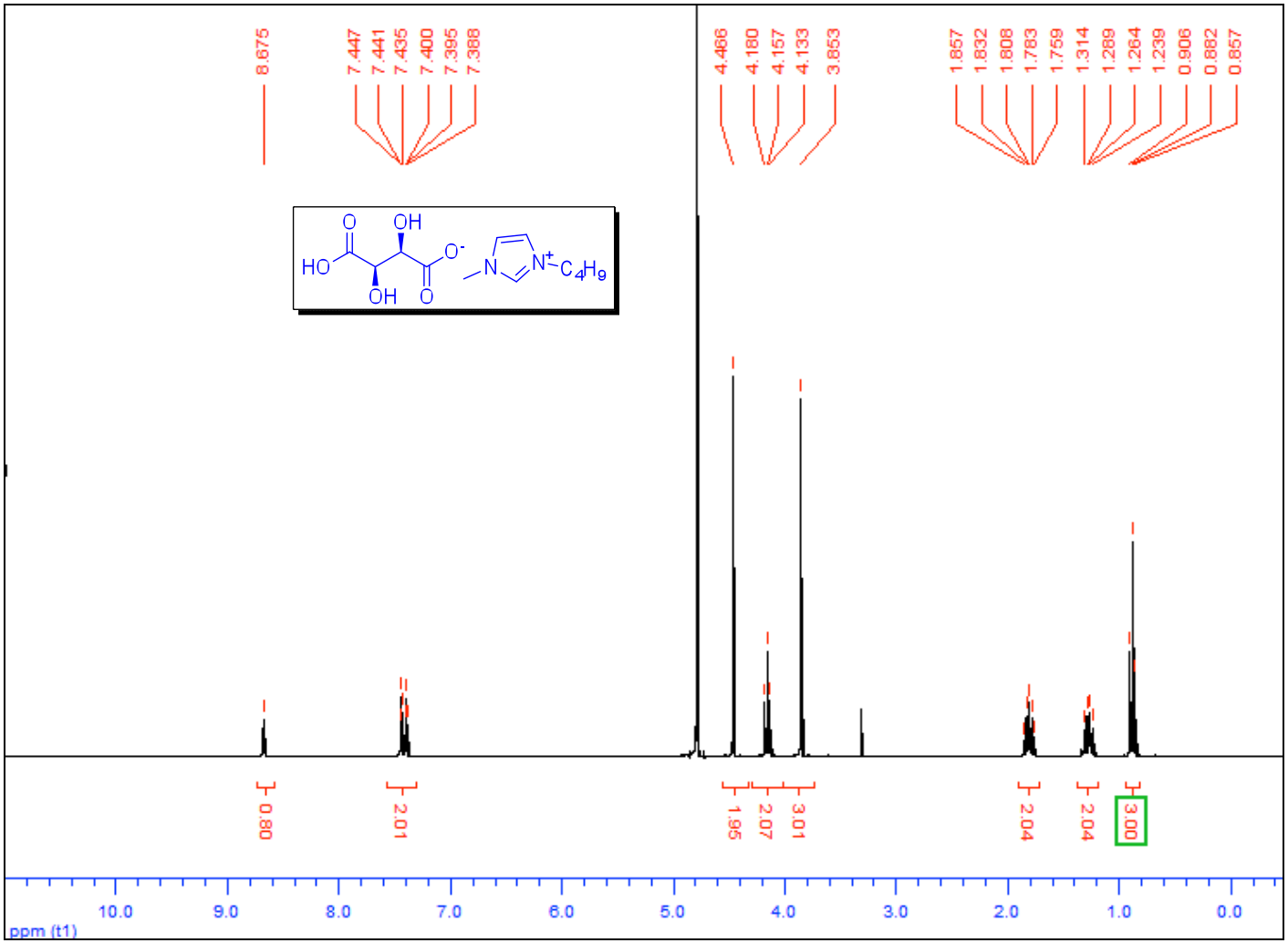
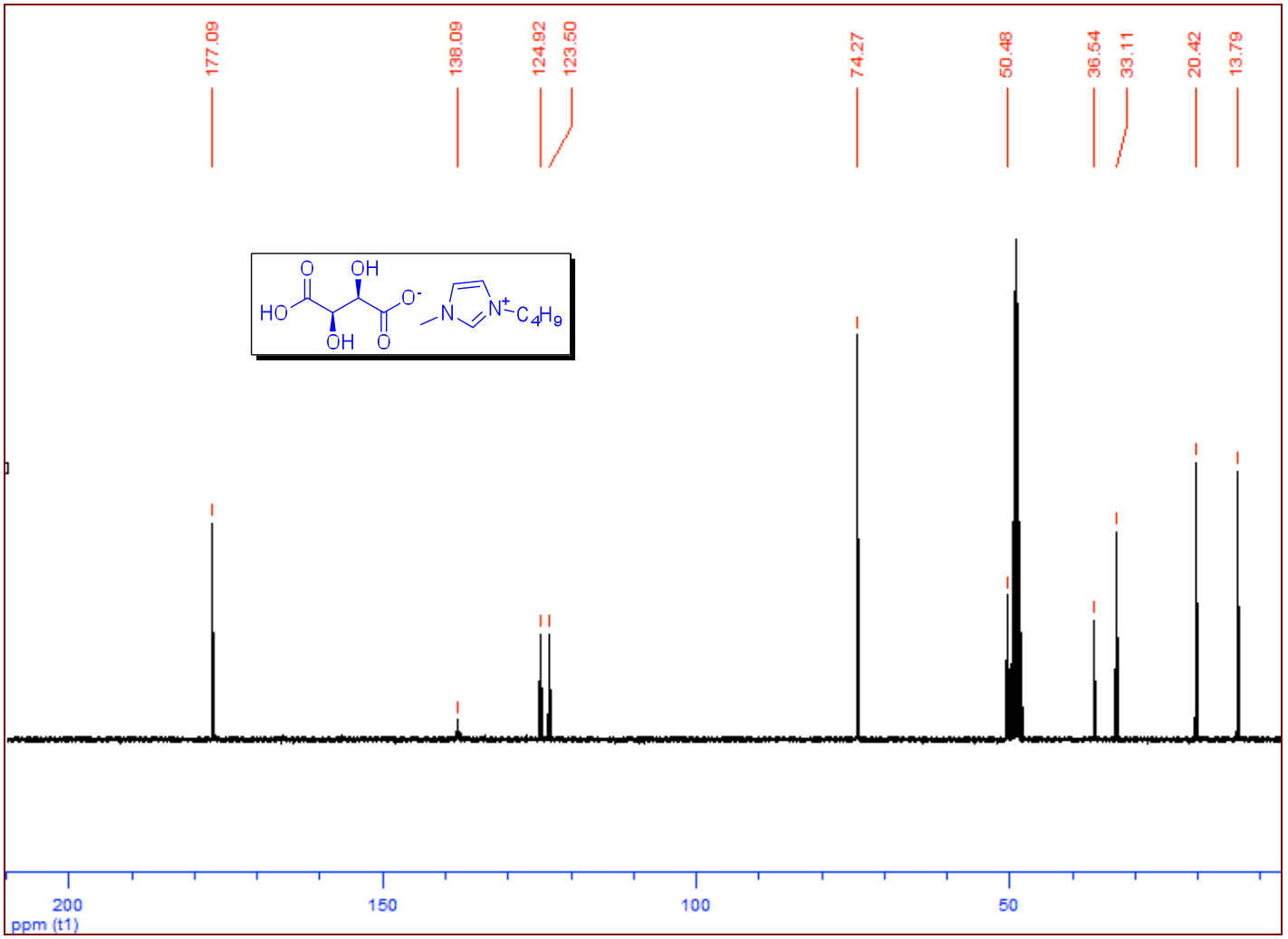
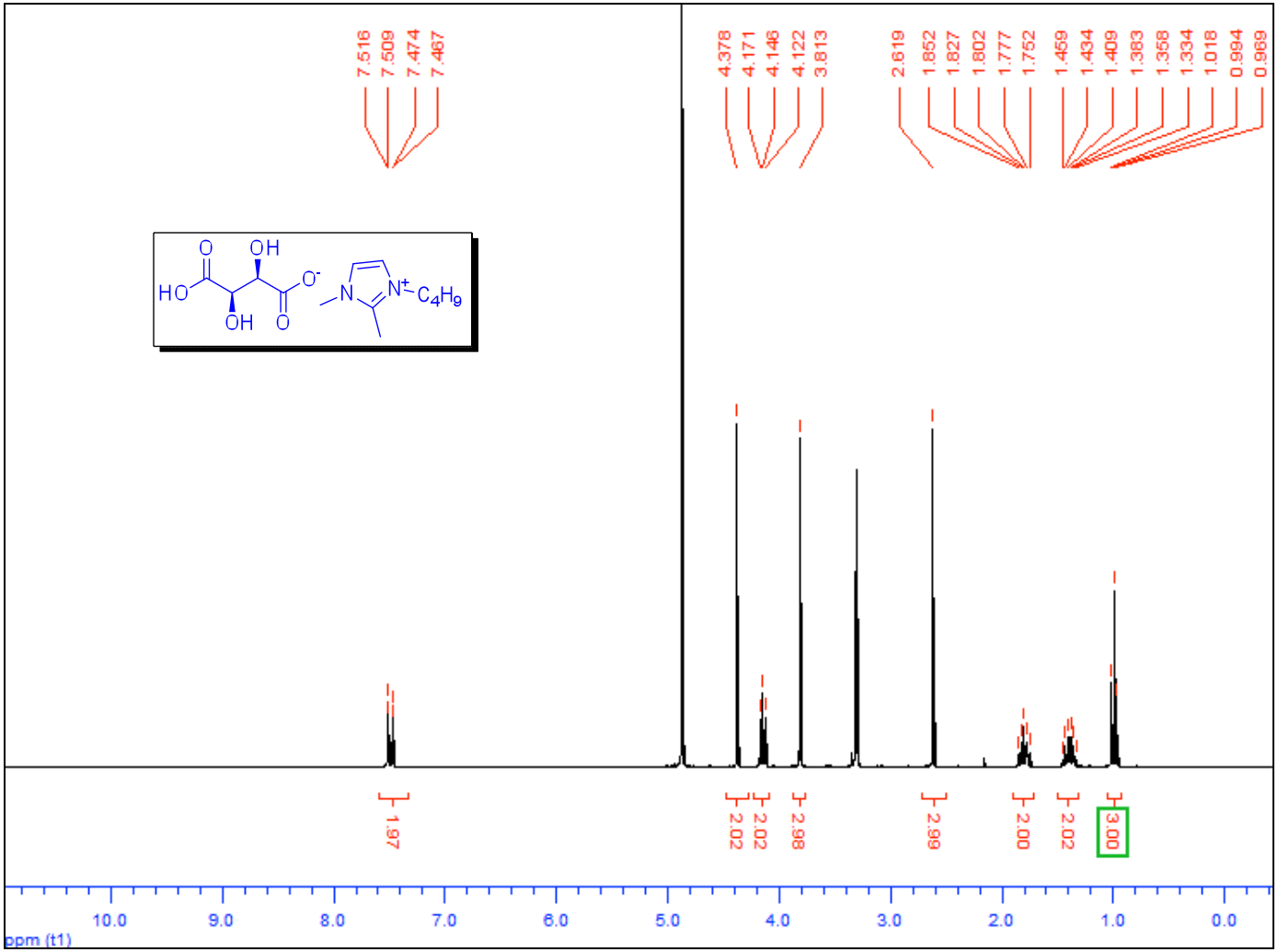


^{1}H-NMR (300 MHz, D_2O) spectrum of [Bmim]D-HTart



^{13}C-NMR (75 MHz, CD_3OD) spectrum of [Bmim]D-HTart



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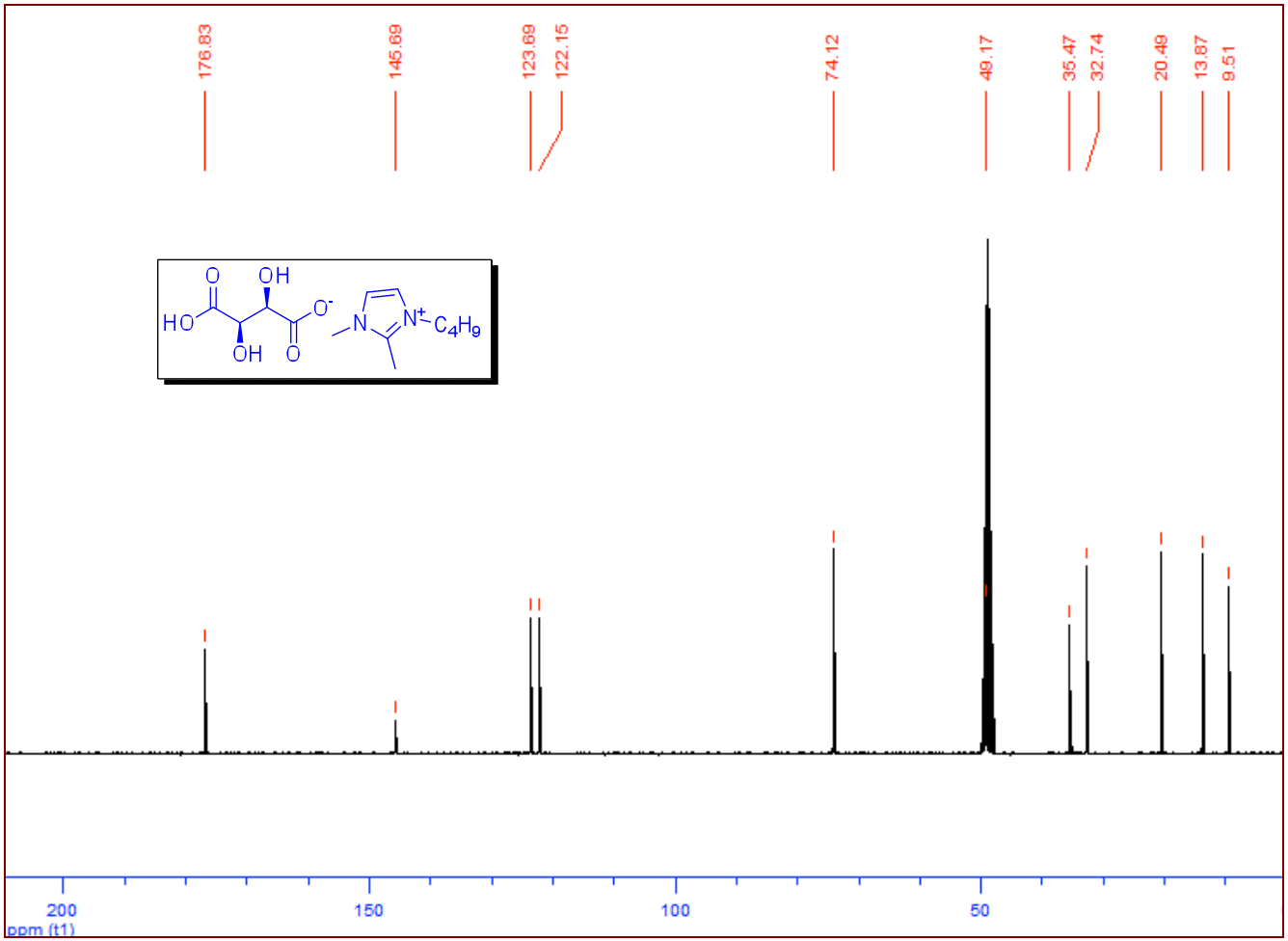

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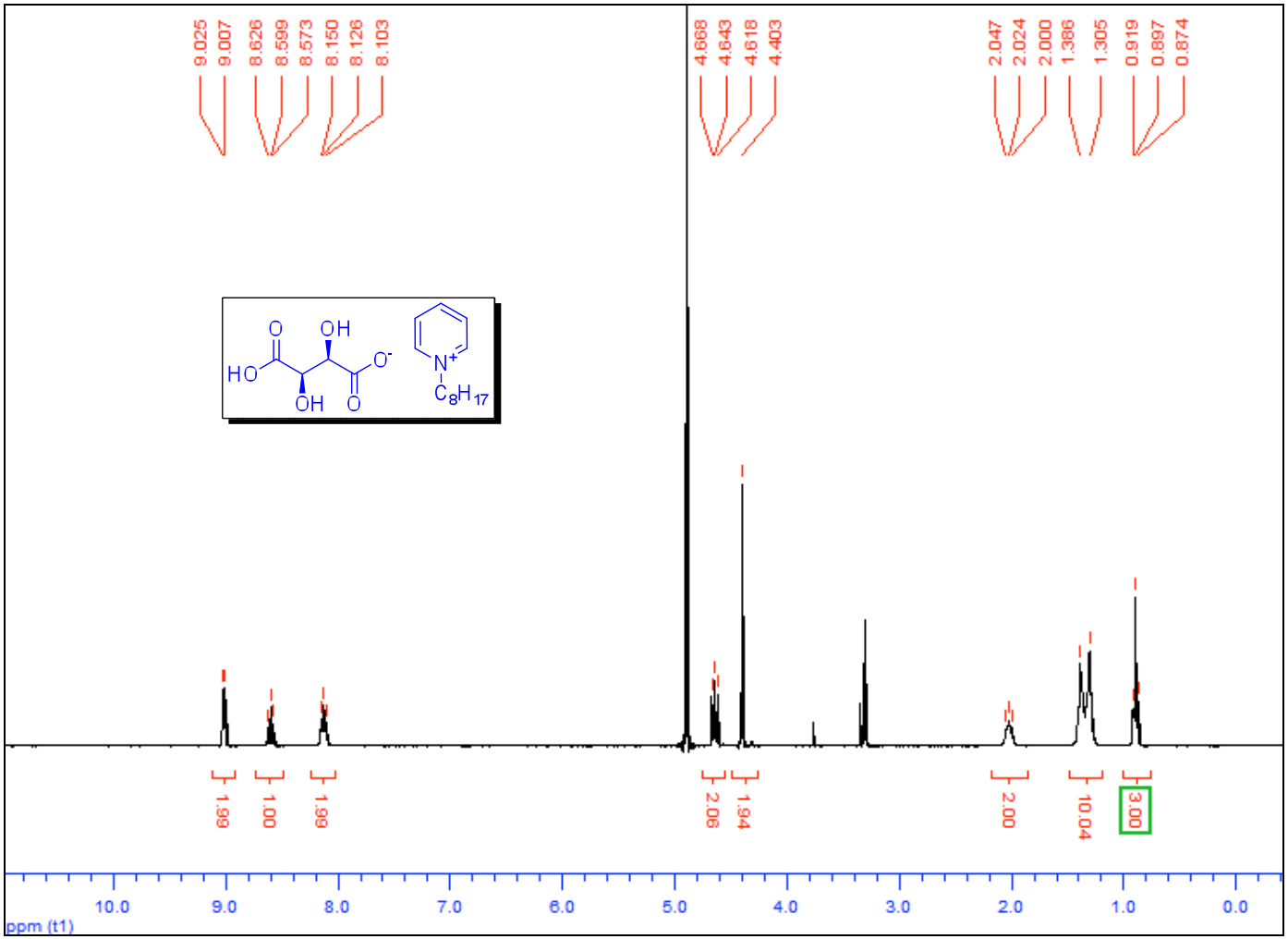

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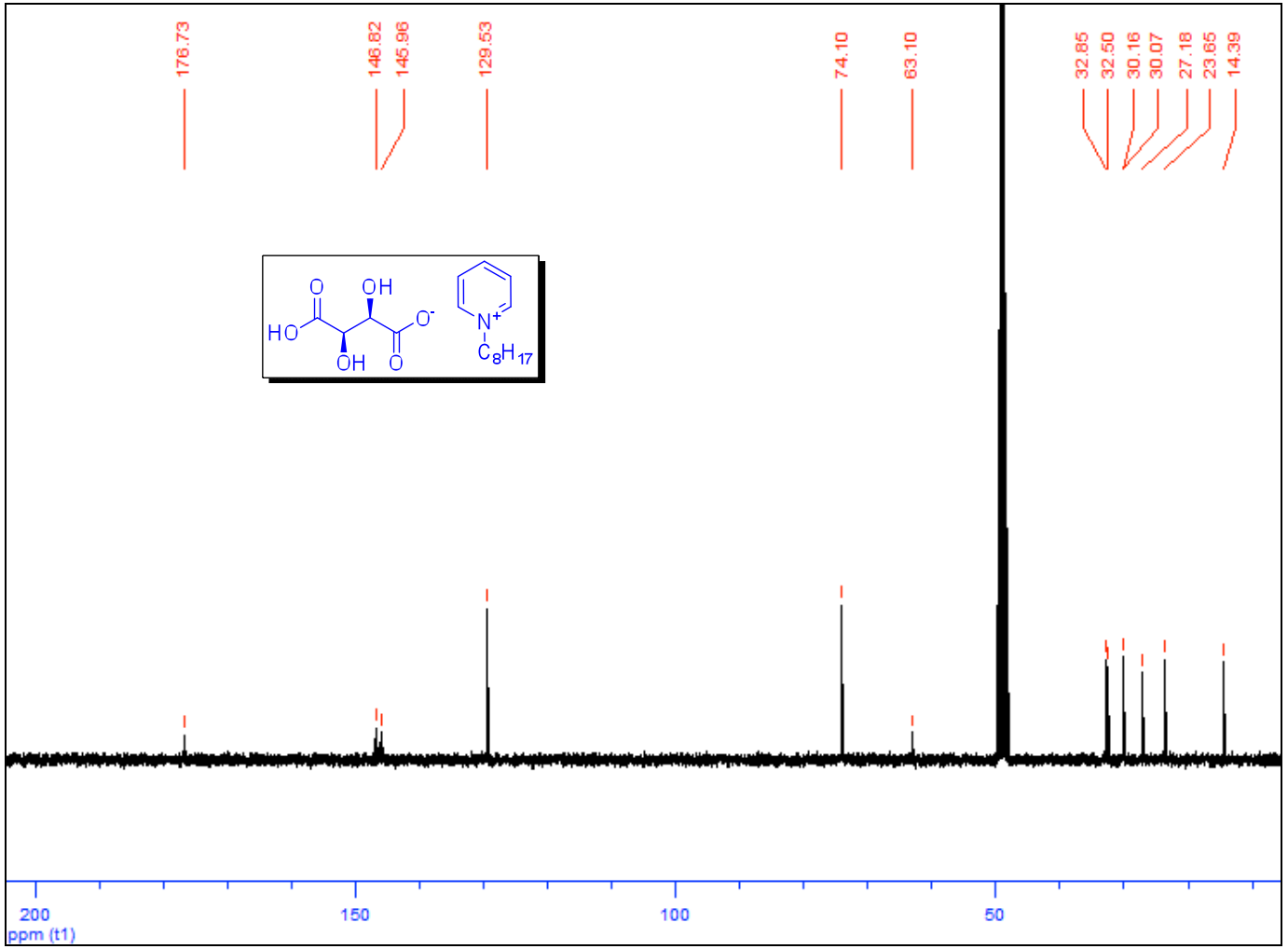

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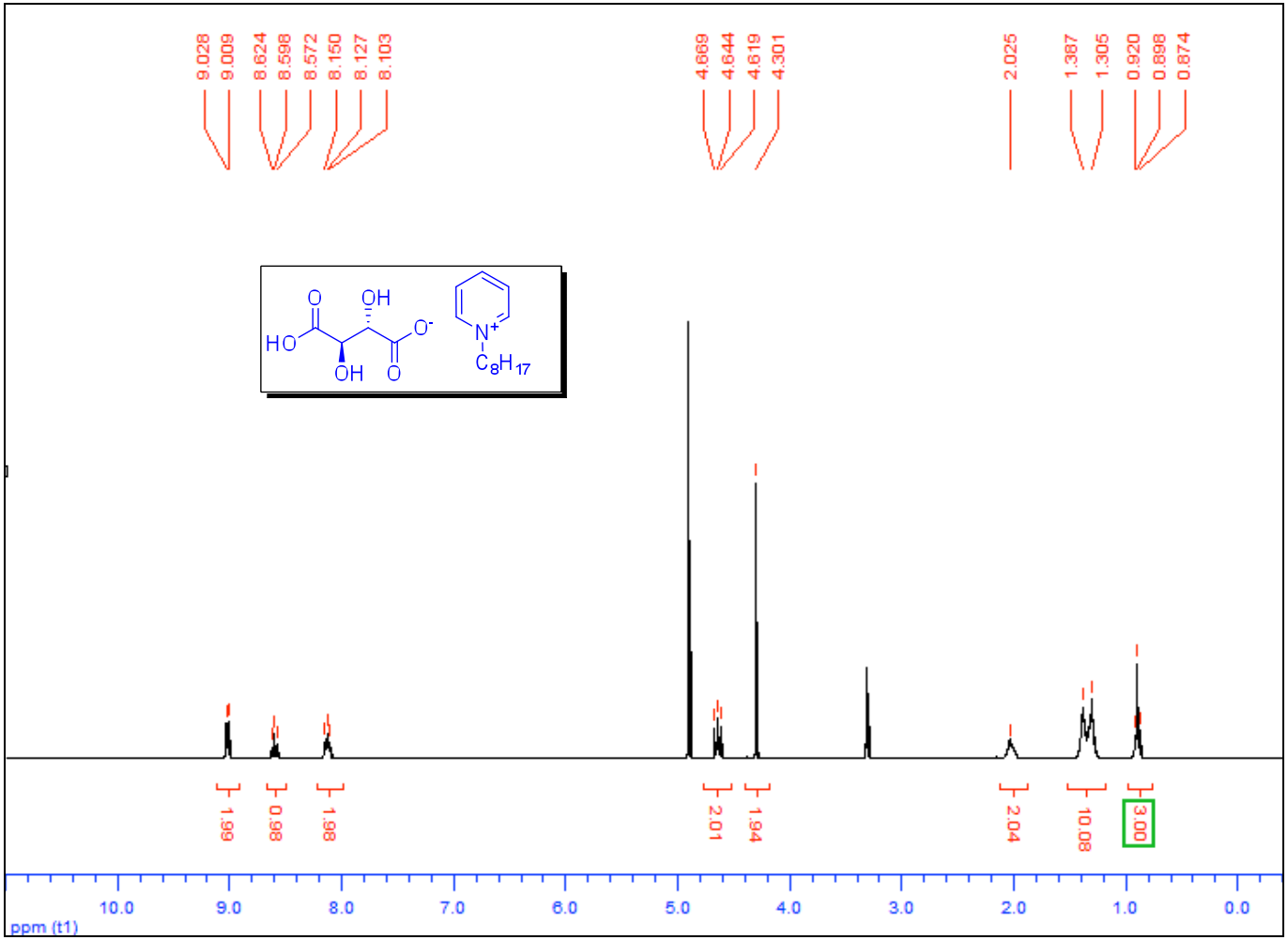
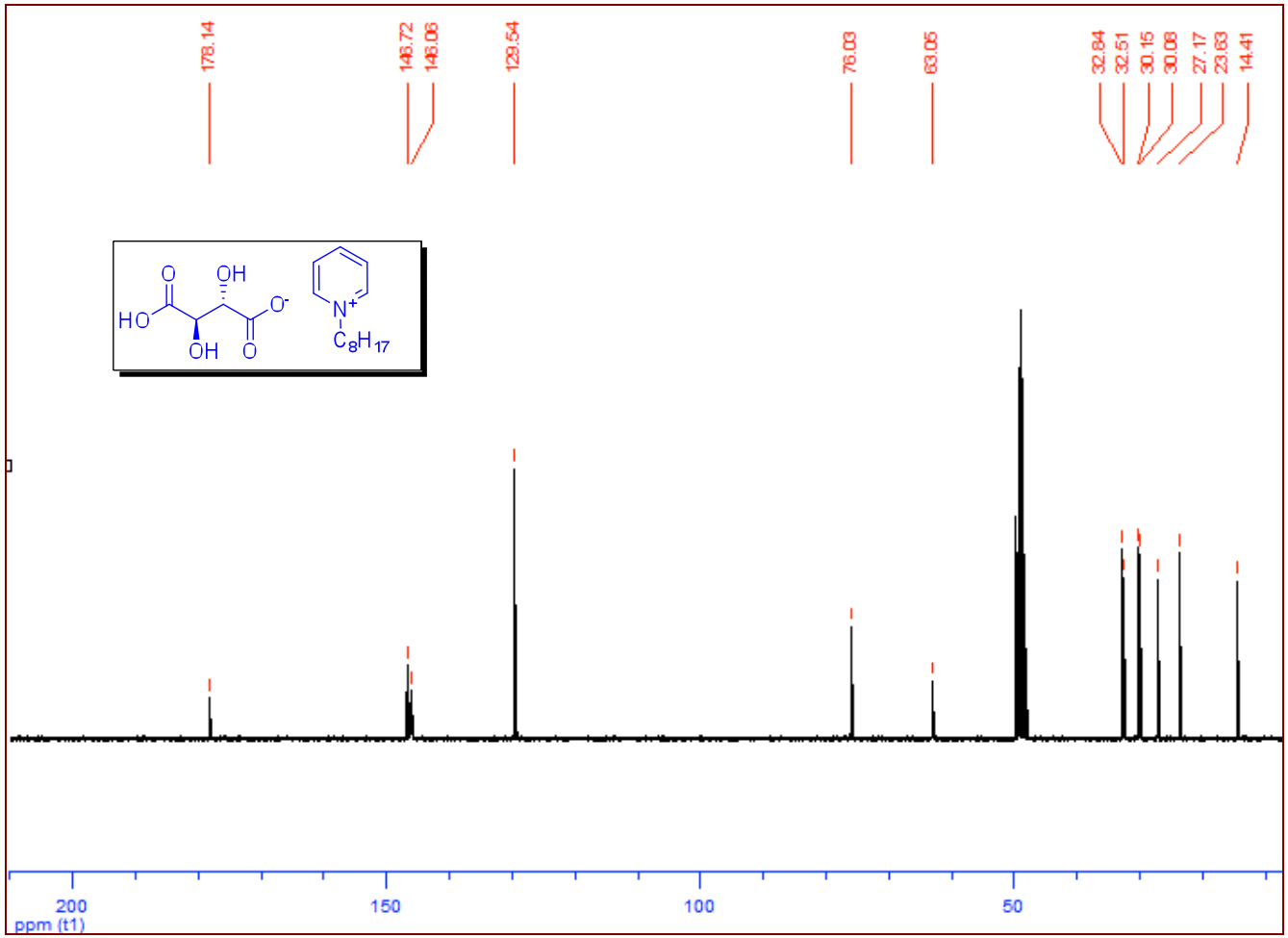


^{1}H-NMR (300 MHz, CD_3OD) spectrum of [OctPyr]*meso*-HTart



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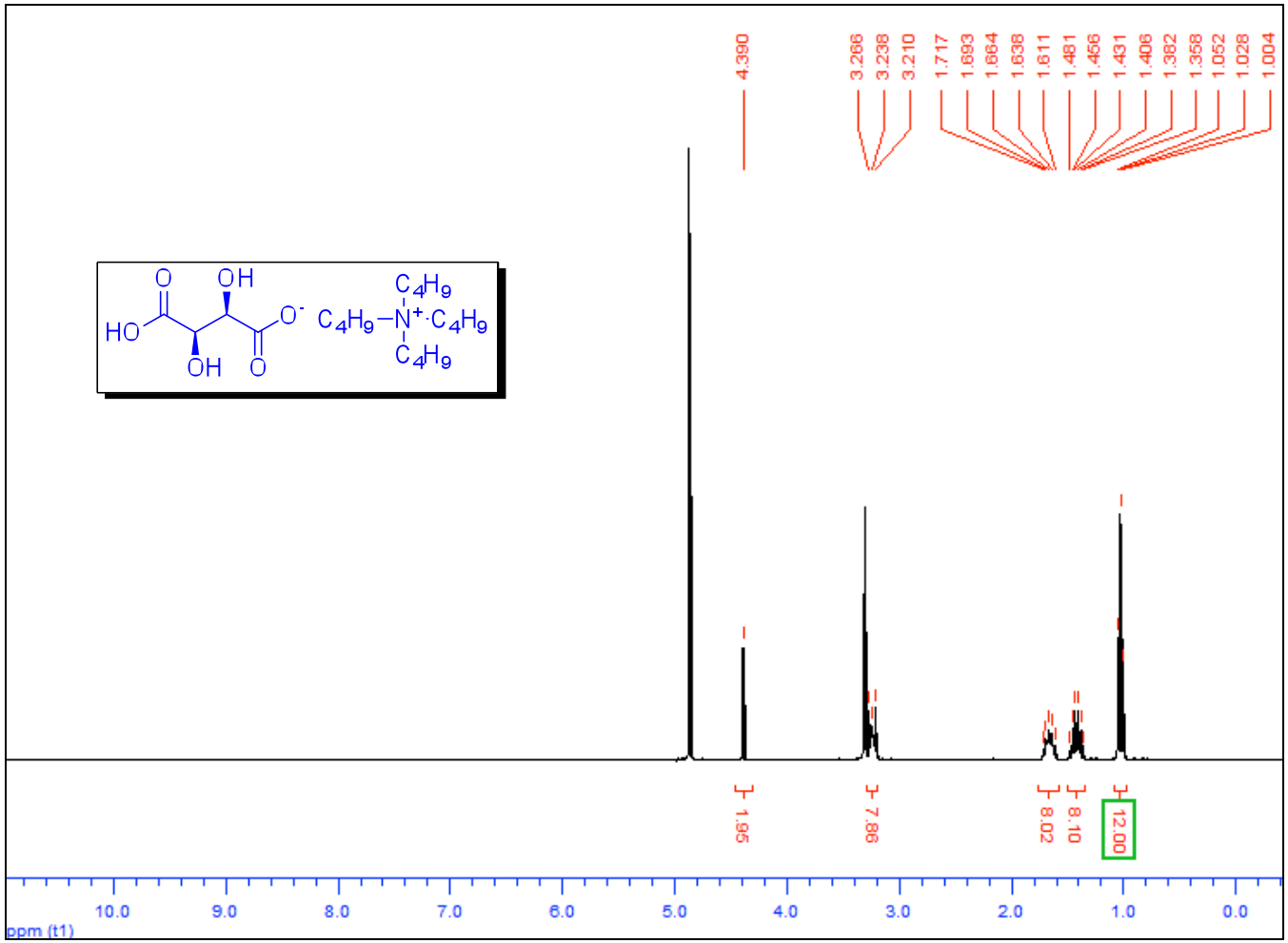
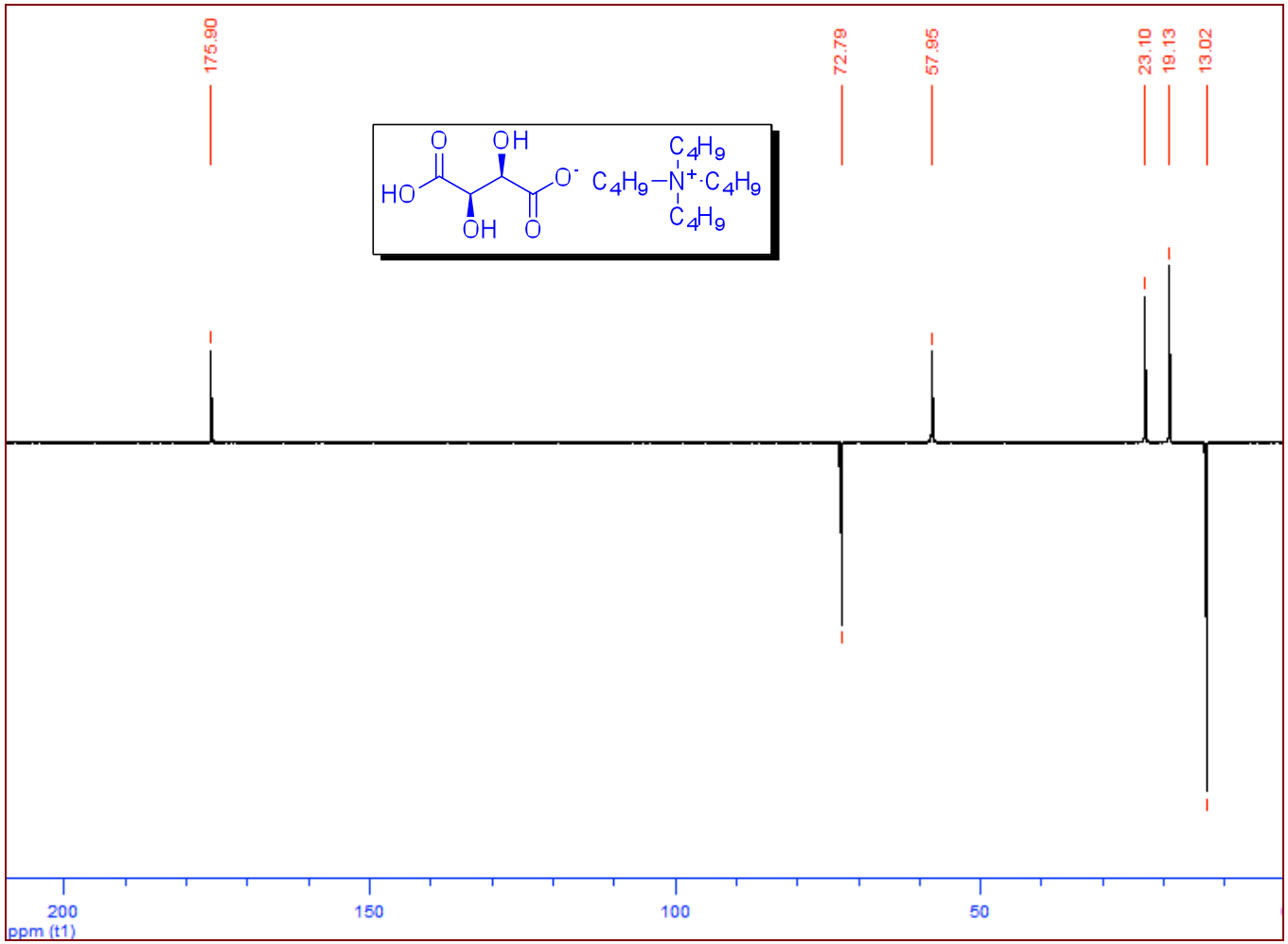
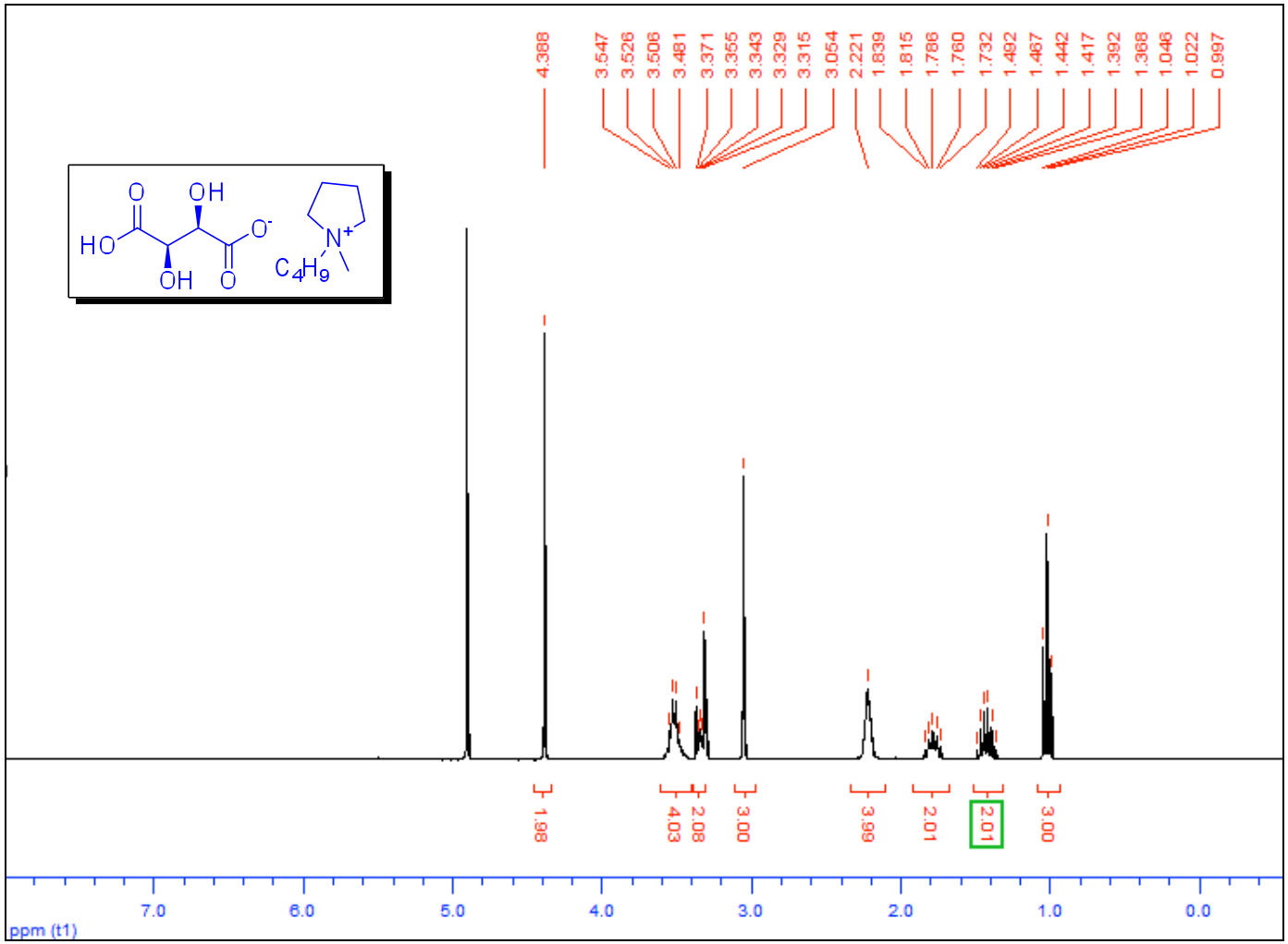


^{1}H-NMR (300 MHz, CD_3OD) spectrum of [TBA]D-HTart



^{13}C-NMR (75 MHz, D_2O) spectrum of [TBA]D-HTart



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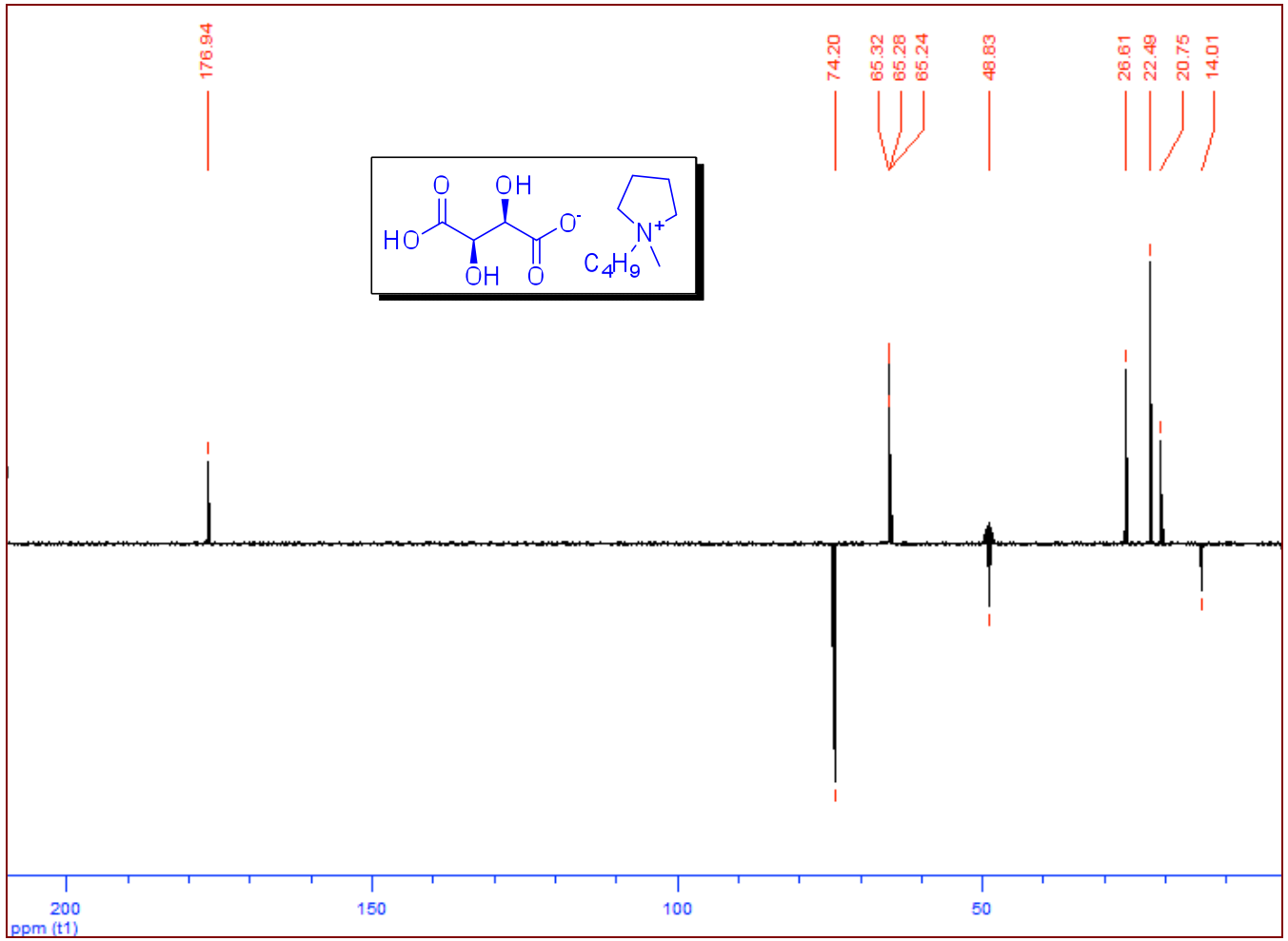

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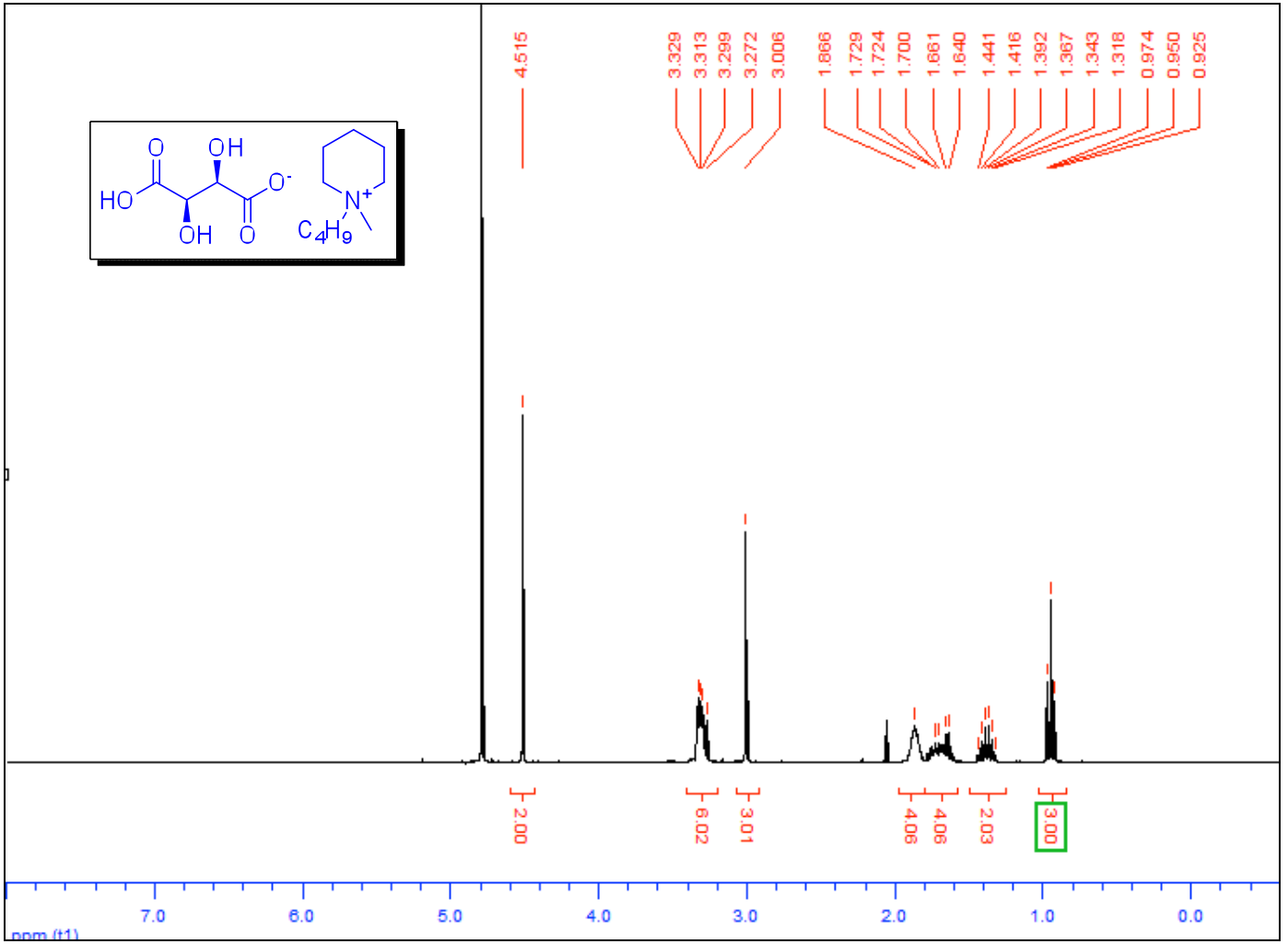

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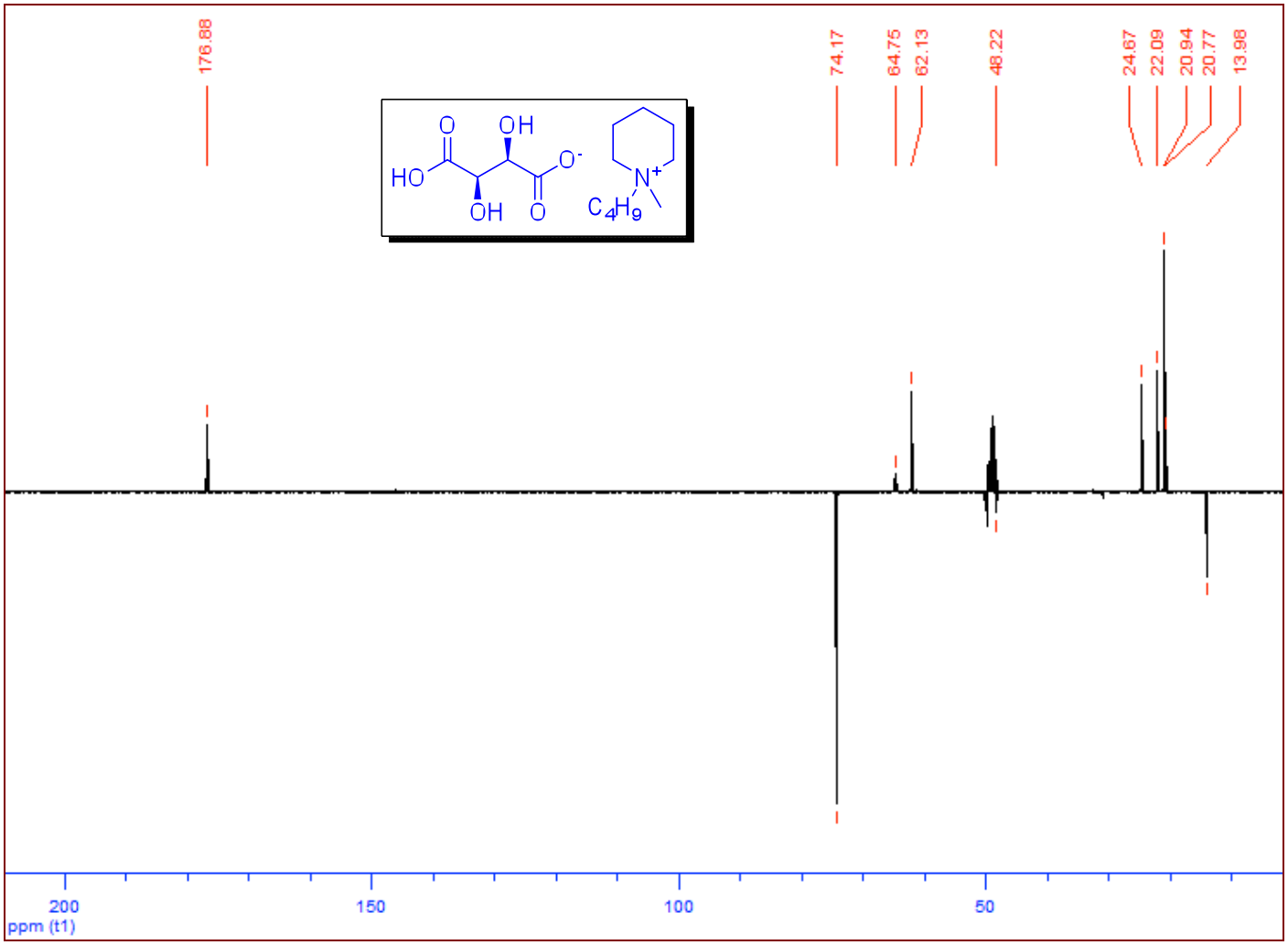

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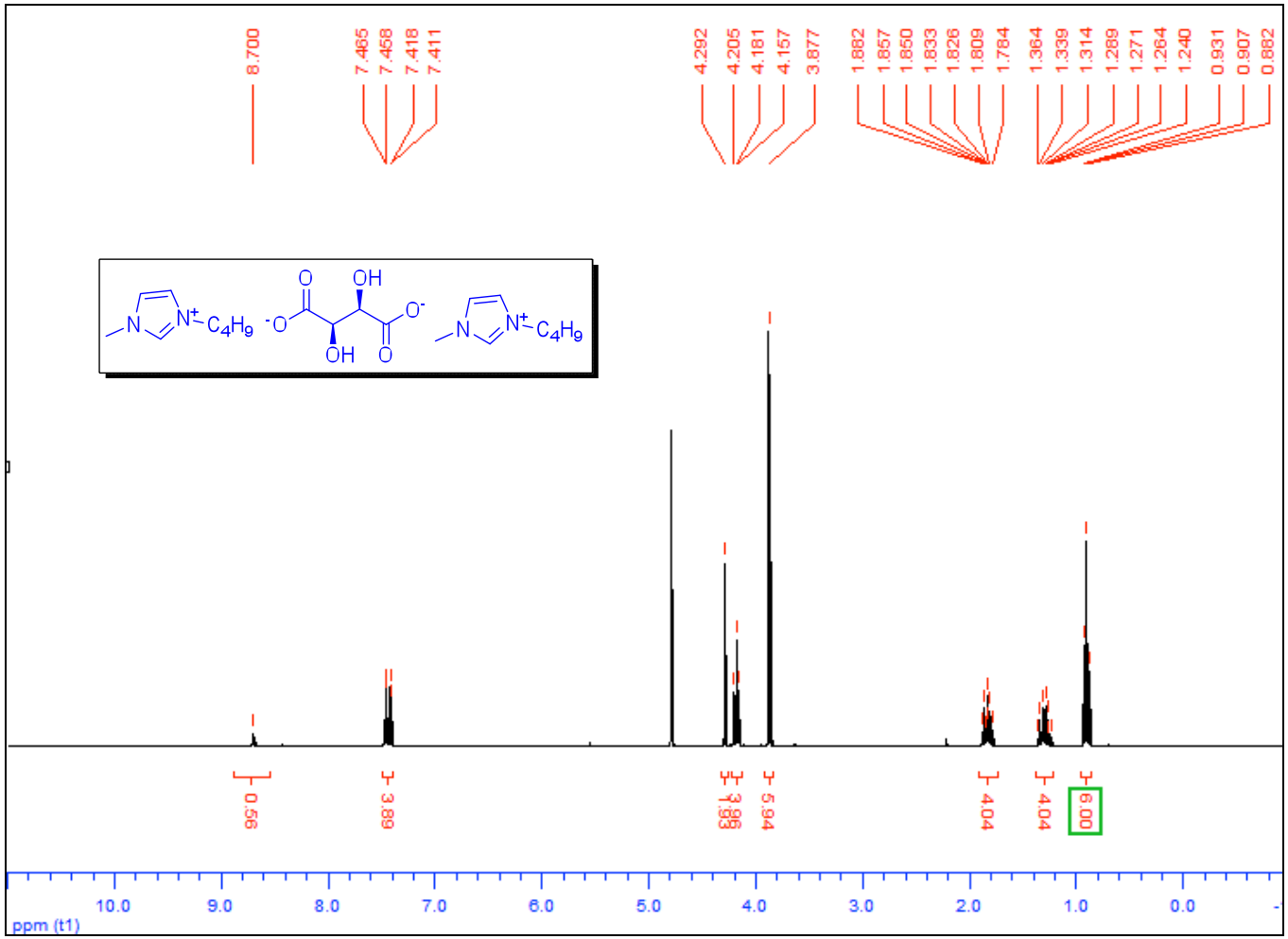
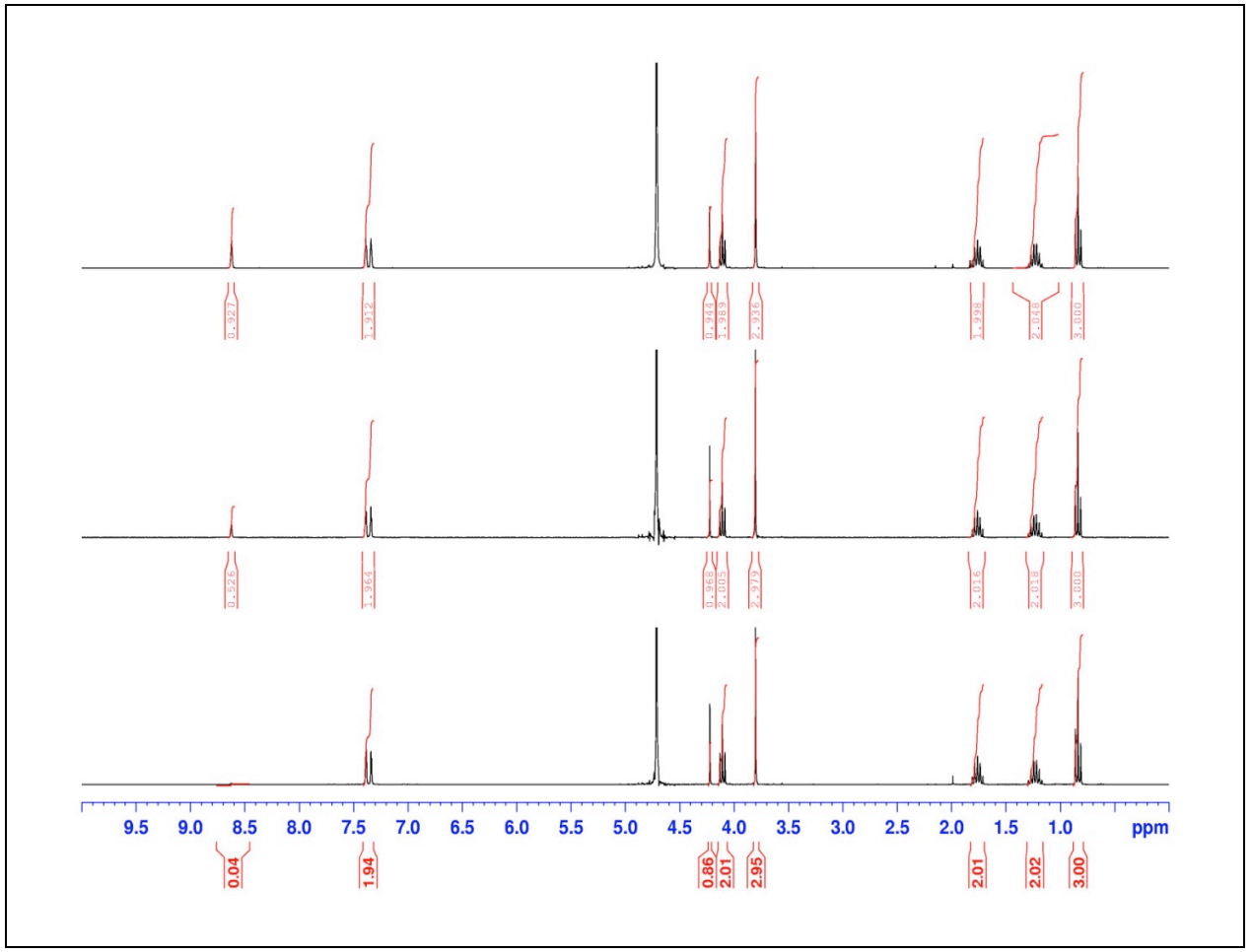
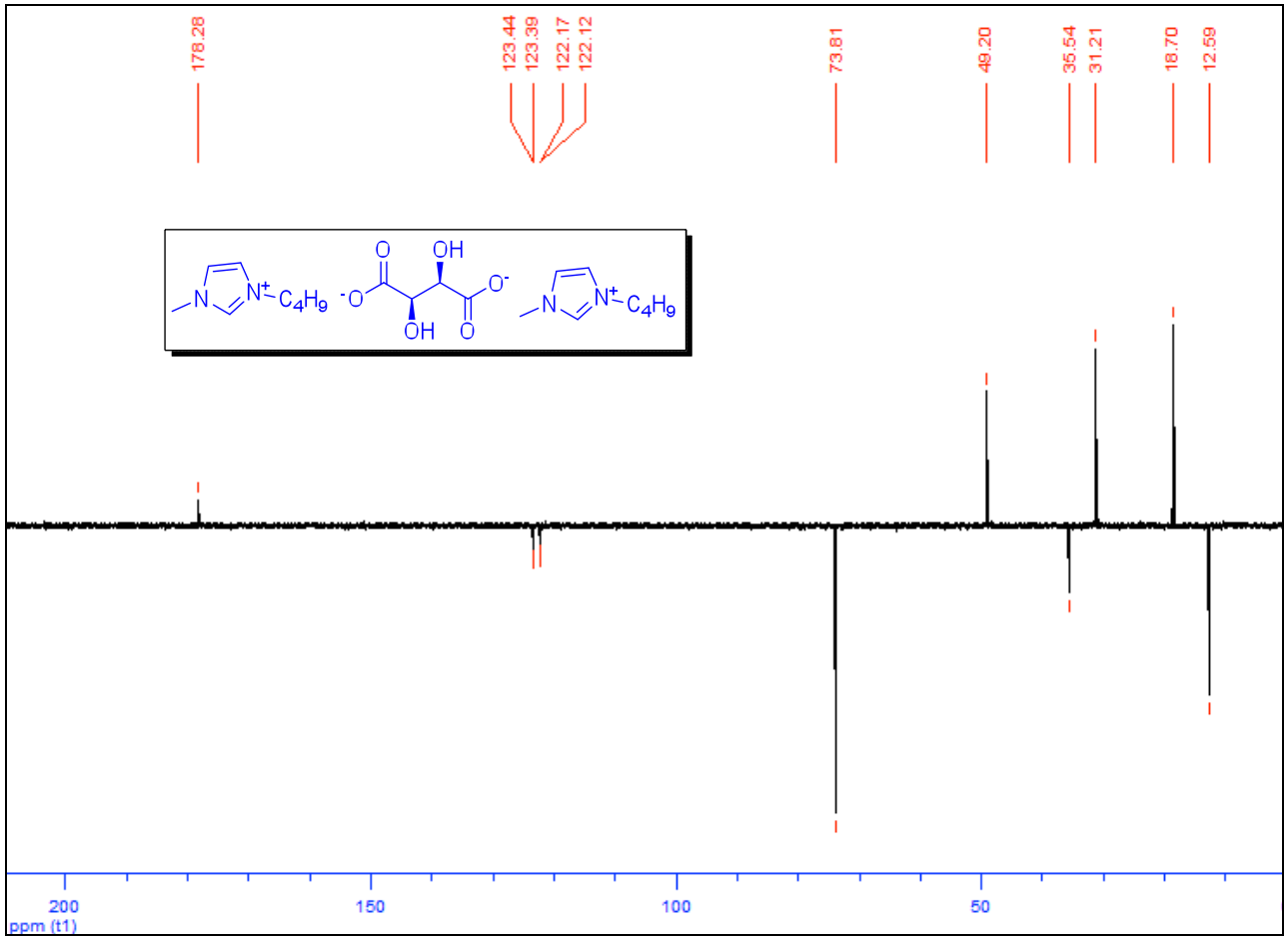


^{1}H-NMR (300 MHz, D_2O) spectrum of $[Bmim]_2$D-Tart

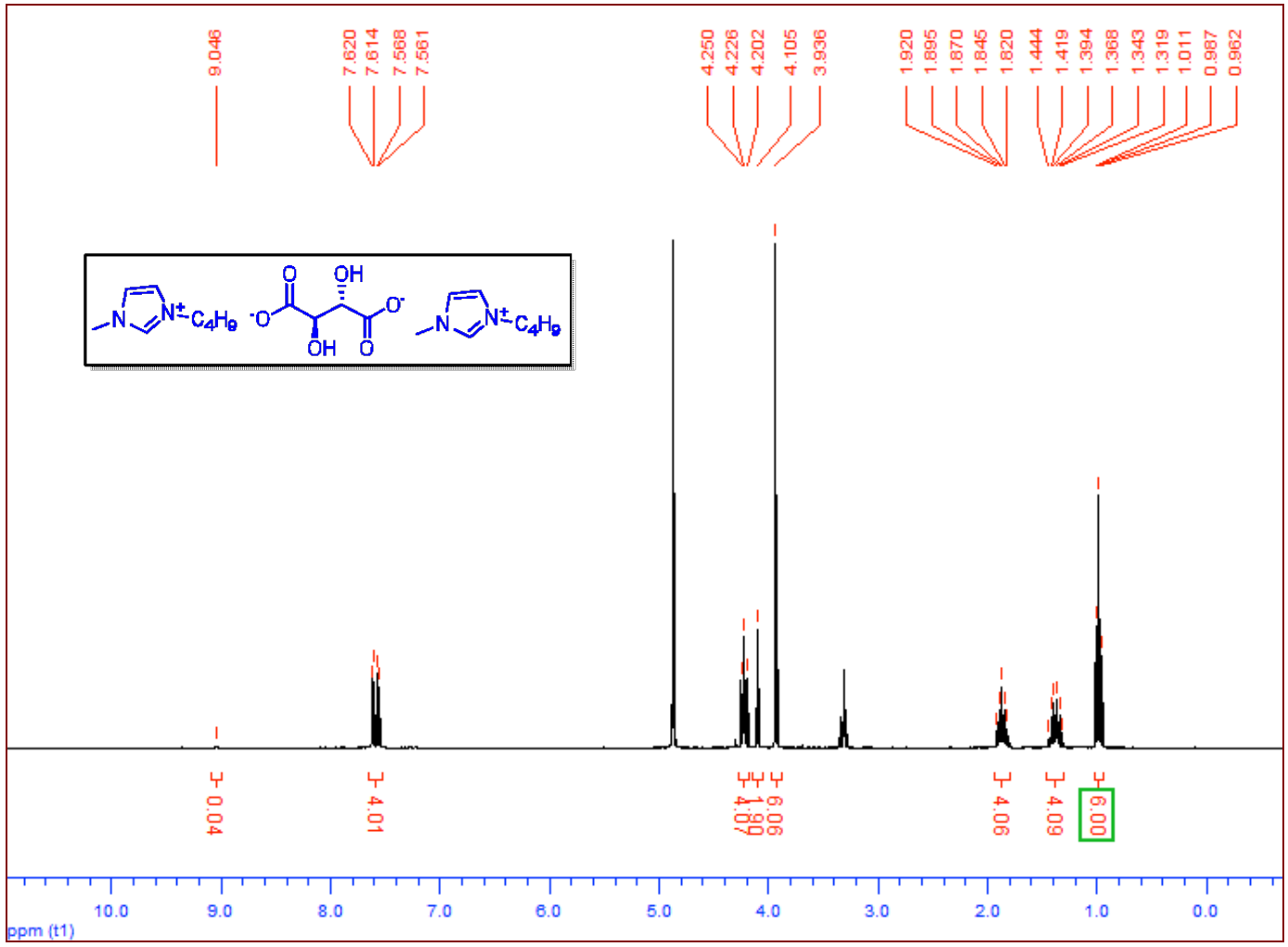


^{1}H-NMR (300 MHz, D_2O) spectra of $[Bmim]_2$D-Tart

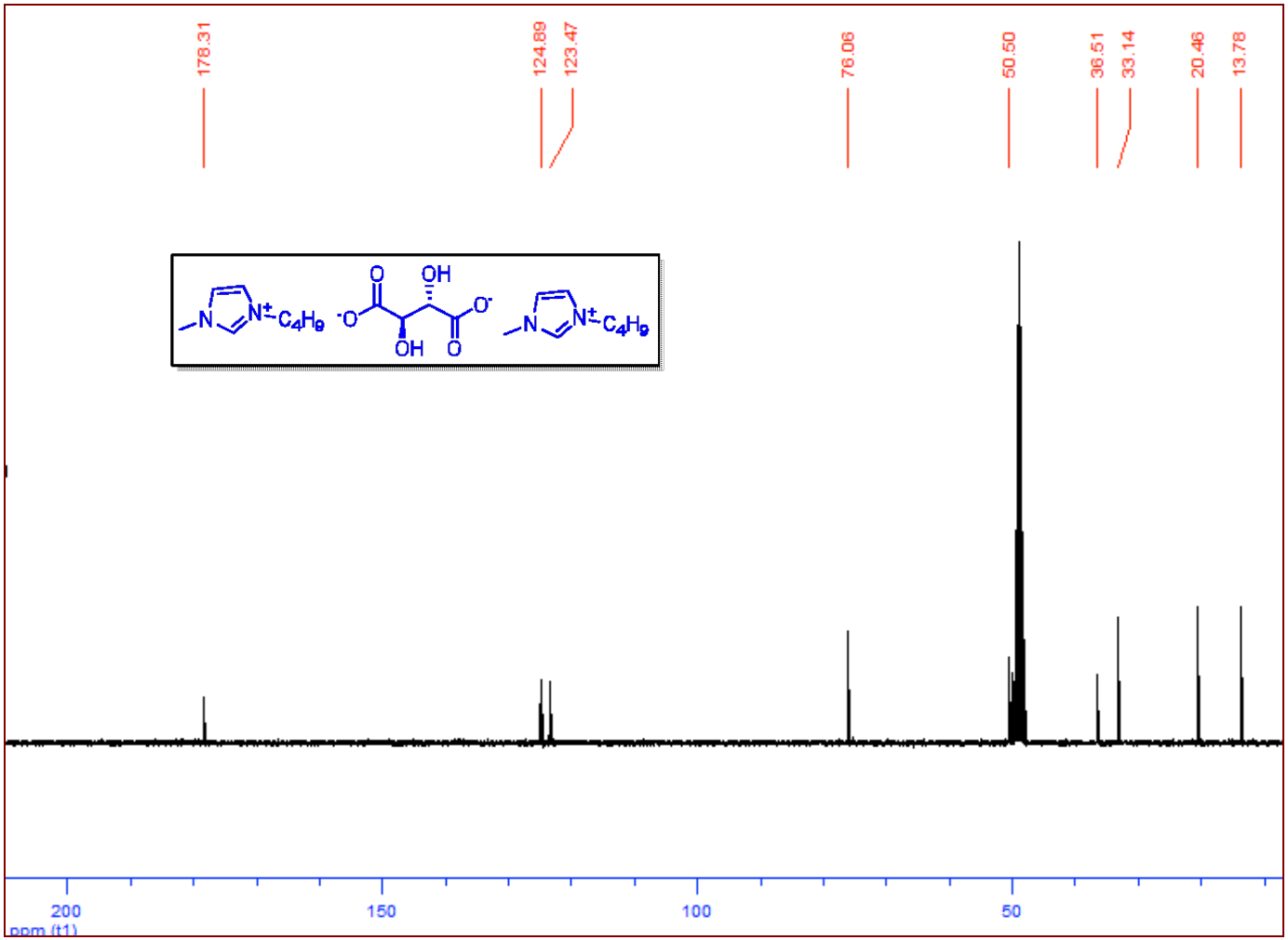
(showing variable extents of deuteration of the C-2 position)



^{13}C-NMR (75 MHz, D_2O) spectrum of $[Bmim]_2$D-Tart



^{1}H-NMR (300 MHz, CD_3OD) spectrum of [Bmim]$_2$*meso*-Tart



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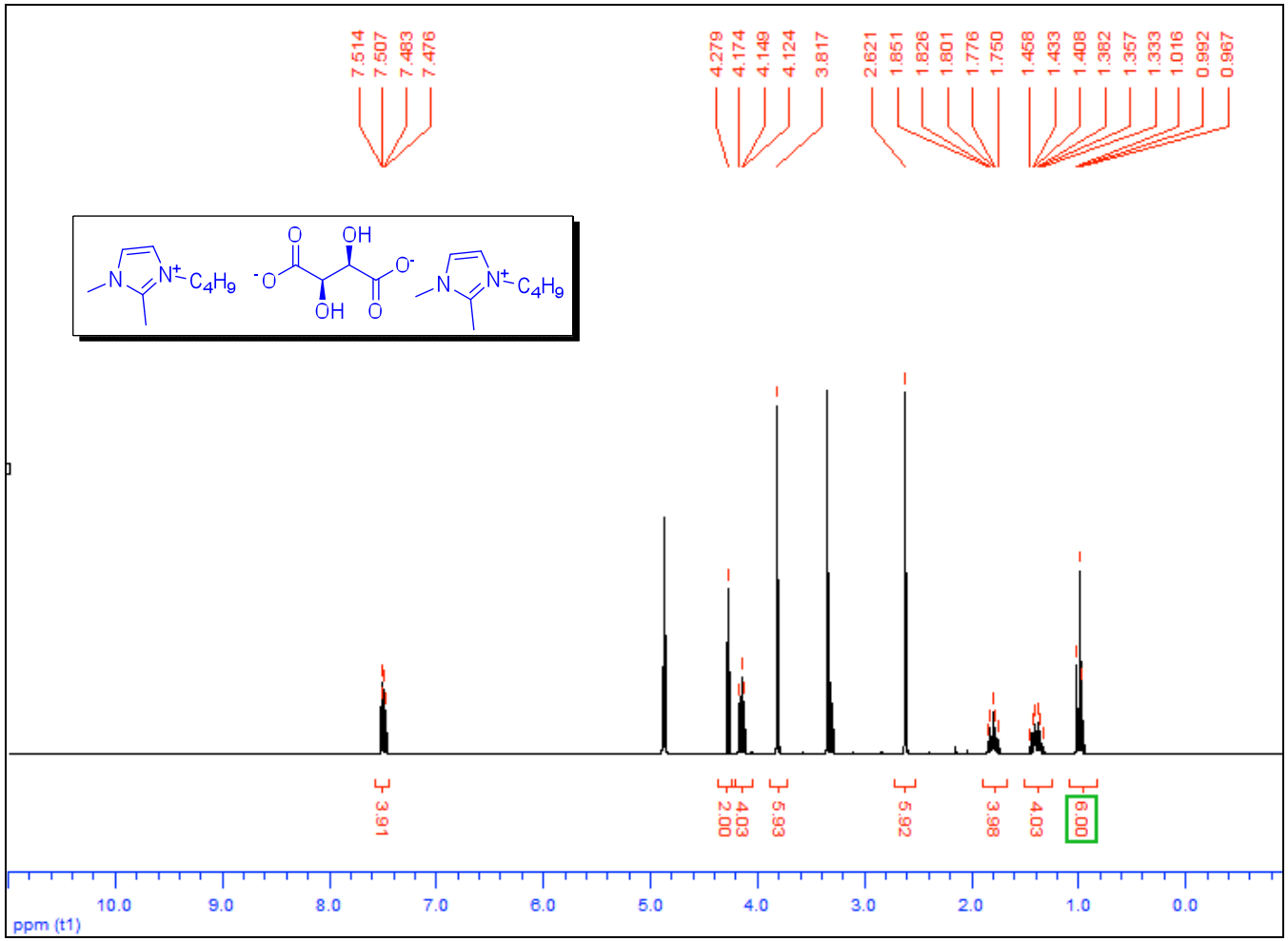

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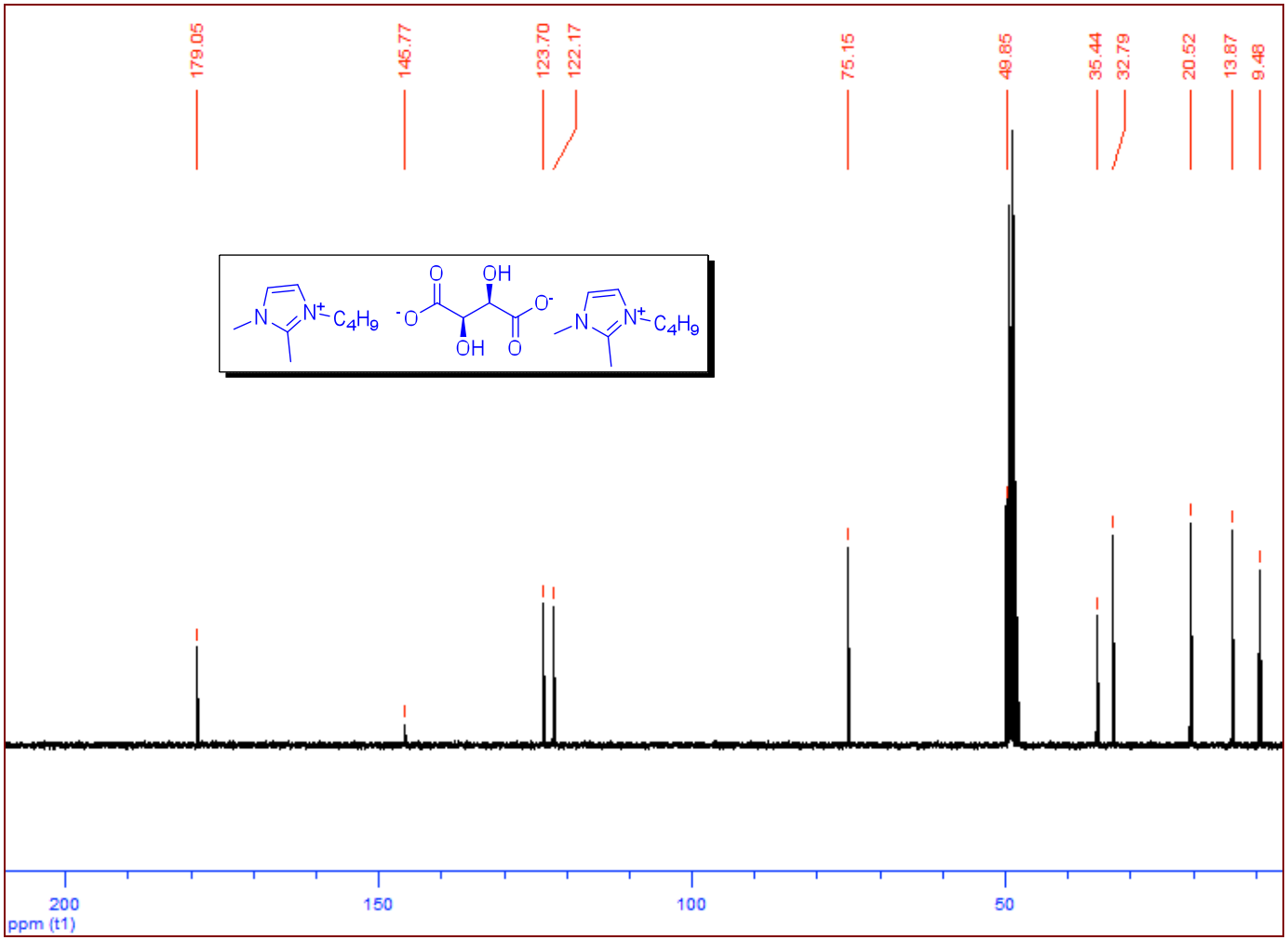
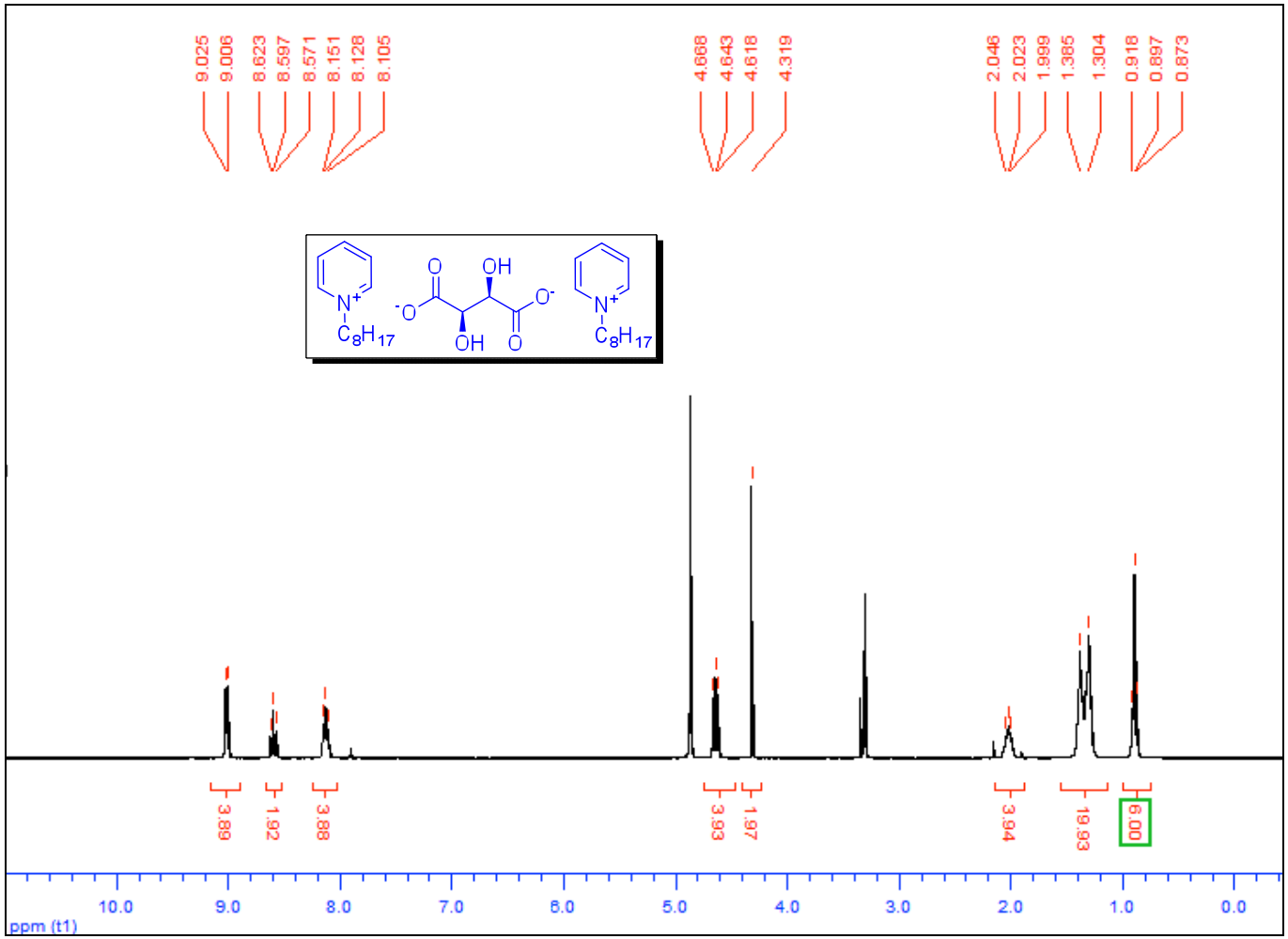


^{13}C-NMR (75 MHz, CD_3OD) spectrum of $[Bmmim]_2D$-Tart



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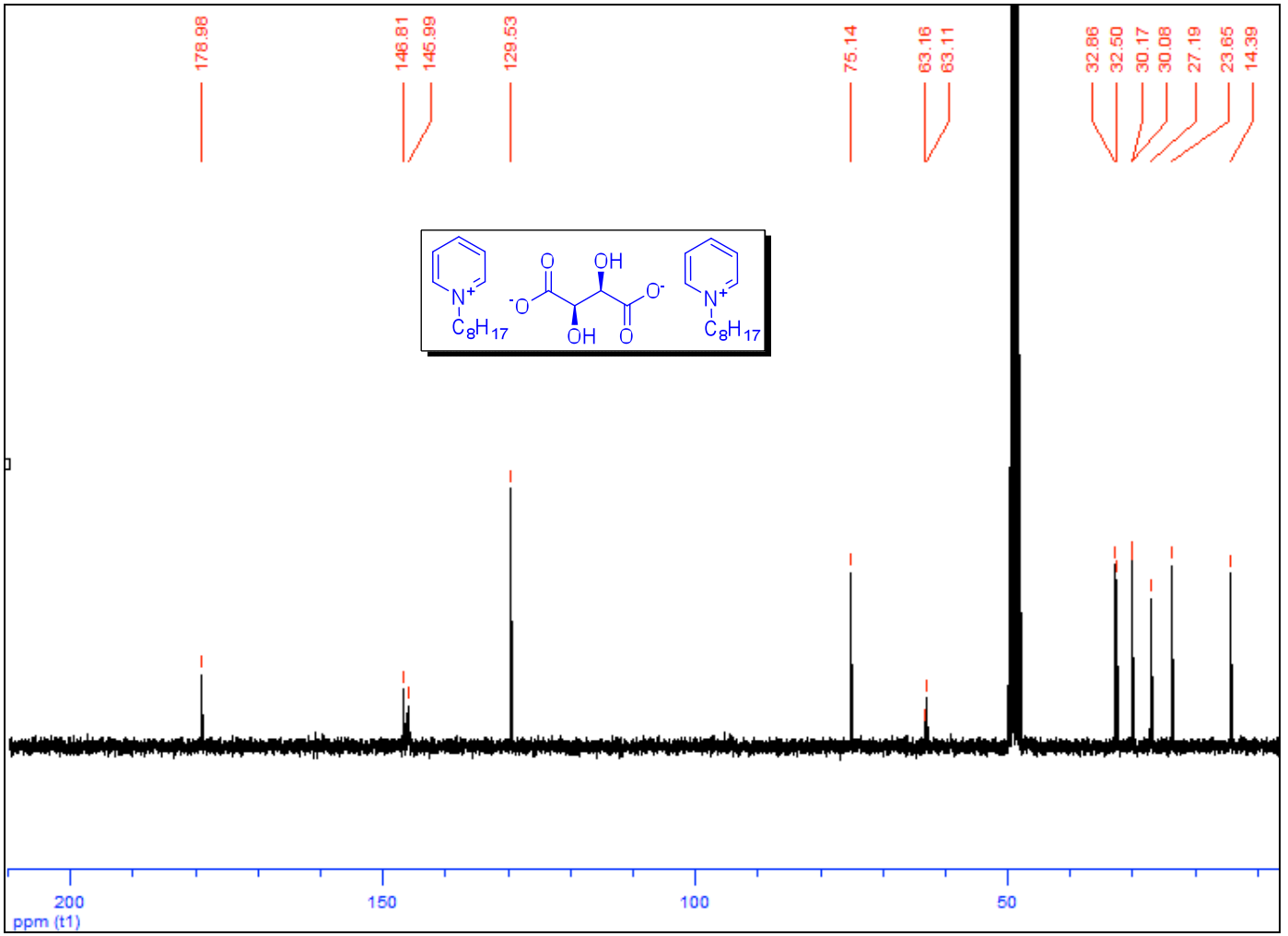
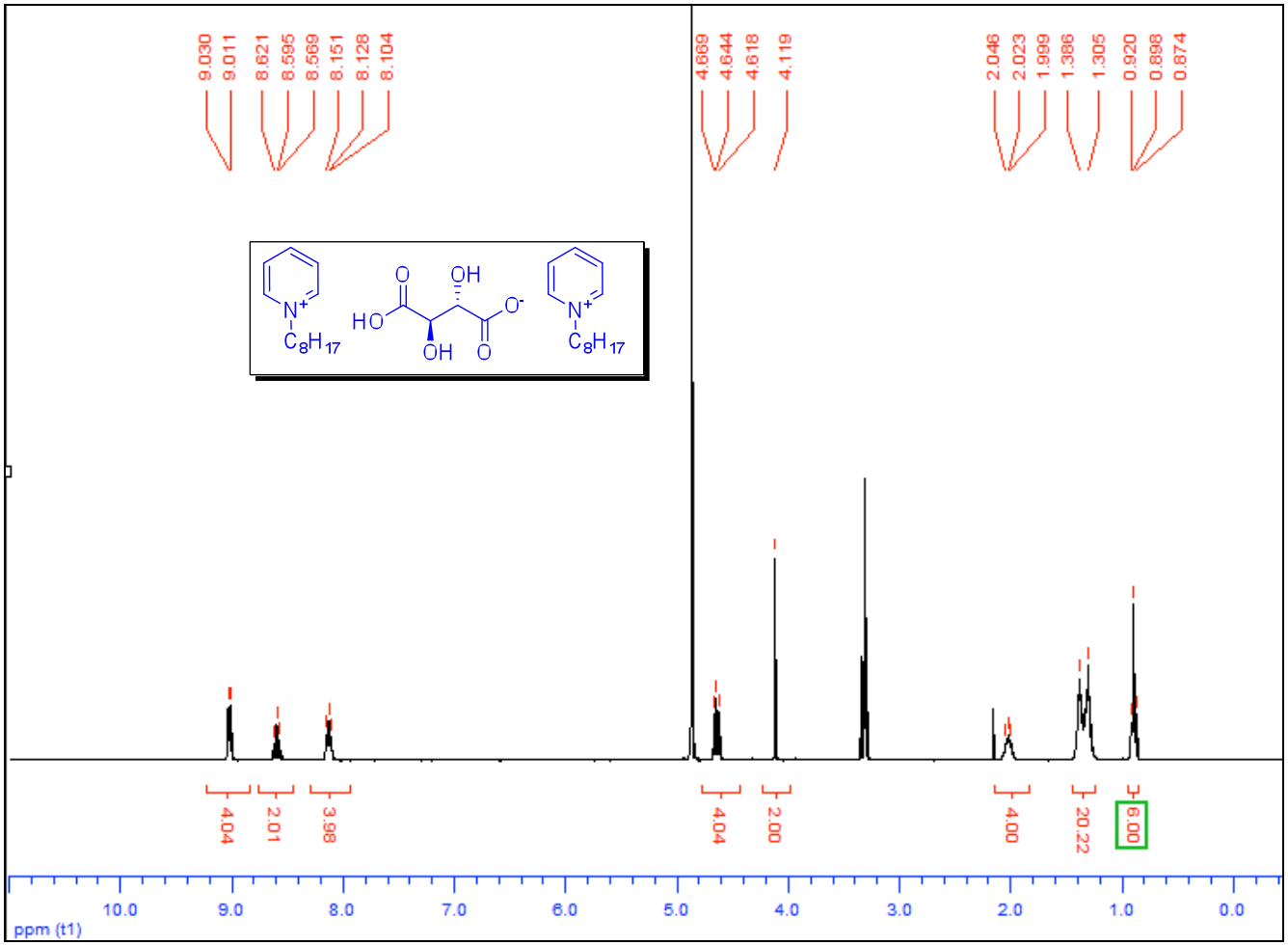
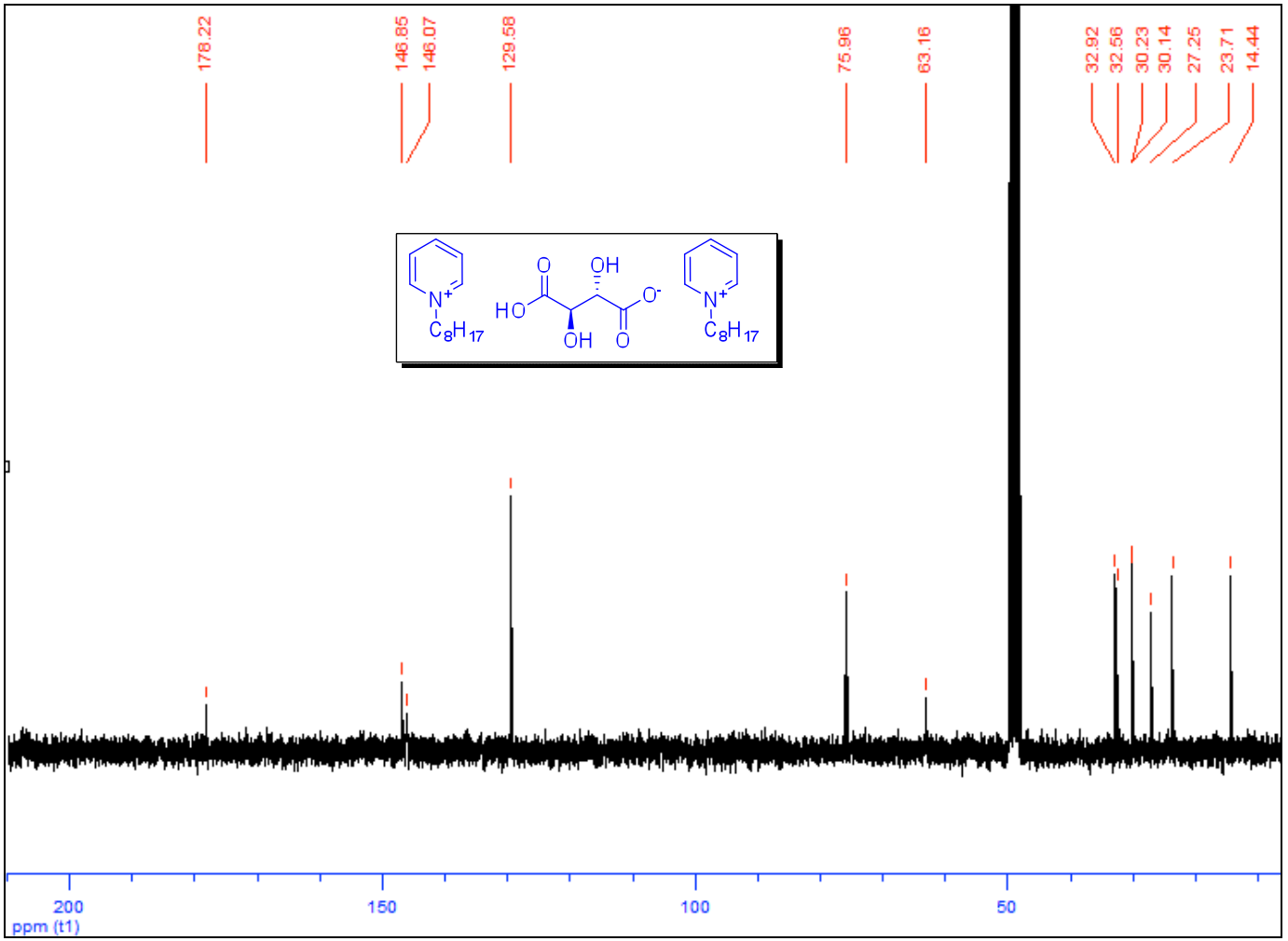


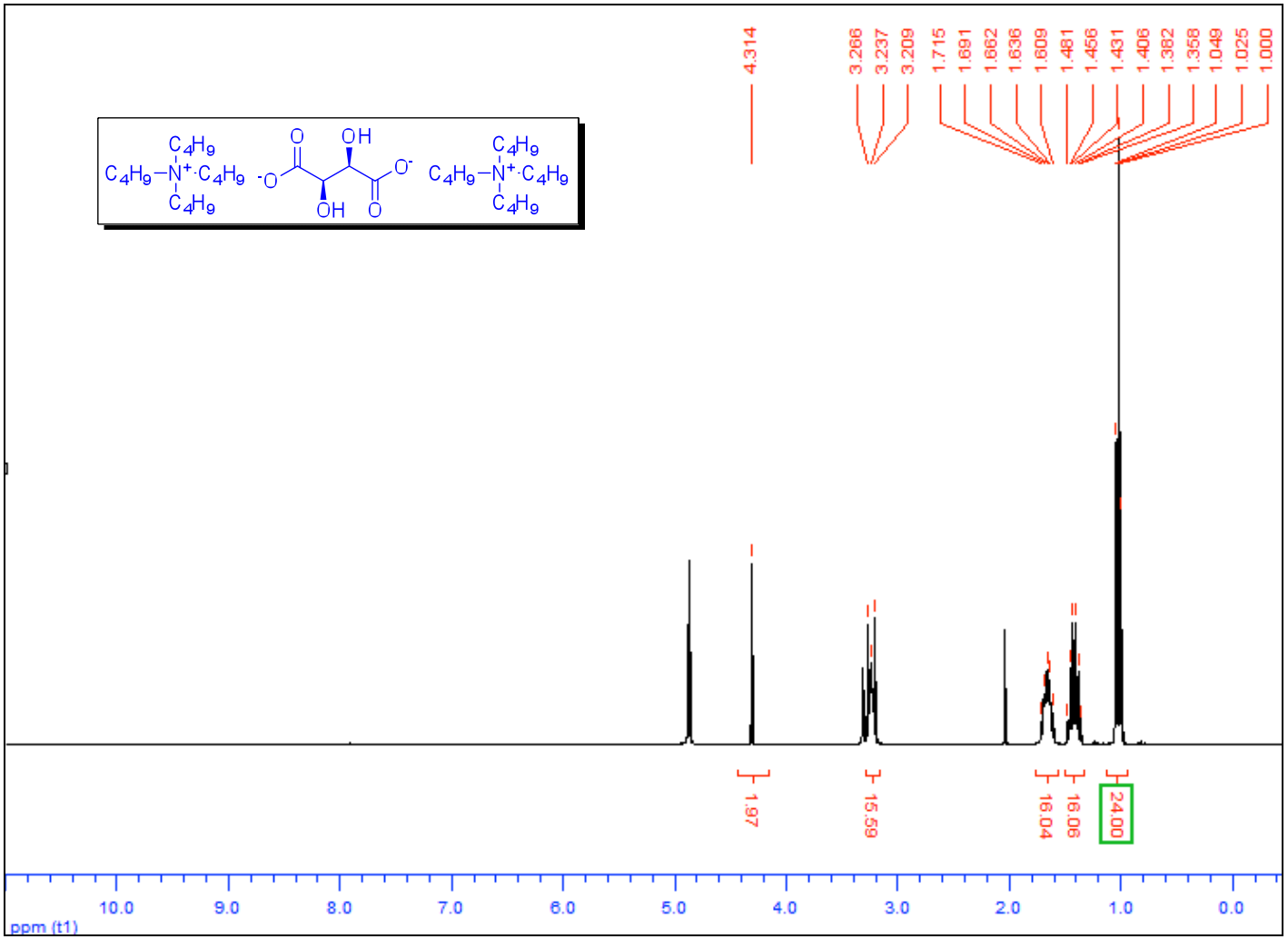
^{13}C-NMR (75 MHz, CD_3OD) spectrum of $[OctPyr]_2D$-Tart



^{1}H-NMR (300 MHz, CD_3OD) spectrum of $[OctPyr]_2$*meso*-Tart



^{13}C-NMR (75 MHz, CD_3OD) spectrum of [OctPyr]$_2$*meso*-Tart



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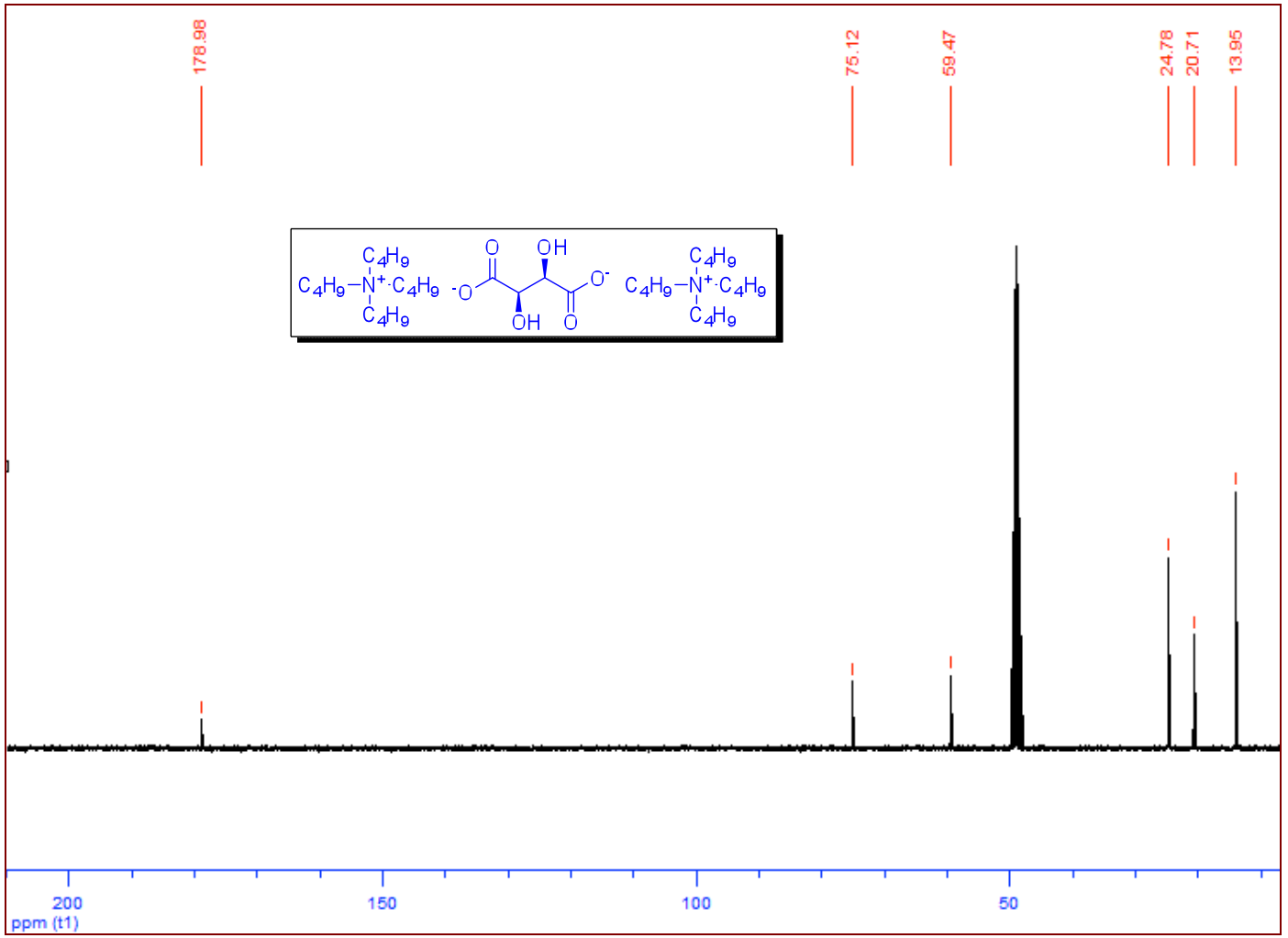

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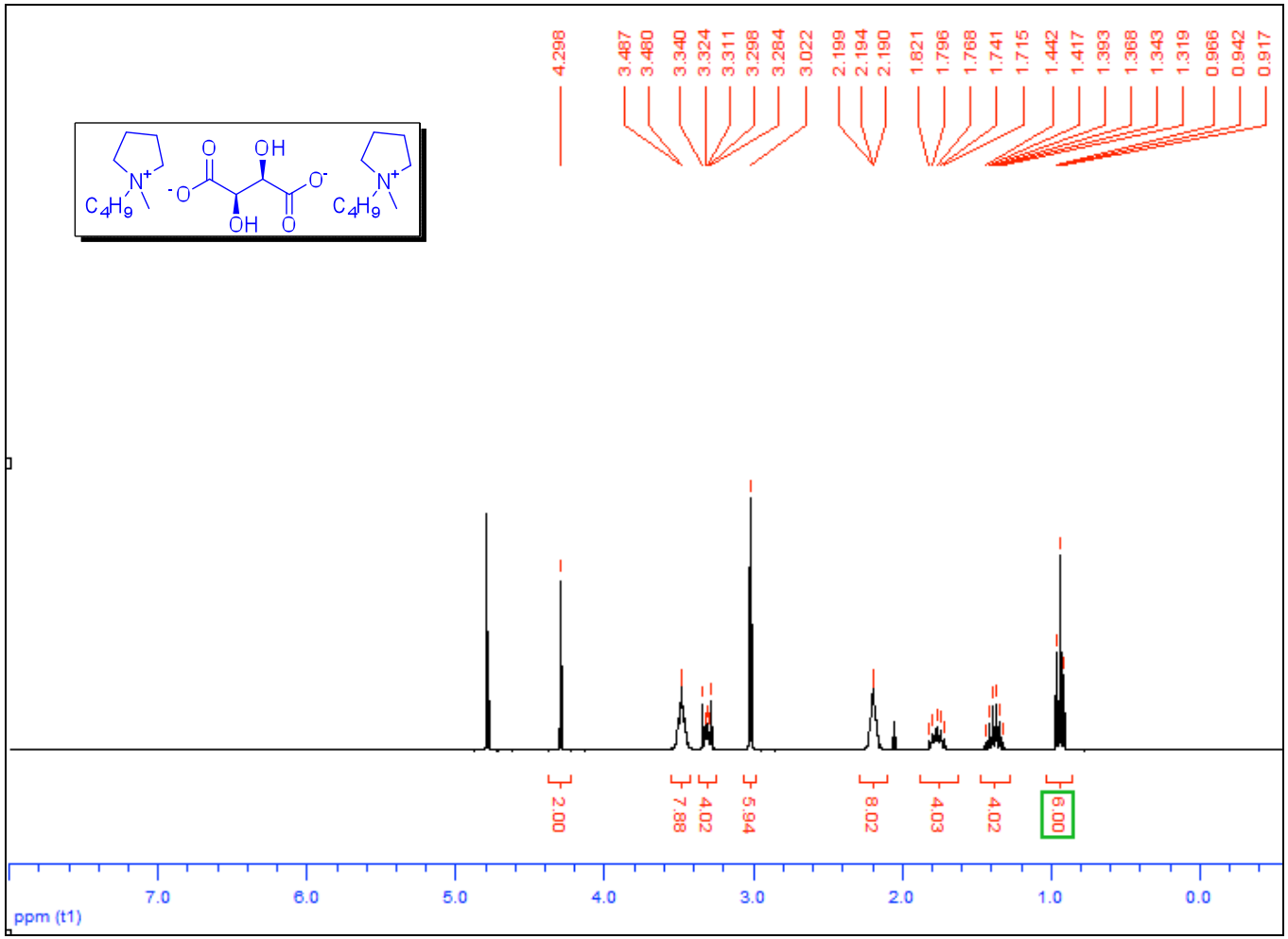

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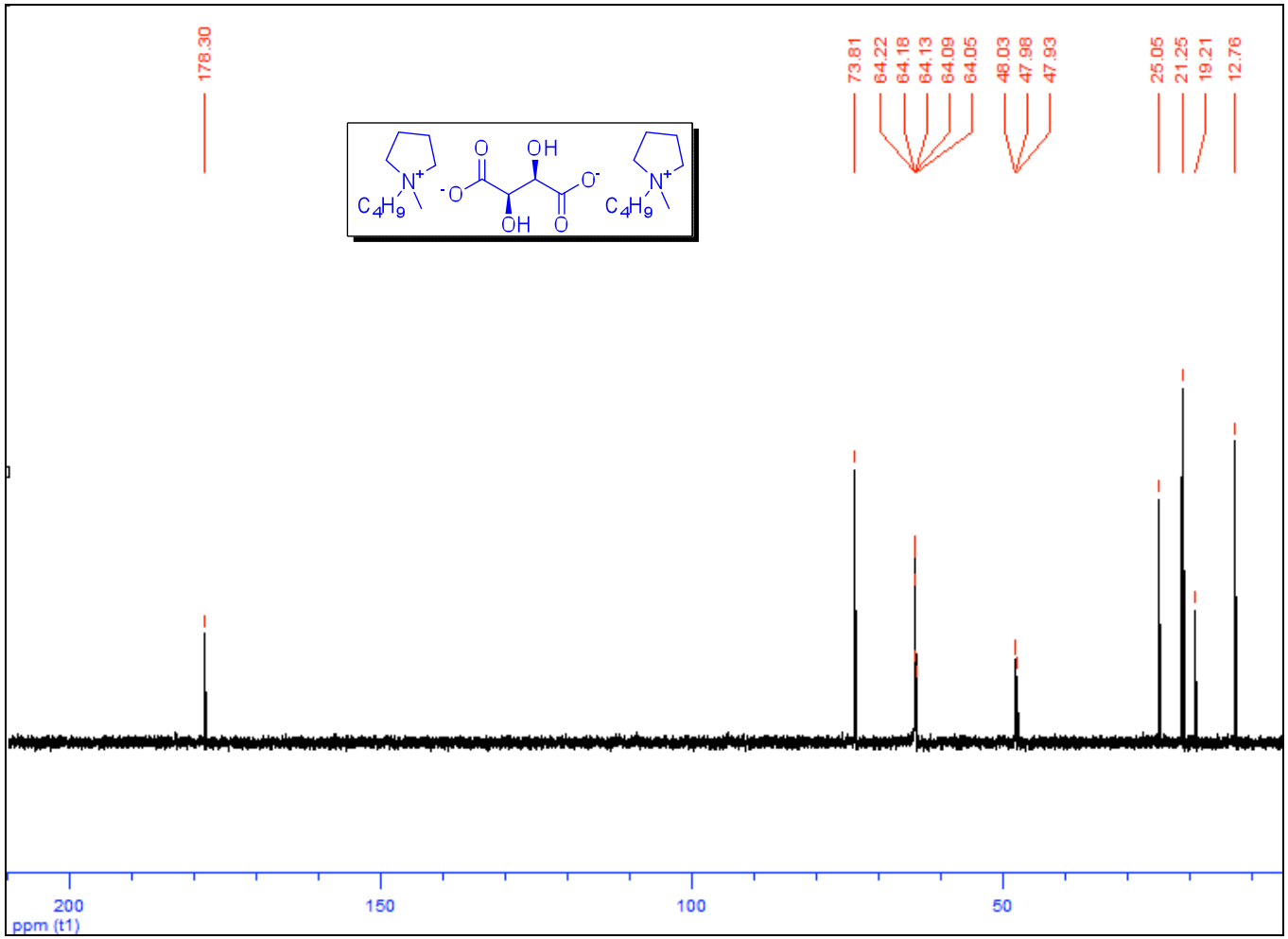
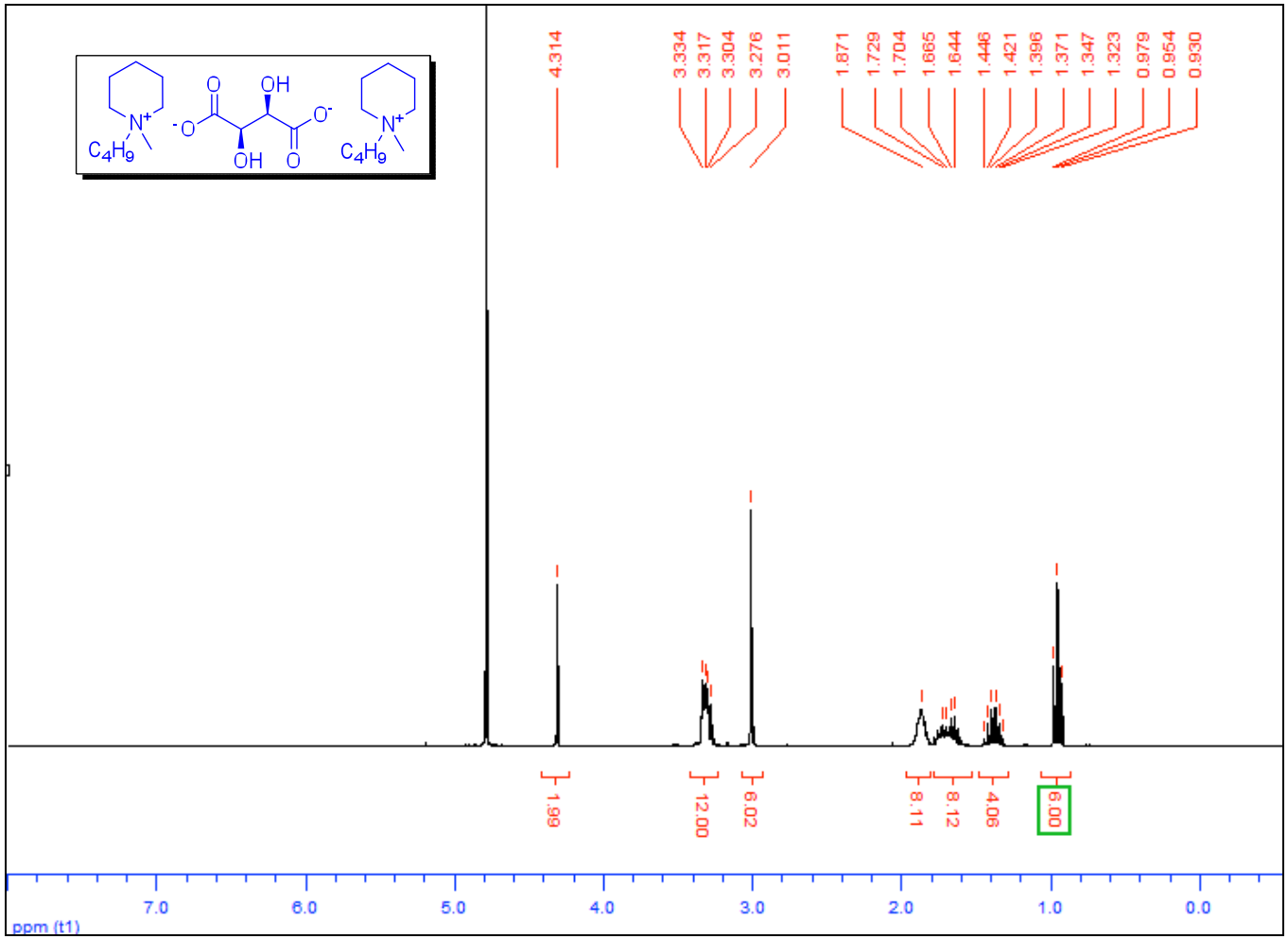


^{13}C-NMR (75 MHz, D_2O) spectrum of $[Bmpyr]_2$D-Tart



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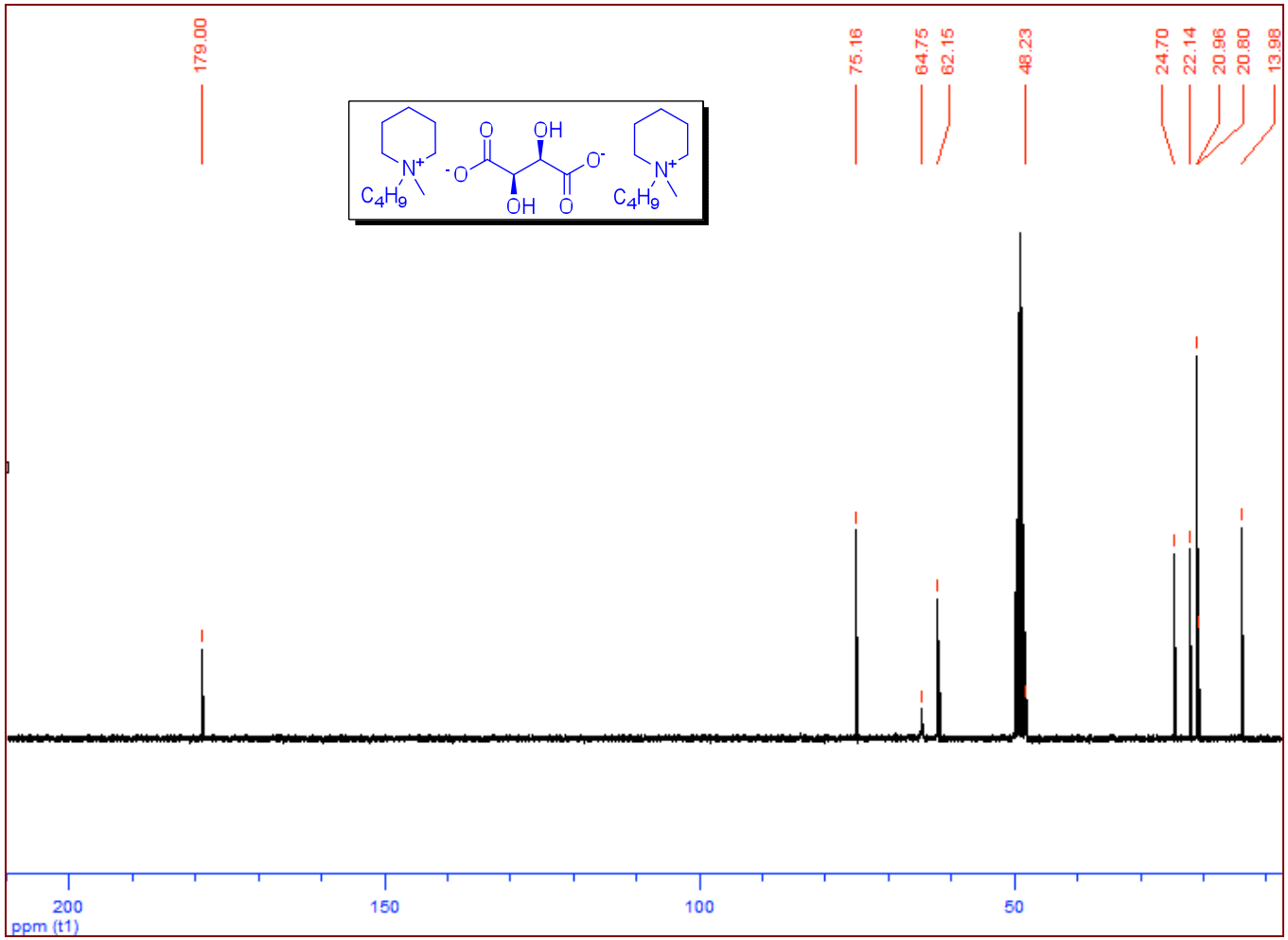

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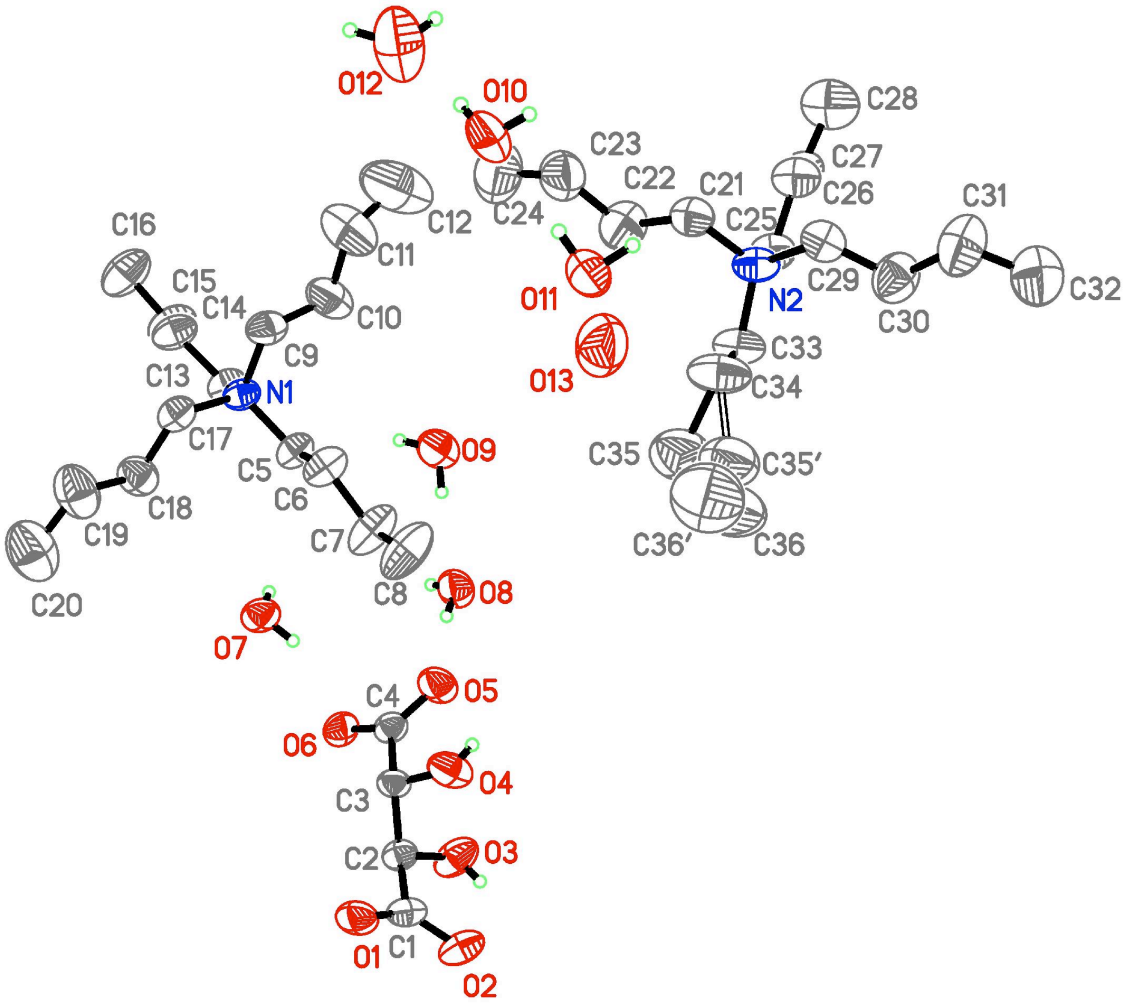

Molecular view of $[TBA]_2$L-Tart (+)-4b in the solid state (thermal ellipsoids at 50% probability)

Table 1. Crystal data and structure refinement for $[TBA]_2$L-Tart (+)-4b.

Identification code	tc83m	
Empirical formula	$C_{36}\ H_{90}\ N_2\ O_{13}$	
Formula weight	759.10	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 9.5730(5) Å	α= 90°.
	b = 15.2408(9) Å	β= 91.996(2)°.
	c = 16.3095(10) Å	γ = 90°.
Volume	2378.1(2) $Å^3$	
Z	2	
Density (calculated)	1.060 Mg/m^3	
Absorption coefficient	0.078 mm^{-1}	
F(000)	848	
Crystal size	0.60 x 0.10 x 0.10 mm^3	

Theta range for data collection	5.13 to 24.71°.
Index ranges	-11<=h<=11, -17<=k<=17, -19<=l<=19
Reflections collected	18337
Independent reflections	8021 [R(int) = 0.0338]
Completeness to theta = 24.71°	98.9 %
Max. and min. transmission	0.9922 and 0.9545
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8021 / 69 / 534
Goodness-of-fit on F^2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0625, wR2 = 0.1579
R indices (all data)	R1 = 0.0953, wR2 = 0.1808
Largest diff. peak and hole	0.388 and -0.224 e.$Å^{-3}$

Table 2. Hydrogen bonds for $[TBA]_2$L-Tart (+)-4b. [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3A)...O(2)	0.75(5)	2.05(5)	2.590(4)	129(5)
O(4)-H(4A)...O(5)	0.74(5)	2.10(5)	2.584(3)	124(5)
O(7)-H(7C)...O(6)	0.82(3)	2.03(3)	2.797(3)	156(4)
O(7)-H(7D)...O(1)#1	0.81(3)	1.93(3)	2.729(3)	169(4)
O(8)-H(8D)...O(5)	0.75(3)	2.02(3)	2.755(4)	168(6)
O(8)-H(8E)...O(2)#1	0.74(3)	2.04(3)	2.778(4)	174(5)
O(9)-H(9D)...O(8)	0.87(4)	2.00(4)	2.854(5)	166(5)
O(9)-H(9E)...O(4)#1	0.89(4)	2.11(4)	2.874(4)	143(4)
O(10)-H(10D)...O(12)	1.01(7)	1.80(7)	2.805(7)	168(5)

O(10)-H(10E)...O(7)#2	0.794(10)	1.940(18)	2.719(4)	166(6)
O(11)-H(11C)...O(10)	0.91(4)	2.24(5)	2.954(5)	135(5)
O(11)-H(11D)...O(6)#2	0.92(4)	1.81(4)	2.733(4)	174(5)
O(12)-H(12D)...O(13)#1	0.916(10)	1.75(3)	2.641(6)	163(8)
O(13)-H(13D)...O(11)	0.81(5)	2.18(6)	2.856(6)	142(7)
O(13)-H(13E)...O(1)#2	0.80(5)	1.95(5)	2.750(5)	173(7)

Symmetry transformations used to generate equivalent atoms: #1 x-1,y,z #2 x,y+1,z