

Name:	IsoMetronidazole-D4 Hydrochloride
Lot#:	GR-9-163-1
Test Date:	01/22/2020 (re-test date:01/22/2025)
CAS No.:	705-19-1 (free base unlabelled)
MF:	C ₆ H ₆ D ₄ ClN ₃ O ₃
MW:	211.64
Appearance:	Off-White Solid
Purity:	95.7% by HPLC; 99.3% atom D
¹H-NMR:	Conforms
MS-ESI (+)	Conforms (shows peak at m/z = 175.09 [M _(free base) +H] ⁺)

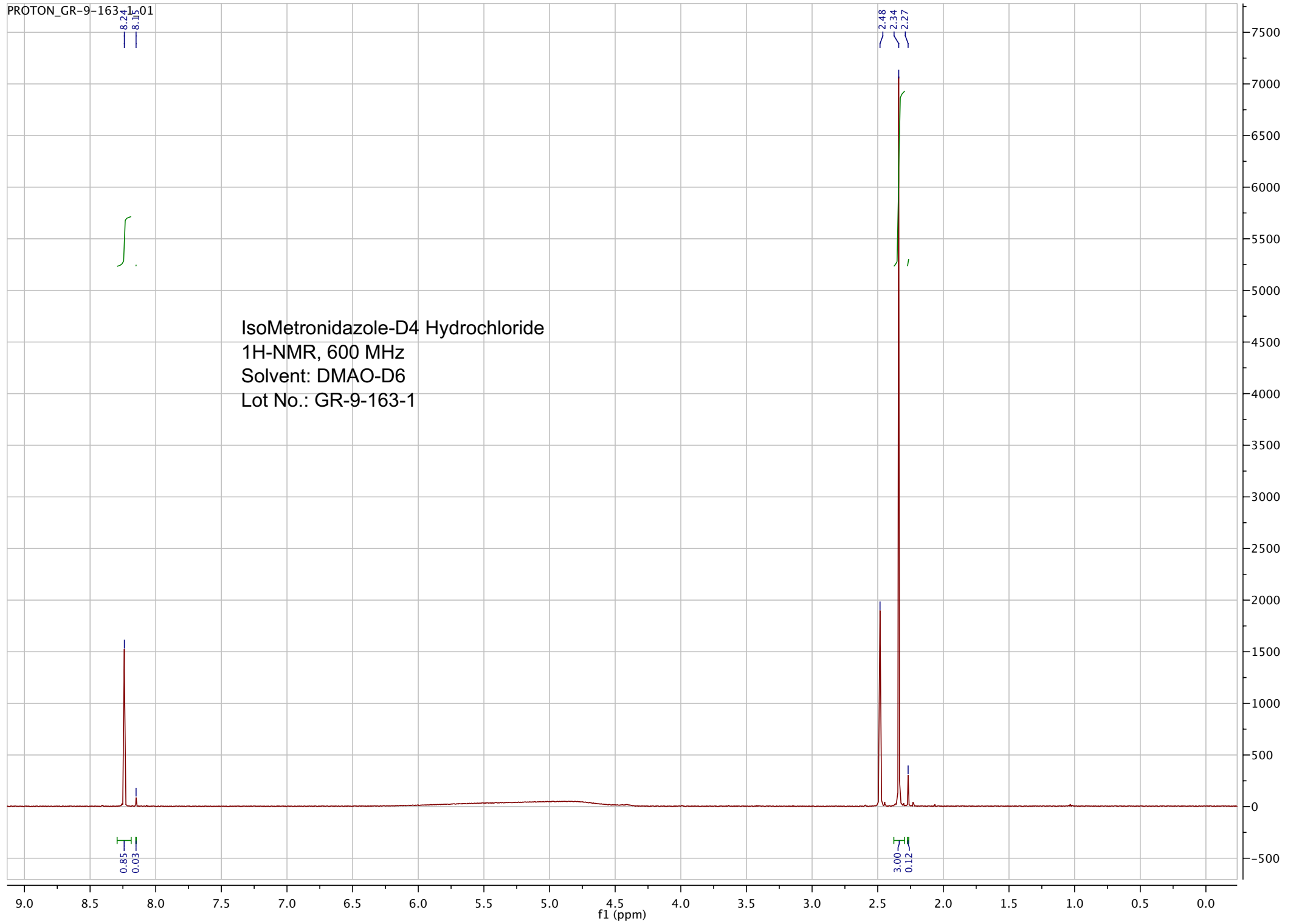
Approved by:

Date: 01/24/2020



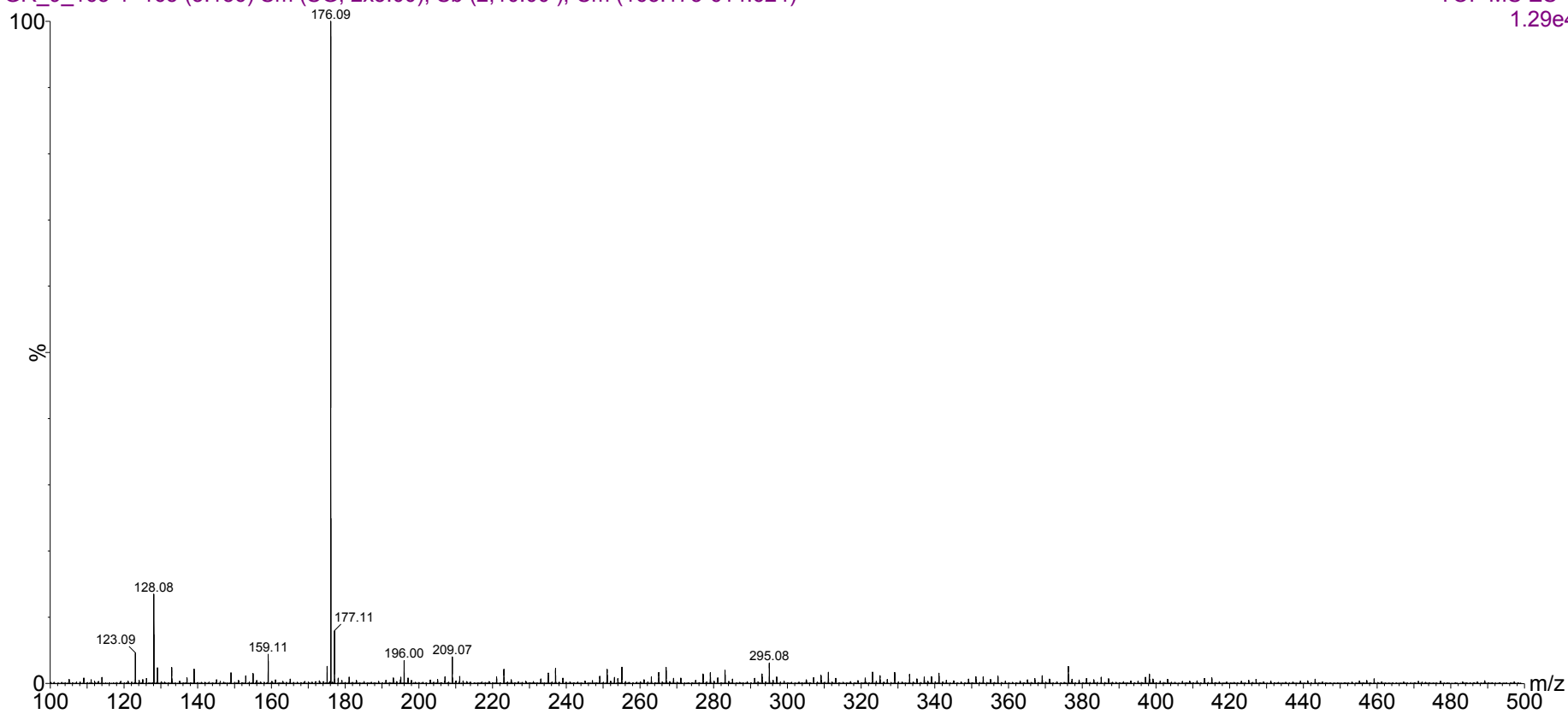
Viorica Rusu, QC/QA Manager

IsoMetronidazole-D4 Hydrochloride
1H-NMR, 600 MHz
Solvent: DMAO-D6
Lot No.: GR-9-163-1



GR_9_163-1 165 (3.156) Sm (SG, 2x5.00); Sb (2,10.00); Cm (163:173-614:624)

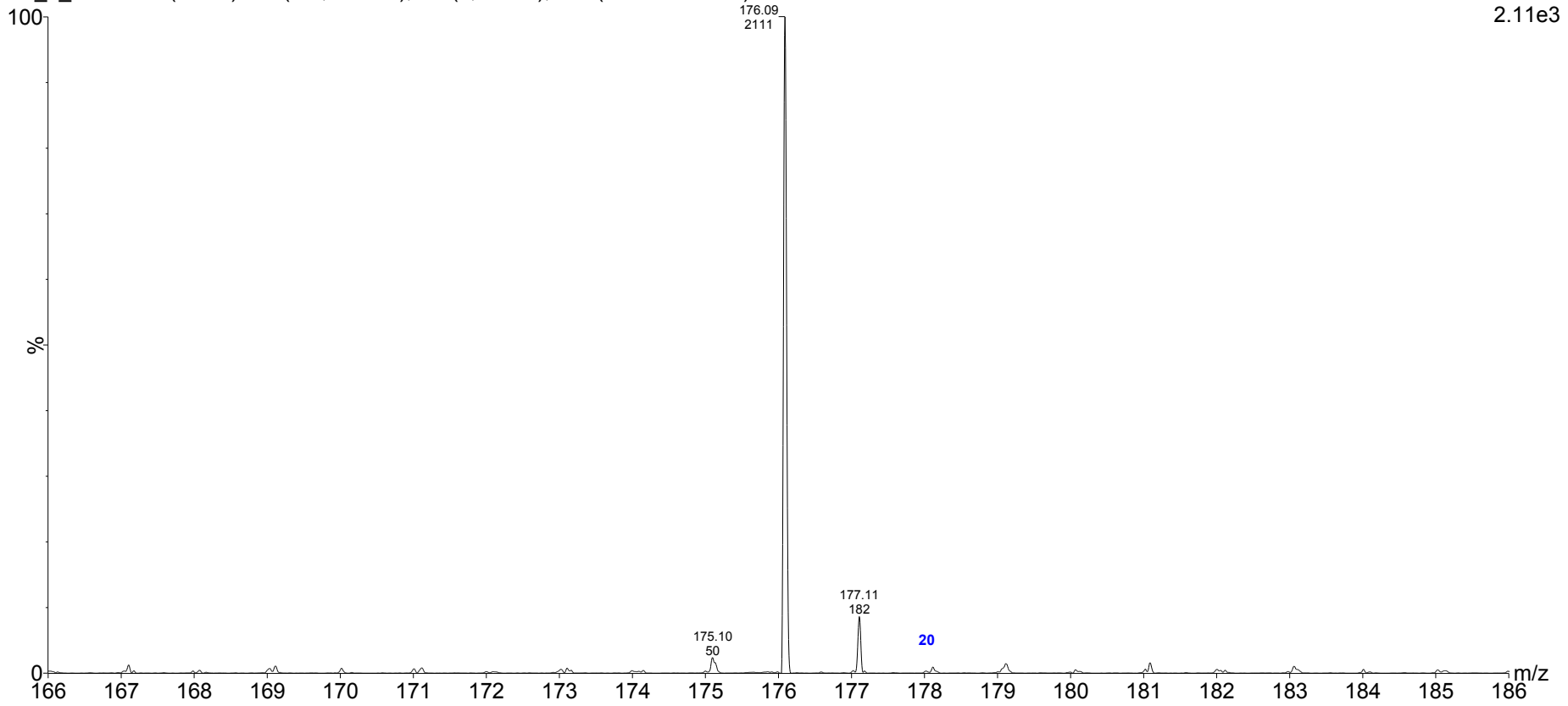
TOF MS ES+
1.29e4



Raw ESI-MS spectrum for sample GR-9-163-1. Shows monoisotopic $[M+H]^+$ mass.

GR_9_163-1 32 (0.613) Sm (SG, 2x5.00); Sb (2,10.00); Cm (31:32-8x2.000)

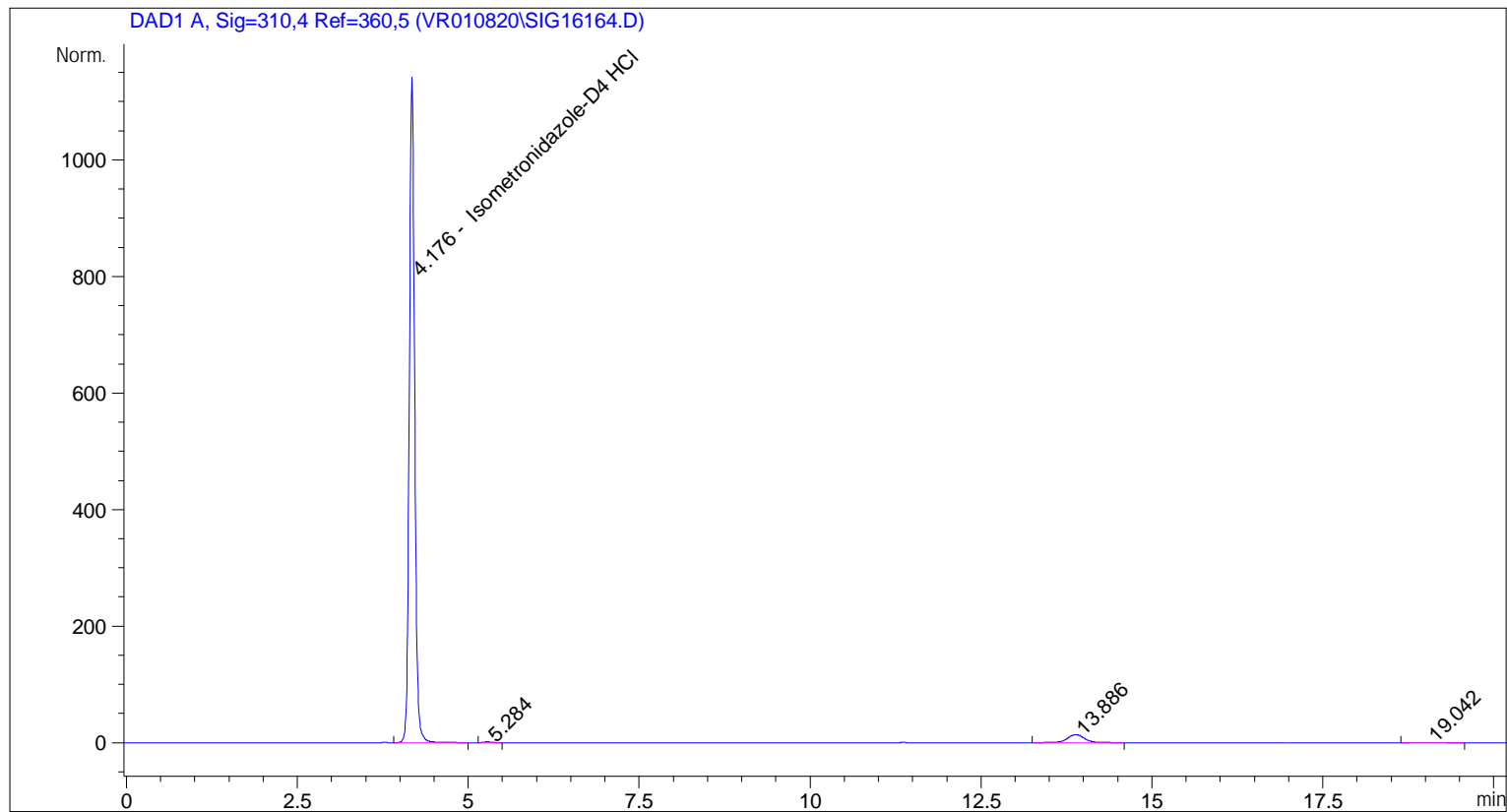
TOF MS ES+
2.11e3



Expansion of above with intensity labels.

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Acq. Operator   : vrusu
Acq. Instrument : Instrument 1                Location : Vial 22
Injection Date  : 1/22/2020 1:00:05 PM
                                           Inj Volume : 5.0 µl
Acq. Method     : C:\CHEM32\1\METHODS\VR012220_163-1.M
Last changed    : 1/22/2020 12:59:02 PM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR012420_163-1PM.M
Last changed    : 1/24/2020 11:38:17 AM by vrusu
  
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 Area Percent Report
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Sorted By       : Signal
Calib. Data Modified : 1/24/2020 11:36:32 AM
Multiplier:     : 1.0000
Dilution:       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
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Signal 1: DAD1 A, Sig=310,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	4.176	BB	0.0835	6236.51807	95.7117	Isometronidazole-D4 HCl
2	5.284	BB	0.1073	9.45320	0.1451	?
3	13.886	BB	0.2658	246.91811	3.7894	?
4	19.042	BB	0.2664	23.05422	0.3538	?

Totals : 6515.94359

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*** End of Report ***