

Agilent QTOF 7200

Mass Spectrometer Operators: Moya McCarron and Jean Ellis.

Room B21, Donnan Laboratories Basement

Tel: 0151 794 3609

e-mail: moy@liv.ac.uk

jmelis@liv.ac.uk

Sample Supplied By: N. PERRI

Date Run: 14/12/15

Sample Reference: NESI 2PH2OH

Sample Run By: M.M.

Log Book No: 2015-12-14-C745

Inlet

☒ Solids Probe

☐ GC-MS

Polarity

☒ Positive

☐ Negative

Analysis Type

☐ Nominal Mass Low resolution

☒ Accurate Mass High resolution

Ionisation Mode

☐ EI Electron Ionisation

☒ CI Chemical Ionisation

CI Gas

☐ Ammonia

☒ Methane

☐ Iso Butane

Operator Comments :

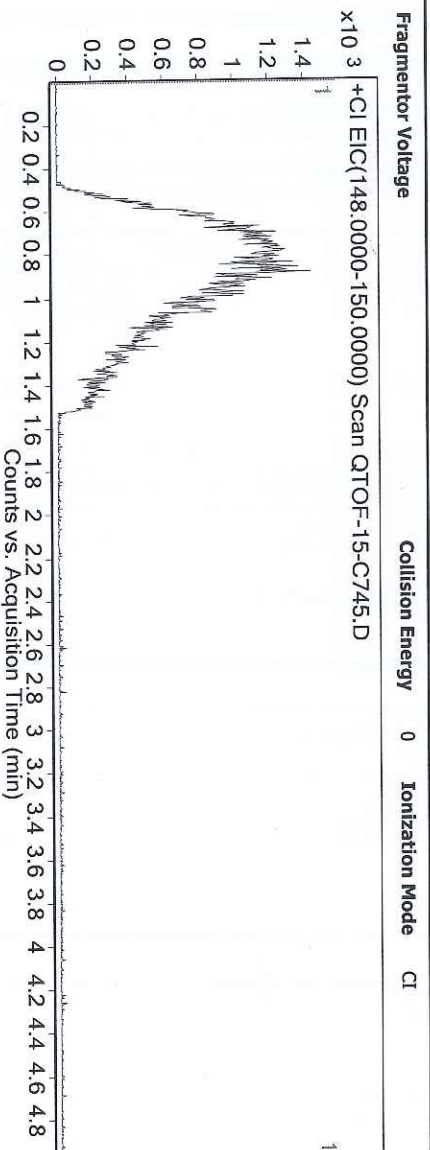
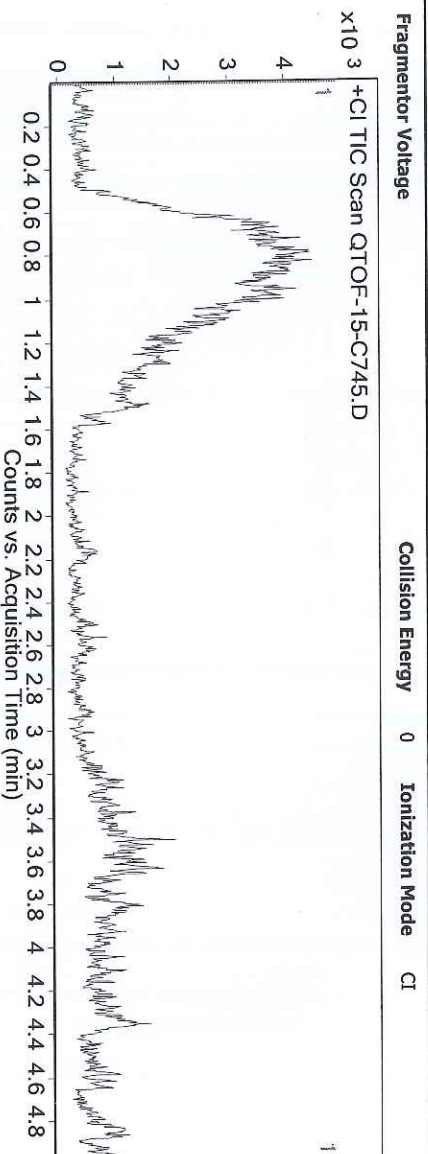
$$[(M - H_2O) + H]^+ @ 149 Da$$

ACCMASS OK

Qualitative Analysis Report

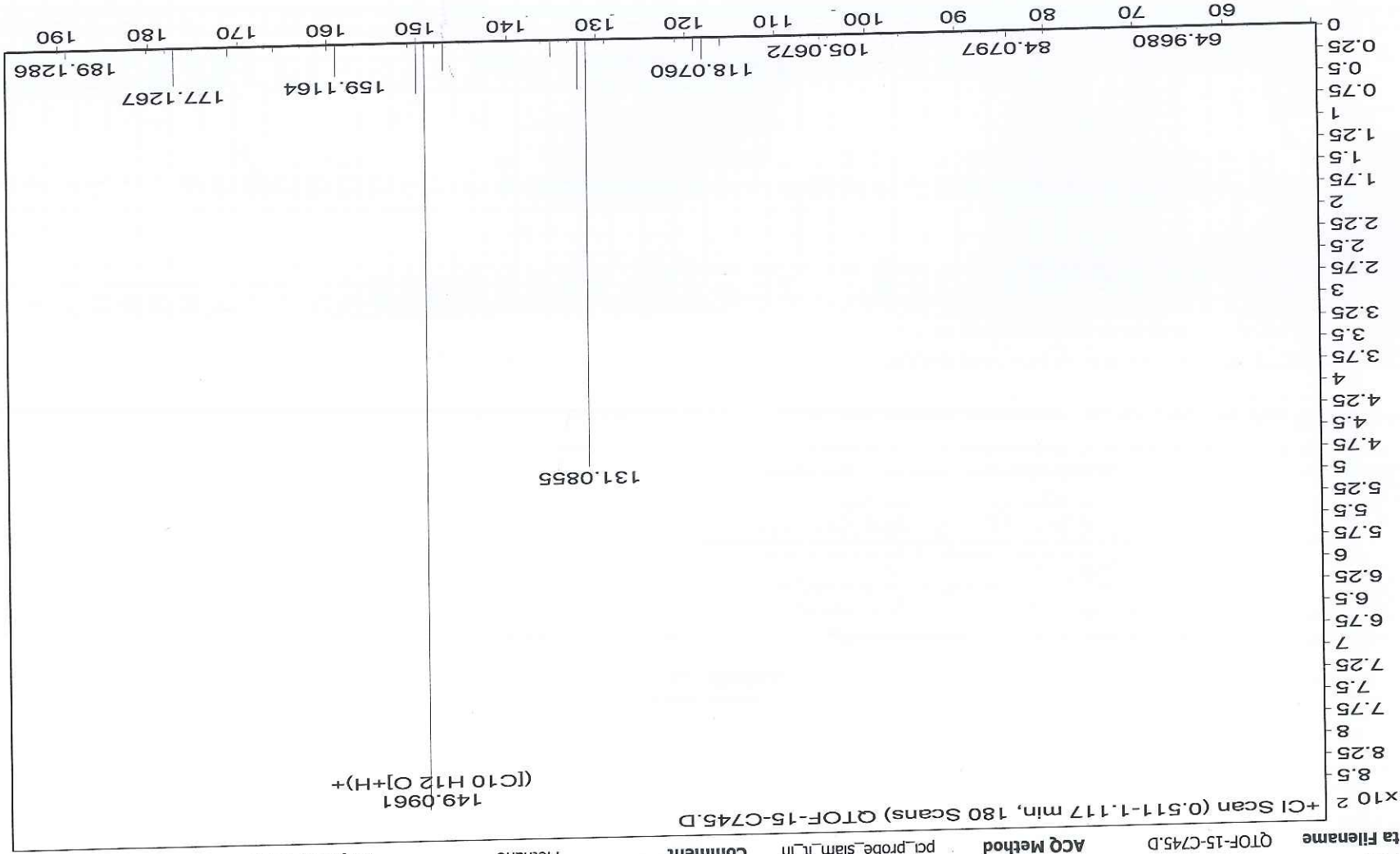
Data Filename	QTOF-15-C745.D	Sample Name	NF51 2PH2OH
Sample Type		Position	1
Instrument Name		User Name	agilent-PC\admin
Acq Method	GCQTOF	Acquired Time	12/14/2015 12:29:12 PM
IRM Calibration Status	pc_probe_slam_it_in.M	DA Method	Default.m
Comment	Success		
Expected Barcode	Methane		
Dual Inj Vol		Sample Amount	
		TuneName	atunes_2ghz.pci.tune.xml
TunePath	D:\MassHunter\GCMS\1\7200	TuneDateStamp	42352.84435
MSFirmwareVersion	G.7200.01.09	OperatorName	agilent-PC\admin
RunCompletedFlag	TRUE		

User Chromatograms



--- End Of Report ---

Sample Name	Inj Vol	Data Filename	Position	Acq Method	SampleType	Instrument Name	User Name	Acquired Time
NF51 2PH2OH	0	QTOF-15-C745.D	1	pd_probe_slam_it_in		GCQTOF	agilent-PC\admin	12/14/2015 12:29:12 PM



MS Peaks One: + Scan (0.511-1.117 min) (QTOF-15-C745.D)

m/z	Abund	Abund %
80.048	3.98	0.46
84.0797	6.44	0.74
105.0672	3.59	0.41
105.0716	3.18	0.37
116.0842	8.26	0.95
116.0891	6.18	0.71
118.076	23.25	2.69
118.0788	19.56	2.26
119.0821	14.04	1.62
119.0866	12.58	1.45
121.0619	3.43	0.4
129.0675	3.52	0.41
131.0855	481.9	55.66
132.0885	55.52	6.41
135.0788	17.33	2
135.0834	5.17	0.6
147.0786	30.93	3.57
147.0817	28.35	3.27
148.0814	5.49	0.63
148.0887	2.66	0.31
149.0961	865.82	100
150.098	55.89	6.46
150.1004	43.65	5.04
151.1012	3.7	0.43
159.1164	34.34	3.97
160.1175	4.41	0.51
166.0987	5.12	0.59
171.1118	2.8	0.32
171.117	8.32	0.96
177.1267	41.22	4.76
178.1269	3.82	0.44
180.0559	4.12	0.48
189.1228	5.39	0.62
189.1286	6.93	0.8
227.1517	13.41	1.55
227.1563	16.75	1.94
228.1569	4.58	0.53
245.1464	3.47	0.4
247.1545	2.65	0.31
247.1603	16.58	1.91
247.1657	7.23	0.84
248.1688	2.57	0.3

Spectrum Identification Results: + Scan (0.511-1.117 min) (QTOF-15-C745.D)

Best	ID Source	Formula	Species	m/z	Score	Diff (ppm)	Diff (mDa)
	MFG	C10 H12 O	(M+H)+	149.0961	79.43	0.54	0.08

Ion Formula	Species	m/z	Score (mass)	Score (MS)	Score (MFG)	Height
C10H13O	(M+H)+	149.0961	99.92	79.43	79.43	865.8

Height (Calc)	Height Sum% (Calc)	Height % (Calc)	100	149.0961	0	865.8	100	93.9	149.0961	-0.08
Height (Calc)	Height Sum% (Calc)	Height % (Calc)	m/z (Calc)	Diff (mDa)	Height	Height	Height %	Height Sum	m/z	Diff (ppm)