Walkup MS Report

Data File	SE-522 (AC-2)_Pos_5mins_MS_07376.d	**Sample Name**	SE-522 (AC-2)
Sample Type	Sample	**Position**	P1-C7
Instrument Name	6545 QTof	**User Name**	Susana Estopina-Duran
Acq Method	Pos_5mins_MS.m	**Acquired Time**	8/29/2019 9:23:22 PM
IRM Calibration Status	Success	**DA Method**	Pos_5mins_MS.m
Comment			

Sample Group		**Info.**	
Walkup Sample Description		**Walkup Method**	Pos_5Mins_C18
Formula	C20H22O3	**Walkup Method Description**	Positive mode ionization using C18 column chromatography
Stream Name	LC 1	**Acquisition SW Version**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)

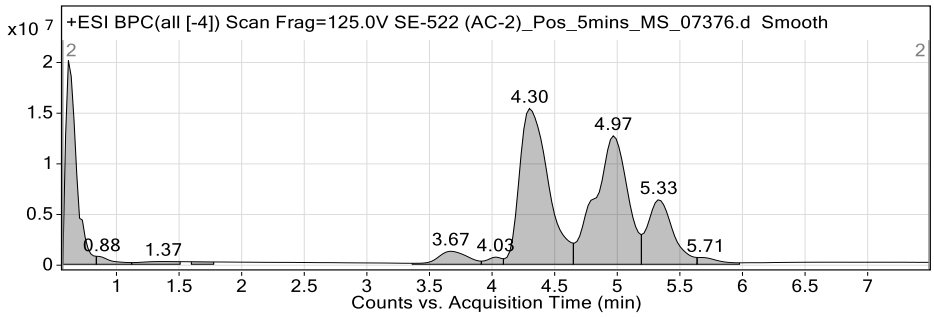

Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.62	120584616	48.76	16.34	102.1295	0.100
0.88	6510678	2.63	0.88	203.0920	0.140
1.37	5537381	2.24	0.75	921.9990	0.310
1.64	2541596	1.03	0.34	921.9986	0.150
3.67	21140377	8.55	2.86	201.0516	0.270
4.03	5706642	2.31	0.77	203.0921	0.120
4.30	247305310	100.00	33.52	215.0688	0.250
4.97	230099653	93.04	31.18	333.1463	0.270
5.33	90599643	36.63	12.28	446.2668	0.210
5.71	7864784	3.18	1.07	419.3141	0.190

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)	Error flag
Cpd 1: C20 H22 O3	4.98	333.1468	310.1586	310.1569	5.50	98.43	No H adduct

Mass errors of between -5.00 and 5.00 ppm with isotope match scores above 60% are considered confirmation of molecular formulae

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Compound specific information

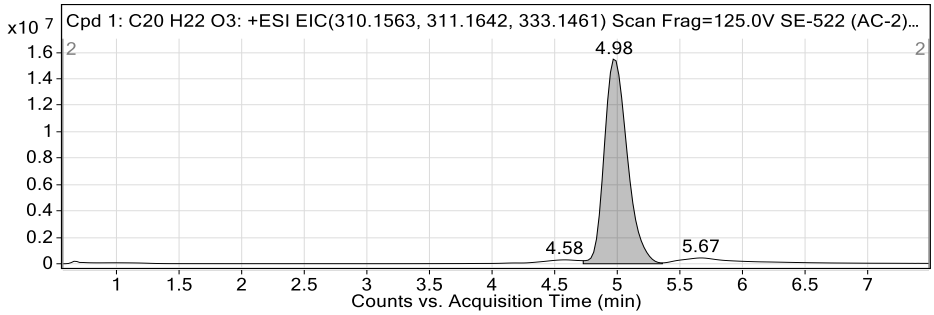

Figure: Extracted ion chromatogram (EIC) of compound.

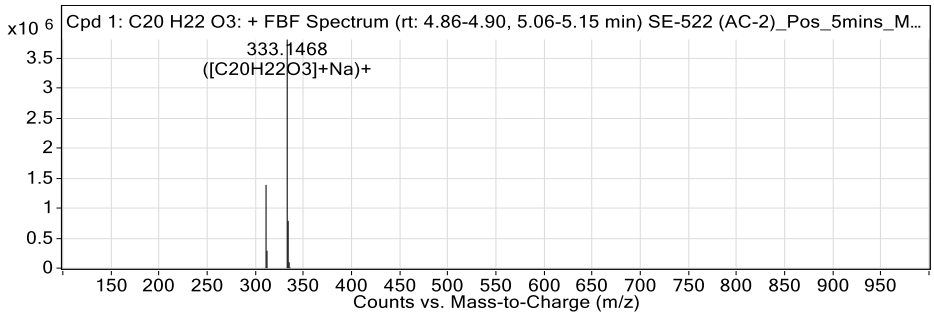

Figure: Full range view of Compound spectra and potential adducts.

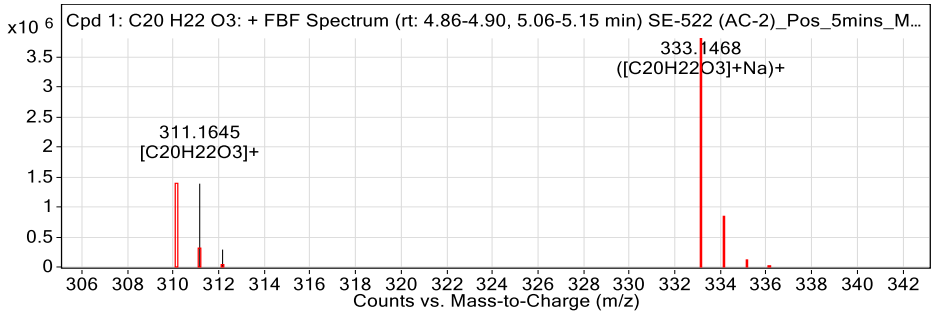

Figure: Zoomed Compound spectra view
(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
310.1605	1	1301.4	C20H22O3	M+
311.1645	1	1388610.9	C20H22O3	M+
312.1680	1	289940.8	C20H22O3	M+
333.1468	1	3810358.5	C20H22O3	(M+Na)+
334.1499	1	787815.4	C20H22O3	(M+Na)+
335.1525	1	98618.6	C20H22O3	(M+Na)+
336.1554	1	9757.9	C20H22O3	(M+Na)+

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