

Walkup MS Report



Data File	ESIPT-DI + ONOO-_Neg_5mins_MS_04509.d	Sample Name	ESIPT-DI + ONOO-
Sample Type	Sample	Position	P1-A5
Instrument Name	6545 QTof	User Name	Maria Odyniec
Acq Method	Neg_5mins_MS.m	Acquired Time	5/30/2019 3:45:40 PM
IRM Calibration Status	Success	DA Method	Neg_5mins_MS.m
Comment			

Sample Group		Info.	
Walkup Sample Description		Walkup Method	Neg_5Mins_C18
Formula	C20H14N4O	Walkup Method Description	Negative 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)

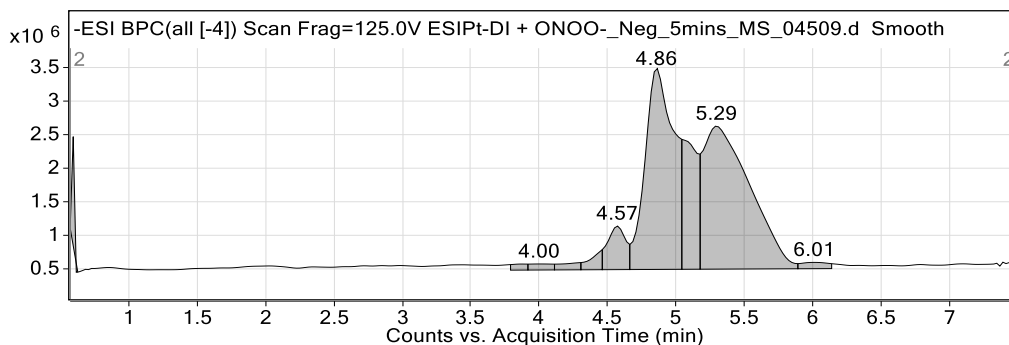


Figure 1: Base peak chromatogram

User Chromatogram Peak List

RT (min)	Area	Area %	Area Sum (%)	Base Peak (m/z)	Width (min)
0.59	2040656	4.04	1.67	1033.9821	0.020
3.87	671171	1.33	0.55	1033.9865	0.110
4.00	1035827	2.05	0.85	1033.9868	0.170
4.26	1091505	2.16	0.89	1033.9869	0.150
4.42	1686112	3.34	1.38	1033.9869	0.130
4.57	5930808	11.74	4.84	1033.9870	0.130
4.86	43453140	86.01	35.49	265.1575	0.200
5.09	14715285	29.13	12.02	277.1844	0.120
5.29	50521667	100.00	41.27	291.2002	0.360
6.01	1279009	2.53	1.04	1033.9874	0.210

Compound Table

Compound Label	RT (min)	Observed mass (m/z)	Neutral observed mass (Da)	Theoretical mass (Da)	Mass error (ppm)	Isotope match score (%)
Cpd 1: C20 H14 N4 O	4.63	325.1110	326.1160	326.1168	-2.25	51.22

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

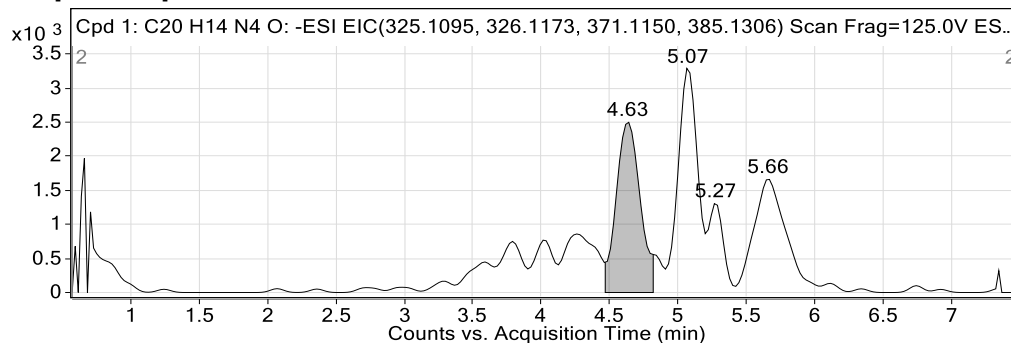


Figure: Extracted ion chromatogram (EIC) of compound.

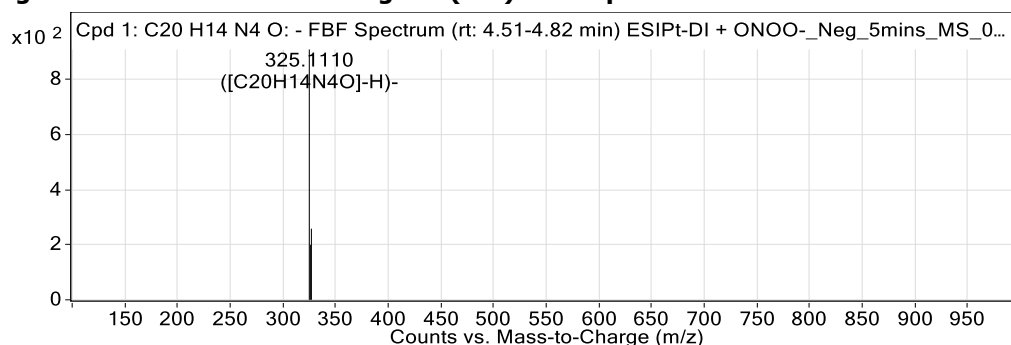


Figure: Full range view of Compound spectra and potential adducts.

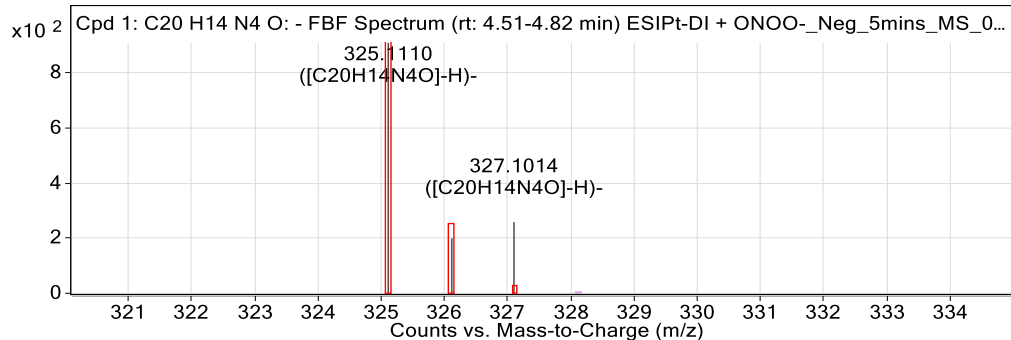


Figure: Zoomed Compound spectra view
(red boxes indicating expected theoretical isotope spacing and abundance)

Compound isotope peak List

m/z	z	Abund	Formula	Ion
325.1110	1	910.2	C ₂₀ H ₁₄ N ₄ O	(M-H)-
326.1187	1	199.9	C ₂₀ H ₁₄ N ₄ O	(M-H)-
327.1014	1	258.8	C ₂₀ H ₁₄ N ₄ O	(M-H)-

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