

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
 Data File : BF101512.D
 Acq On : 19 Dec 2017 6:58
 Operator : SJ/JU
 Sample : I6910-04
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 121317-TIDO-E-U-M

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	496	499	512	rBV	74675	106173	3.04%	0.465%
2	5.434	566	569	588	rBV	1052955	1293417	37.09%	5.667%
3	6.451	739	742	761	rBV2	557147	864888	24.80%	3.790%
4	6.581	761	764	777	rVV	2196288	2158751	61.91%	9.459%
5	6.810	799	803	811	rBV	864007	803377	23.04%	3.520%
6	6.963	825	829	845	rBV	2826326	2953258	84.70%	12.940%
7	7.381	895	900	903	rBV	2325466	2197390	63.02%	9.628%
8	7.487	914	918	925	rVB	82323	90173	2.59%	0.395%
9	8.092	1017	1021	1033	rBV	1024632	1033837	29.65%	4.530%
10	8.810	1140	1143	1149	rBV	74062	68159	1.95%	0.299%
11	8.904	1154	1159	1165	rVB	45113	44617	1.28%	0.195%
12	9.169	1199	1204	1207	rBV	3647277	3486844	100.00%	15.278%
13	9.563	1269	1271	1277	rVB	51084	43851	1.26%	0.192%
14	9.828	1313	1316	1317	rBV	117756	98951	2.84%	0.434%
15	9.845	1317	1319	1323	rVV2	849107	810873	23.26%	3.553%
16	9.880	1323	1325	1333	rVB	116489	101596	2.91%	0.445%
17	10.057	1352	1355	1359	rBV	49952	46923	1.35%	0.206%
18	10.398	1410	1413	1419	rVB	66682	63464	1.82%	0.278%
19	10.516	1430	1433	1438	rBV	199249	168808	4.84%	0.740%
20	10.563	1438	1441	1446	rVB3	31161	35308	1.01%	0.155%
21	10.645	1451	1455	1468	rBV	1039712	1156153	33.16%	5.066%
22	11.339	1569	1573	1576	rBV	788270	724072	20.77%	3.173%
23	11.363	1576	1577	1582	rVB	172697	113283	3.25%	0.496%
24	12.557	1777	1780	1785	rBV	81930	84808	2.43%	0.372%
25	12.792	1813	1820	1824	rBV	48449	65779	1.89%	0.288%
26	12.921	1838	1842	1845	rBV	2771690	2608724	74.82%	11.430%
27	13.804	1989	1992	2000	rBV3	34762	47143	1.35%	0.207%
28	13.986	2020	2023	2031	rVB	868024	842826	24.17%	3.693%
29	15.462	2269	2274	2281	rVB	521302	709364	20.34%	3.108%

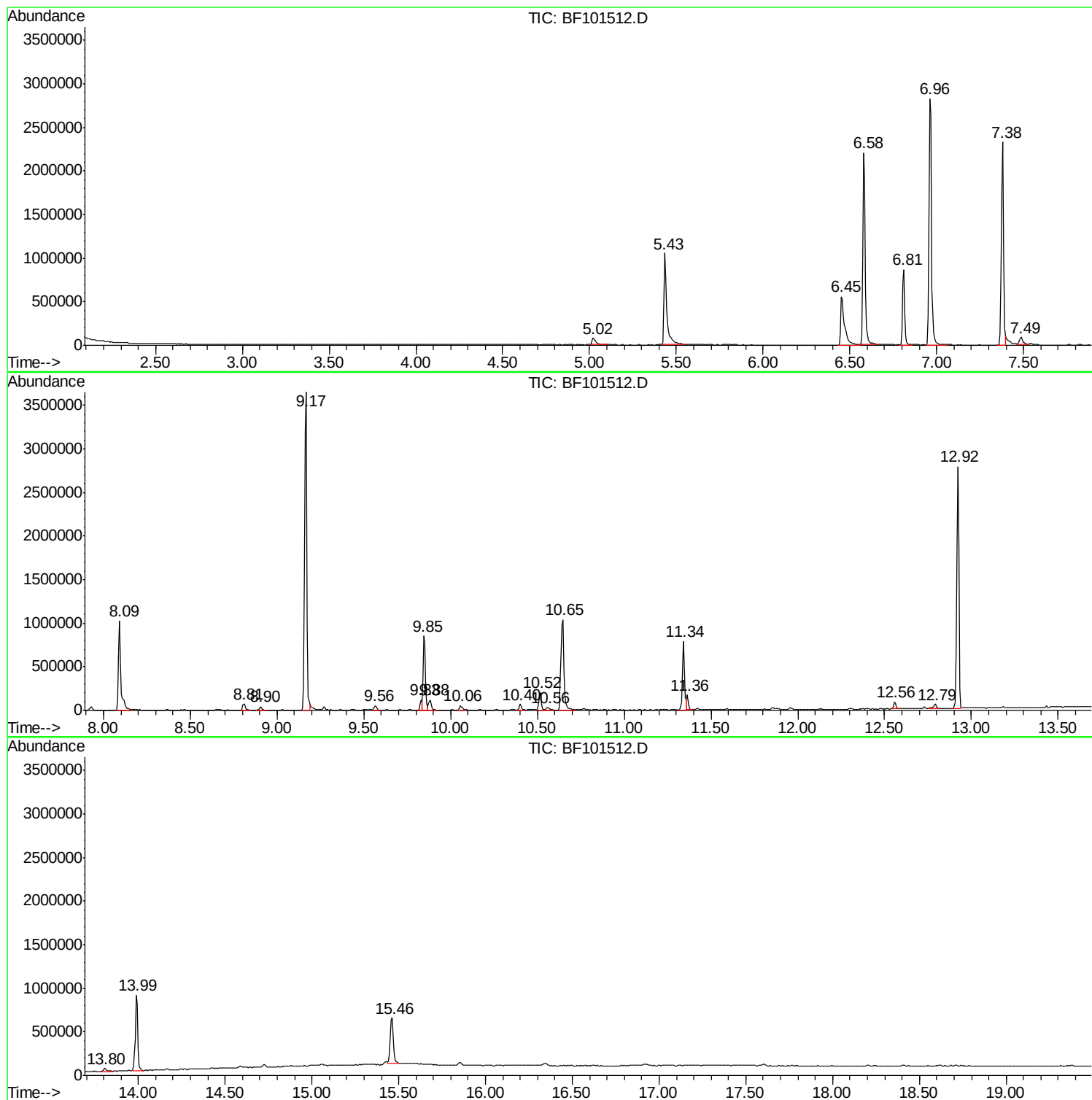
Sum of corrected areas: 22822810

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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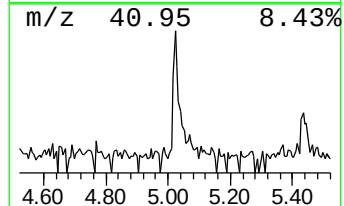
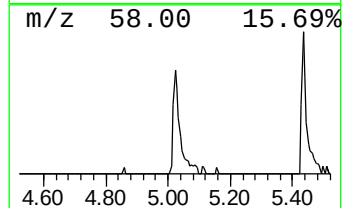
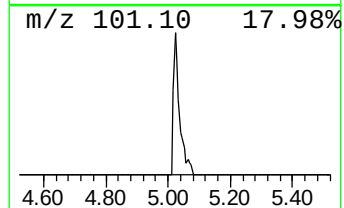
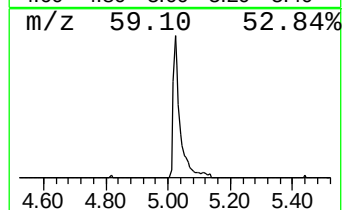
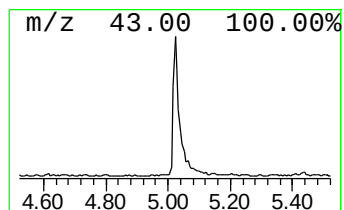
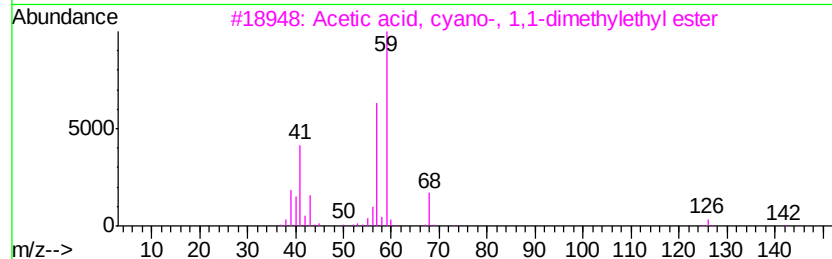
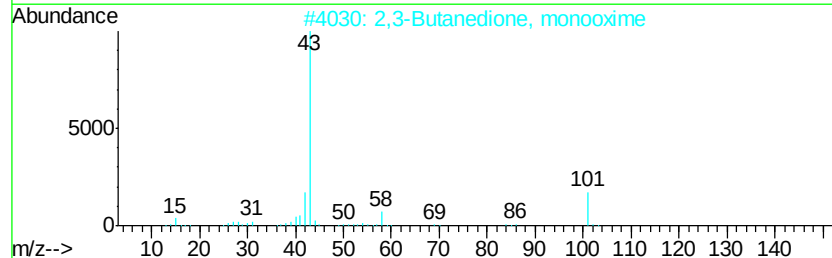
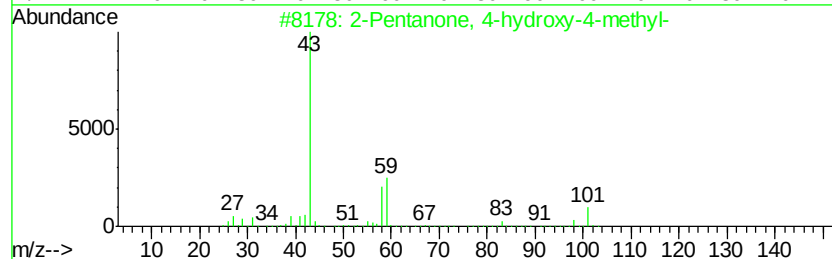
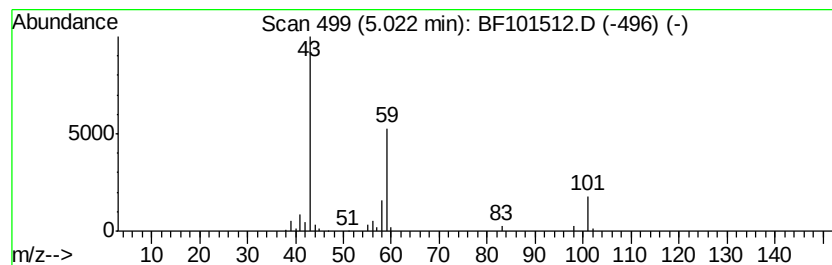
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.02	2.64 ng	106173	1,4-Dichlorobenzene-d4	6.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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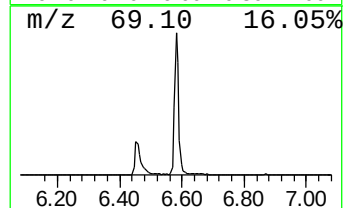
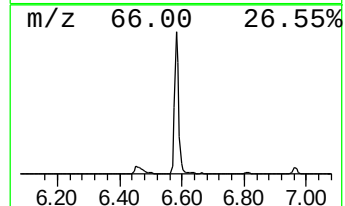
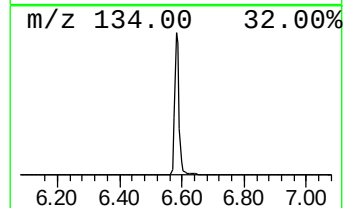
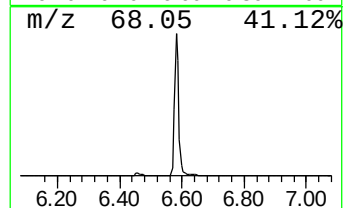
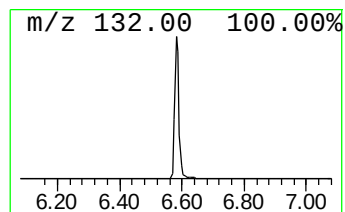
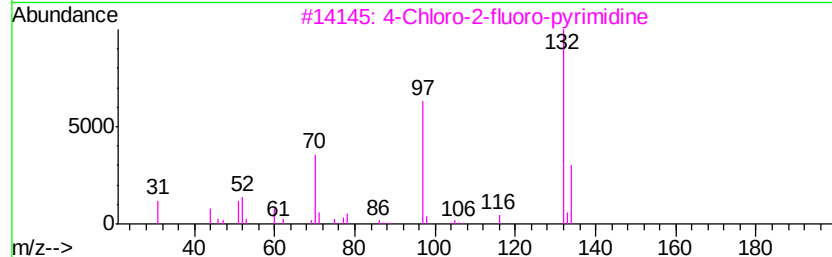
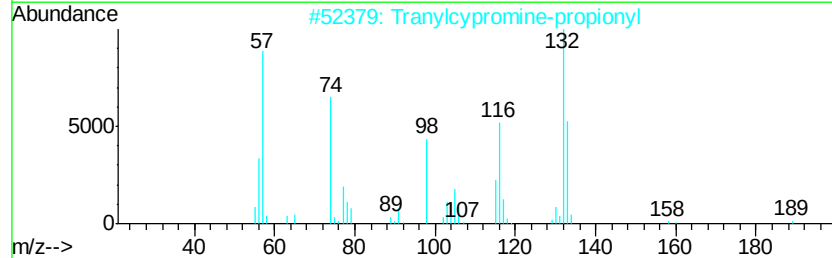
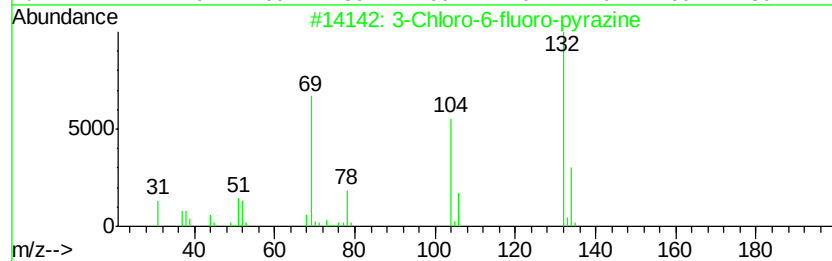
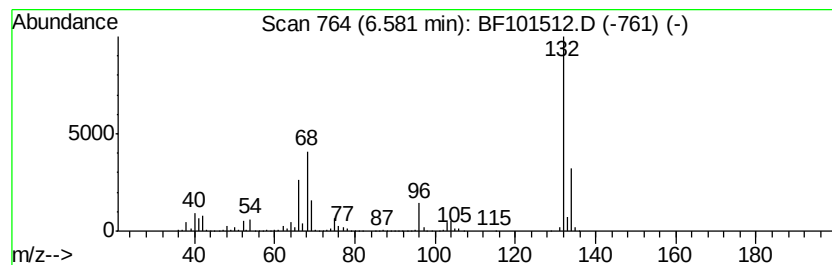
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Peak Number 2 unknown6.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	53.74 ng	2158750	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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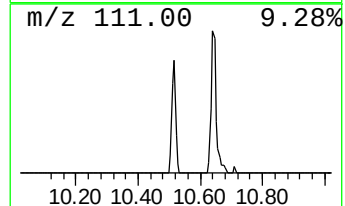
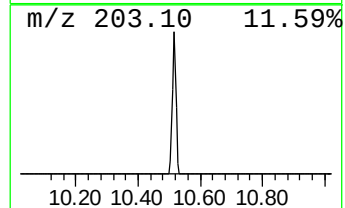
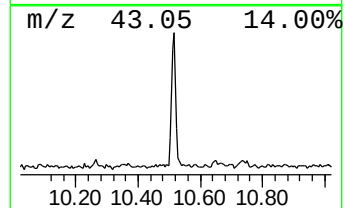
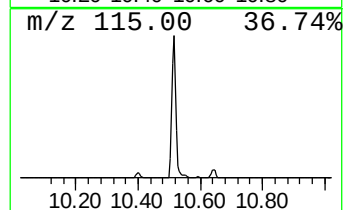
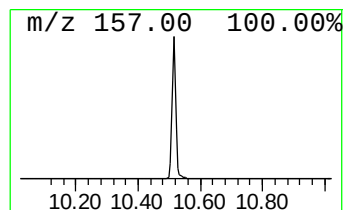
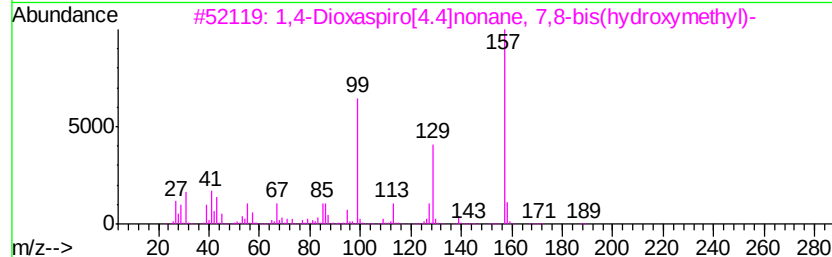
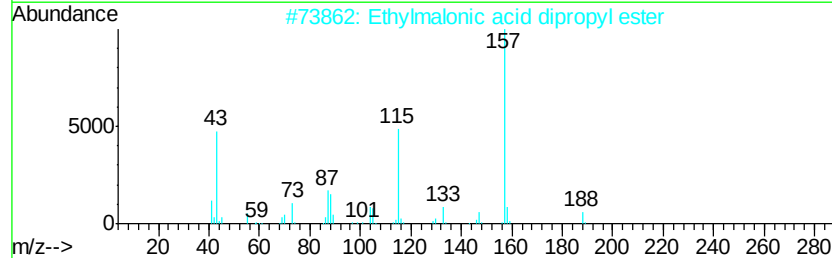
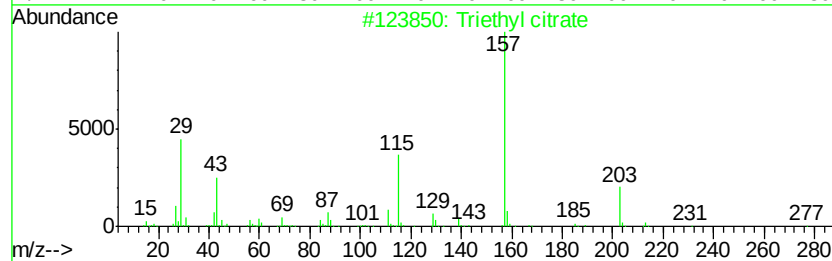
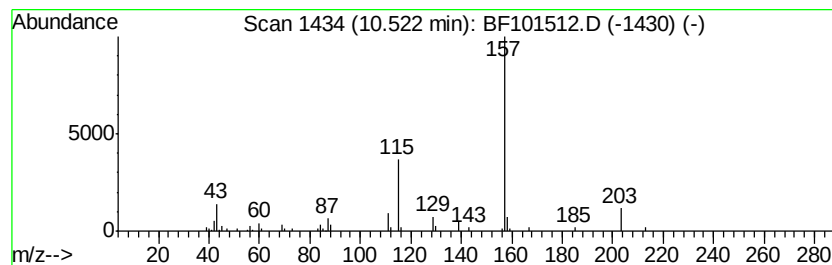
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Peak Number 4 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	4.16 ng	168808	Acenaphthene-d10	9.85
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Triethyl citrate	276 C12H20O7	000077-93-0 91
2		Ethylmalonic acid dipropyl ester	216 C11H20O4	001113-91-3 64
3		1,4-Dioxaspiro[4.4]nonane, 7,8-b...	188 C9H16O4	1000155-54-9 33
4		2-Chlorobenzoic acid, tridecyl e...	338 C20H31ClO2	1000292-42-8 33
5		Piperazine-1-carboxylic acid, 4-...	362 C14H19ClN2O5S	1000303-79-9 33



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	2.6	ng	106173	1	6.81	803377	20.0
unknown6.58	6.58	53.7	ng	2158750	1	6.81	803377	20.0
Triethyl citrate	10.52	4.2	ng	168808	3	9.85	810873	20.0