

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\
Data File : BF104516.D
Acq On : 14 Apr 2018 10:12
Operator : JU/SJ
Sample : J2368-10
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
041118-DBRI-E-U-S

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-BF040618.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	5.004	493	496	506	rVB	116472	119347	3.29%	0.531%
2	5.422	563	567	570	rBV	1356543	1158787	31.90%	5.159%
3	6.028	667	670	681	rBV	54776	61211	1.68%	0.273%
4	6.433	736	739	748	rBV	745518	731184	20.13%	3.256%
5	6.575	759	763	767	rBV	2454050	2243775	61.76%	9.990%
6	6.804	799	802	806	rBV	967527	840569	23.14%	3.743%
7	6.963	825	829	833	rBV	2968230	2871816	79.05%	12.786%
8	7.375	893	899	902	rBV	2075192	2060161	56.71%	9.173%
9	8.092	1017	1021	1024	rBV	1089348	918250	25.28%	4.088%
10	9.169	1198	1204	1207	rBV	3785686	3632880	100.00%	16.175%
11	9.557	1266	1270	1273	rBV	62269	60290	1.66%	0.268%
12	9.774	1304	1307	1310	rBV	62168	50948	1.40%	0.227%
13	9.845	1315	1319	1328	rVB	1203686	1114233	30.67%	4.961%
14	10.274	1385	1392	1395	rBV2	85264	97107	2.67%	0.432%
15	10.639	1450	1454	1457	rBV	1450523	1398647	38.50%	6.227%
16	10.745	1470	1472	1474	rBV	66216	60913	1.68%	0.271%
17	10.774	1474	1477	1487	rVB2	462730	500511	13.78%	2.228%
18	11.333	1568	1572	1576	rBV	938596	774250	21.31%	3.447%
19	12.739	1808	1811	1818	rVB	81452	65892	1.81%	0.293%
20	12.927	1838	1843	1846	rBV	2709795	2505029	68.95%	11.153%
21	13.445	1928	1931	1934	rBV	54077	46402	1.28%	0.207%
22	13.821	1991	1995	2003	rBV	36130	40809	1.12%	0.182%
23	13.980	2018	2022	2028	rVB	633754	629320	17.32%	2.802%
24	15.445	2266	2271	2279	rVB	351166	477426	13.14%	2.126%

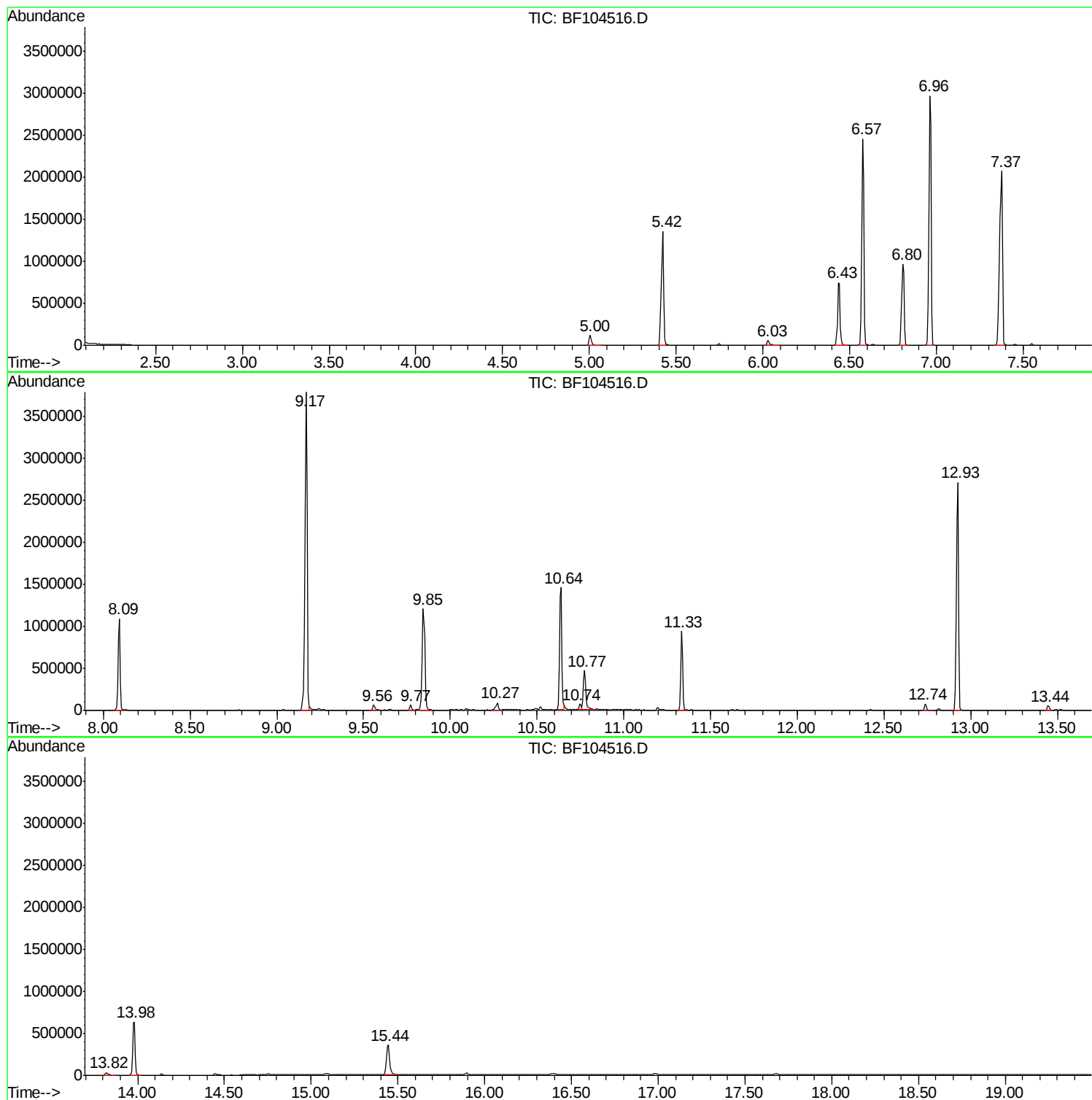
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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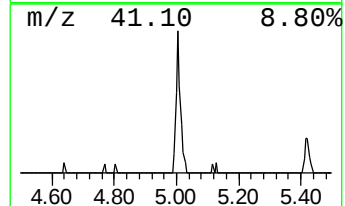
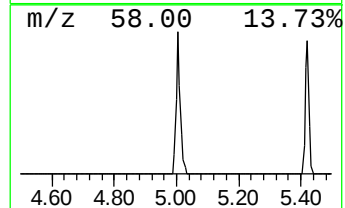
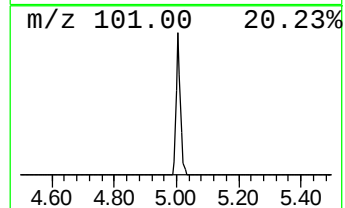
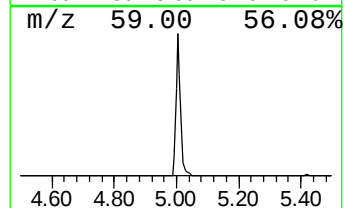
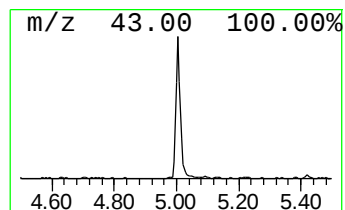
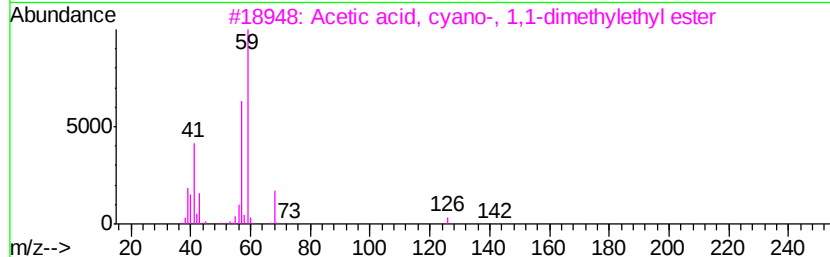
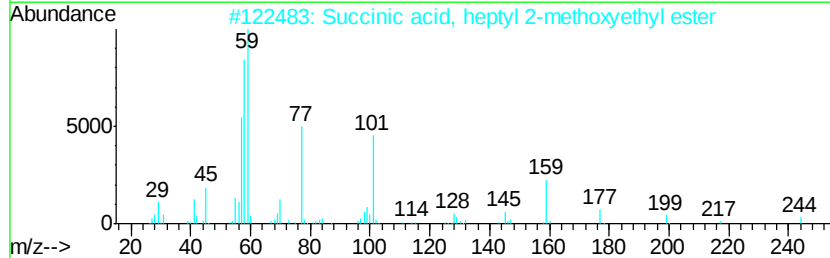
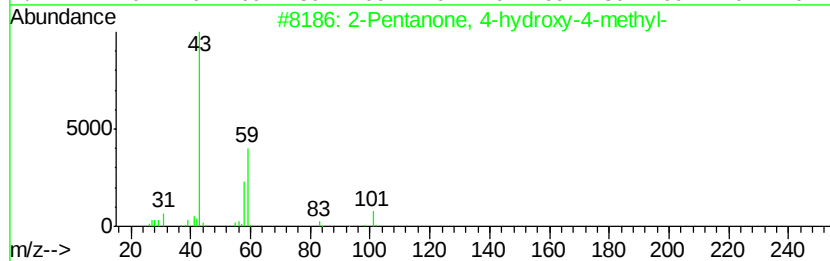
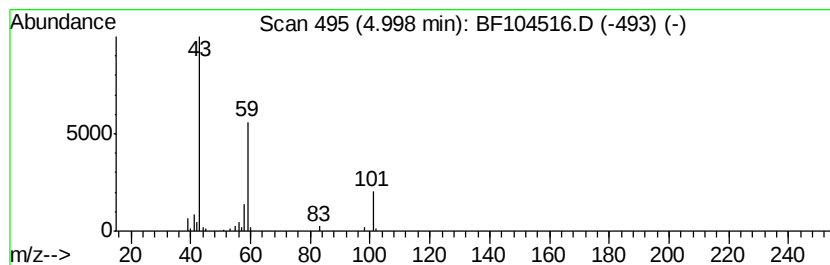
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.00	2.84 ng	119347	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Succinic acid, heptyl 2-methoxyethyl ester	274	C14H26O5	1000325-80-7	28
3			Acetic acid, cyano-, 1,1-dimethylethyl ester	141	C7H11NO2	001116-98-9	25
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5			Acetone	58	C3H6O	000067-64-1	9



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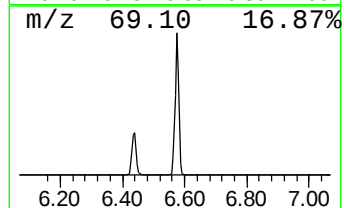
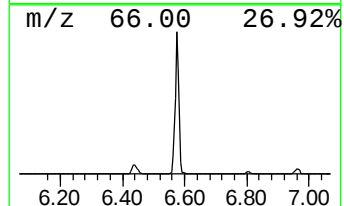
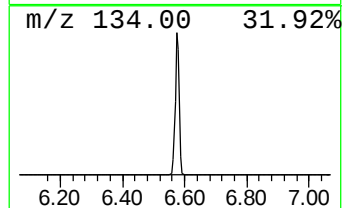
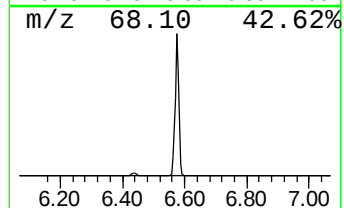
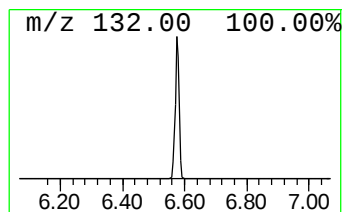
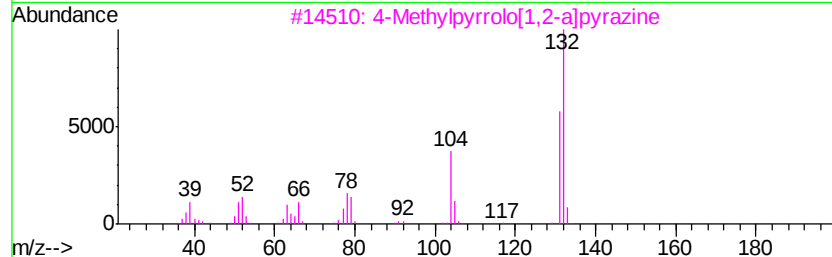
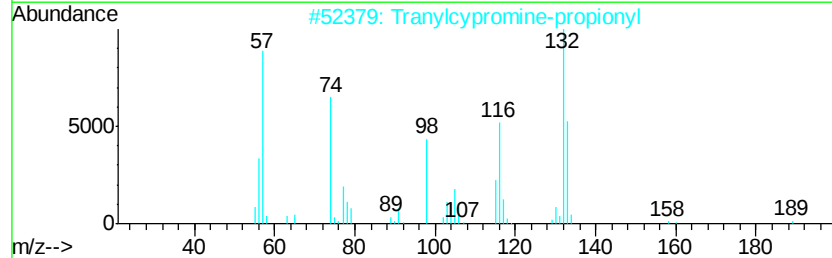
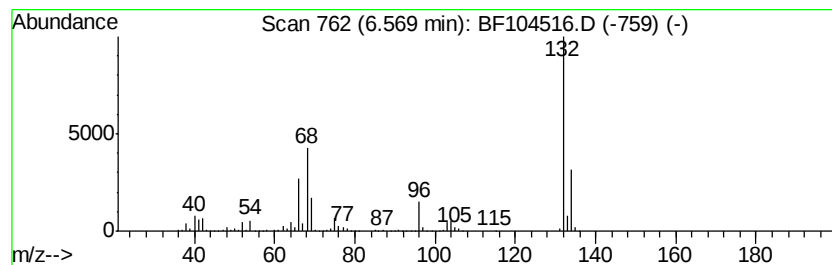
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Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	53.39 ng	2243780	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		5-Aminoindole	132	C8H8N2	005192-03-0	9



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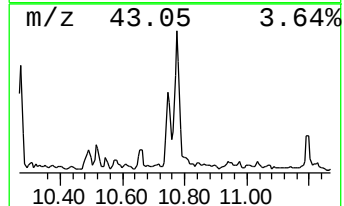
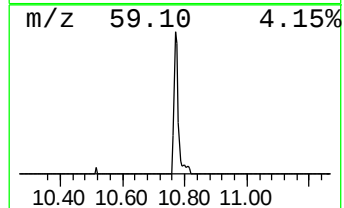
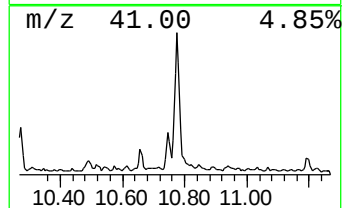
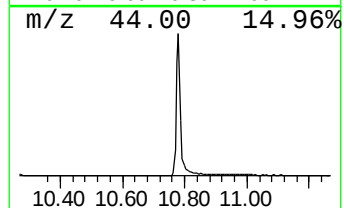
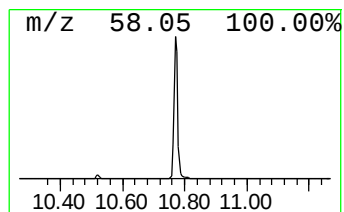
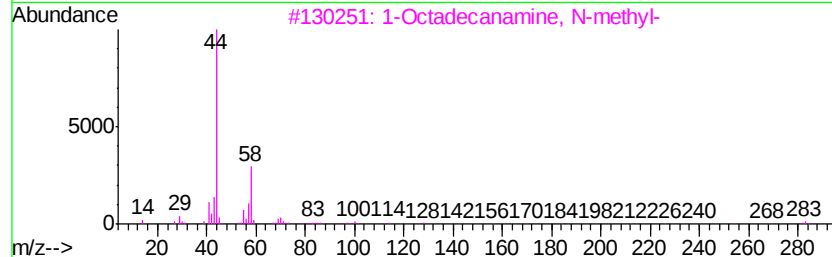
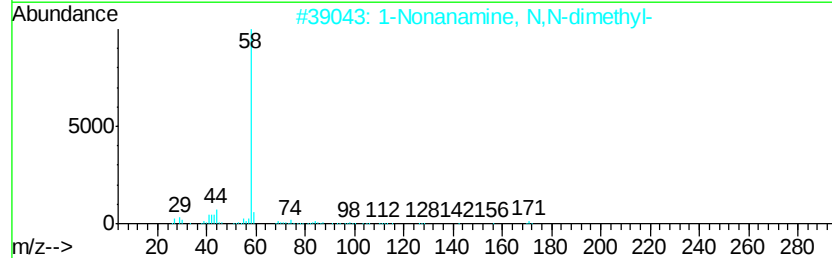
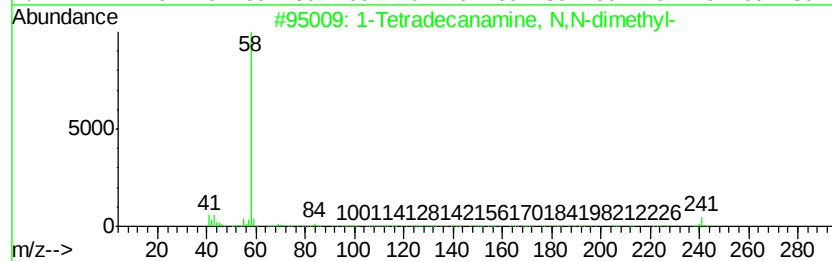
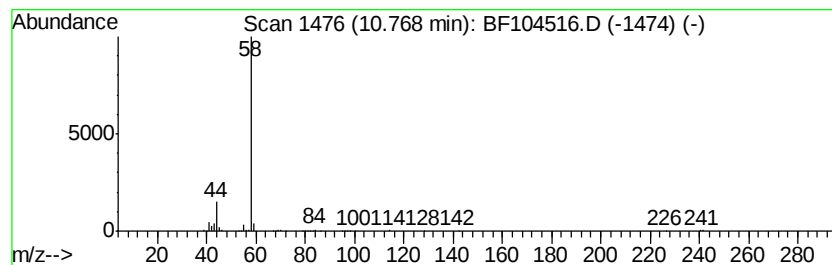
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Peak Number 4 unknown10.77 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	12.93 ng	500511	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	43
2		1-Nonanamine, N,N-dimethyl-	171	C11H25N	017373-27-2	38
3		1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	37
4		Dodecyltrimethylammonium bromide	307	C15H34BrN	001119-94-4	32
5		N,N-Dimethyl-6-benzyloxyhexylamine	235	C15H25NO	071126-72-2	32



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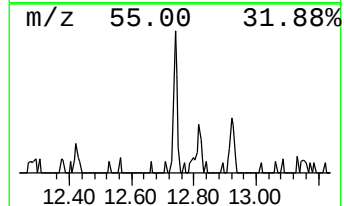
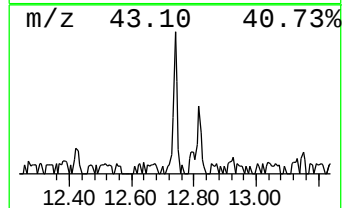
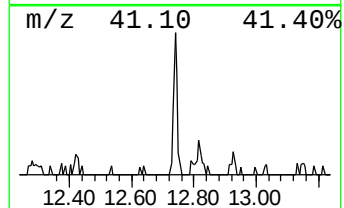
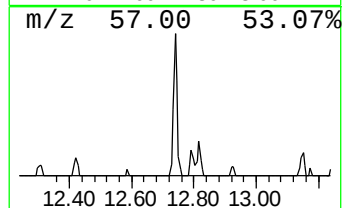
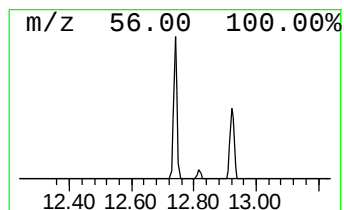
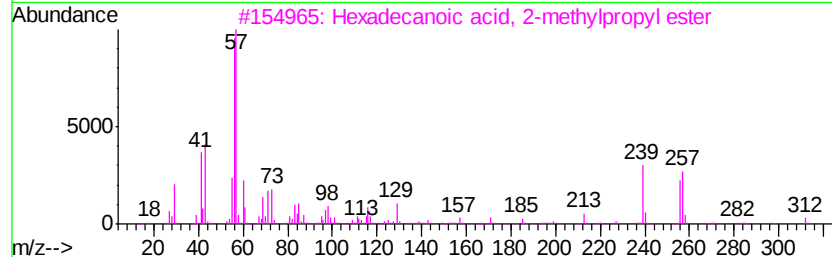
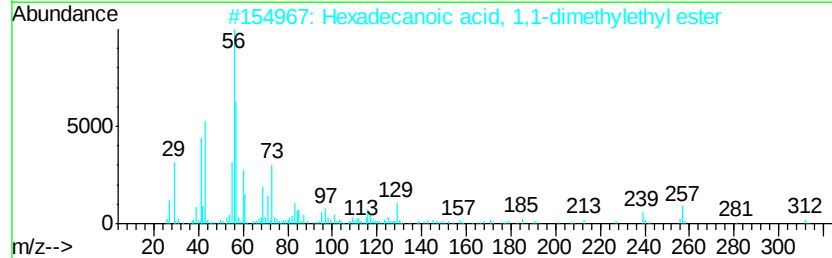
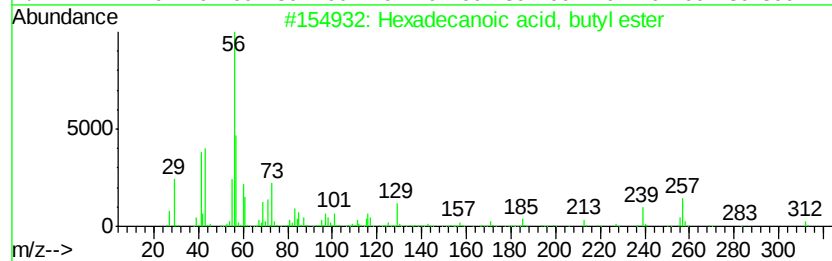
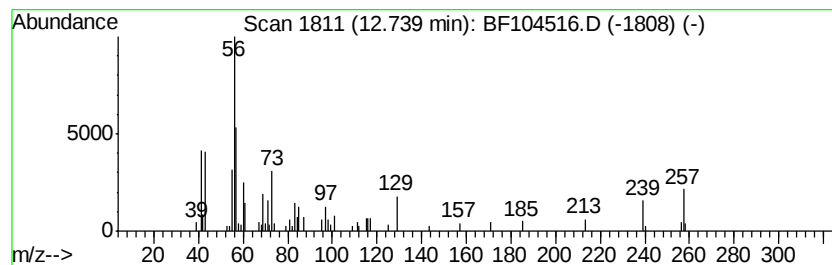
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.09 ng	65892	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	42
4		Hexanoic acid, butyl ester	172	C10H20O2	000626-82-4	38
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	2.8	ng	119347	1	6.80	840569	20.0
unknown6.57	6.57	53.4	ng	2243780	1	6.80	840569	20.0
unknown10.77	10.77	12.9	ng	500511	4	11.33	774250	20.0
Hexadecanoic acid...	12.74	2.1	ng	65892	5	13.98	629320	20.0