

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120918\
 Data File : BF111233.D
 Acq On : 10 Dec 2018 11:01
 Operator : JU/SJ
 Sample : PB115080BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB115080BL

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:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.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	493	499	511	rBV	486957	695120	5.33%	0.612%
2	5.422	562	567	571	rBV	10382364	11492689	88.05%	10.114%
3	6.428	732	738	741	rBV	10713331	11797446	90.38%	10.382%
4	6.569	757	762	765	rBV	11625696	11663696	89.36%	10.264%
5	6.798	797	801	805	rBV	4462512	3693579	28.30%	3.250%
6	6.957	823	828	831	rBV	9950845	9186413	70.38%	8.084%
7	7.357	890	896	899	rBV	7715298	7896179	60.49%	6.949%
8	8.081	1014	1019	1022	rBV	5192157	4942624	37.87%	4.350%
9	9.157	1196	1202	1206	rBV	12148416	13053193	100.00%	11.487%
10	9.833	1311	1317	1321	rBV2	5839779	5391225	41.30%	4.744%
11	10.622	1444	1451	1454	rBV	7736775	7372185	56.48%	6.488%
12	11.316	1565	1569	1573	rBV	5869896	5158599	39.52%	4.540%
13	11.474	1592	1596	1600	rBV2	166277	138274	1.06%	0.122%
14	11.845	1654	1659	1666	rBV2	91690	148590	1.14%	0.131%
15	12.733	1807	1810	1814	rBV	652094	577351	4.42%	0.508%
16	12.810	1821	1823	1827	rVB	177621	142462	1.09%	0.125%
17	12.910	1835	1840	1843	rBV	11088040	11439640	87.64%	10.067%
18	13.439	1927	1930	1934	rBV	529417	444931	3.41%	0.392%
19	13.951	2011	2017	2021	rBV	4665897	4448751	34.08%	3.915%
20	14.739	2148	2151	2157	rVB	147888	152967	1.17%	0.135%
21	15.068	2204	2207	2214	rVB	150882	187885	1.44%	0.165%
22	15.392	2256	2262	2267	rBV	2643800	3265174	25.01%	2.873%
23	15.445	2267	2271	2278	rVB	155845	214609	1.64%	0.189%
24	15.868	2339	2343	2347	rVB3	88756	130991	1.00%	0.115%

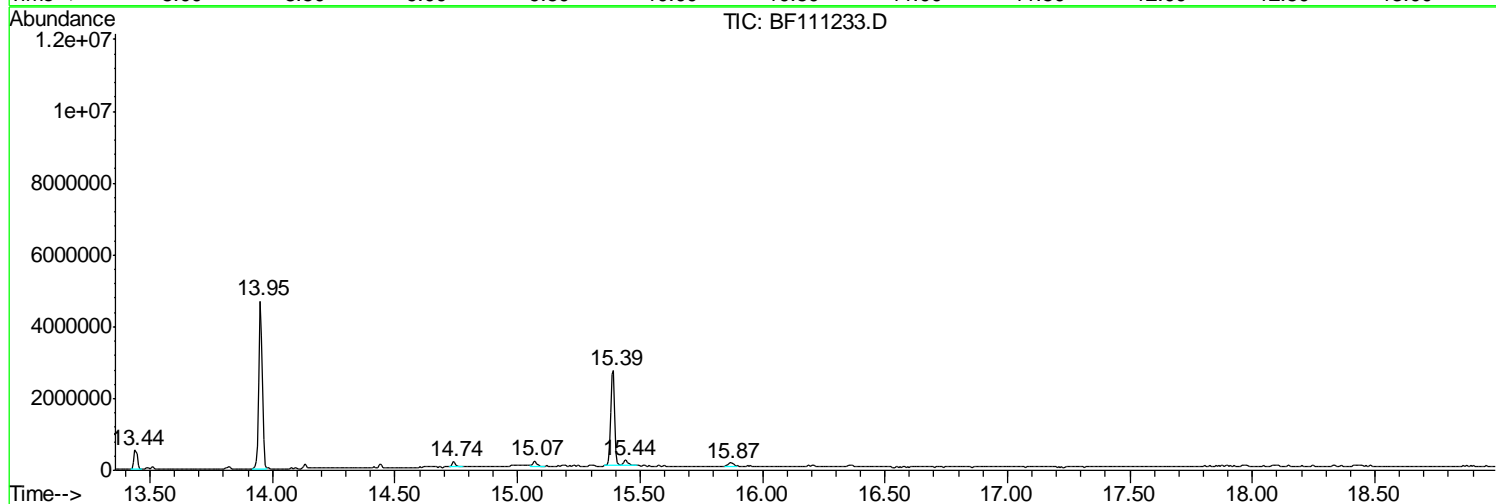
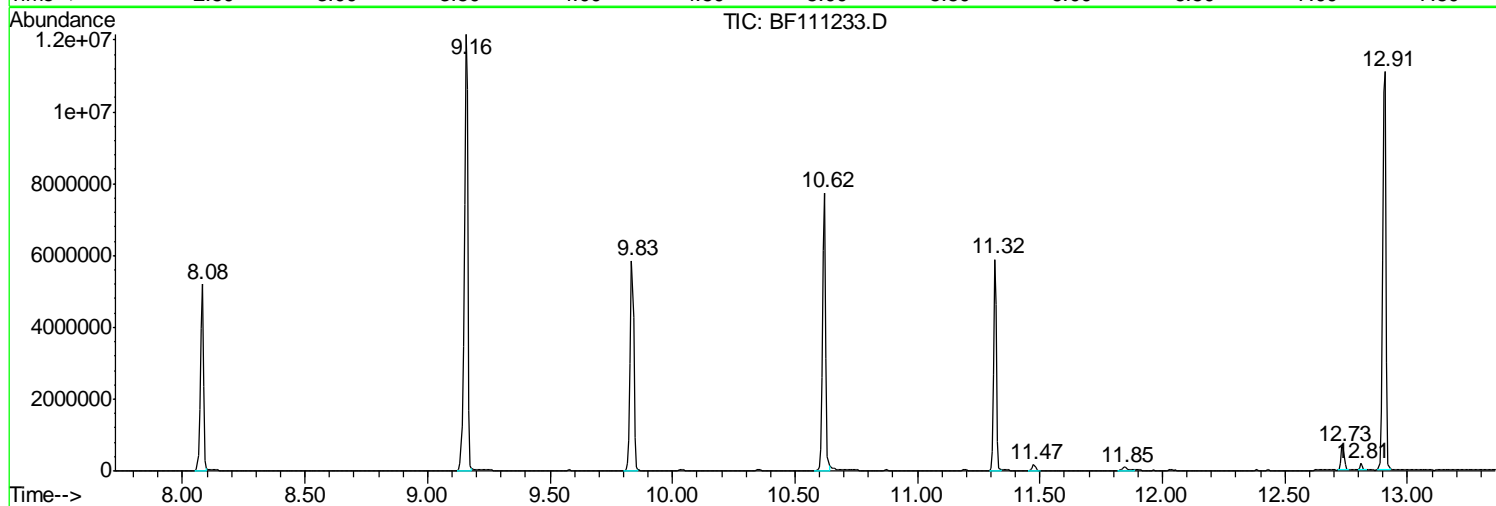
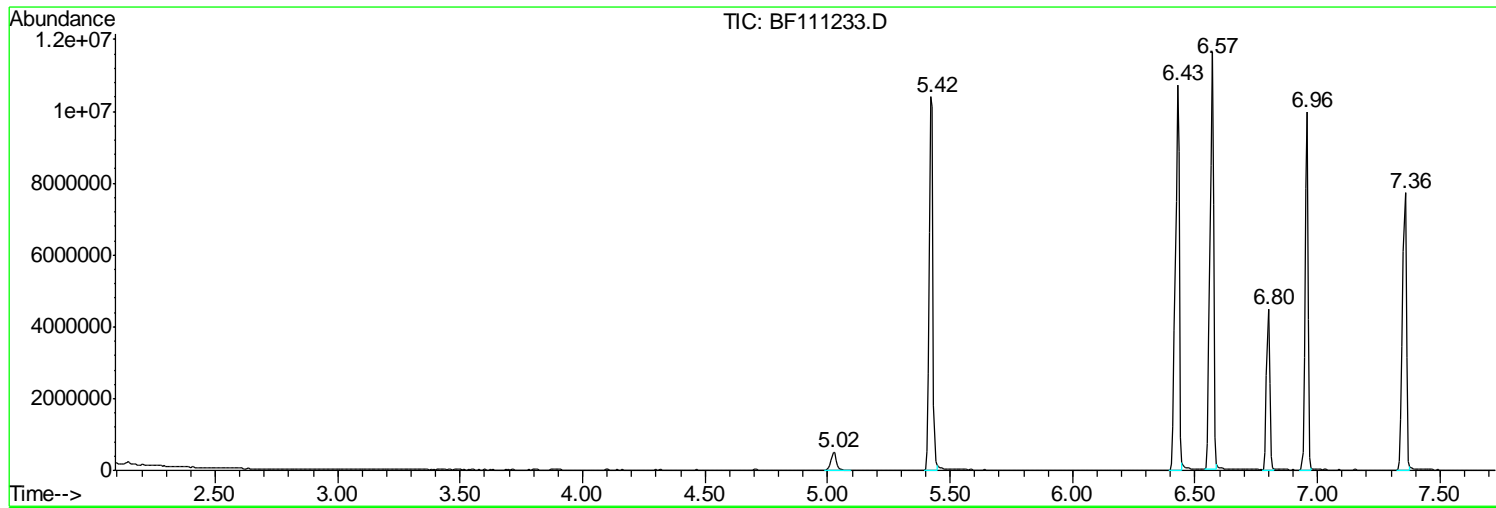
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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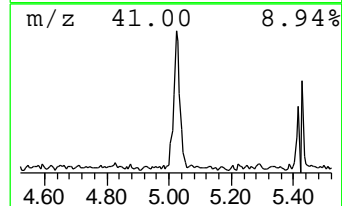
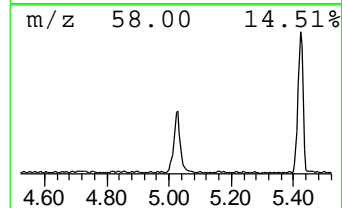
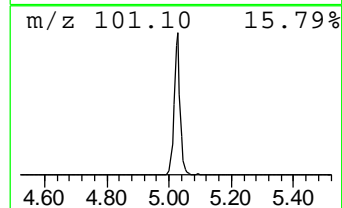
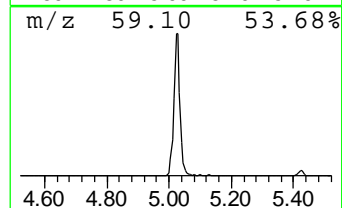
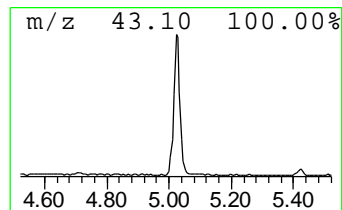
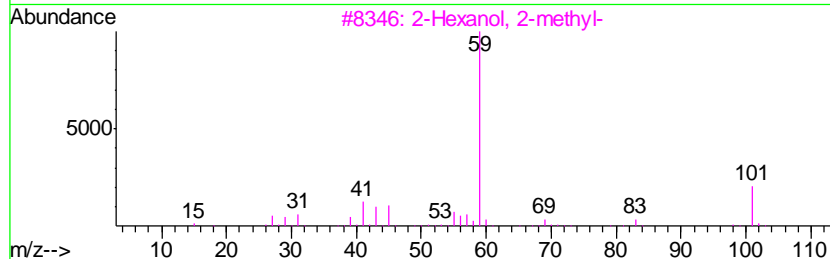
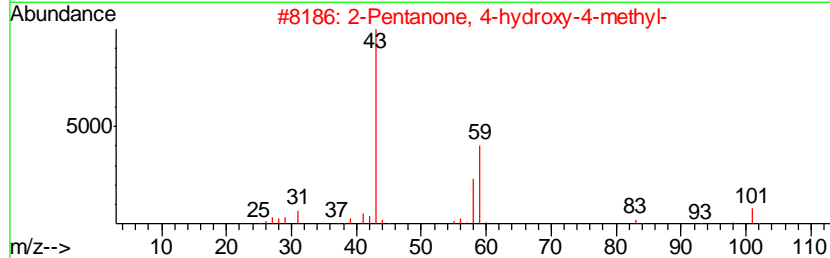
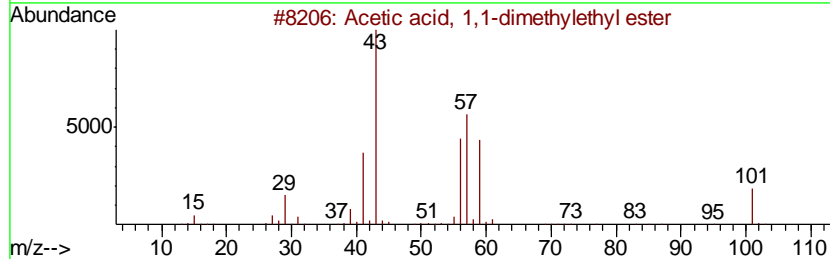
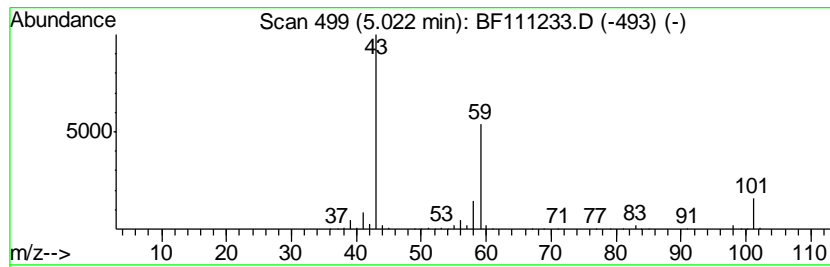
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.76 ng	695120	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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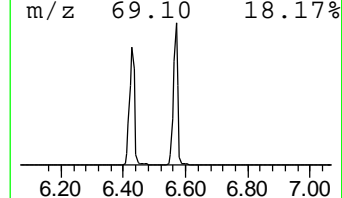
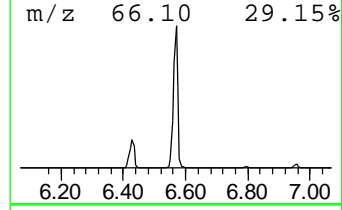
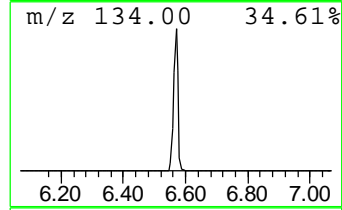
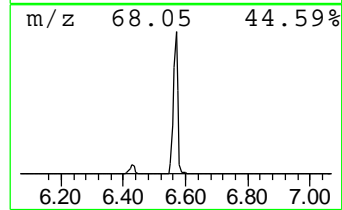
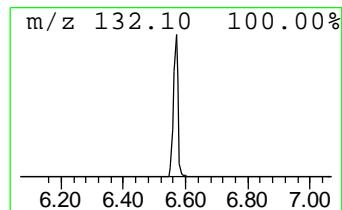
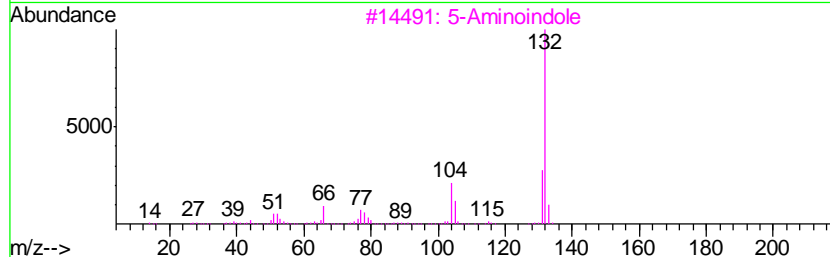
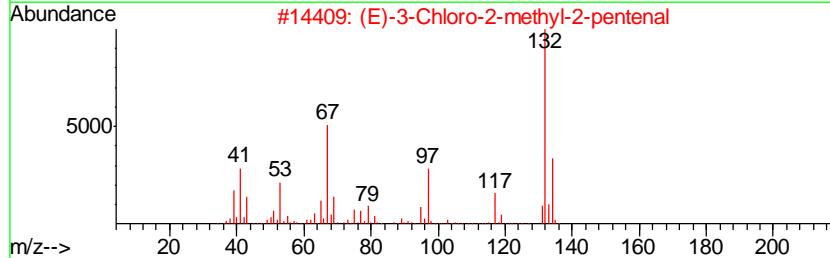
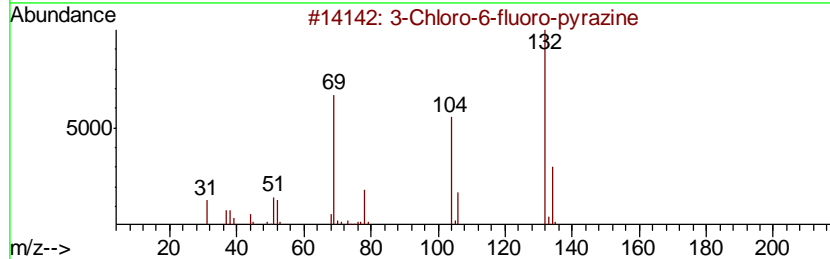
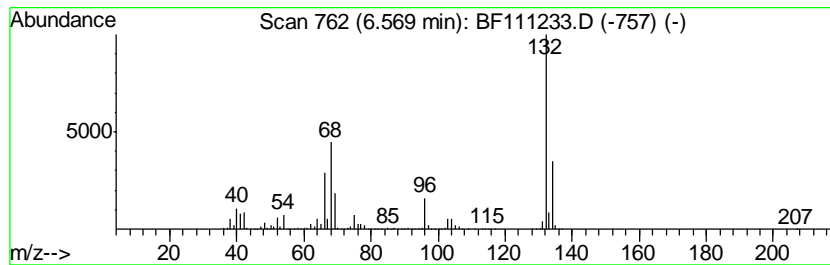
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 Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	63.16 ng	11663700	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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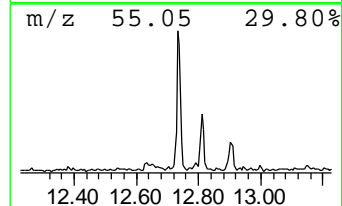
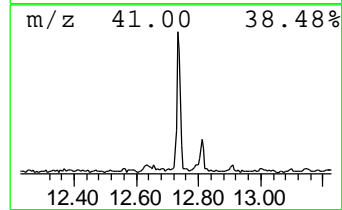
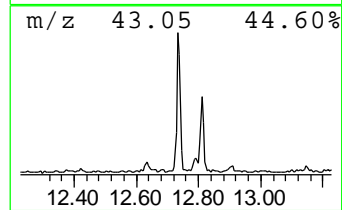
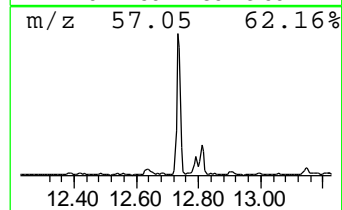
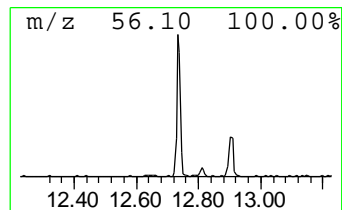
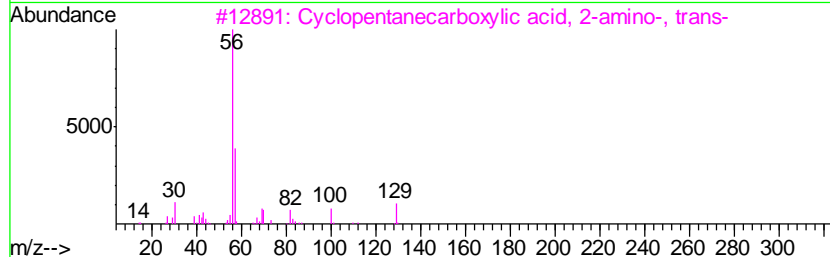
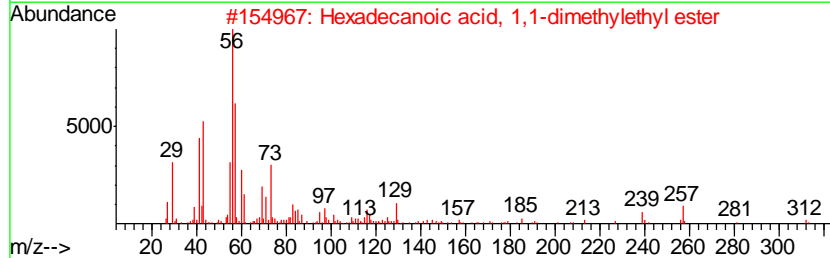
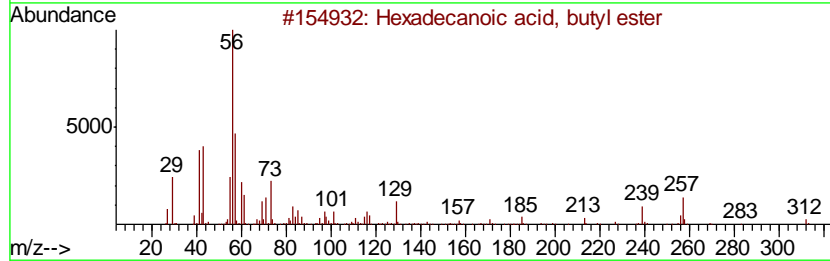
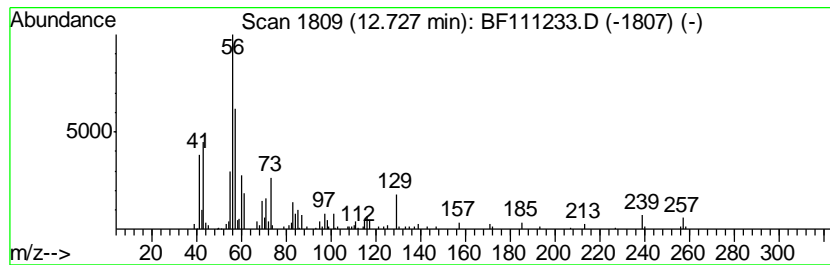
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 Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	2.60 ng	577351	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5		Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	40



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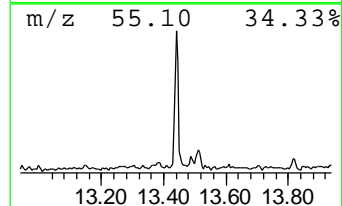
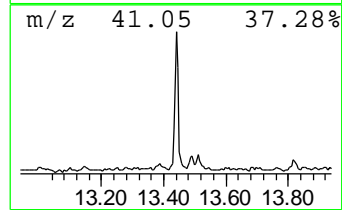
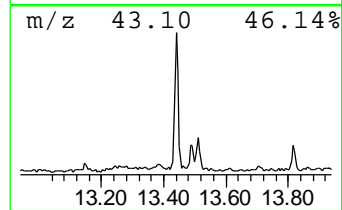
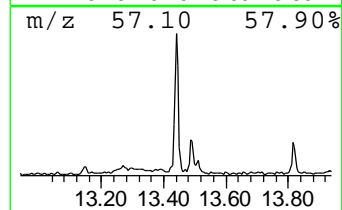
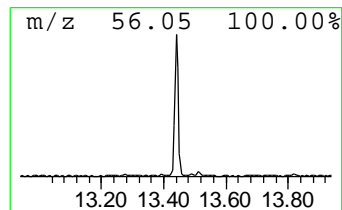
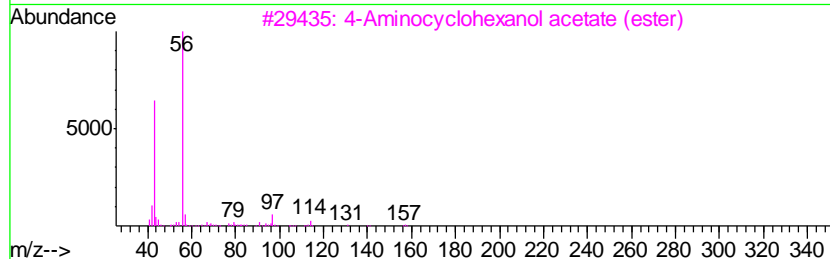
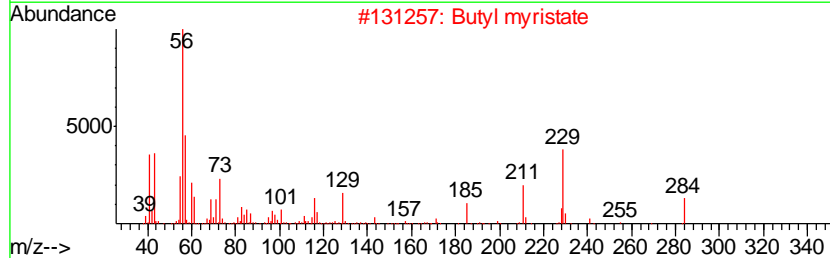
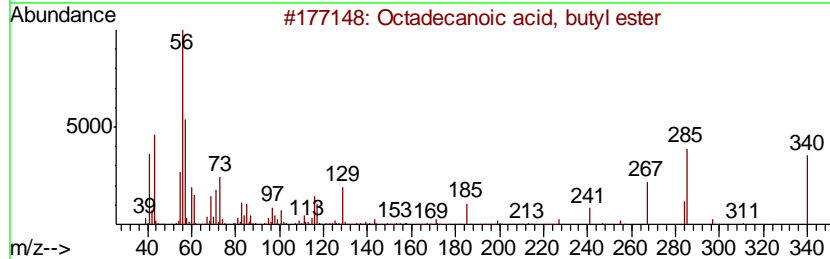
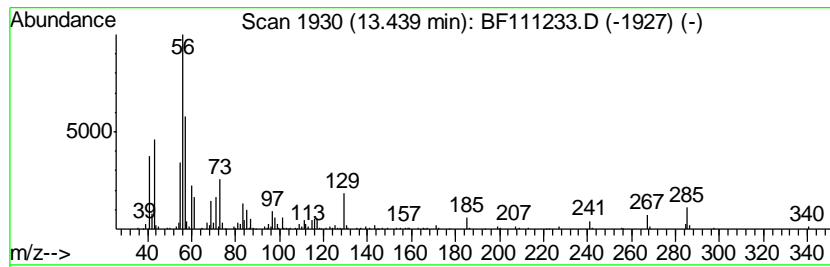
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 Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	2.00 ng	444931	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2		Butyl myristate	284	C18H36O2	000110-36-1	86
3		4-Aminocyclohexanol acetate (ester)	157	C8H15NO2	1000130-62-8	43
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	43
5		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	3.8	ng	695120	1	6.80	3693580	20.0
unknown6.57	6.57	63.2	ng	11663700	1	6.80	3693580	20.0
Hexadecanoic acid...	12.73	2.6	ng	577351	5	13.95	4448750	20.0
Octadecanoic acid...	13.44	2.0	ng	444931	5	13.95	4448750	20.0