

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100817\
 Data File : BF099230.D
 Acq On : 8 Oct 2017 14:14
 Operator : SJ/JU
 Sample : I5604-06
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-B-100217

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-BF092317.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	2.934	140	144	151	rVB	39265	56301	1.42%	0.183%
2	5.116	511	515	525	rVB	561347	817743	20.65%	2.664%
3	5.504	576	581	585	rBV	2739129	2979857	75.25%	9.708%
4	6.504	746	751	754	rBV	2598375	2578237	65.11%	8.399%
5	6.640	769	774	777	rBV	3177627	3325787	83.99%	10.834%
6	6.698	781	784	797	rVB	47992	55587	1.40%	0.181%
7	6.863	809	812	816	rBV	845890	736001	18.59%	2.398%
8	7.022	834	839	843	rBV	2774746	2733091	69.02%	8.904%
9	7.434	903	909	912	rBV	2074763	2217296	55.99%	7.223%
10	8.145	1026	1030	1033	rBV	1206381	1039618	26.25%	3.387%
11	9.222	1207	1213	1216	rBV	3827779	3959875	100.00%	12.900%
12	9.898	1323	1328	1332	rBV	1161817	1123352	28.37%	3.660%
13	10.692	1458	1463	1478	rBV	2043256	2251060	56.85%	7.333%
14	11.386	1577	1581	1585	rBV	1247373	1142744	28.86%	3.723%
15	12.780	1815	1818	1821	rBV	179694	136304	3.44%	0.444%
16	12.974	1846	1851	1854	rBV2	3387295	3732896	94.27%	12.161%
17	13.486	1934	1938	1941	rBV	122674	99026	2.50%	0.323%
18	14.027	2026	2030	2034	rBV	1101858	981327	24.78%	3.197%
19	15.504	2276	2281	2291	rBV	588295	730320	18.44%	2.379%

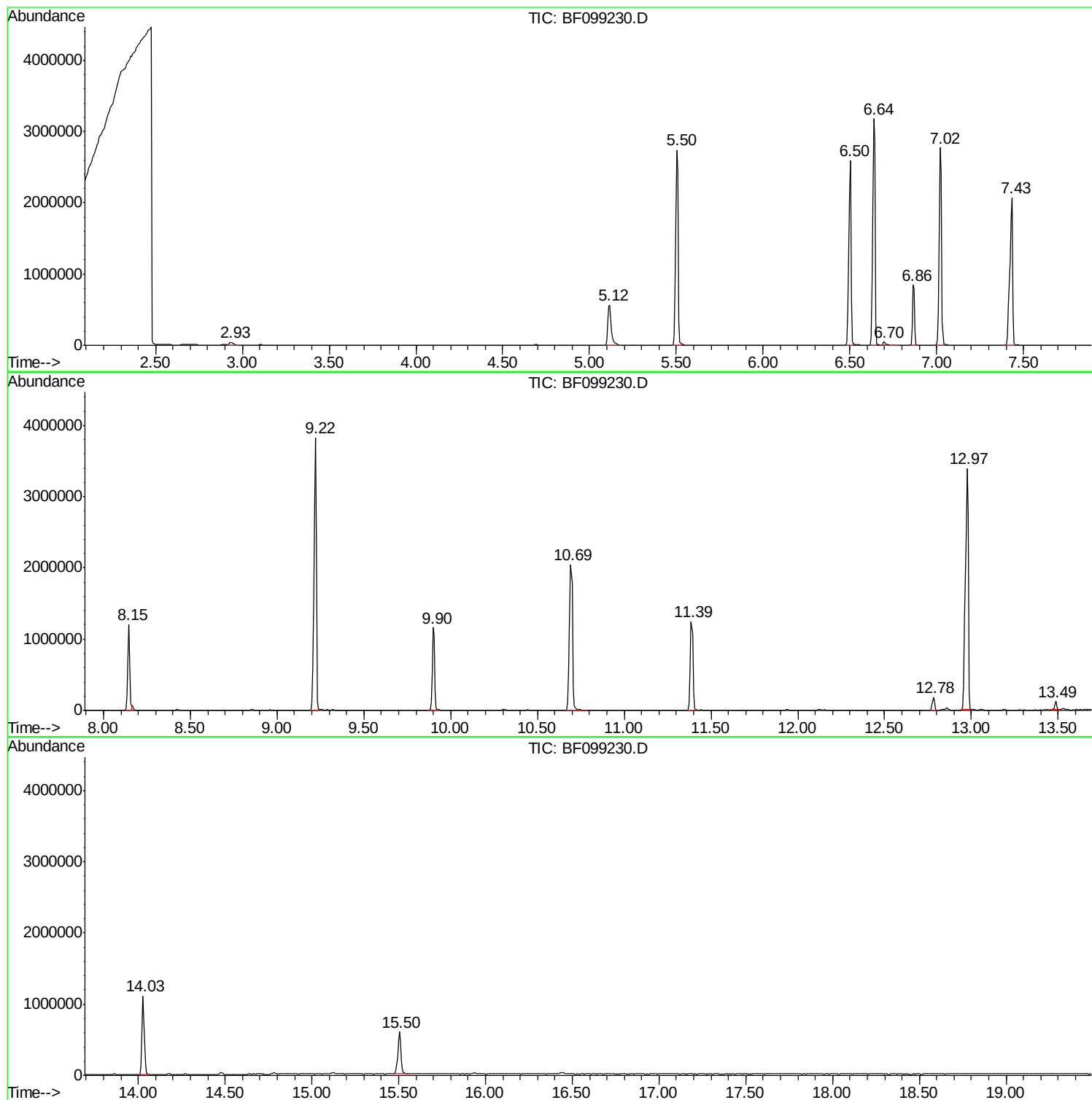
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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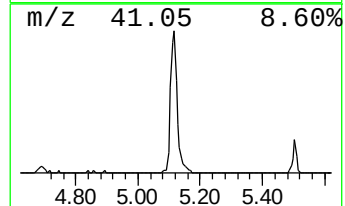
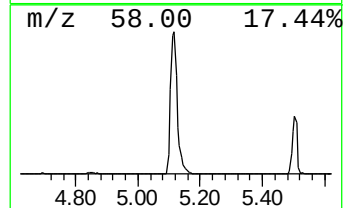
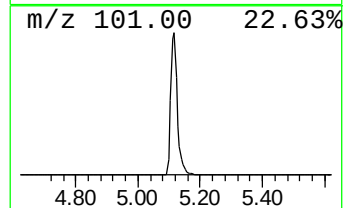
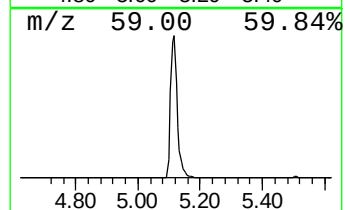
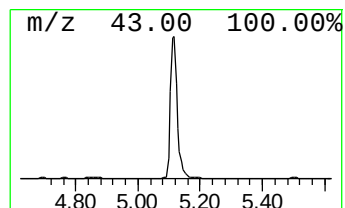
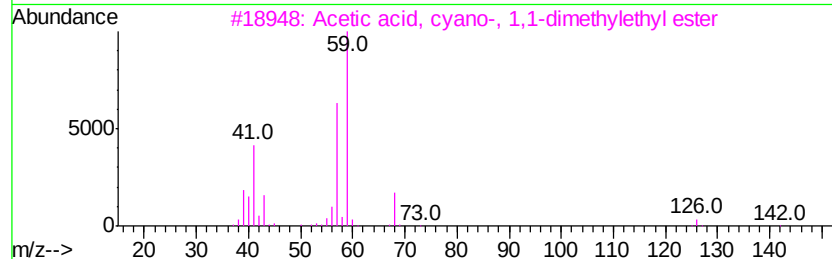
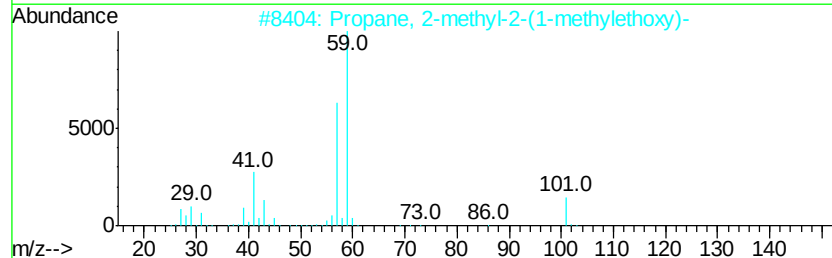
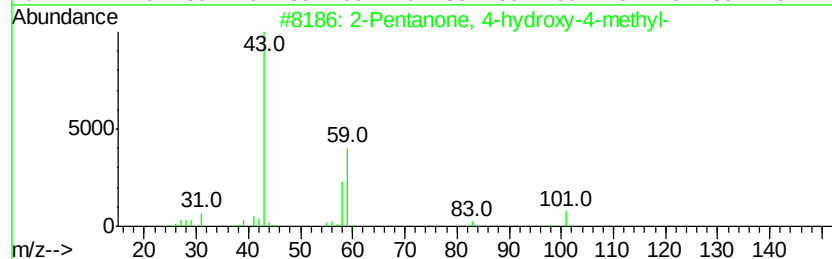
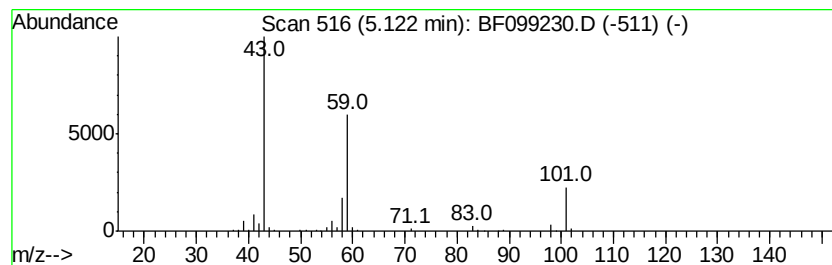
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	22.22 ng	817743	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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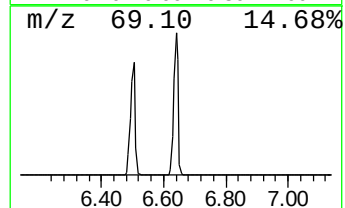
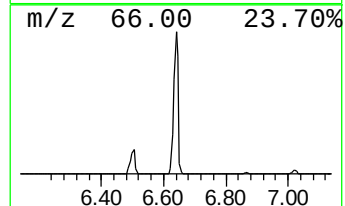
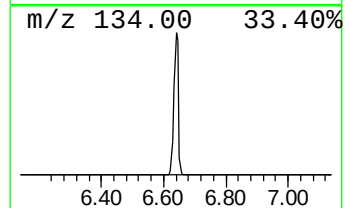
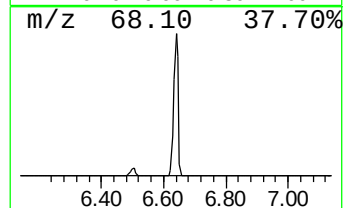
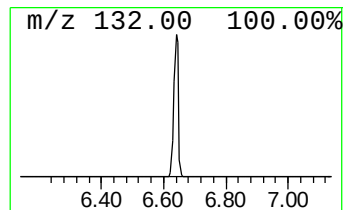
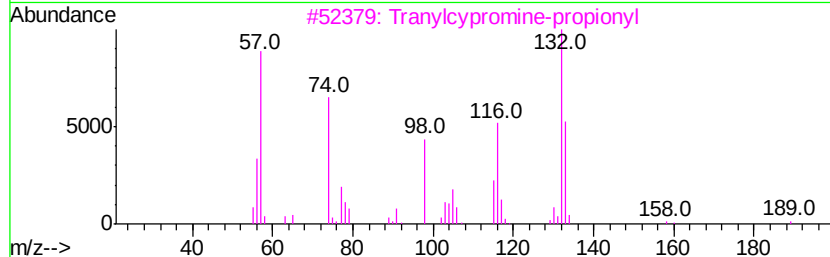
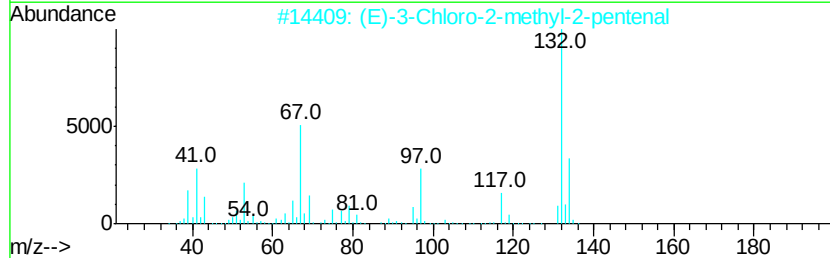
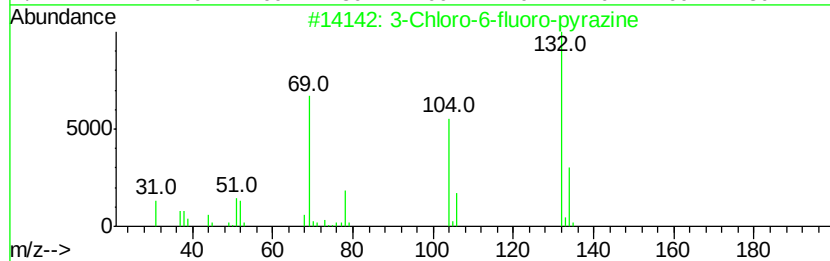
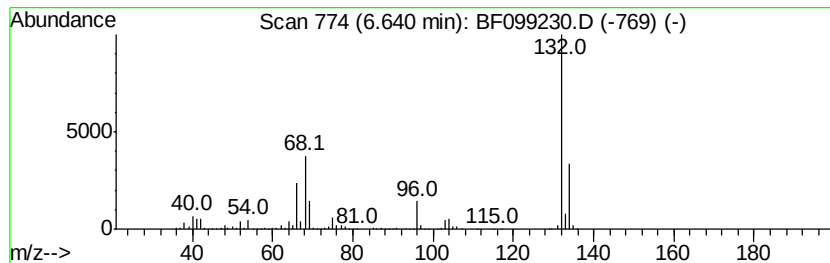
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Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	90.37 ng	3325790	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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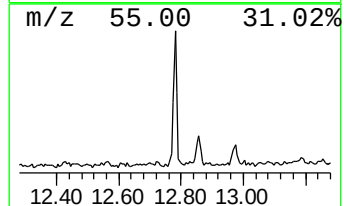
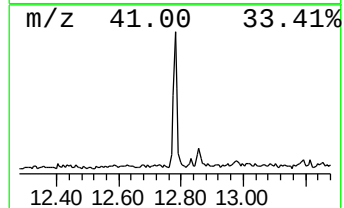
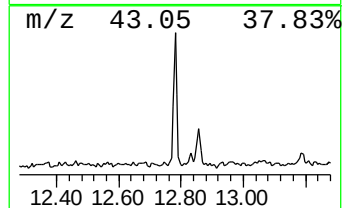
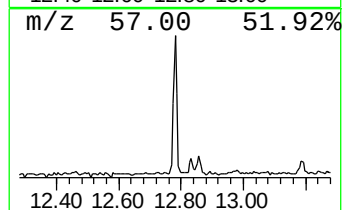
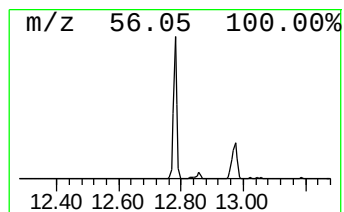
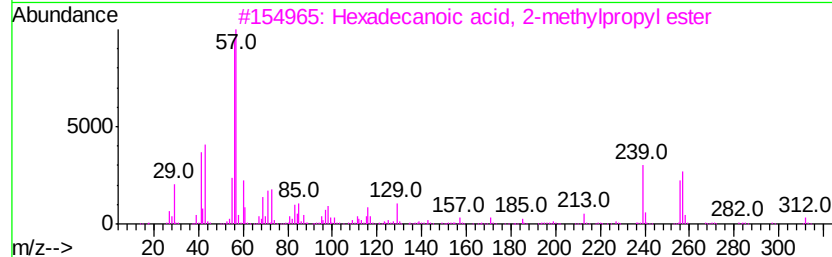
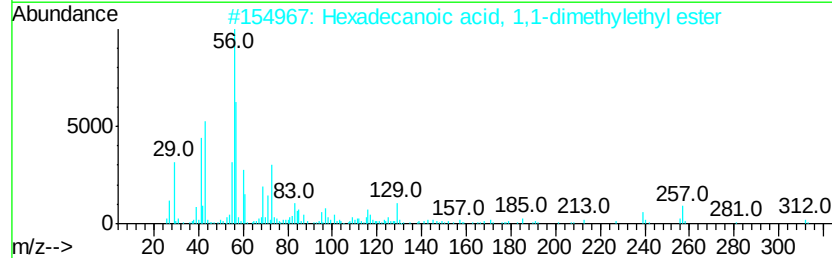
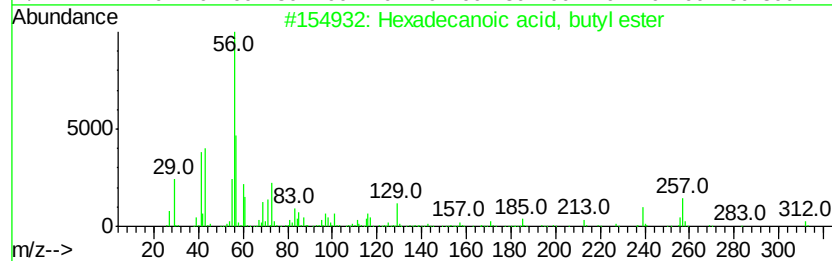
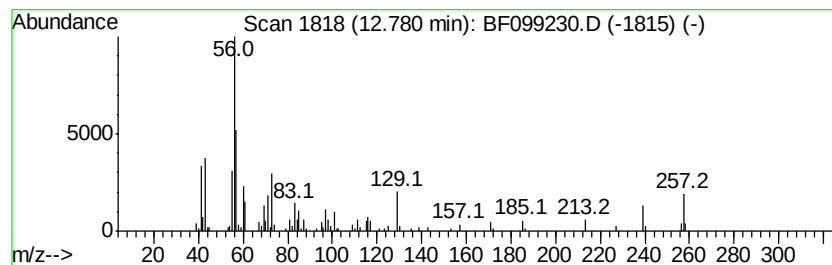
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	2.78 ng	136304	Chrysene-d12	14.03

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	74
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	45
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	37



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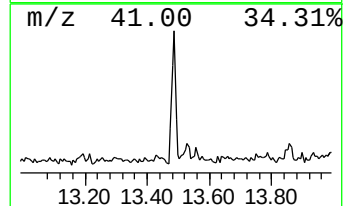
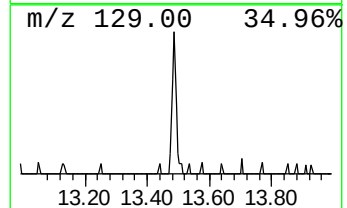
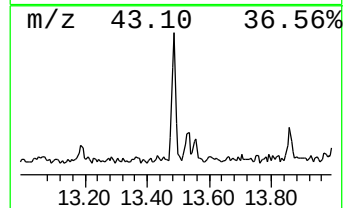
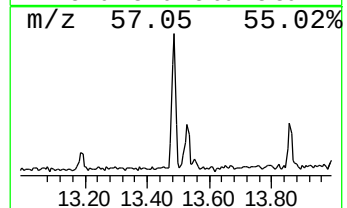
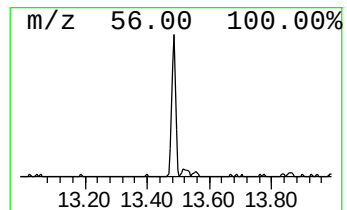
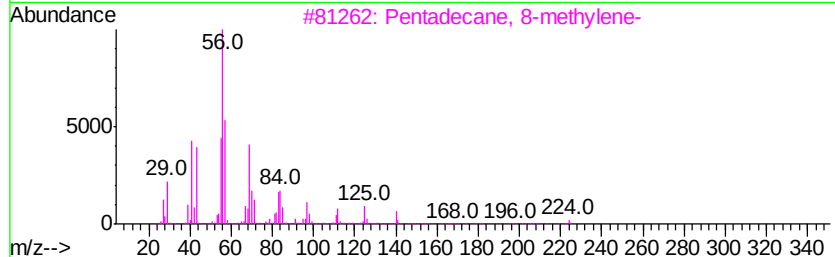
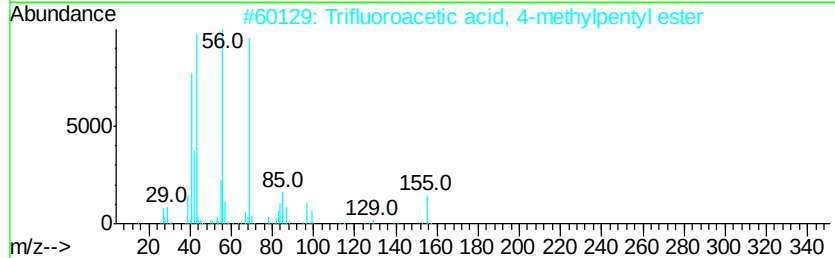
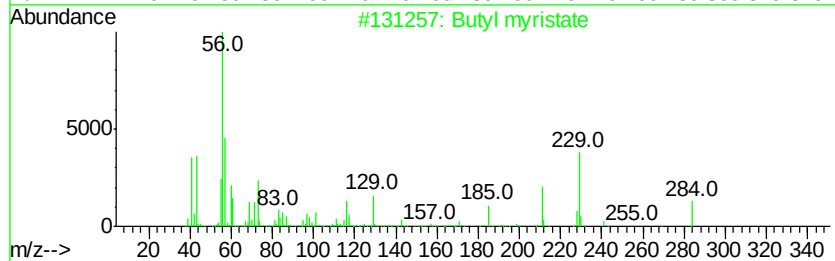
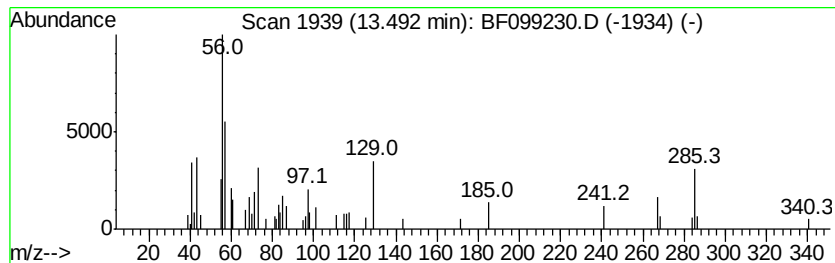
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Peak Number 5 Butyl myristate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.49	2.02 ng	99026	Chrysene-d12	14.03	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	64
2	Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	32
3	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
4	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	32
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.12	22.2	ng	817743	1	6.86	736001	20.0
unknown6.64	6.64	90.4	ng	3325790	1	6.86	736001	20.0
Hexadecanoic acid...	12.78	2.8	ng	136304	5	14.03	981327	20.0
Butyl myristate	13.49	2.0	ng	99026	5	14.03	981327	20.0