

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062118\
 Data File : BF106655.D
 Acq On : 21 Jun 2018 12:18
 Operator : JU/SJ
 Sample : J3575-21 2X
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-13

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF061918.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	5.184	480	484	494	rBV	83483	86732	7.40%	0.655%
2	5.595	551	554	566	rBV	1056630	984990	84.06%	7.435%
3	6.601	721	725	736	rBV	1228023	1060939	90.54%	8.008%
4	6.736	744	748	751	rBV	1223344	1075784	91.81%	8.120%
5	6.960	782	786	789	rBV	725810	571838	48.80%	4.316%
6	7.113	808	812	816	rBV	978393	814707	69.53%	6.149%
7	7.519	877	881	884	rBV	801263	690782	58.95%	5.214%
8	8.242	1000	1004	1007	rBV	970585	760403	64.89%	5.740%
9	9.313	1183	1186	1190	rBV	1397282	1171767	100.00%	8.844%
10	9.707	1248	1253	1259	rVB	141245	114737	9.79%	0.866%
11	9.913	1284	1288	1292	rBV2	34822	30492	2.60%	0.230%
12	10.001	1299	1303	1307	rBV2	1013767	882727	75.33%	6.663%
13	10.413	1370	1373	1376	rVB	44865	33226	2.84%	0.251%
14	10.630	1405	1410	1413	rBV	13791	16557	1.41%	0.125%
15	10.713	1421	1424	1428	rVB	17940	14803	1.26%	0.112%
16	10.795	1434	1438	1441	rBV	856673	771545	65.84%	5.824%
17	10.883	1450	1453	1458	rBV	43563	48104	4.11%	0.363%
18	11.336	1527	1530	1532	rBV	24281	21166	1.81%	0.160%
19	11.495	1553	1557	1560	rBV	949208	857668	73.19%	6.474%
20	12.171	1669	1672	1674	rBV	14372	14734	1.26%	0.111%
21	12.542	1732	1735	1737	rBV	13679	16078	1.37%	0.121%
22	12.707	1760	1763	1767	rBV	93715	86340	7.37%	0.652%
23	12.877	1789	1792	1796	rVB	179497	162824	13.90%	1.229%
24	12.942	1796	1803	1809	rBV	100845	163902	13.99%	1.237%
25	12.995	1809	1812	1815	rVV	18105	18758	1.60%	0.142%
26	13.077	1822	1826	1829	rBV	1145582	1029333	87.84%	7.769%
27	13.154	1836	1839	1841	rBV4	12153	16554	1.41%	0.125%
28	13.371	1873	1876	1878	rBV2	27796	28187	2.41%	0.213%
29	13.465	1890	1892	1894	rBV	36755	28143	2.40%	0.212%
30	13.589	1909	1913	1916	rBV	121669	105045	8.96%	0.793%
31	13.630	1918	1920	1923	rVV	24655	21622	1.85%	0.163%
32	13.842	1953	1956	1959	rBV	28641	25080	2.14%	0.189%
33	13.877	1960	1962	1964	rBV	34271	32656	2.79%	0.246%
34	13.960	1973	1976	1980	rBV3	66064	75311	6.43%	0.568%

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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

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35	14.148	2004	2008	2011	rBV	787818	767448	65.49%	5.793%
36	14.289	2030	2032	2035	rVB	35579	25585	2.18%	0.193%
37	15.695	2266	2271	2277	rBV	470090	621990	53.08%	4.695%

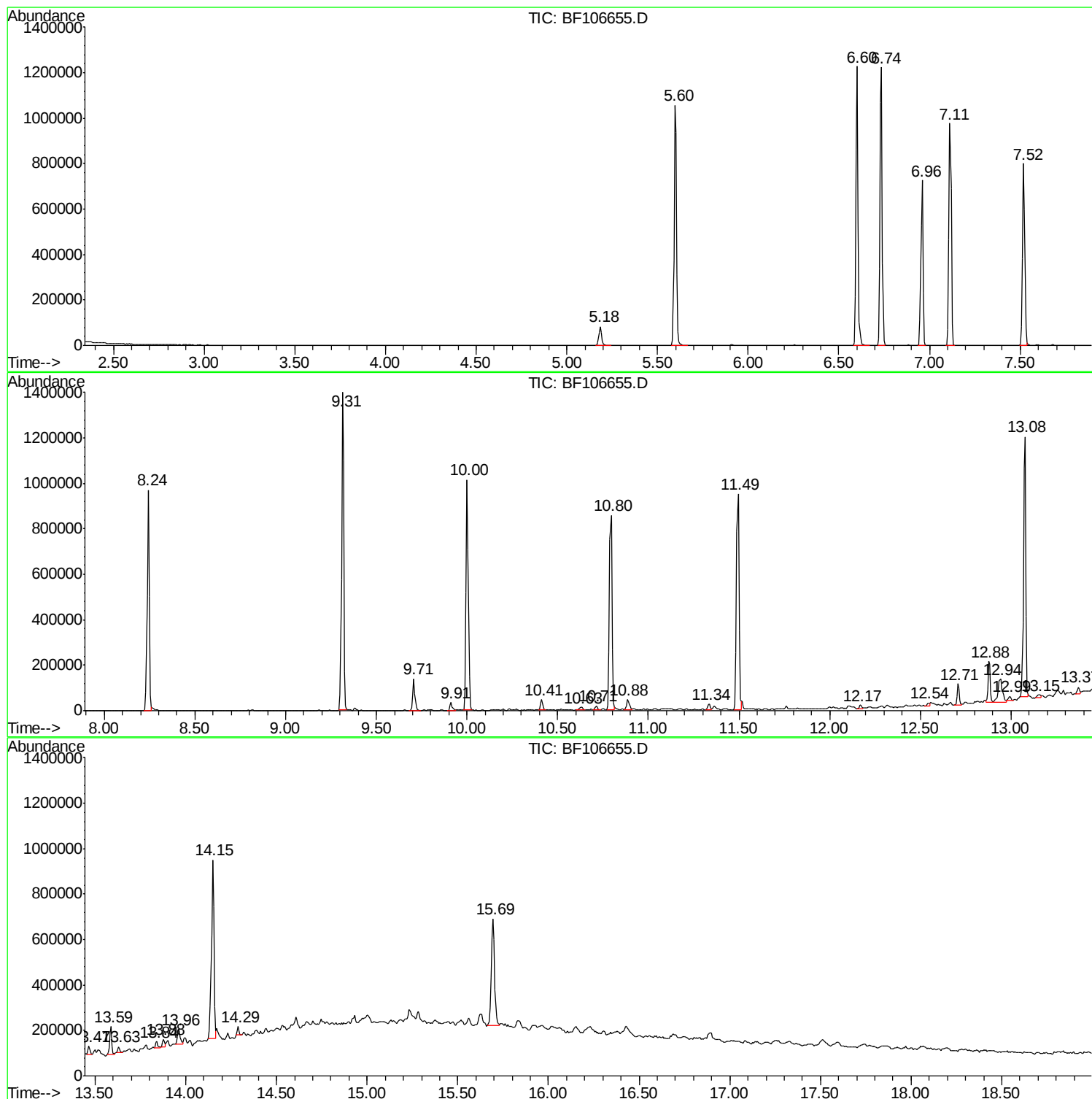
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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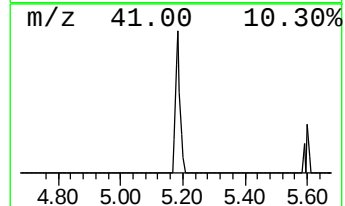
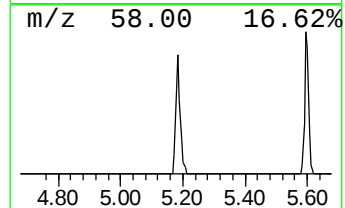
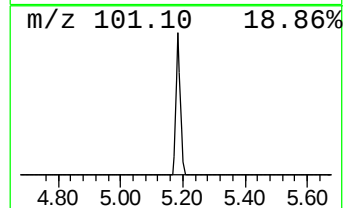
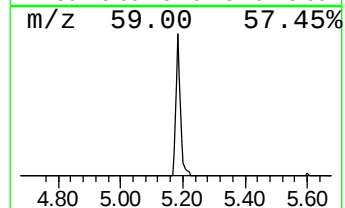
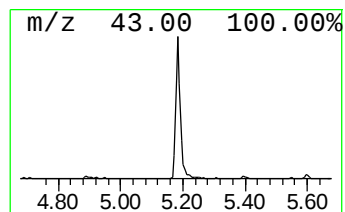
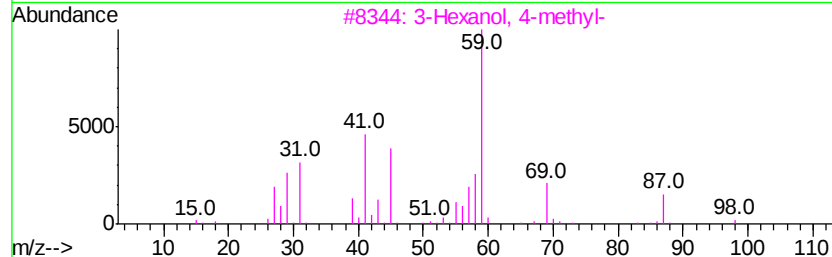
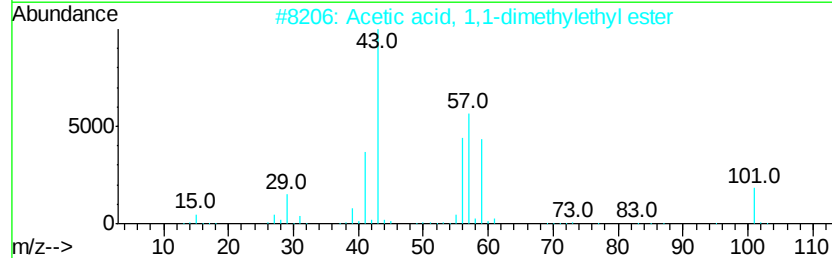
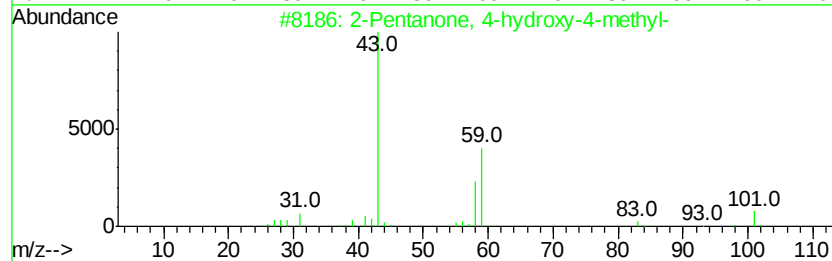
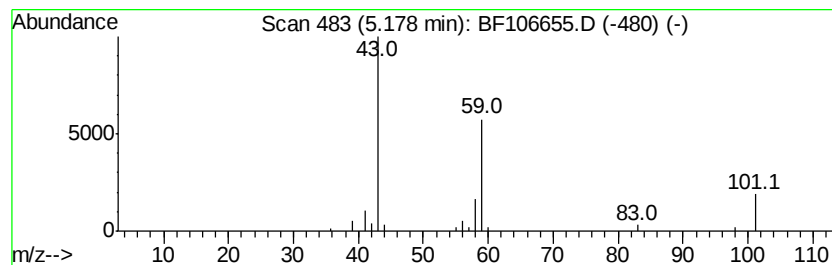
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	3.03 ng	86732	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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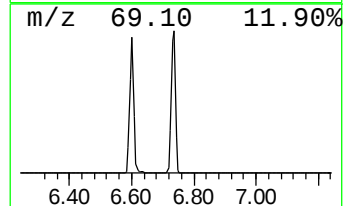
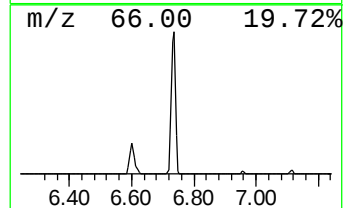
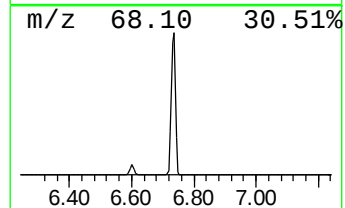
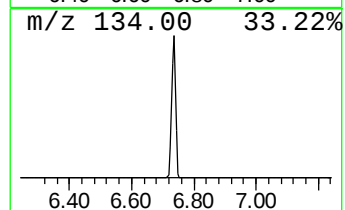
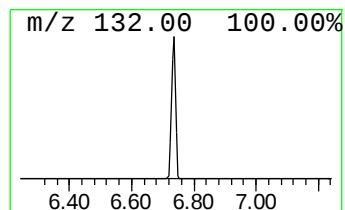
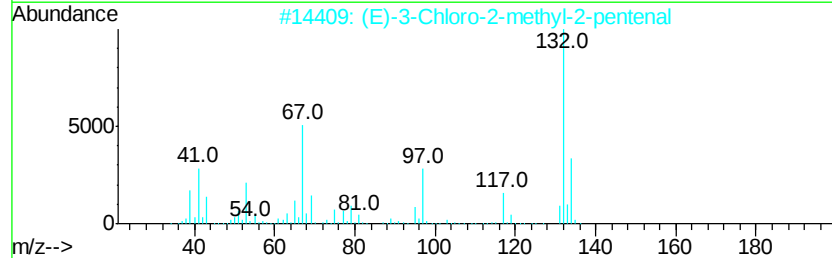
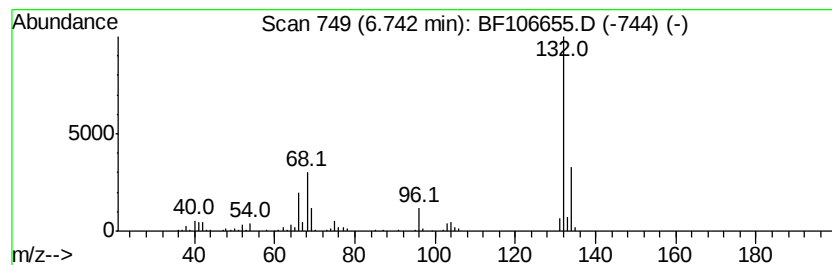
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	37.63 ng	1075780	1,4-Dichlorobenzene-d4	6.96

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	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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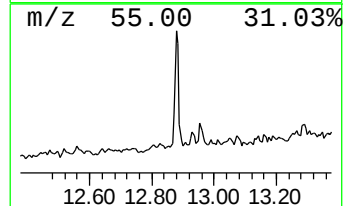
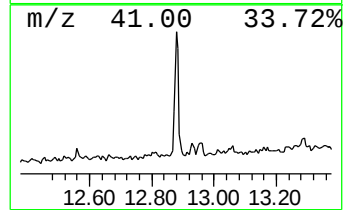
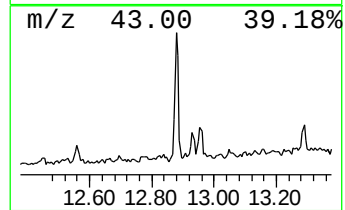
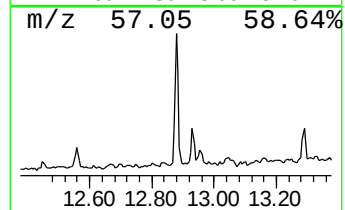
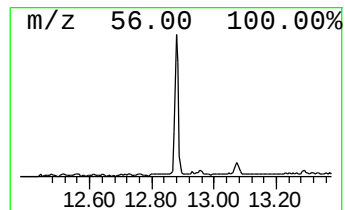
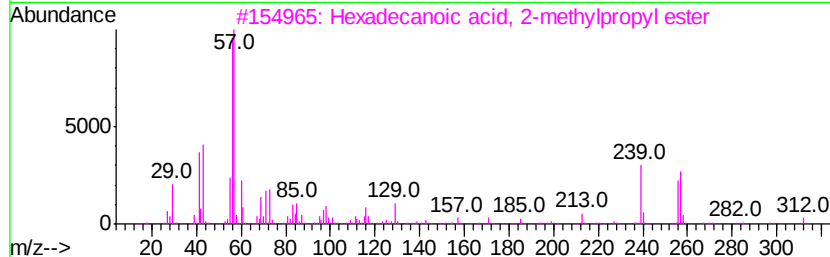
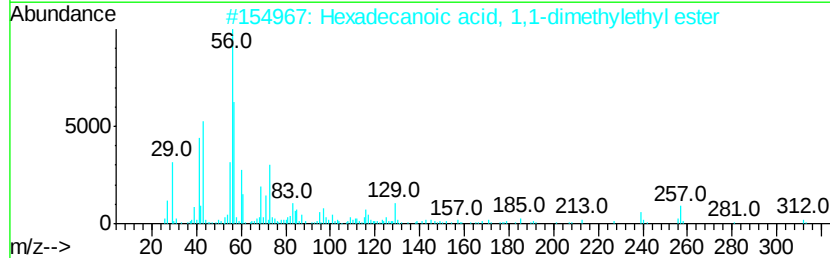
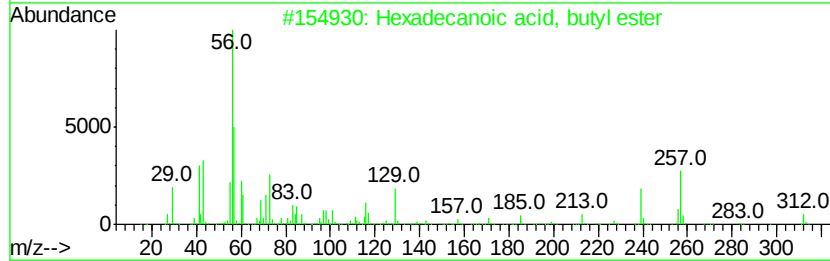
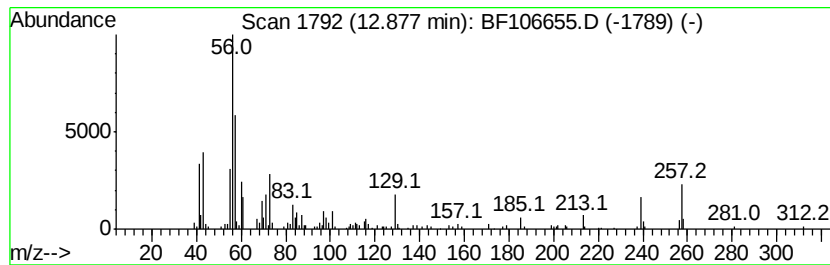
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.88	4.24 ng	162824	Chrysene-d12	14.15

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	41
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	38
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	35



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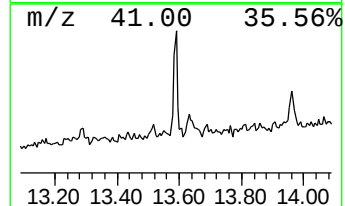
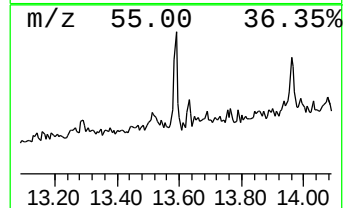
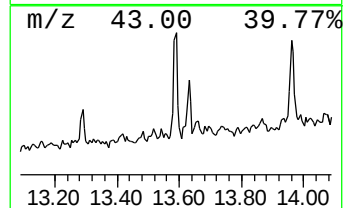
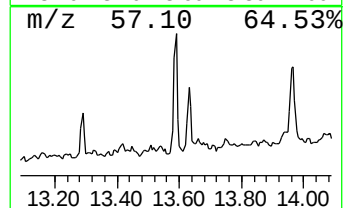
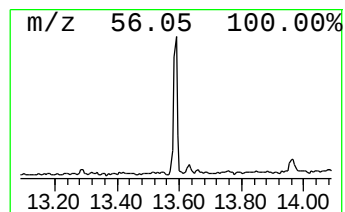
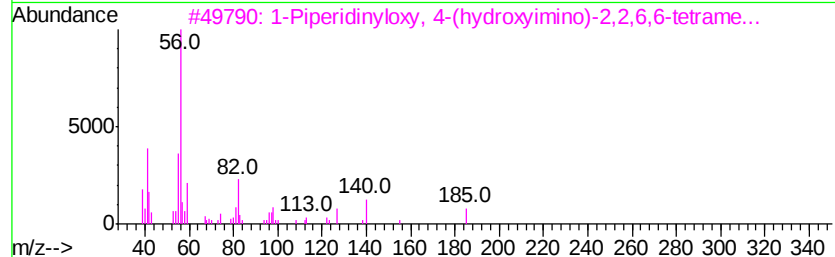
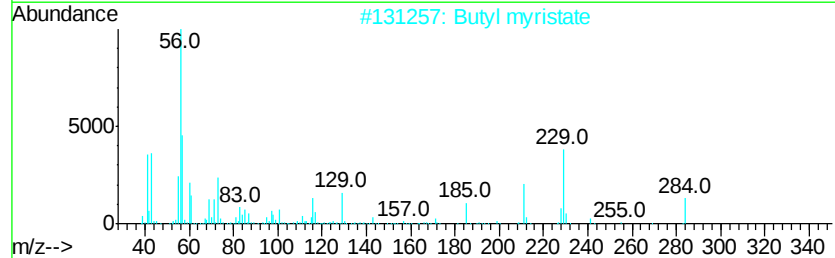
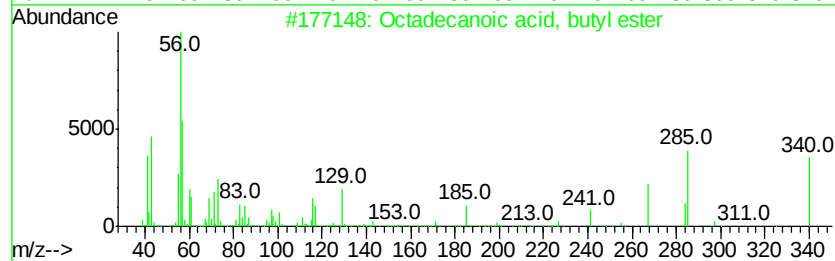
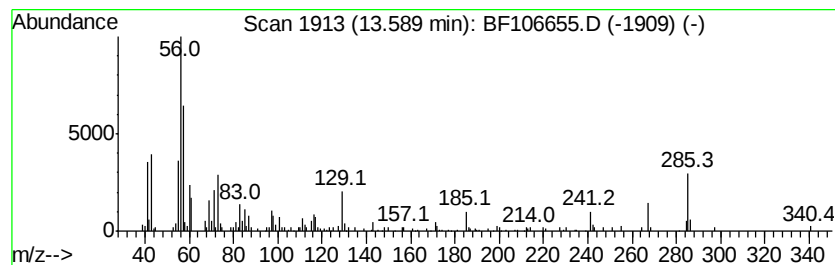
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	2.74 ng	105045	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	87
2		Butyl myristate	284	C18H36O2	000110-36-1	64
3		1-Piperidinylloxv, 4-(hydroximin...	185	C9H17N2O2	003229-75-2	35
4		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	30
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.18	3.0	ng	86732	1	6.96	571838	20.0
unknown6.74	6.74	37.6	ng	1075780	1	6.96	571838	20.0
Hexadecanoic acid...	12.88	4.2	ng	162824	5	14.15	767448	20.0
Octadecanoic acid...	13.59	2.7	ng	105045	5	14.15	767448	20.0