

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123020\
 Data File : BF122880.D
 Acq On : 30 Dec 2020 15:56
 Operator : JU/CG
 Sample : L5235-01 5X
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-05-122920

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-BF120520.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122880.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.440	566	570	587	rBV	225056	297981	15.62%	2.668%
2	6.457	740	743	757	rBV	211533	296551	15.55%	2.655%
3	6.816	801	804	813	rBV	676816	644668	33.79%	5.771%
4	7.381	897	900	905	rBV	167792	169463	8.88%	1.517%
5	8.104	1019	1023	1029	rBV	878757	741727	38.88%	6.640%
6	9.175	1202	1205	1216	rBV	382765	376976	19.76%	3.375%
7	9.575	1269	1273	1276	rBV2	19780	22383	1.17%	0.200%
8	9.786	1306	1309	1313	rBV2	29907	28420	1.49%	0.254%
9	9.857	1317	1321	1336	rVB	1061028	908480	47.62%	8.133%
10	10.286	1391	1394	1397	rVB	35412	26238	1.38%	0.235%
11	10.645	1453	1455	1466	rVB	201415	219881	11.53%	1.968%
12	10.757	1472	1474	1480	rBV2	35971	43326	2.27%	0.388%
13	11.210	1544	1551	1554	rBV2	29347	33637	1.76%	0.301%
14	11.345	1570	1574	1581	rBV	1015398	876632	45.95%	7.848%
15	11.633	1620	1623	1626	rBV	29400	23727	1.24%	0.212%
16	11.733	1637	1640	1643	rBV	531746	396249	20.77%	3.547%
17	11.869	1660	1663	1671	rVB3	65987	71111	3.73%	0.637%
18	12.039	1689	1692	1697	rBV	32612	33131	1.74%	0.297%
19	12.421	1753	1757	1759	rBV	2208255	1907664	100.00%	17.077%
20	12.445	1759	1761	1767	rVB	1178758	1033307	54.17%	9.250%
21	12.527	1771	1775	1778	rBV	232420	194843	10.21%	1.744%
22	12.563	1778	1781	1782	rBV	63464	62182	3.26%	0.557%
23	12.580	1782	1784	1793	rVV4	69752	96898	5.08%	0.867%
24	12.657	1794	1797	1803	rVV6	22332	30504	1.60%	0.273%
25	12.798	1817	1821	1827	rVB2	46242	74960	3.93%	0.671%
26	12.927	1839	1843	1850	rVB	545870	489743	25.67%	4.384%
27	13.157	1879	1882	1886	rBV2	45262	65155	3.42%	0.583%
28	13.251	1896	1898	1903	rVB3	28248	27949	1.47%	0.250%
29	13.498	1938	1940	1943	rVB	35098	26188	1.37%	0.234%
30	13.986	2019	2023	2027	rBV	921179	889048	46.60%	7.959%
31	15.451	2268	2272	2283	rBV	819566	1061688	55.65%	9.504%

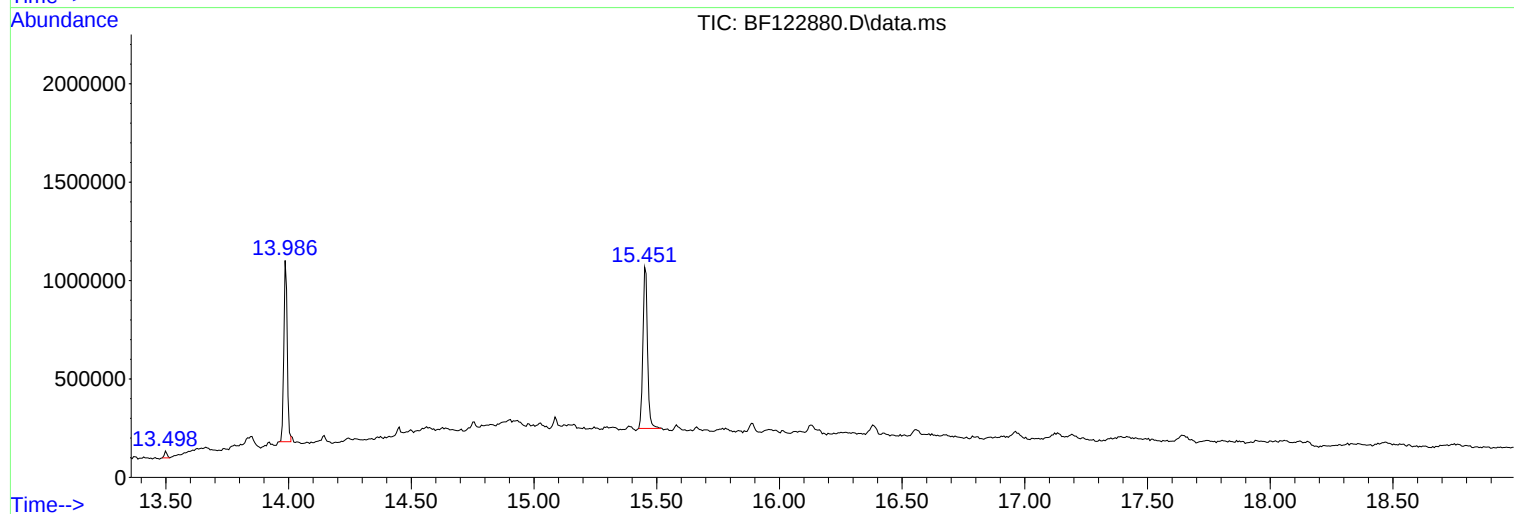
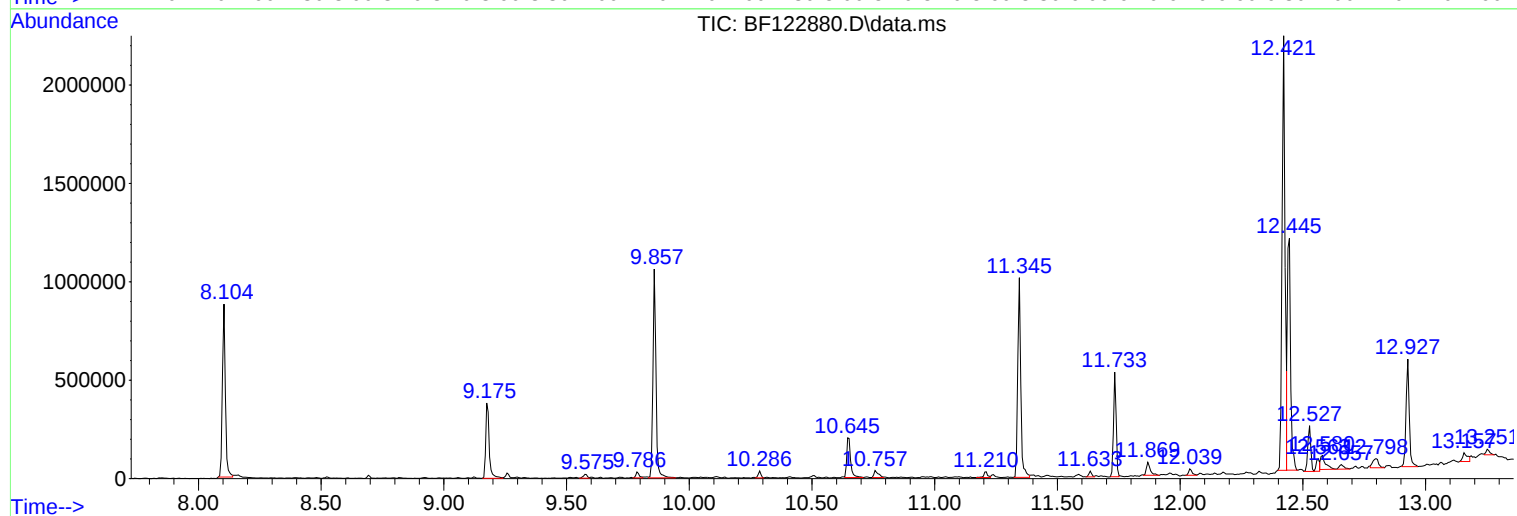
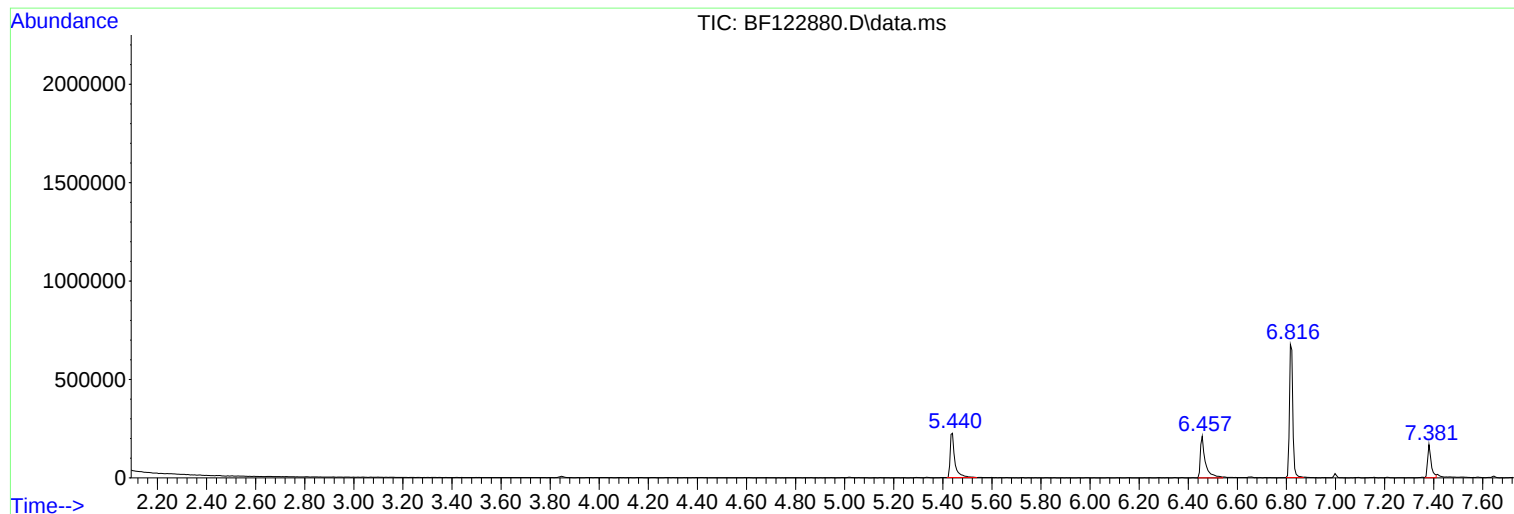
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-05-122920

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.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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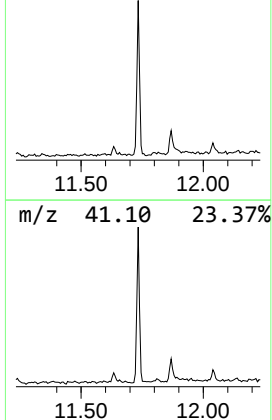
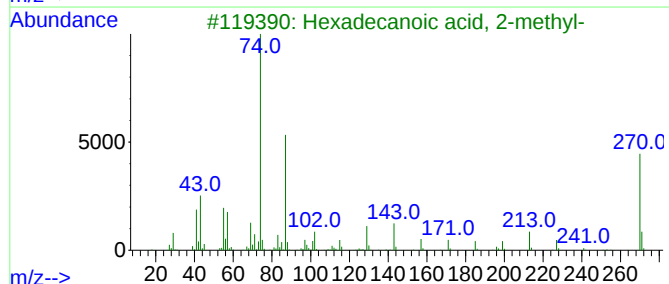
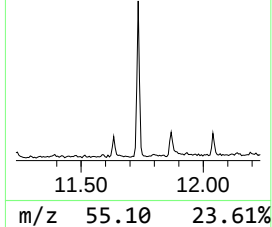
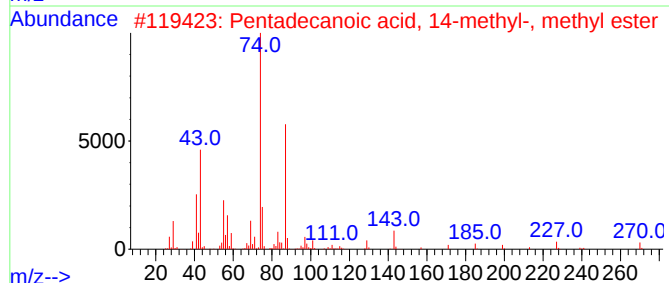
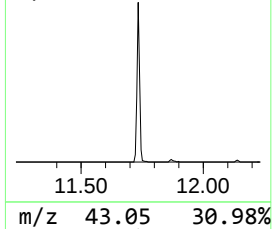
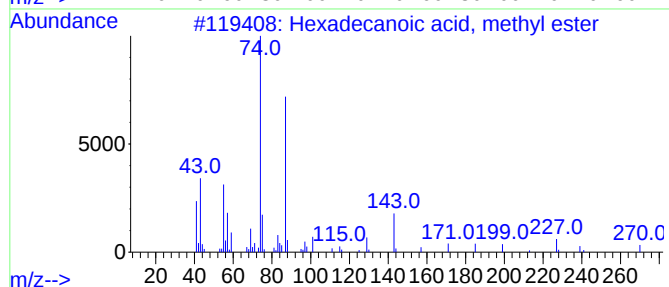
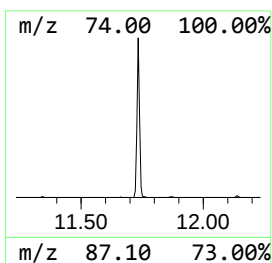
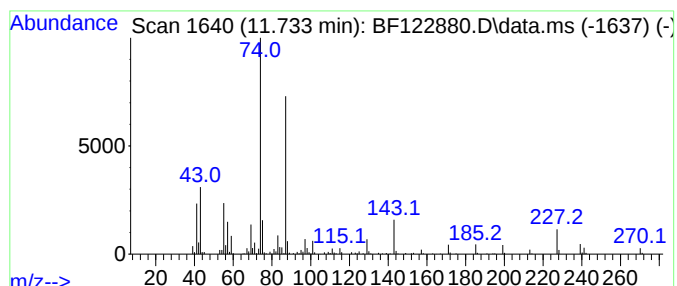
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.733	9.04 ng	396249	Phenanthrene-d10	11.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3			Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	87
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	83



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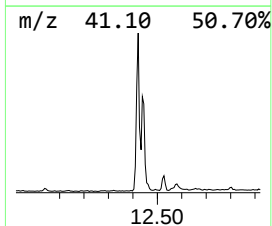
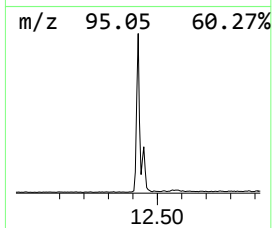
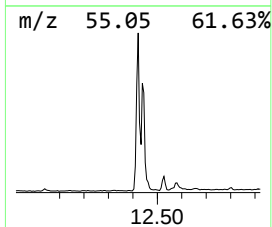
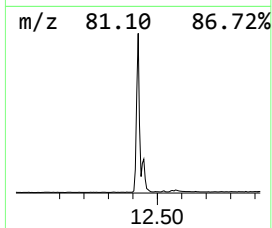
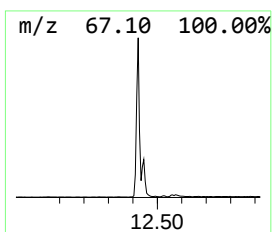
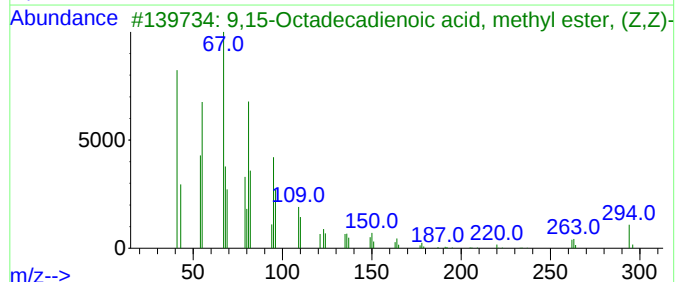
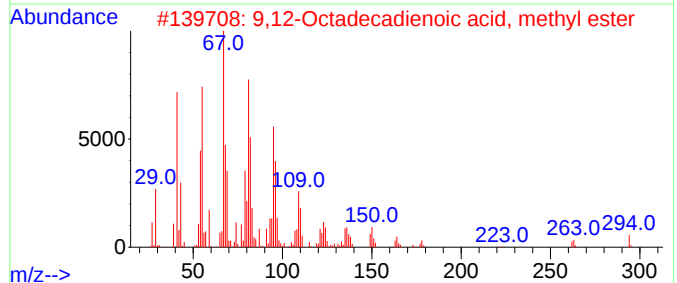
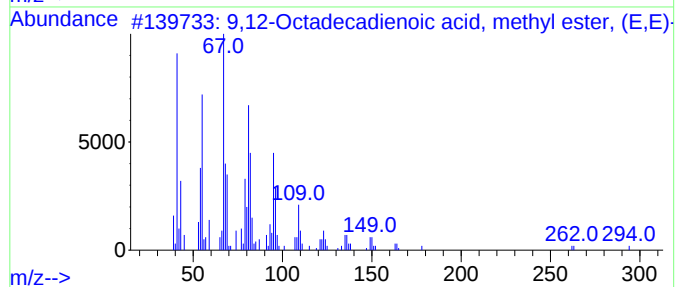
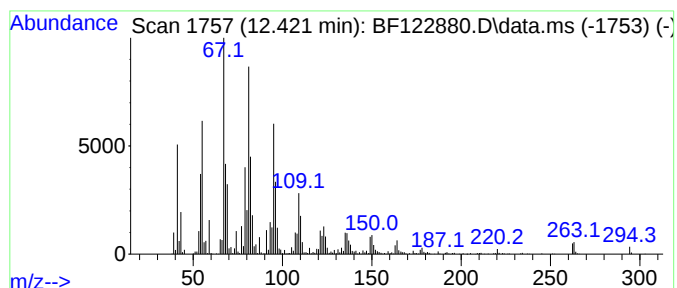
Instrument :
BNA_F
ClientSampleId :
TR-05-122920

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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 2 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.421	43.52 ng	1907660	Phenanthrene-d10	11.345	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99



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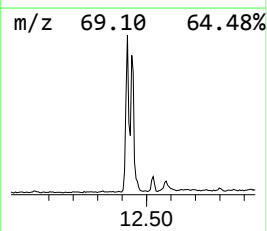
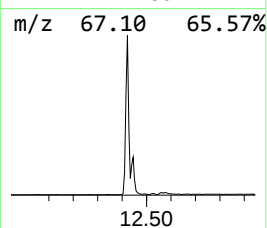
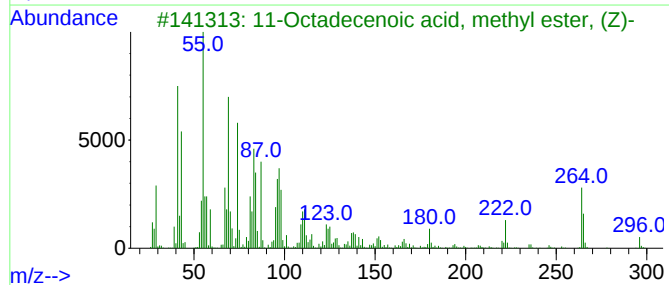
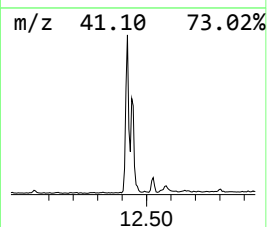
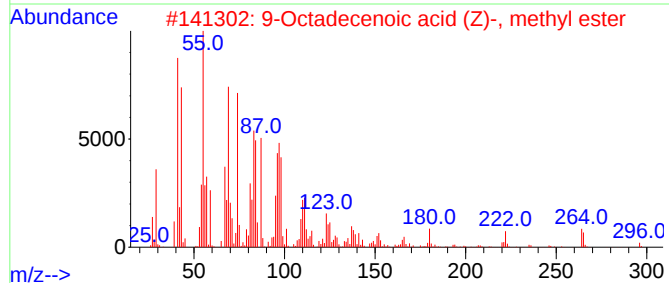
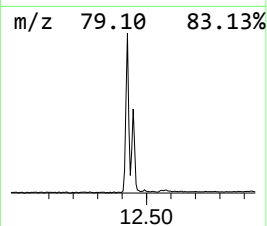
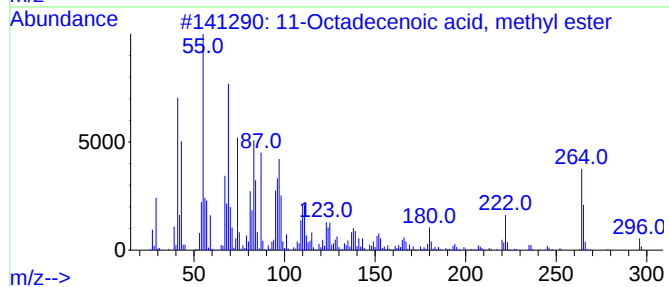
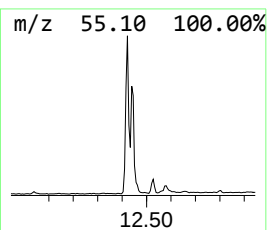
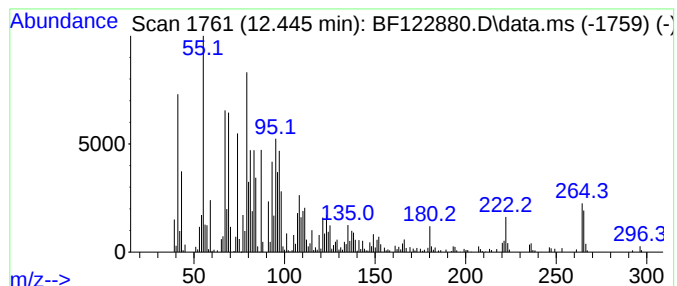
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 11-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.445	23.57 ng	1033310	Phenanthrene-d10	11.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	97
2			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	96
3			11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	96
4			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	95
5			6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	95



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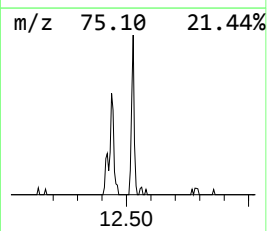
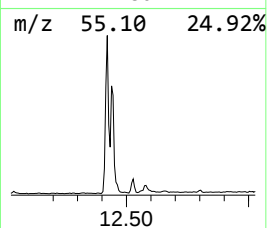
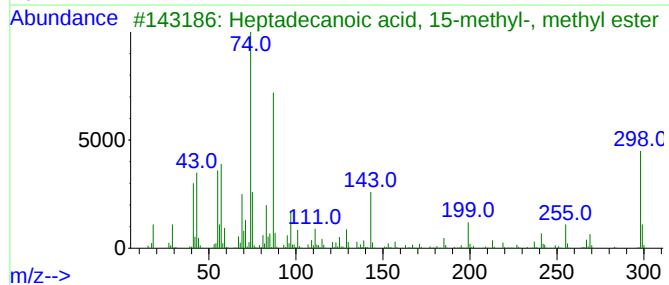
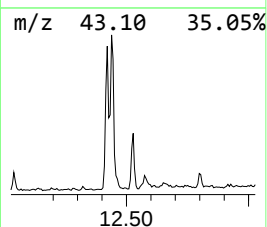
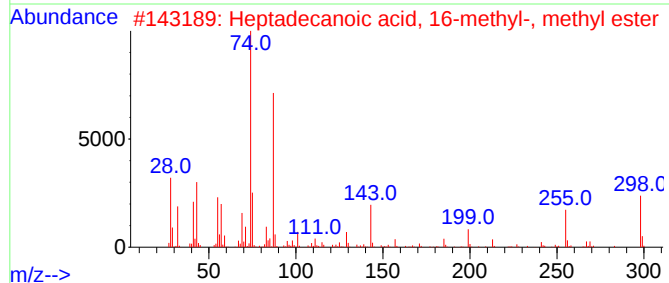
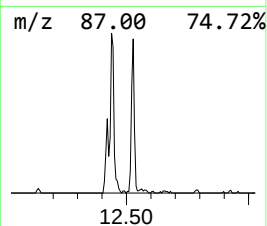
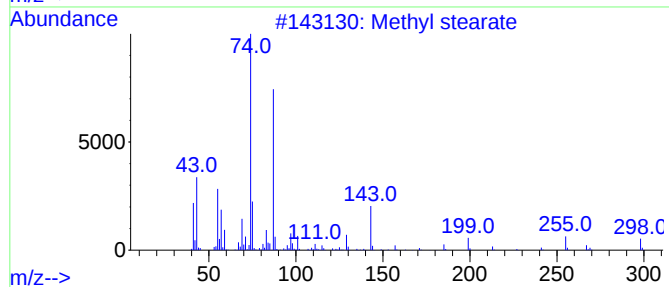
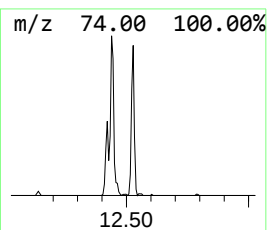
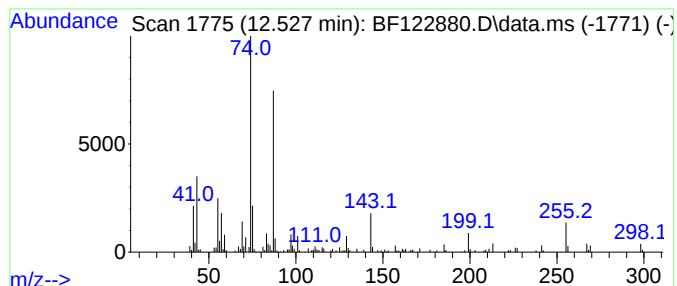
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Peak Number 4 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	4.45 ng	194843	Phenanthrene-d10	11.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	92
3			Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	91
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87



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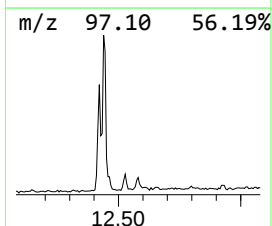
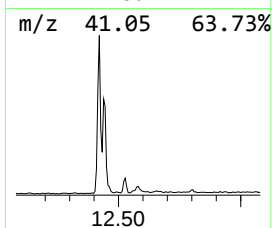
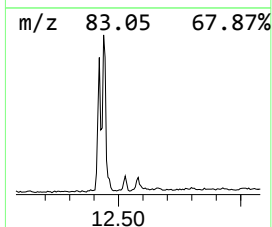
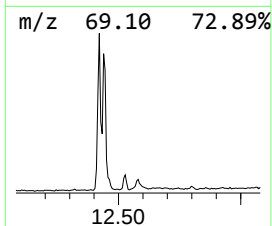
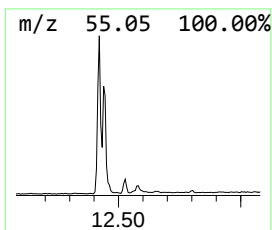
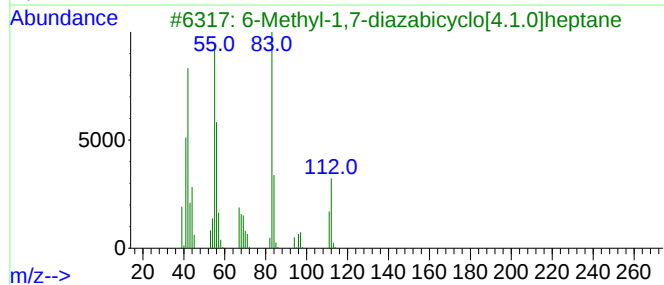
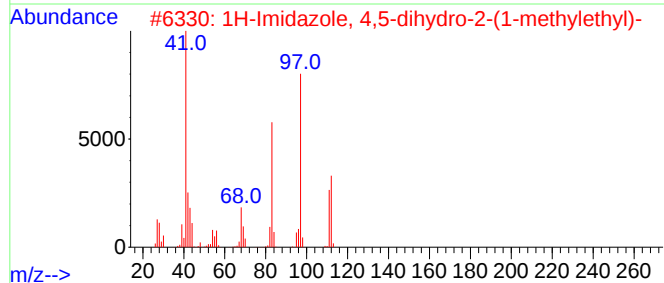
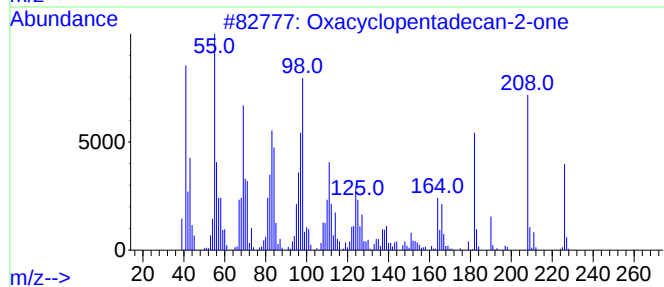
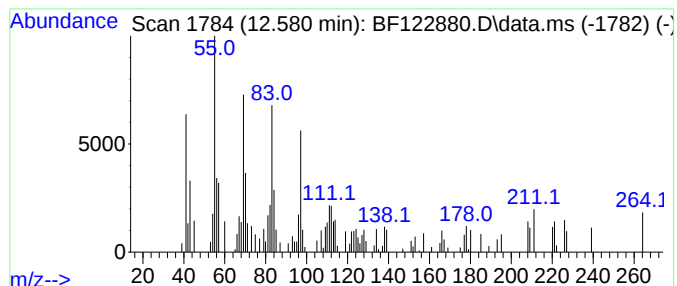
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Oxacyclopentadecan-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.580	2.21 ng	96898	Phenanthrene-d10	11.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxacyclopentadecan-2-one	226	C14H26O2	003537-83-5	50
2			1H-Imidazole, 4,5-dihydro-2-(1-m...	112	C6H12N2	040029-86-5	38
3			6-Methyl-1,7-diazabicyclo[4.1.0]...	112	C6H12N2	108602-71-7	38
4			Z-9-Pentadecenol	226	C15H30O	1000130-76-9	30
5			Cyclohexane, 1-(cyclohexylmethyl)...	208	C15H28	054934-94-0	30



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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
Hexadecanoic ac...	11.733	9.0	ng	396249	4	11.345	876632	20.0
9,12-Octadecadi...	12.421	43.5	ng	1907660	4	11.345	876632	20.0
11-Octadecenoic...	12.445	23.6	ng	1033310	4	11.345	876632	20.0
Methyl stearate	12.527	4.5	ng	194843	4	11.345	876632	20.0
Oxacyclopentade...	12.580	2.2	ng	96898	4	11.345	876632	20.0