

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051019\
 Data File : BF114143.D
 Acq On : 11 May 2019 1:26
 Operator : JU/SJ
 Sample : K2647-07 5X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SU-02-050919-B

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-BF051019.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	5.475	573	576	588	rBV	650478	625794	27.17%	2.626%
2	6.487	744	748	765	rBV	830892	831427	36.10%	3.489%
3	6.622	768	771	776	rBV	818899	720528	31.29%	3.024%
4	6.857	807	811	814	rBV	1837018	1674421	72.71%	7.027%
5	7.010	833	837	844	rVB	594762	484348	21.03%	2.033%
6	7.410	901	905	911	rBV	441705	391365	16.99%	1.642%
7	8.133	1025	1028	1032	rBV	2589784	2096183	91.03%	8.797%
8	8.728	1127	1129	1133	rBV2	32213	29625	1.29%	0.124%
9	9.204	1207	1210	1214	rBV	1111424	913779	39.68%	3.835%
10	9.292	1222	1225	1231	rBV	47437	49865	2.17%	0.209%
11	9.598	1274	1277	1281	rBV	104166	101388	4.40%	0.425%
12	9.751	1300	1303	1306	rBV	41890	44287	1.92%	0.186%
13	9.792	1306	1310	1313	rVV2	38338	63292	2.75%	0.266%
14	9.822	1313	1315	1319	rVB	71427	56207	2.44%	0.236%
15	9.886	1323	1326	1330	rBV	2485859	2212175	96.06%	9.284%
16	10.322	1397	1400	1402	rVB	63549	52734	2.29%	0.221%
17	10.433	1416	1419	1426	rVB4	19396	32772	1.42%	0.138%
18	10.539	1432	1437	1443	rBV	29359	46250	2.01%	0.194%
19	10.674	1454	1460	1467	rBV	600480	557417	24.21%	2.339%
20	10.792	1477	1480	1488	rVB	77719	97712	4.24%	0.410%
21	11.239	1553	1556	1559	rBV2	71977	71902	3.12%	0.302%
22	11.269	1559	1561	1568	rVB2	41731	47091	2.04%	0.198%
23	11.374	1575	1579	1581	rBV	2635735	2302832	100.00%	9.664%
24	11.392	1581	1582	1586	rVV	131780	104771	4.55%	0.440%
25	11.445	1589	1591	1594	rVB	45023	41961	1.82%	0.176%
26	11.669	1625	1629	1631	rBV	53775	56085	2.44%	0.235%
27	11.763	1642	1645	1648	rBV	795312	599665	26.04%	2.517%
28	11.874	1661	1664	1665	rBV2	33172	27081	1.18%	0.114%
29	11.898	1665	1668	1672	rVB3	84024	90436	3.93%	0.380%
30	11.986	1680	1683	1685	rBV2	55219	54892	2.38%	0.230%
31	12.074	1695	1698	1701	rVB	45629	43403	1.88%	0.182%
32	12.168	1711	1714	1716	rBV3	45146	43824	1.90%	0.184%
33	12.421	1755	1757	1758	rBV2	37325	27211	1.18%	0.114%
34	12.451	1758	1762	1763	rBV	1753392	1619037	70.31%	6.795%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.468	1763	1765	1768	rVB	2465226	1905248	82.73%	7.996%
36	12.557	1776	1780	1782	rBV	281031	252100	10.95%	1.058%
37	12.586	1782	1785	1788	rVV	316370	281728	12.23%	1.182%
38	12.792	1817	1820	1821	rBV2	90608	89442	3.88%	0.375%
39	12.810	1821	1823	1829	rVB	310593	323452	14.05%	1.357%
40	12.951	1844	1847	1850	rBV	1152023	923328	40.10%	3.875%
41	13.115	1872	1875	1876	rBV3	96972	84277	3.66%	0.354%
42	13.139	1877	1879	1882	rVV2	107664	116932	5.08%	0.491%
43	13.204	1885	1890	1893	rVV3	91312	160821	6.98%	0.675%
44	14.010	2023	2027	2030	rBV	2064164	1919684	83.36%	8.056%
45	15.474	2272	2276	2288	rVB	1182348	1559700	67.73%	6.546%

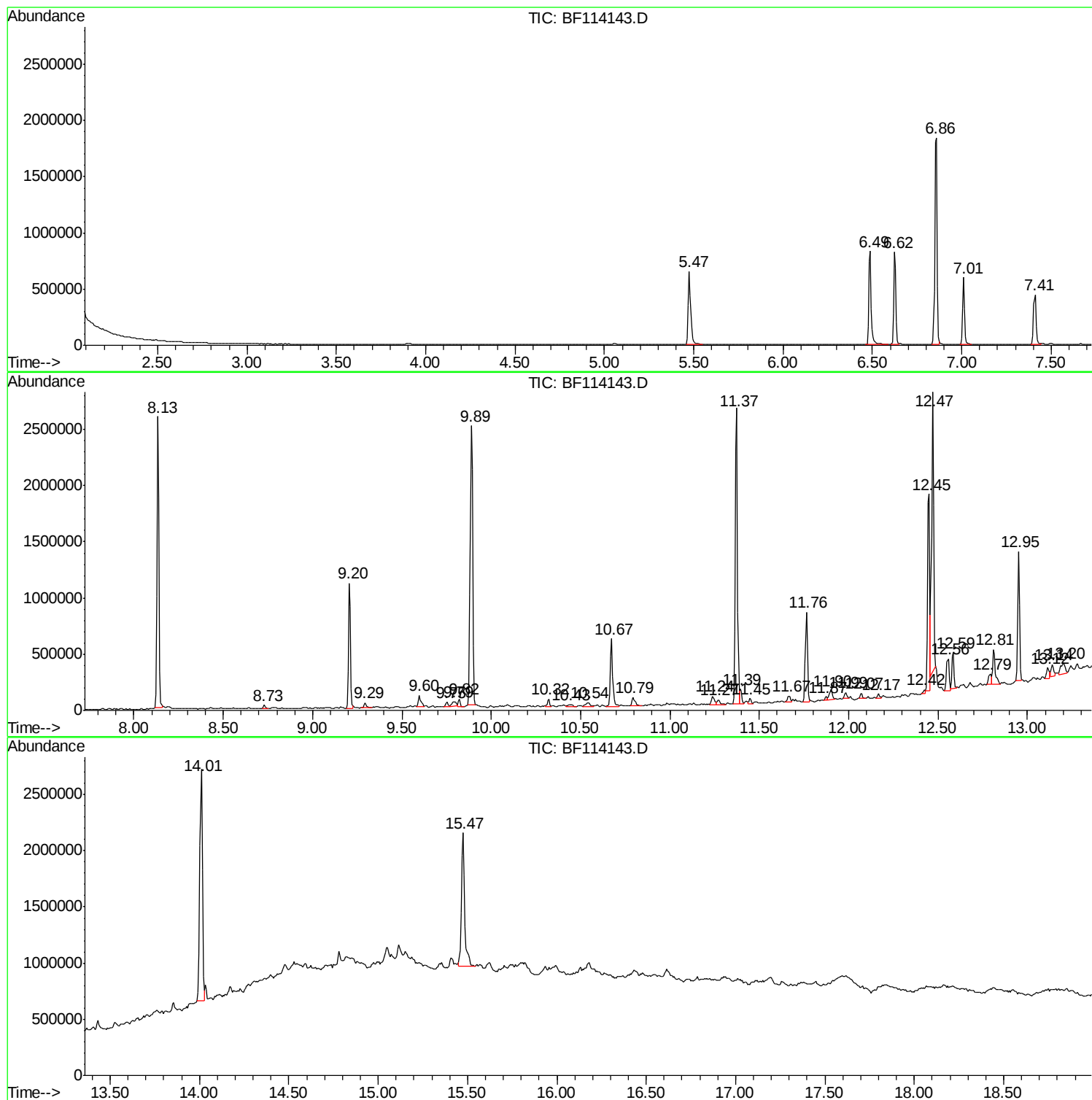
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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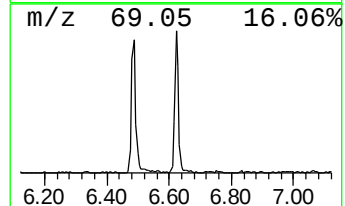
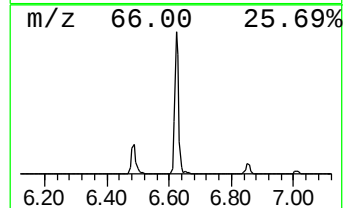
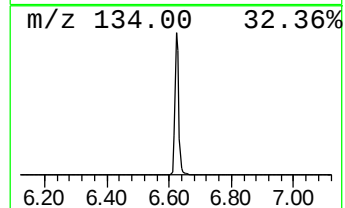
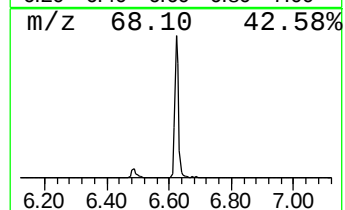
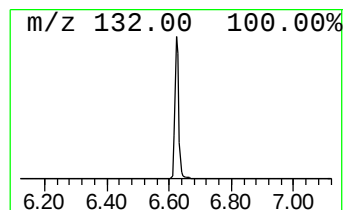
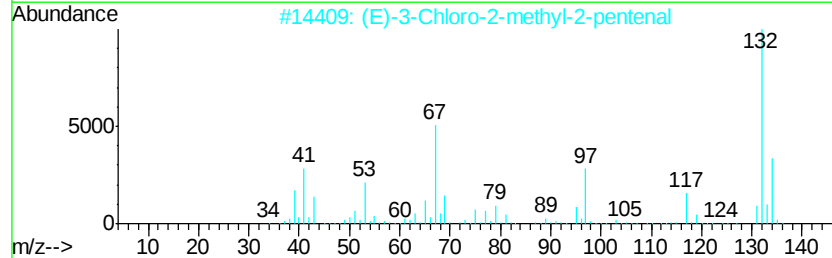
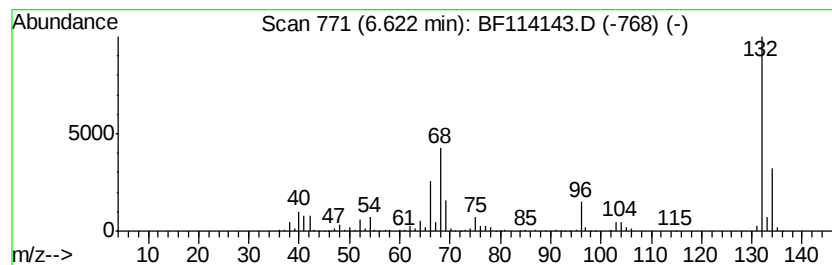
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.62 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	8.61 ng	720528	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5			Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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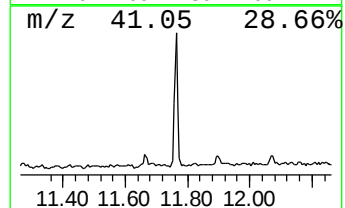
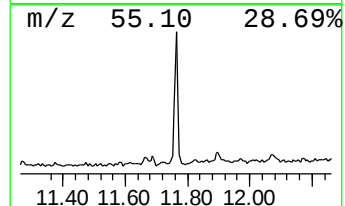
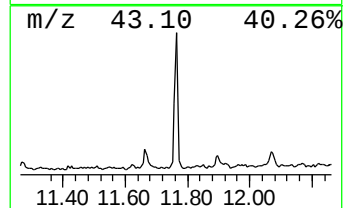
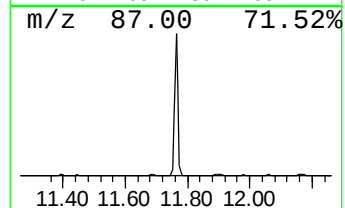
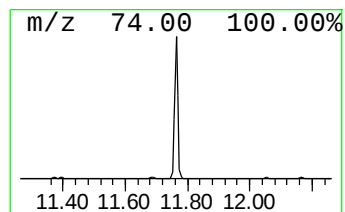
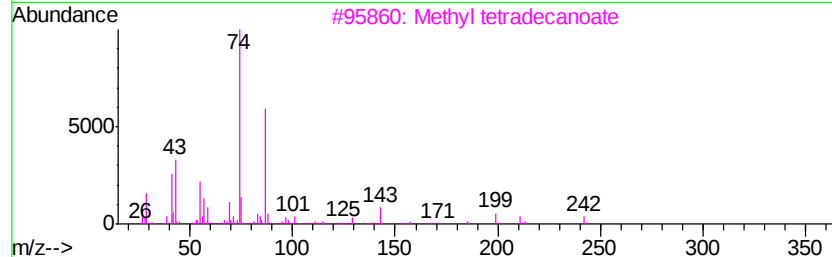
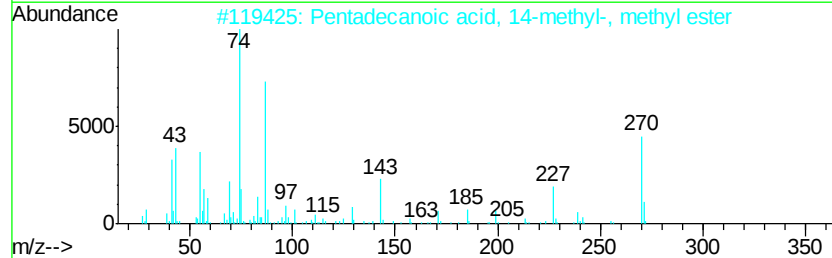
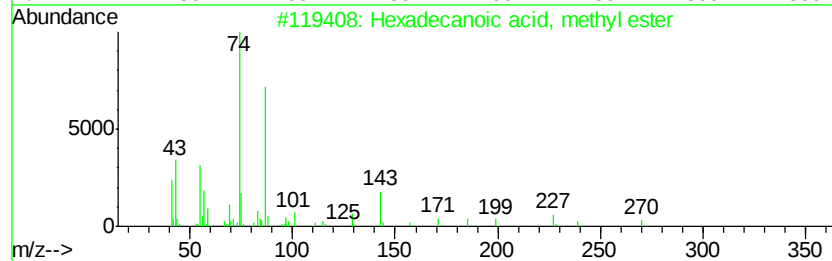
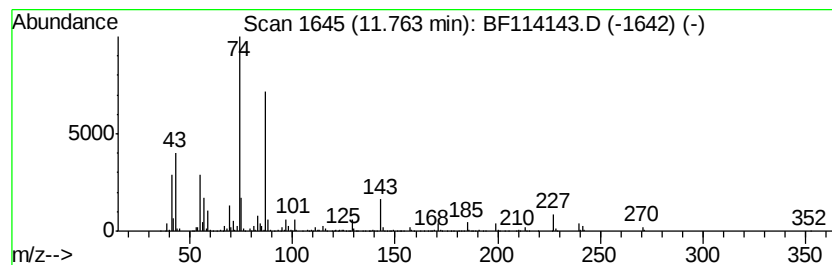
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Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	5.21 ng	599665	Phenanthrene-d10	11.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	99
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3		Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	87



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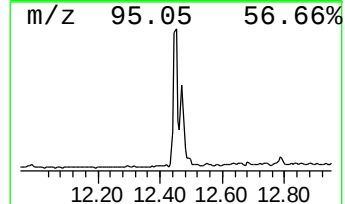
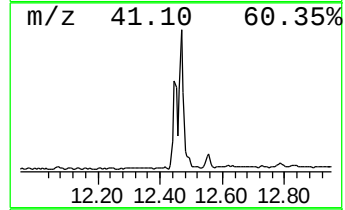
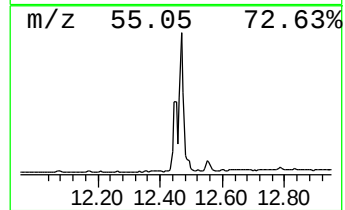
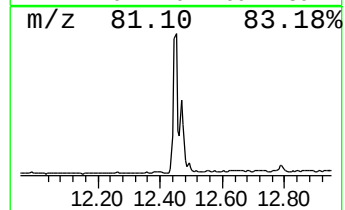
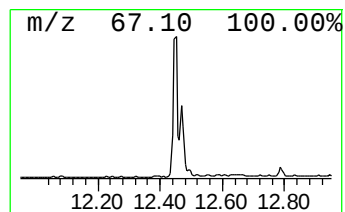
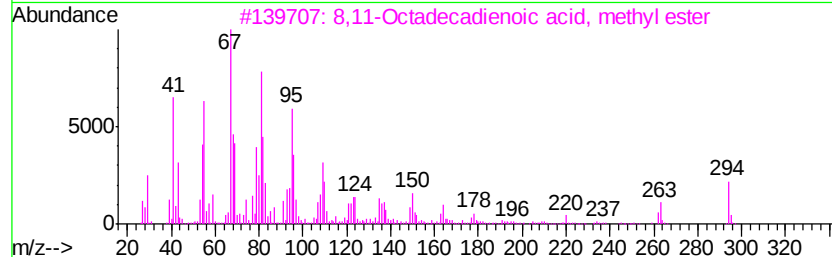
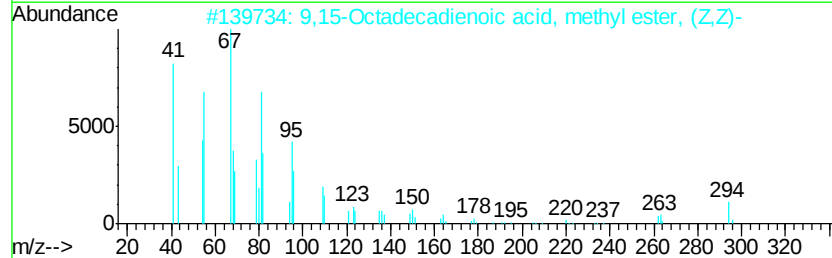
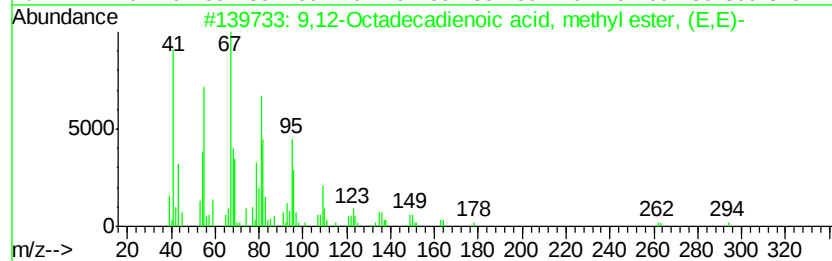
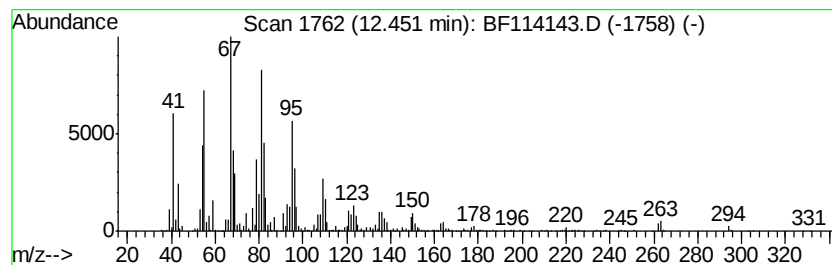
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.45	14.06 ng	1619040	Phenanthrene-d10	11.37		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99	
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99	
3	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99	
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99	
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98	



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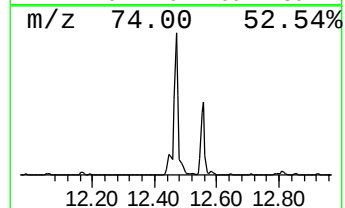
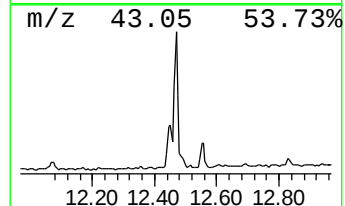
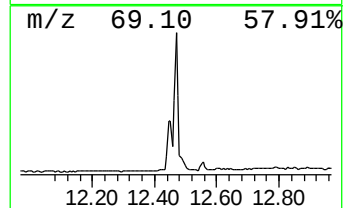
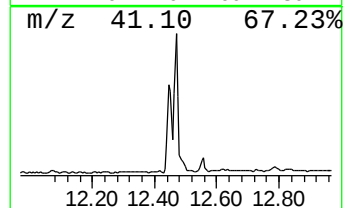
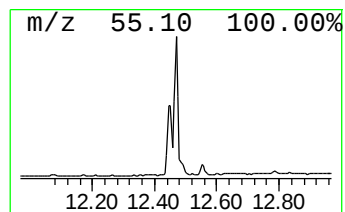
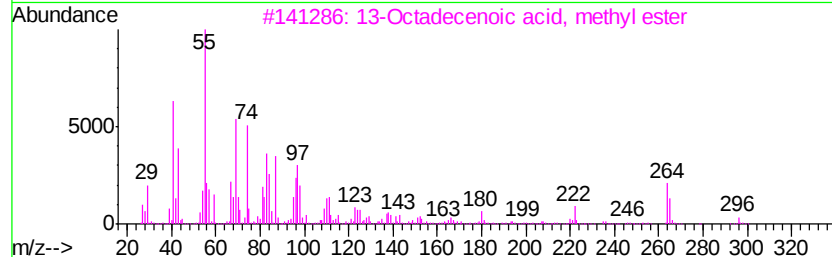
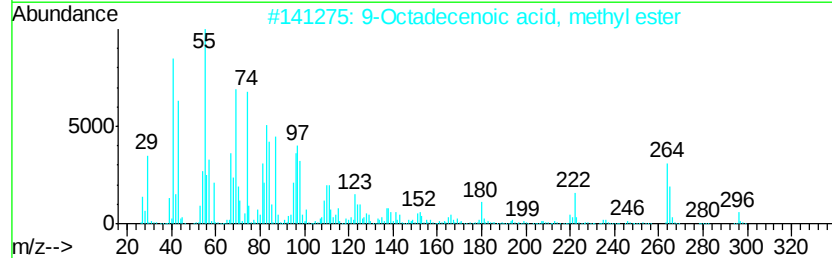
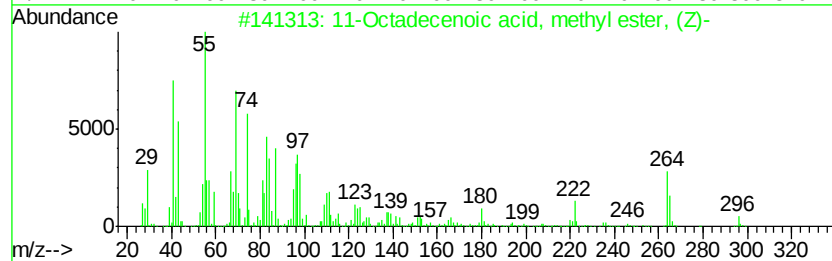
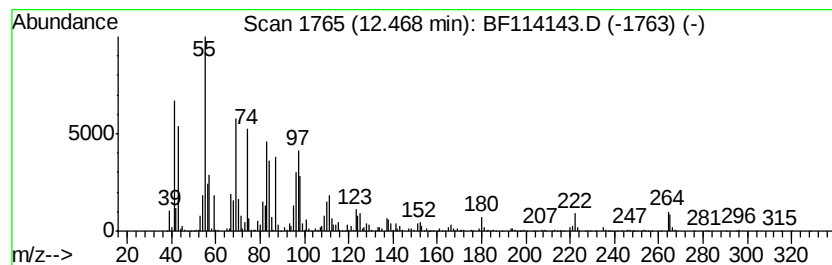
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 11-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	16.55 ng	1905250	Phenanthrene-d10	11.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	98
2		9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	98
3		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	98
4		15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	97
5		11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	94



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
unknown6.62	6.62	8.6	ng	720528	1	6.86	1674420	20.0
Hexadecanoic acid...	11.76	5.2	ng	599665	4	11.37	2302830	20.0
9,12-Octadecadien...	12.45	14.1	ng	1619040	4	11.37	2302830	20.0
11-Octadecenoic a...	12.47	16.6	ng	1905250	4	11.37	2302830	20.0