

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031519\
 Data File : BF113073.D
 Acq On : 15 Mar 2019 18:41
 Operator : JU/SJ
 Sample : K1685-07 5X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AU-05-031419-D

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-BF022719.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	5.334	548	552	564	rBV	523920	560098	6.07%	1.519%
2	6.363	723	727	741	rBV	627124	621059	6.73%	1.684%
3	6.492	746	749	758	rVV	743672	628125	6.81%	1.703%
4	6.728	785	789	801	rBV	849597	804109	8.71%	2.180%
5	6.881	811	815	824	rBV	592621	490658	5.32%	1.330%
6	7.281	880	883	891	rBV	305468	340998	3.69%	0.925%
7	8.010	1003	1007	1013	rBV	920443	973236	10.55%	2.639%
8	9.081	1186	1189	1202	rBV	749300	763404	8.27%	2.070%
9	9.757	1300	1304	1311	rBV	1389106	1243837	13.48%	3.372%
10	10.539	1434	1437	1450	rBV	547081	561565	6.08%	1.523%
11	10.769	1473	1476	1482	rVB	108036	100486	1.09%	0.272%
12	11.233	1551	1555	1563	rVB	1462641	1363888	14.78%	3.698%
13	11.563	1608	1611	1615	rVB	131795	124519	1.35%	0.338%
14	11.639	1620	1624	1627	rBV	3902821	3240876	35.12%	8.787%
15	11.775	1643	1647	1655	rBV	282867	320802	3.48%	0.870%
16	12.327	1736	1741	1743	rBV	7043835	9228794	100.00%	25.021%
17	12.351	1743	1745	1750	rVV2	7518696	7945602	86.10%	21.542%
18	12.392	1750	1752	1755	rVV	155523	181074	1.96%	0.491%
19	12.427	1755	1758	1761	rVV	2235917	1894449	20.53%	5.136%
20	12.457	1761	1763	1765	rVV	228342	235858	2.56%	0.639%
21	12.474	1765	1766	1778	rVB3	192784	311308	3.37%	0.844%
22	12.816	1819	1824	1827	rBV	949006	861766	9.34%	2.336%
23	13.069	1862	1867	1875	rVB2	169957	301091	3.26%	0.816%
24	13.151	1877	1881	1883	rBV	179966	157647	1.71%	0.427%
25	13.251	1895	1898	1902	rVB	103385	97595	1.06%	0.265%
26	13.569	1946	1952	1956	rBV5	60097	119208	1.29%	0.323%
27	13.727	1976	1979	1988	rBV3	98544	164337	1.78%	0.446%
28	13.816	1991	1994	1997	rBV	146059	136870	1.48%	0.371%
29	13.863	1998	2002	2010	rBV	1242968	1241980	13.46%	3.367%
30	14.339	2080	2083	2086	rBV	104715	98376	1.07%	0.267%
31	14.639	2131	2134	2140	rBV	97152	94176	1.02%	0.255%
32	14.951	2184	2187	2192	rVB	123081	135593	1.47%	0.368%
33	15.268	2236	2241	2245	rBV	916449	1138850	12.34%	3.088%
34	15.304	2245	2247	2254	rVB	115777	152508	1.65%	0.413%

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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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35	15.710	2312	2316	2321	rBV	104204	147597	1.60%	0.400%
36	16.174	2392	2395	2401	rVB2	69978	101730	1.10%	0.276%

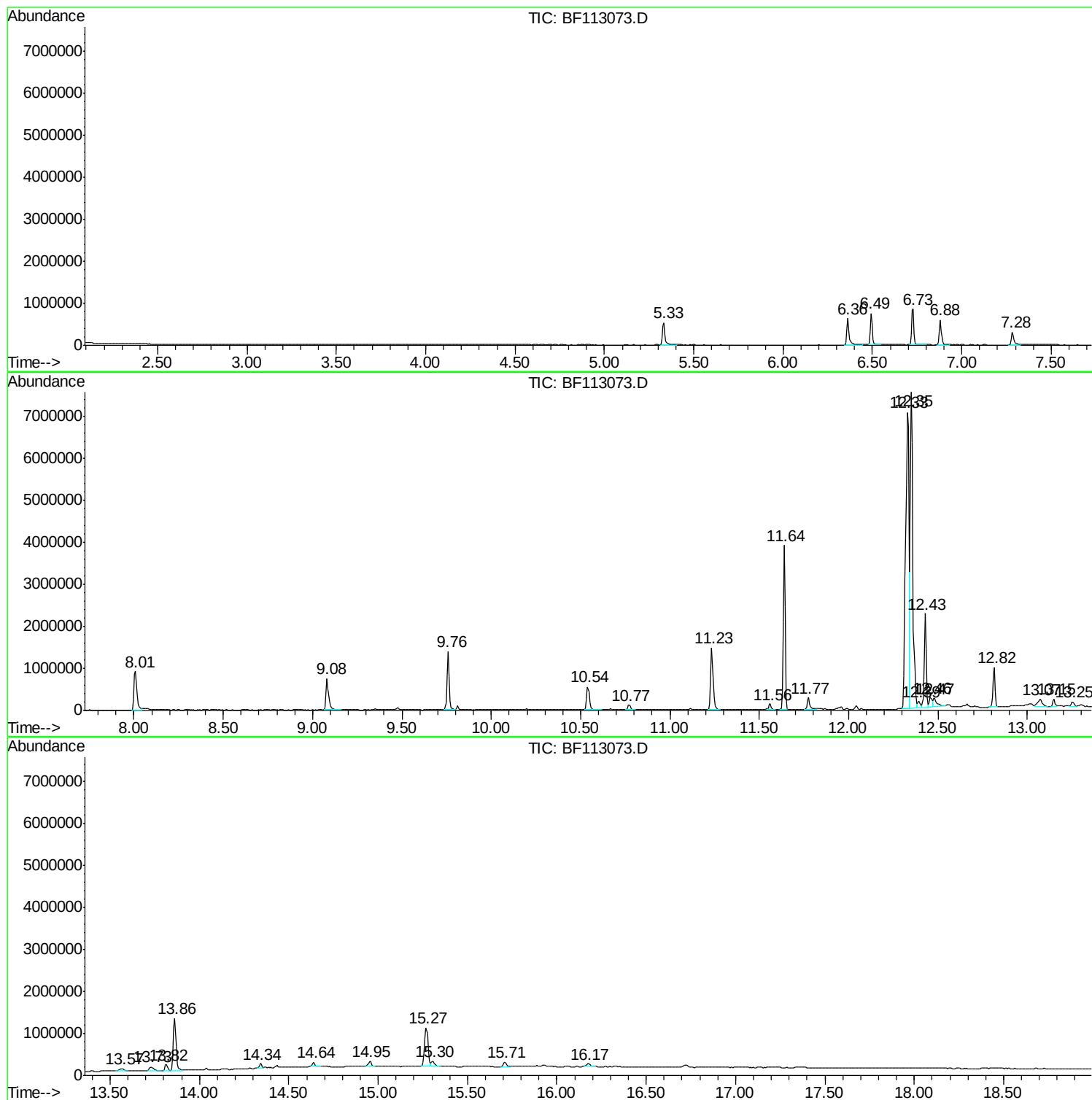
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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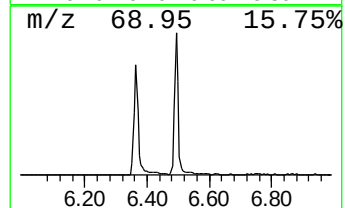
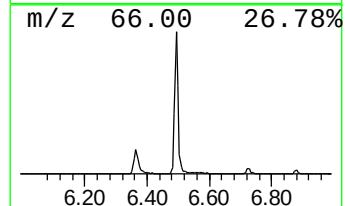
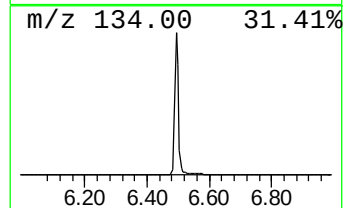
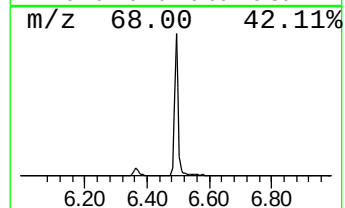
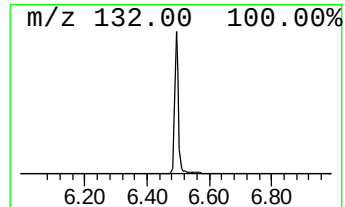
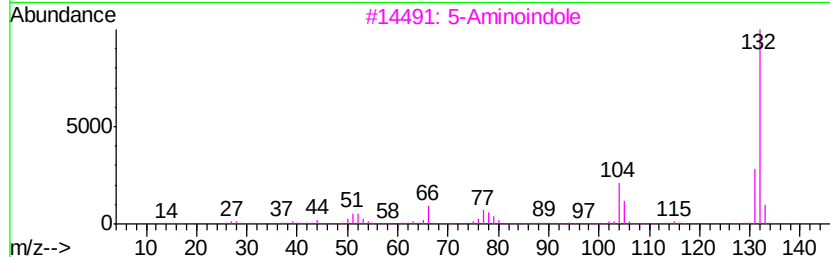
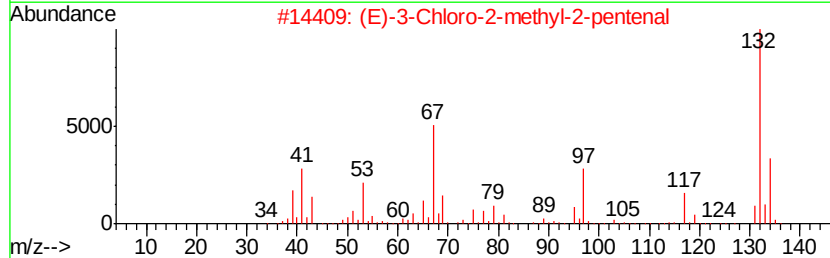
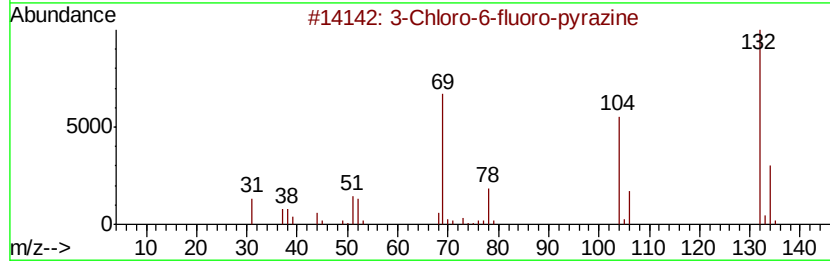
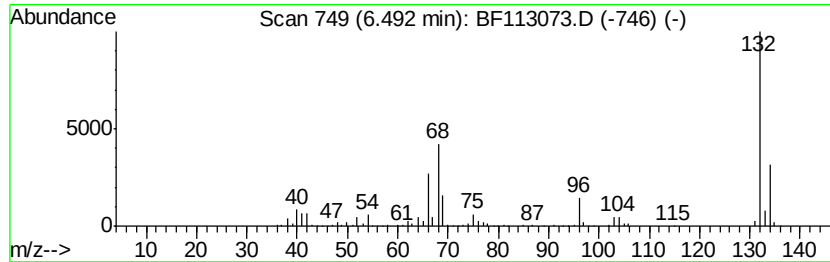
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.49 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	15.62 ng	628125	1,4-Dichlorobenzene-d4	6.73

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Amphetaminil	250	C17H18N2	017590-01-1	10
5		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	10



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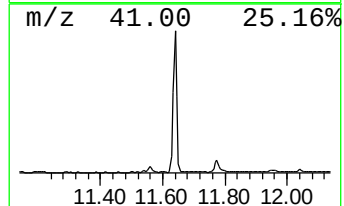
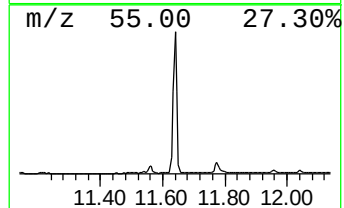
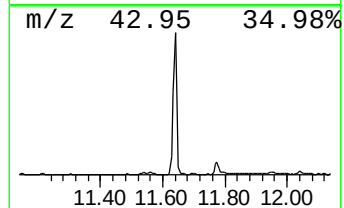
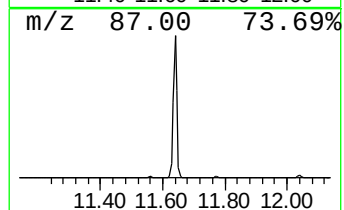
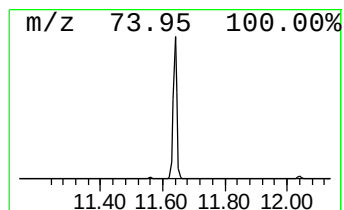
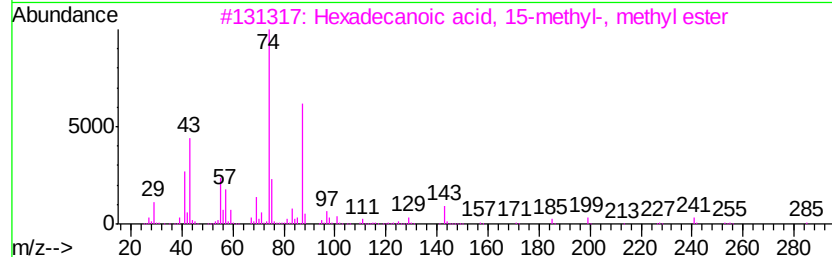
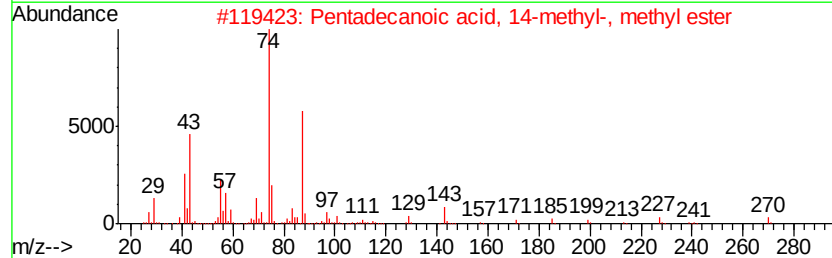
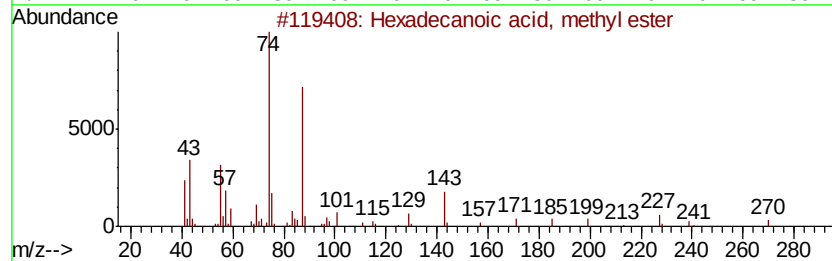
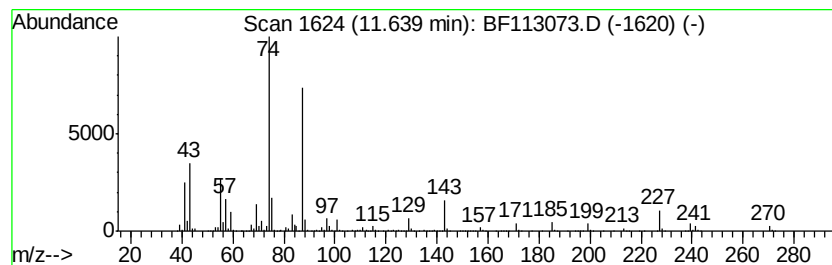
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.64	47.52 ng	3240880	Phenanthrene-d10	11.23	
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	97
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	83



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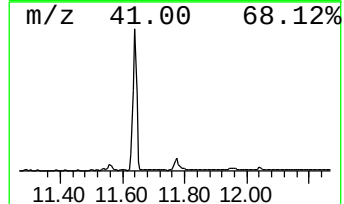
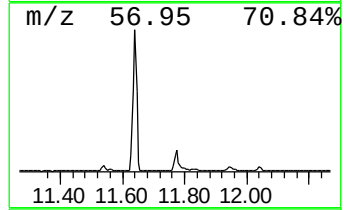
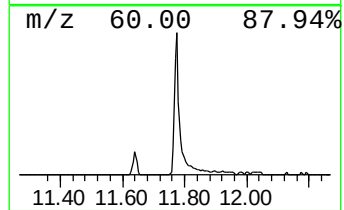
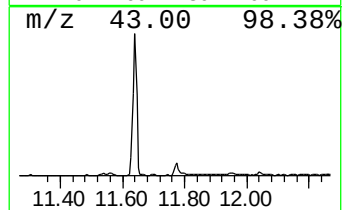
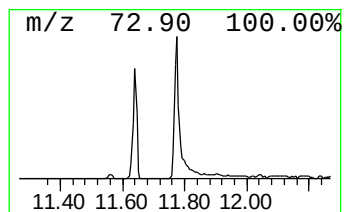
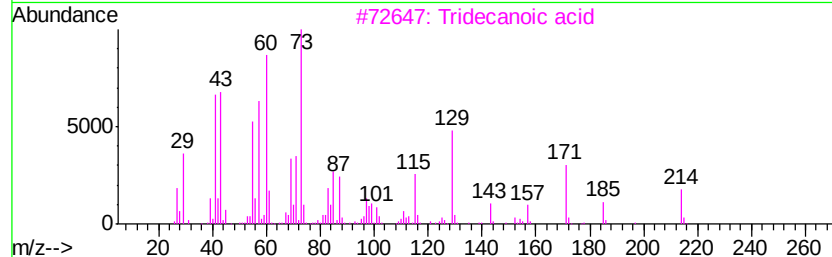
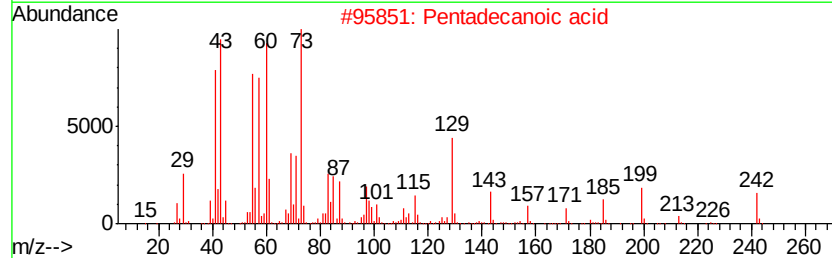
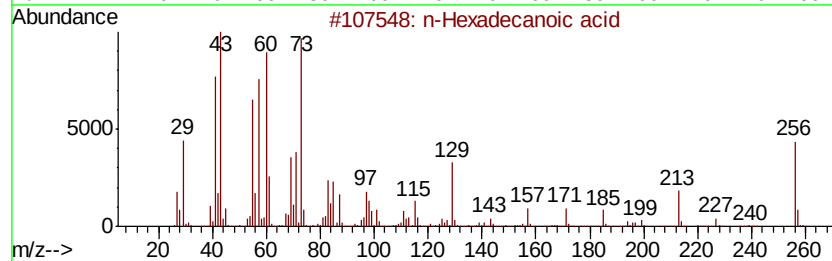
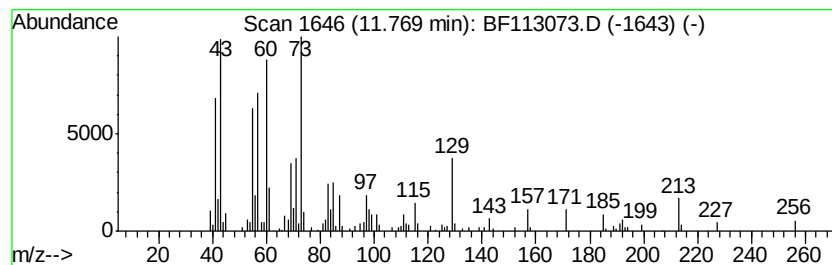
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.77	4.70 ng	320802	Phenanthrene-d10		11.23
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68



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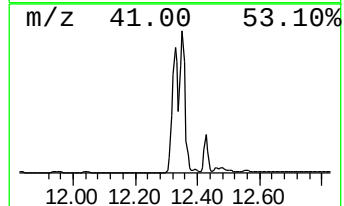
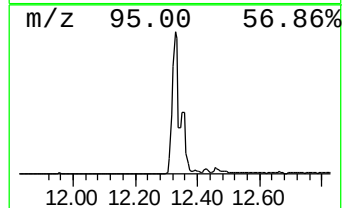
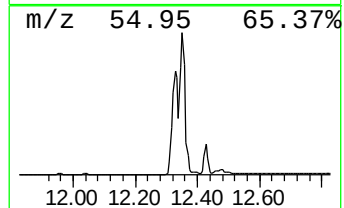
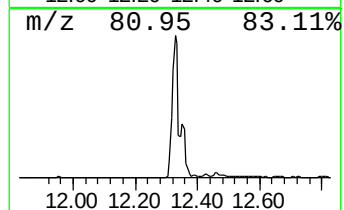
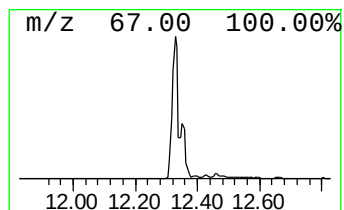
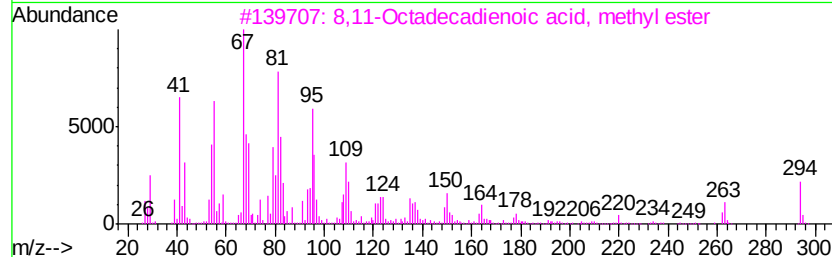
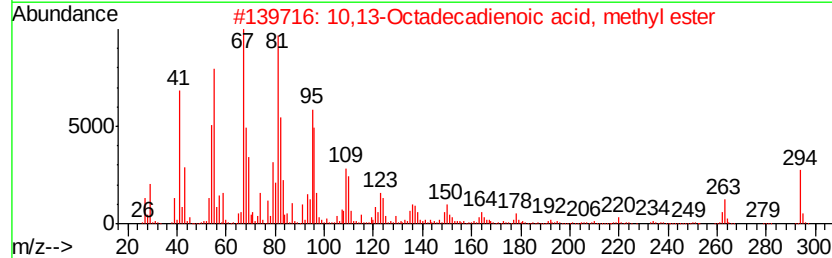
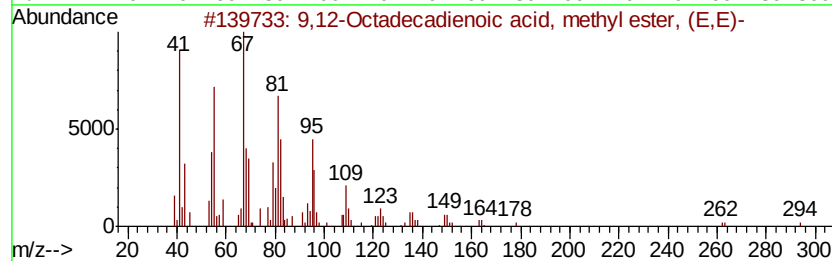
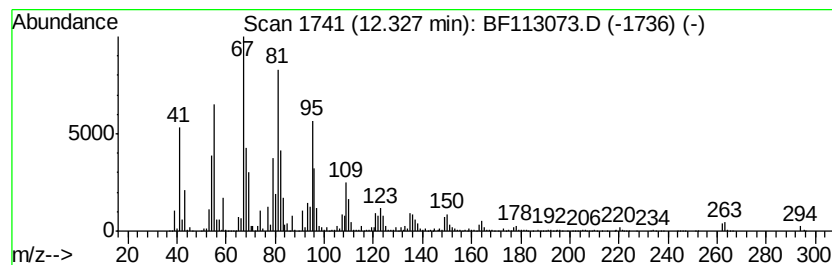
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.33	135.33 ng	9228790	Phenanthrene-d10	11.23		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99	
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99	
3	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99	
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99	
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99	



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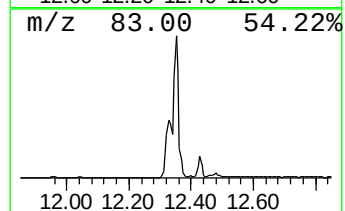
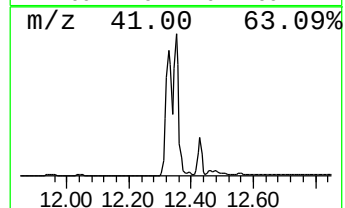
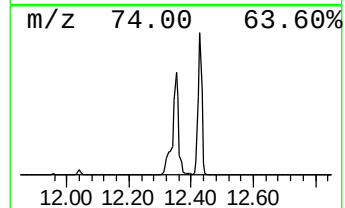
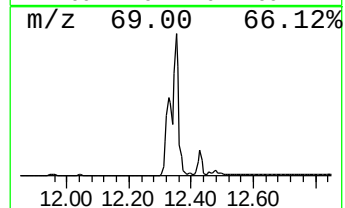
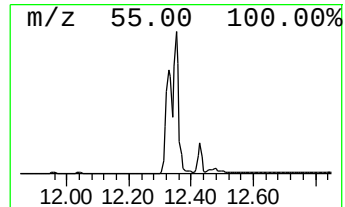
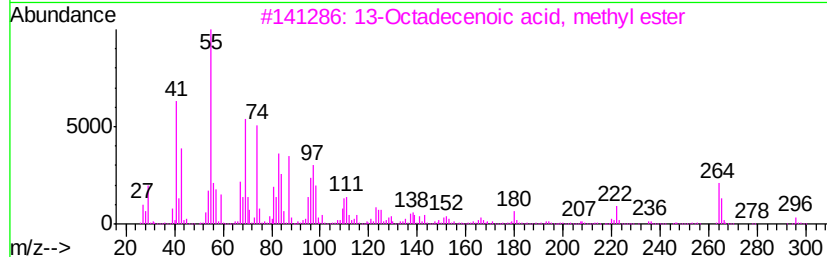
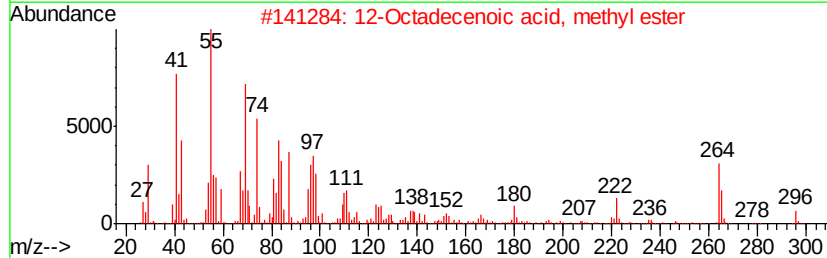
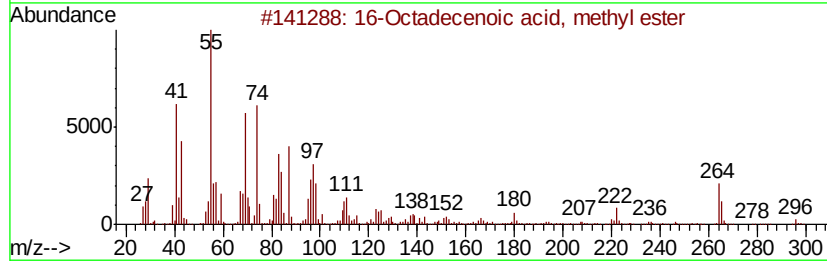
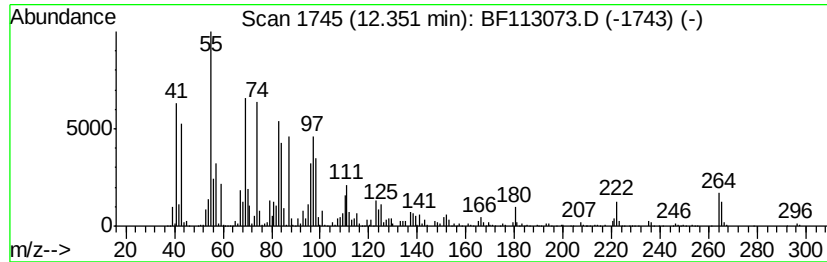
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 16-Octadecenoic acid, methyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.35	116.51 ng	7945600	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	96
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	94
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	94
4	9-Octadecenoic acid (Z)-, methyl ester	296	C19H36O2	000112-62-9	93
5	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	92



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031519\
Data File : BF113073.D
Acq On : 15 Mar 2019 18:41
Operator : JU/SJ
Sample : K1685-07 5X
Misc :
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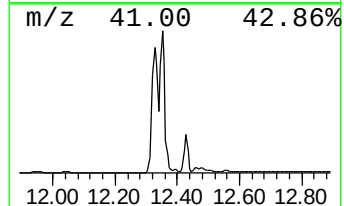
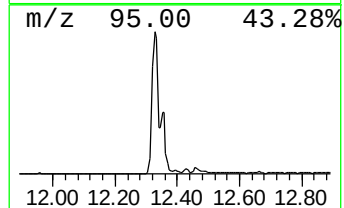
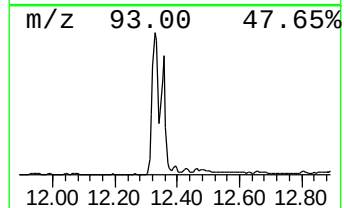
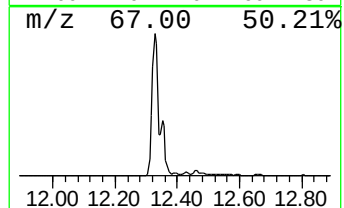
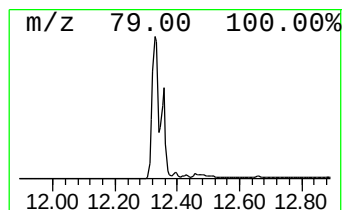
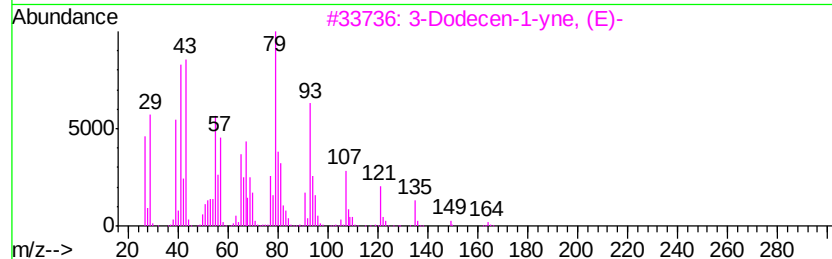
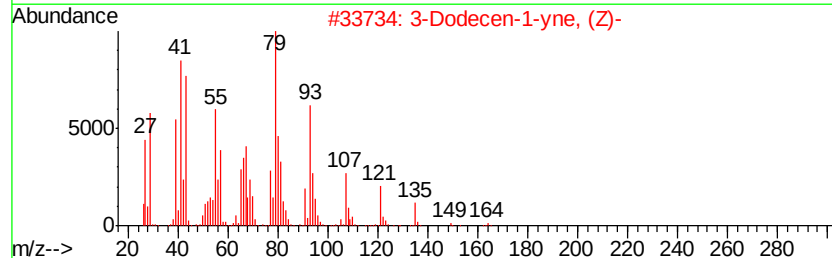
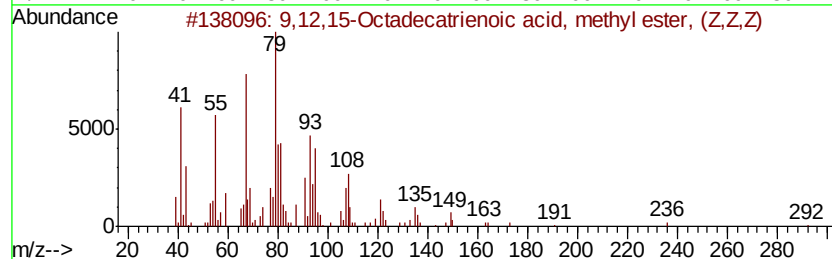
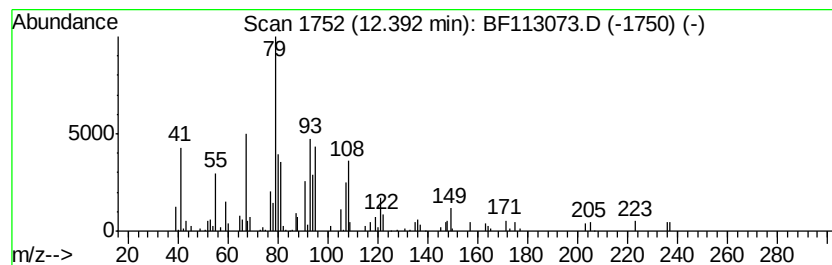
Instrument :
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ClientSampleId :
AU-05-031419-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9,12,15-Octadecatrienoic ac... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.39	2.66 ng	181074	Phenanthrene-d10	11.23		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	91	
2	3-Dodecen-1-yne, (Z)-	164	C12H20	025091-24-1	64	
3	3-Dodecen-1-yne, (E)-	164	C12H20	025091-25-2	64	
4	3-Heptadecen-5-yne, (Z)-	234	C17H30	074744-55-1	64	
5	11,14,17-Eicosatrienoic acid, me...	320	C21H36O2	055682-88-7	64	



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031519\
Data File : BF113073.D
Acq On : 15 Mar 2019 18:41
Operator : JU/SJ
Sample : K1685-07 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleID :
AU-05-031419-D

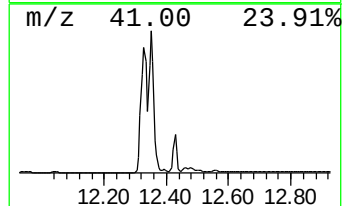
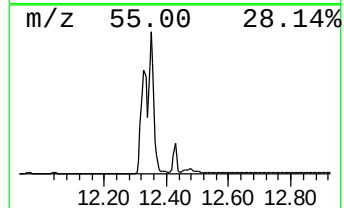
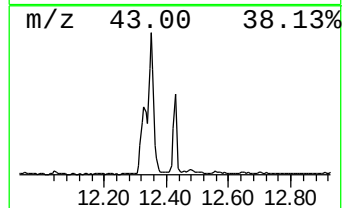
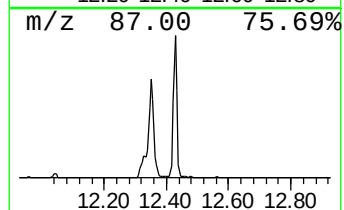
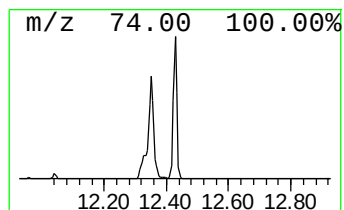
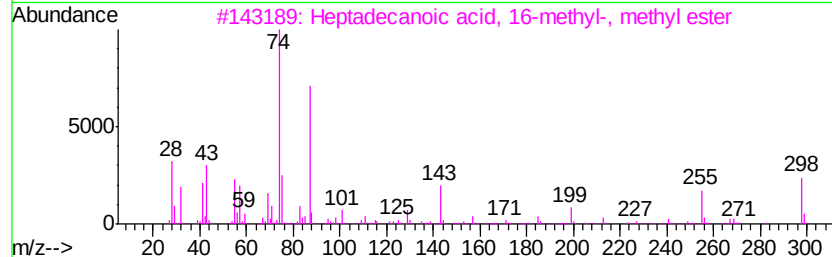
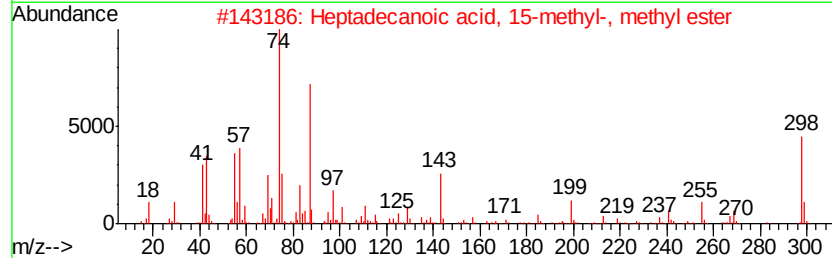
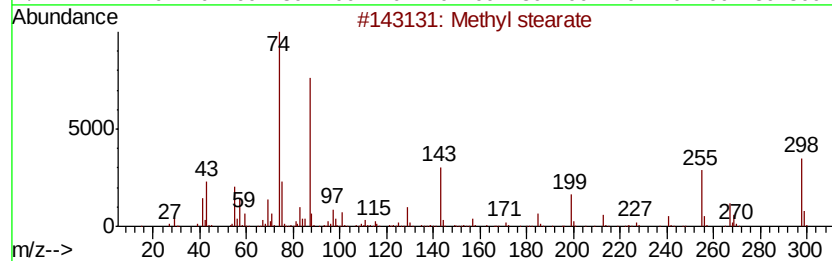
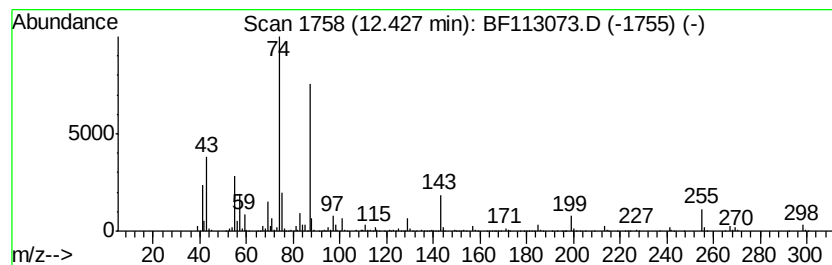
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	27.78 ng	1894450	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl stearate	298	C19H38O2	000112-61-8	98
2		Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	93
3		Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	92
4		Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
5		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031519\
Data File : BF113073.D
Acq On : 15 Mar 2019 18:41
Operator : JU/SJ
Sample : K1685-07 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-05-031419-D

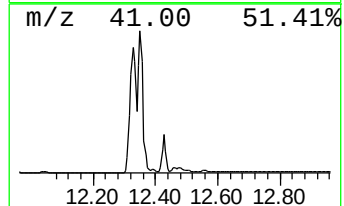
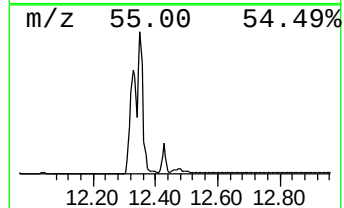
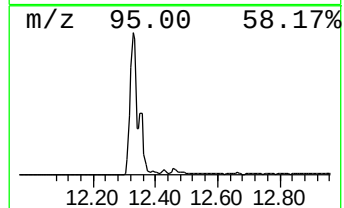
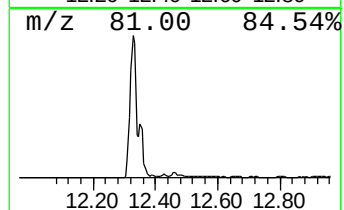
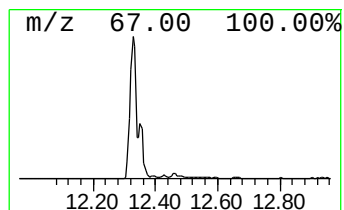
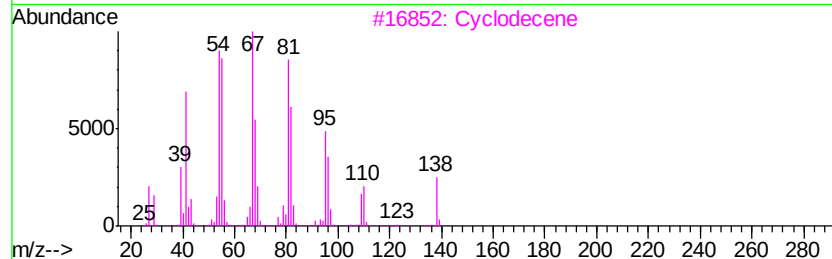
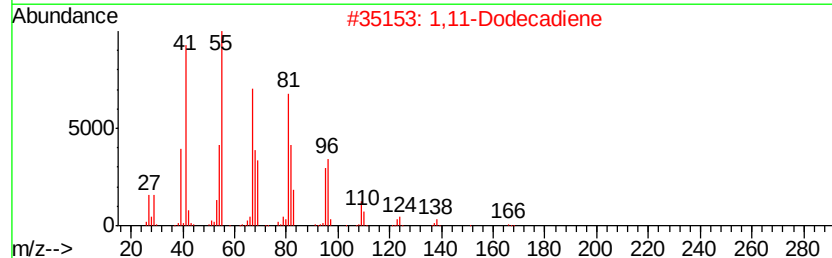
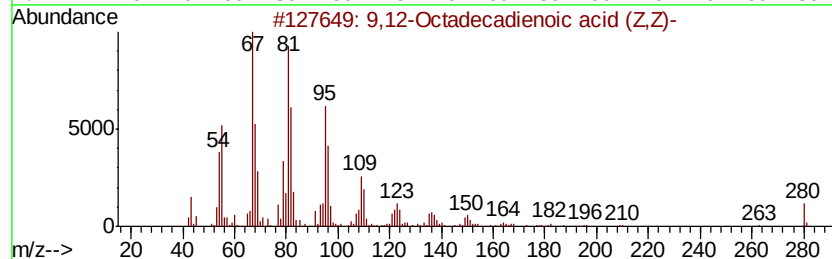
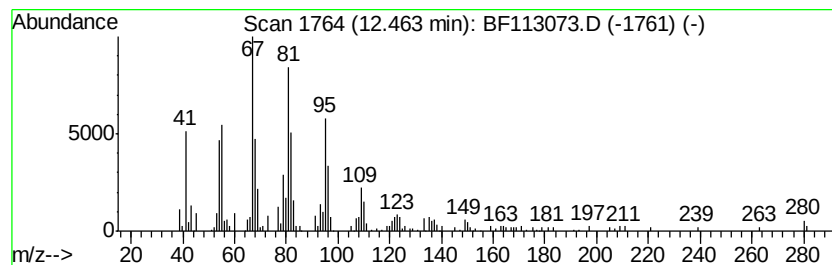
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9,12-Octadecadienoic acid (... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	3.46 ng	235858	Phenanthrene-d10	11.23

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2			1,11-Dodecadiene	166	C12H22	005876-87-9	87
3			Cyclodecene	138	C10H18	003618-12-0	81
4			Bicyclo[4.1.0]heptane, 3-methyl-	110	C8H14	041977-47-3	72
5			9-Eicosyne	278	C20H38	071899-38-2	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031519\
Data File : BF113073.D
Acq On : 15 Mar 2019 18:41
Operator : JU/SJ
Sample : K1685-07 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-05-031419-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Chloroacetic acid, tridecyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	4.57 ng	311308	Phenanthrene-d10	11.23

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	64
2			Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	62
3			1-Hexadecanol	242	C16H34O	036653-82-4	58
4			3-Heptafluorobutyltroxytridecane	396	C17H27F7O2	1000245-49-5	58
5			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	58

