

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102618\
 Data File : BF110225.D
 Acq On : 26 Oct 2018 22:19
 Operator : JU/SJ
 Sample : J5205-05 5X
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-05-102518

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-BF102318.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	5.581	590	594	606	rBV	990724	867133	6.26%	1.609%
2	6.581	760	764	776	rBV	1076788	992902	7.16%	1.843%
3	6.734	786	790	793	rBV	1134067	953952	6.88%	1.770%
4	6.969	826	830	833	rBV	897988	791120	5.71%	1.468%
5	7.122	852	856	865	rBV	850554	694986	5.01%	1.290%
6	7.528	921	925	935	rBV	557662	549067	3.96%	1.019%
7	8.251	1044	1048	1067	rVB	1156600	1022122	7.37%	1.897%
8	9.322	1227	1230	1239	rBV	1238645	1010531	7.29%	1.875%
9	10.010	1343	1347	1350	rBV2	1113301	931547	6.72%	1.729%
10	10.039	1350	1352	1359	rVB	200574	164168	1.18%	0.305%
11	10.798	1478	1481	1486	rBV	462415	420710	3.04%	0.781%
12	11.004	1513	1516	1520	rBV	824961	611365	4.41%	1.135%
13	11.504	1597	1601	1604	rBV	939266	795631	5.74%	1.476%
14	11.804	1649	1652	1655	rVB	1050842	871362	6.29%	1.617%
15	11.886	1661	1666	1669	rVB	7189948	7849545	56.63%	14.567%
16	12.204	1717	1720	1724	rVB	175697	155561	1.12%	0.289%
17	12.280	1730	1733	1739	rVB	263889	224348	1.62%	0.416%
18	12.580	1778	1784	1786	rBV	7352010	11720395	84.56%	21.750%
19	12.610	1786	1789	1794	rVV	9031942	13860131	100.00%	25.721%
20	12.645	1794	1795	1797	rVV	492689	327392	2.36%	0.608%
21	12.680	1797	1801	1804	rVB	5300491	4624726	33.37%	8.582%
22	12.721	1804	1808	1811	rBV	239793	262658	1.90%	0.487%
23	12.910	1836	1840	1843	rBV	235920	211014	1.52%	0.392%
24	12.957	1843	1848	1853	rVB	185794	241017	1.74%	0.447%
25	13.092	1867	1871	1873	rBV	887800	765335	5.52%	1.420%
26	13.268	1893	1901	1905	rBV8	130850	296512	2.14%	0.550%
27	13.321	1905	1910	1917	rVB2	501880	654158	4.72%	1.214%
28	13.398	1919	1923	1932	rVB	330513	312931	2.26%	0.581%
29	13.510	1938	1942	1947	rBV	276112	279583	2.02%	0.519%
30	14.062	2033	2036	2040	rBV	232141	201725	1.46%	0.374%
31	14.151	2046	2051	2054	rBV	739365	730194	5.27%	1.355%
32	15.680	2306	2311	2315	rBV	372212	493149	3.56%	0.915%

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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-05-102518

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-BF102318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

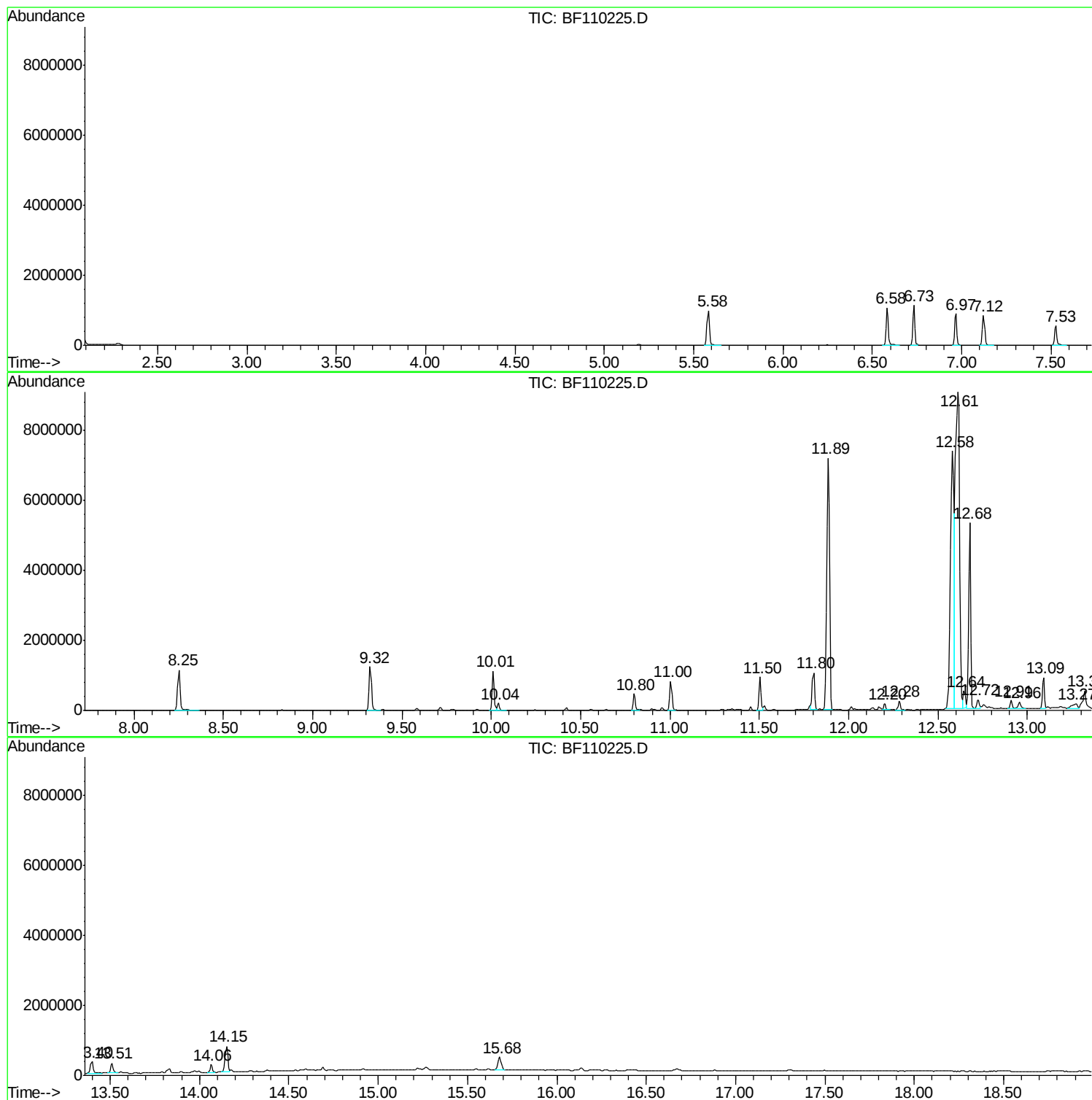
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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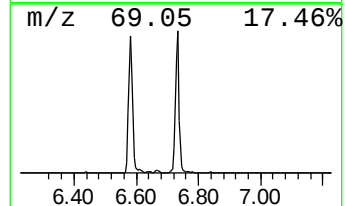
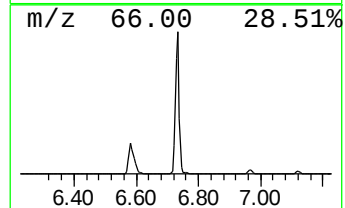
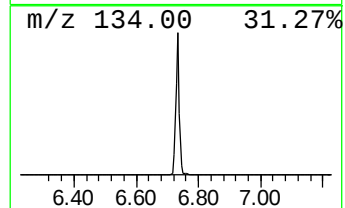
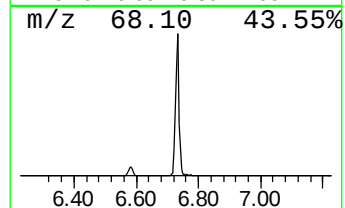
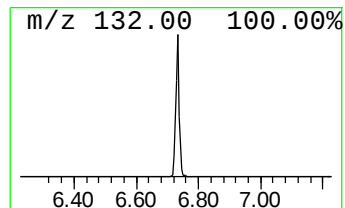
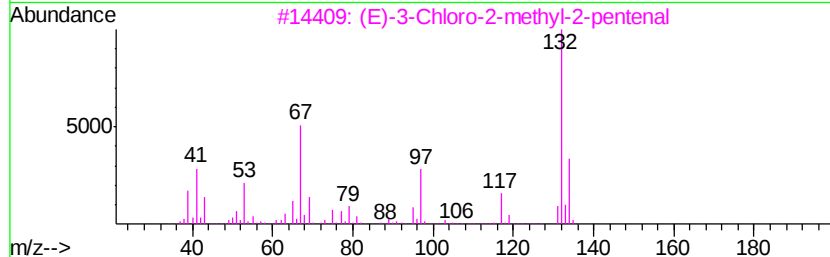
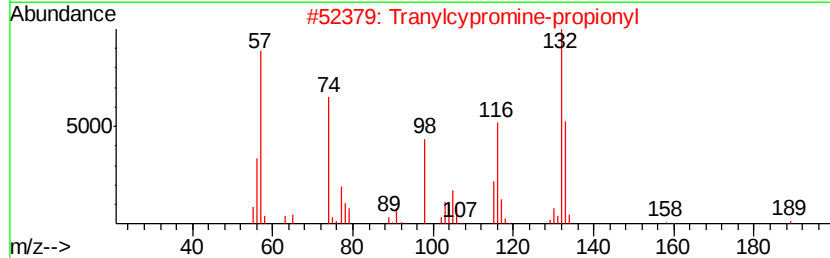
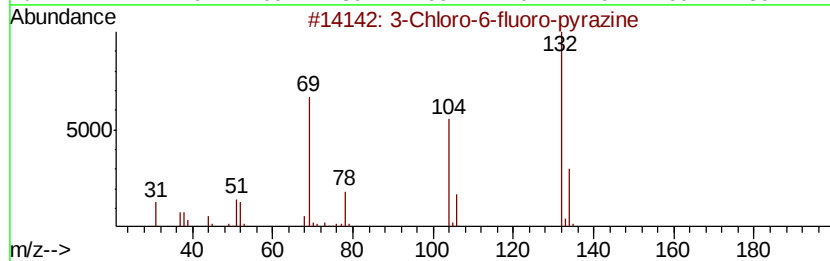
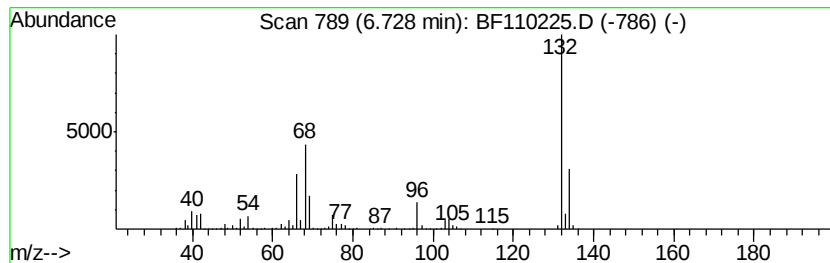
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.73 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	24.12 ng	953952	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4			1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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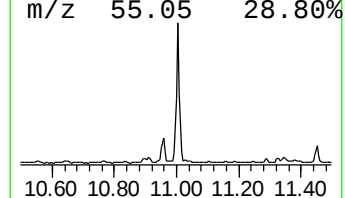
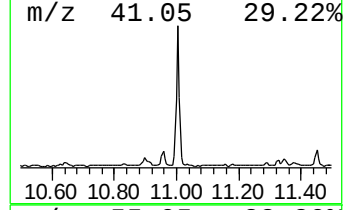
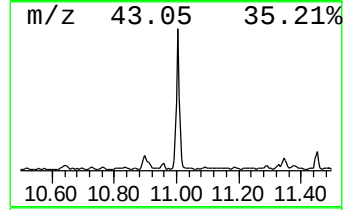
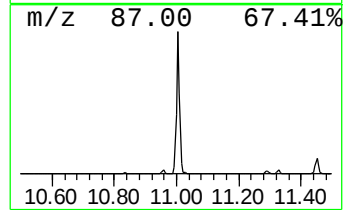
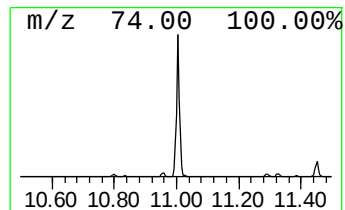
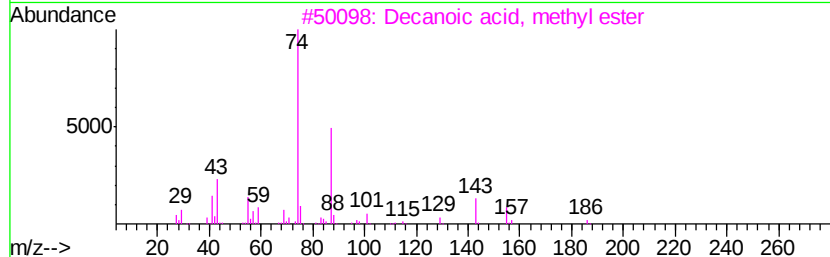
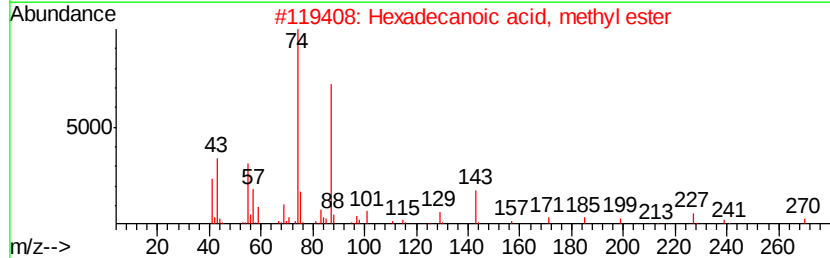
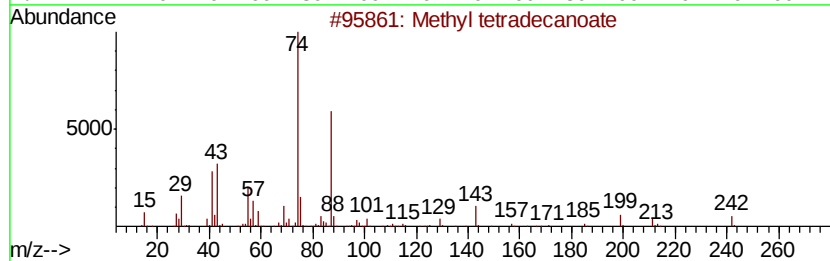
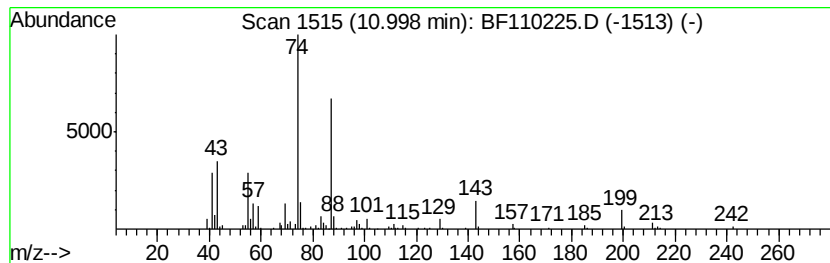
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Methyl tetradecanoate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.00	15.37 ng	611365	Phenanthrene-d10	11.50		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
2		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	87
3		Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	86
4		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86
5		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	86



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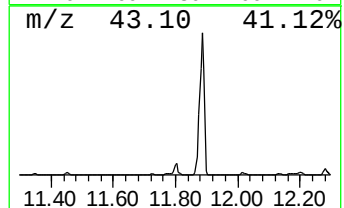
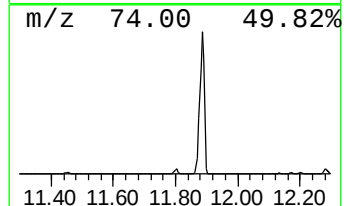
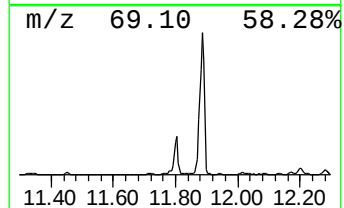
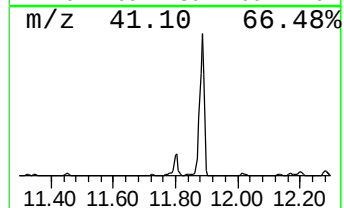
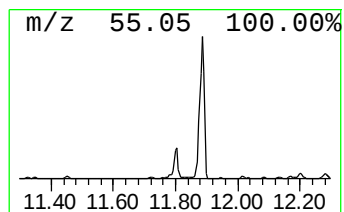
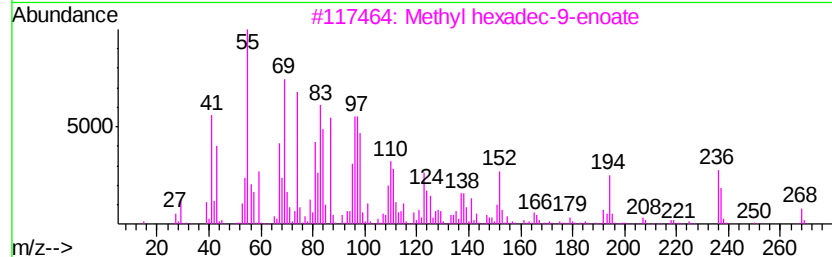
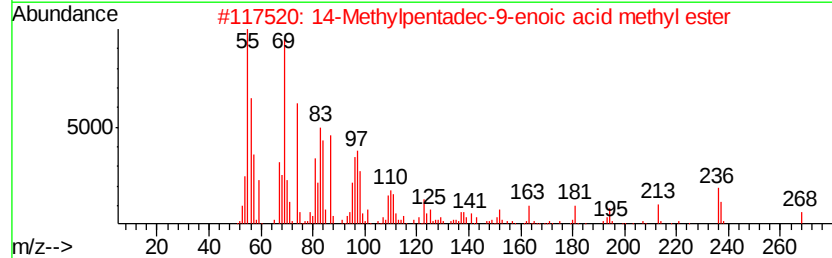
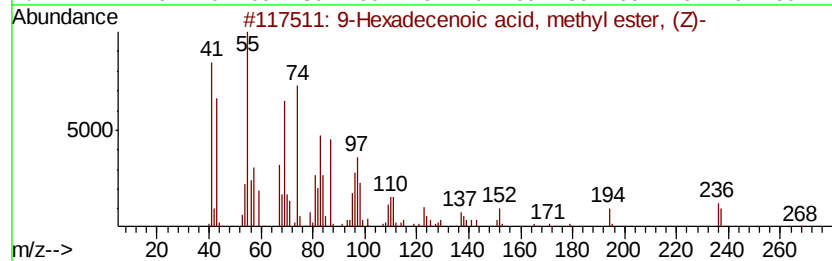
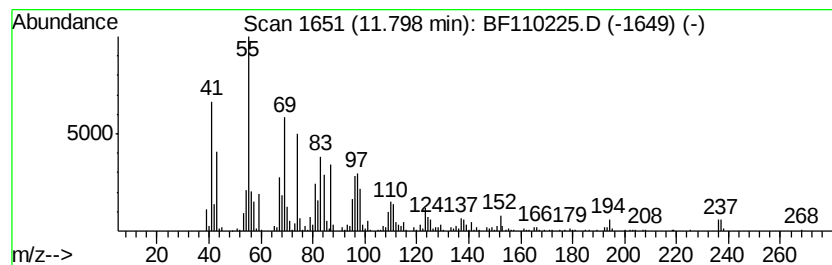
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Hexadecenoic acid, methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	21.90 ng	871362	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	99
2		14-Methylpentadec-9-enoic acid m...	268	C17H32O2	1000365-89-7	91
3		Methyl hexadec-9-enoate	268	C17H32O2	010030-74-7	91
4		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	87
5		Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	87



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Instrument :
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ClientSampleId :
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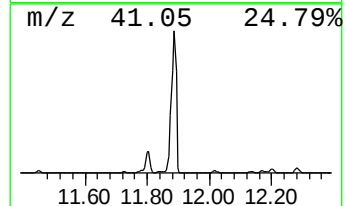
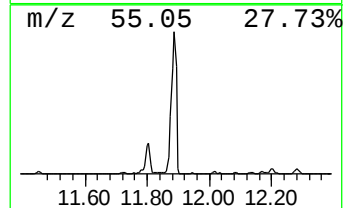
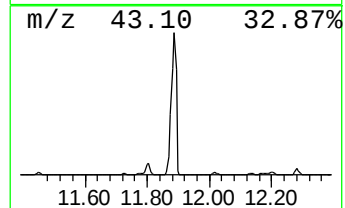
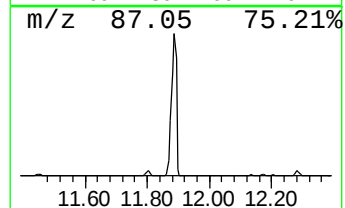
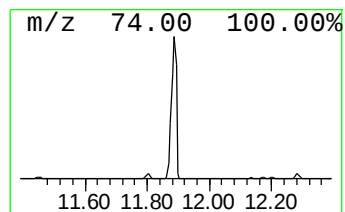
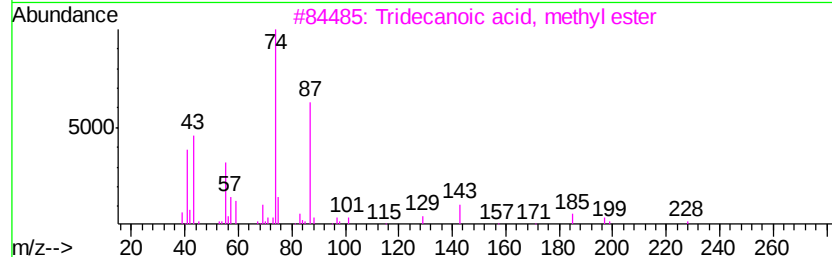
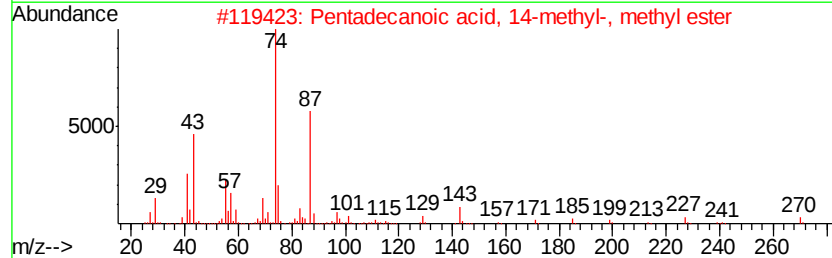
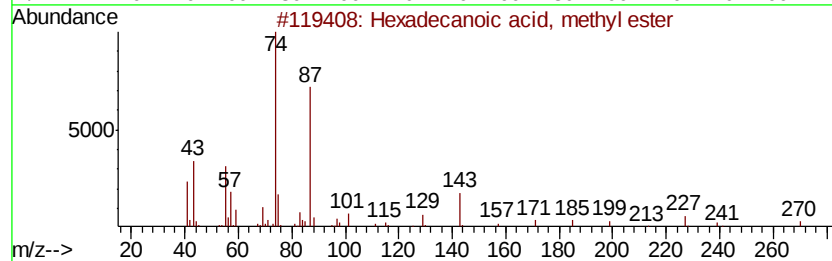
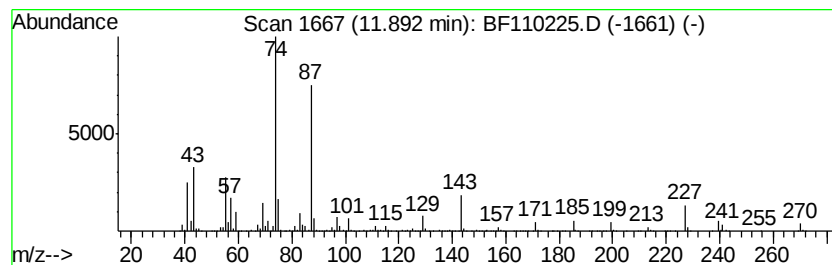
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	197.32 ng	7849550	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
4		Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



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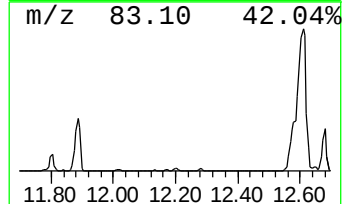
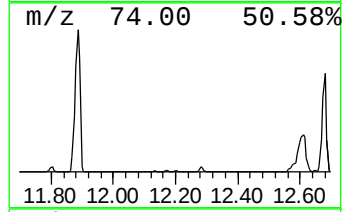
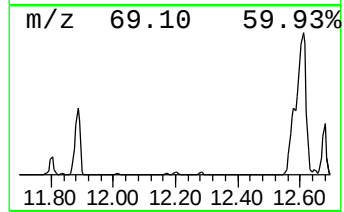
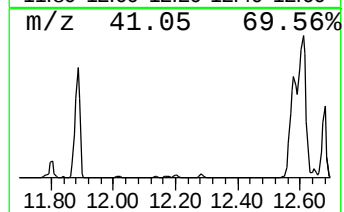
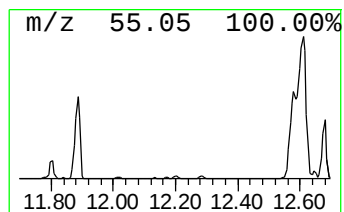
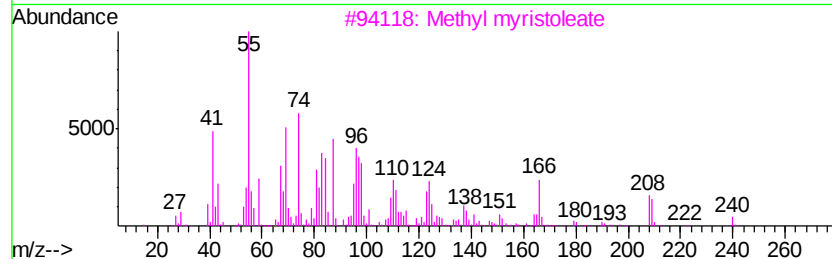
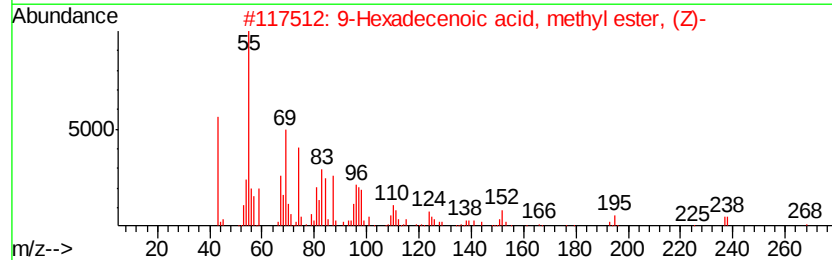
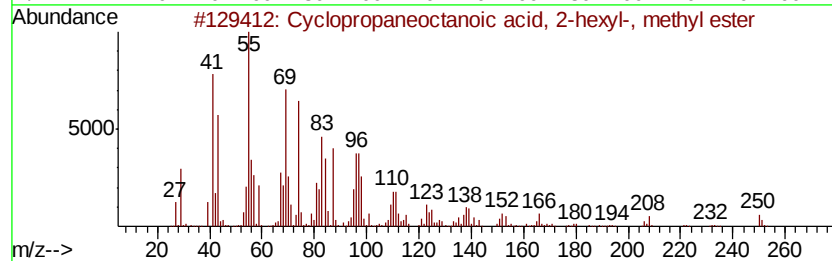
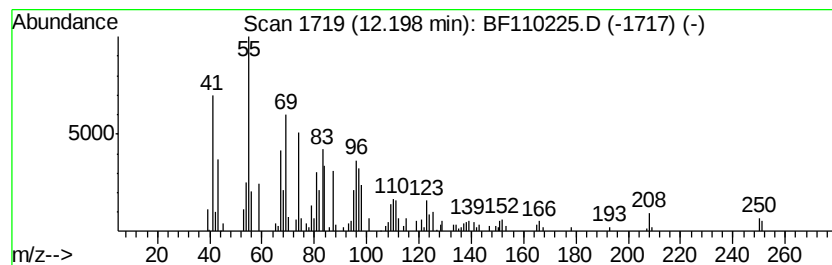
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclopropaneoctanoic acid, ... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.20	3.91 ng	155561	Phenanthrene-d10	11.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	90
2	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	83
3	Methyl myristoleate	240	C15H28O2	056219-06-8	80
4	E-9-Tetradecenoic acid	226	C14H26O2	1000131-35-8	58
5	Z-7-Tetradecenoic acid	226	C14H26O2	1000130-98-4	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102618\
Data File : BF110225.D
Acq On : 26 Oct 2018 22:19
Operator : JU/SJ
Sample : J5205-05 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-102518

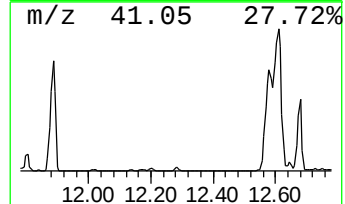
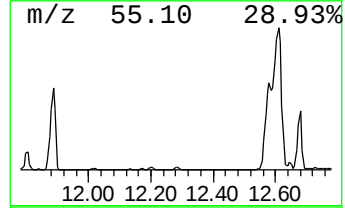
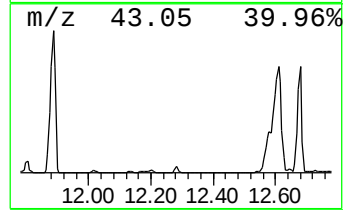
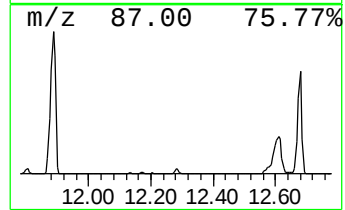
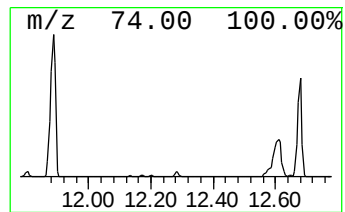
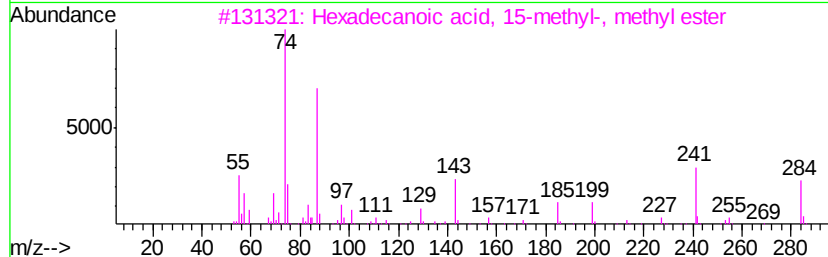
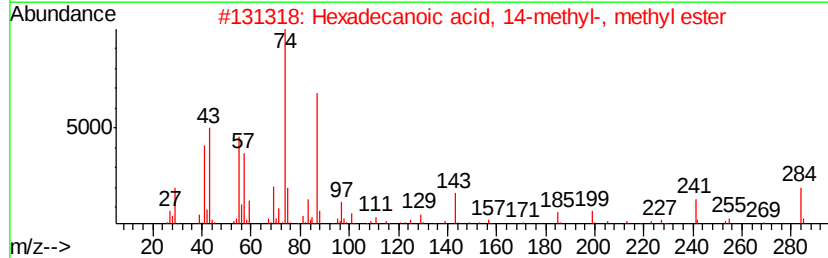
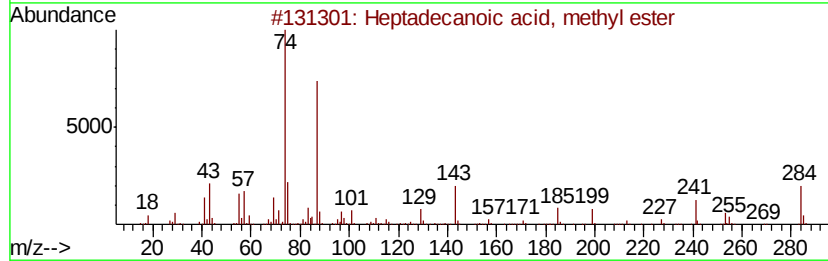
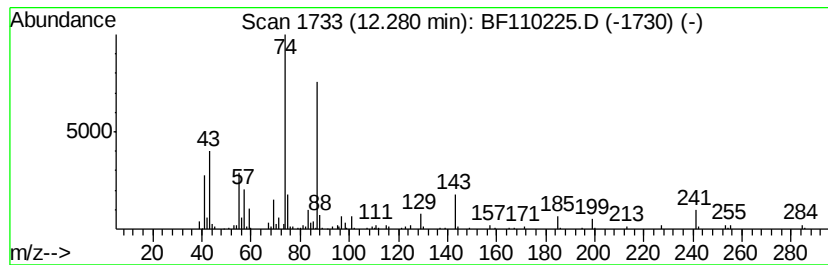
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecanoic acid, methyl ... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	5.64 ng	224348	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	96
2		Hexadecanoic acid, 14-methyl-, m...	284	C18H36O2	002490-49-5	94
3		Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91
4		Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
5		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86



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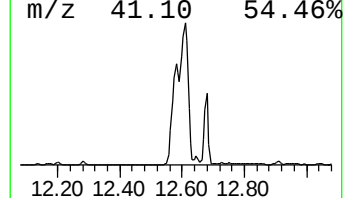
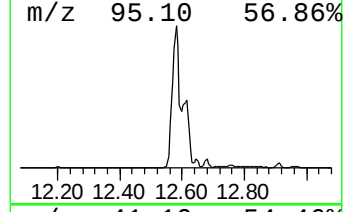
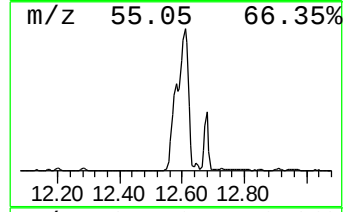
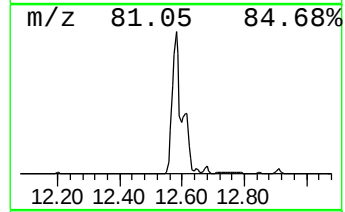
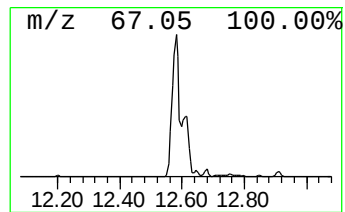
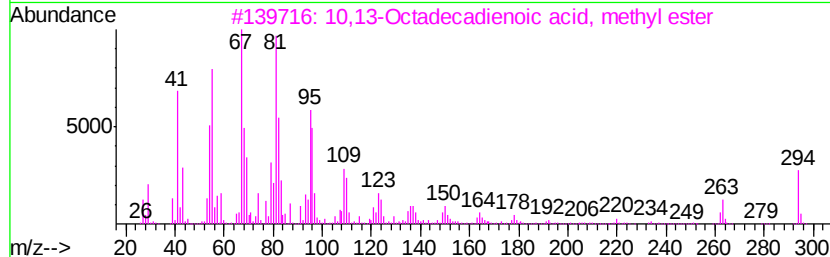
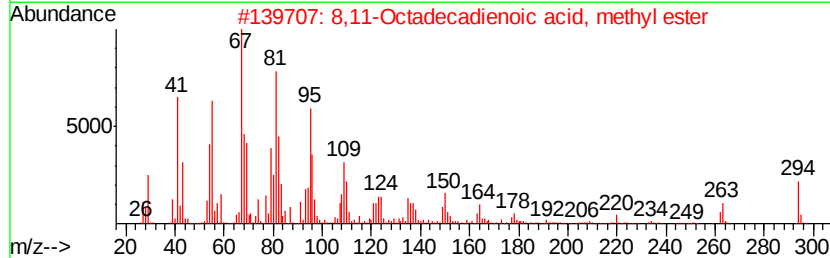
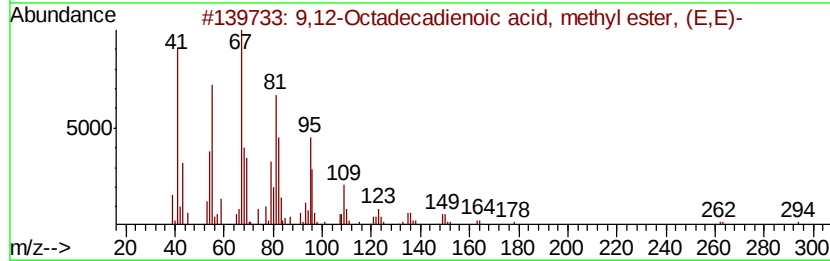
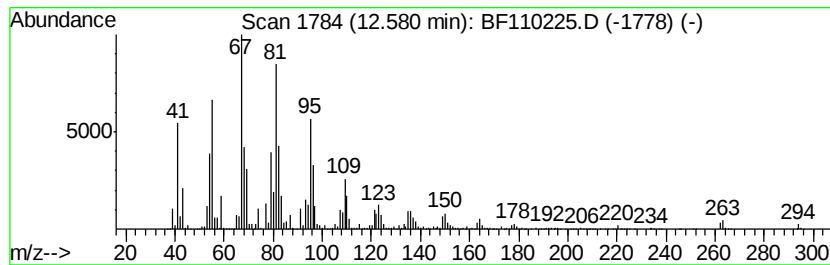
Instrument :
BNA_F
ClientSampleId :
TR-05-102518

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.58	294.62 ng	11720400	Phenanthrene-d10	11.50		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99	
2	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99	
3	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99	
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99	
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99	



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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-102518

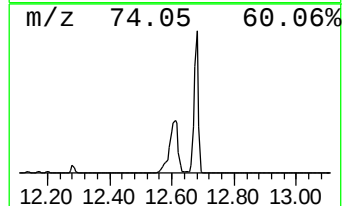
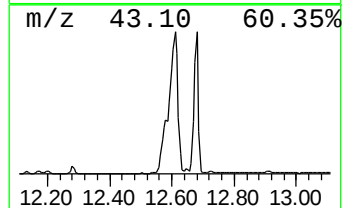
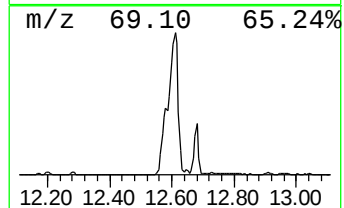
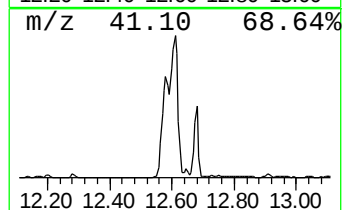
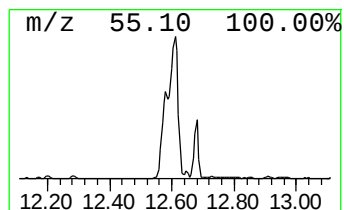
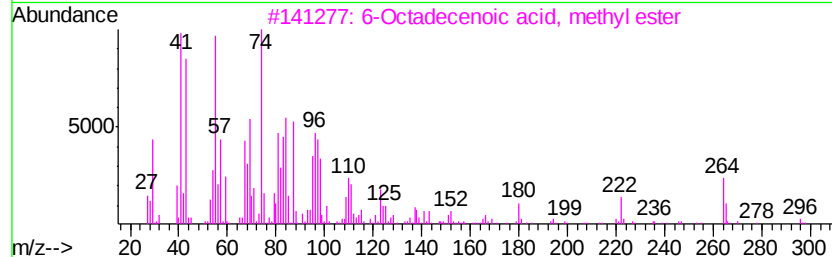
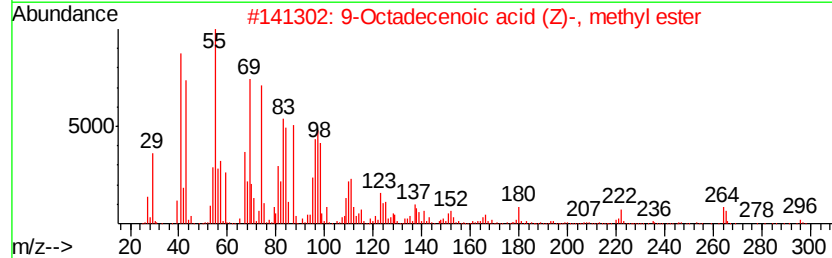
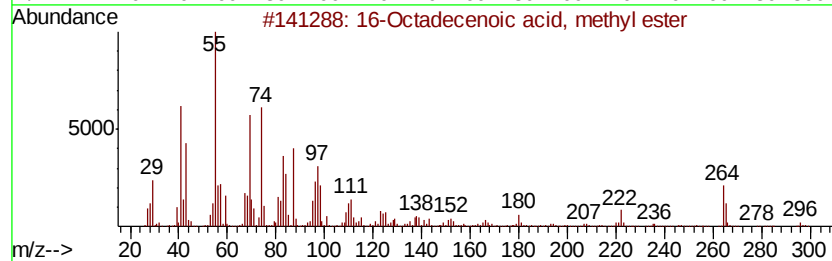
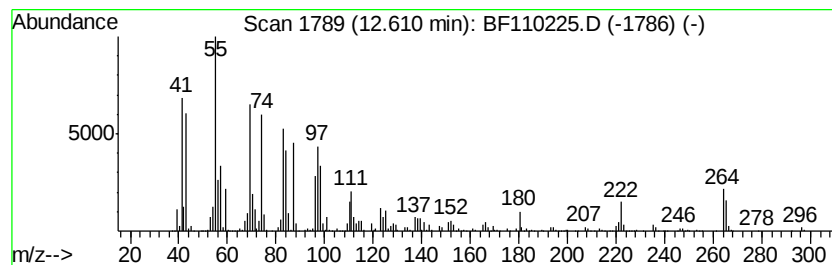
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 16-Octadecenoic acid, methyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.61	348.41 ng	13860100	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
2		9-Octadecenoic acid (Z)-, methyl ester	296	C19H36O2	000112-62-9	99
3		6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	93
4		15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	93
5		14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	93



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Misc :
ALS Vial : 20 Sample Multiplier: 1

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

Peak Number 10 9,12,15-Octadecatrienoic ac... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	8.23 ng	327392	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	99
2		7,10,13-Hexadecatrienoic acid, m...	264	C17H28O2	056554-30-4	91
3		9,12,15-Octadecatrienoic acid, (...	278	C18H30O2	000463-40-1	87
4		9,12,15-Octadecatrien-1-ol, (Z,Z...	264	C18H32O	000506-44-5	86
5		Methyl 8,11,14-heptadecatrienoate	278	C18H30O2	1000336-35-1	81

