

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
 Data File : BF099930.D
 Acq On : 28 Oct 2017 21:14
 Operator : SJ/JU
 Sample : I6146-07 5X
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AU-06-102517-C

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:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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	4.992	492	494	507	rBV	22495	35056	1.28%	0.270%
2	5.416	563	566	587	rBV	159353	255241	9.33%	1.965%
3	6.434	737	739	756	rBV	195046	277693	10.15%	2.137%
4	6.563	758	761	769	rVB	322489	313803	11.48%	2.415%
5	6.786	796	799	810	rBV	635924	560076	20.48%	4.311%
6	6.939	822	825	839	rVB	284229	252876	9.25%	1.946%
7	7.357	893	896	907	rBV	159197	172673	6.31%	1.329%
8	8.069	1013	1017	1034	rBV	902409	750946	27.46%	5.780%
9	9.139	1196	1199	1208	rVB	509166	388131	14.19%	2.987%
10	9.539	1260	1267	1273	rBV	53487	67541	2.47%	0.520%
11	9.822	1311	1315	1321	rVB2	899793	753986	27.57%	5.803%
12	10.457	1417	1423	1426	rBV	26822	30776	1.13%	0.237%
13	10.616	1448	1450	1459	rBV	128143	130491	4.77%	1.004%
14	10.716	1463	1467	1472	rBV2	48903	72085	2.64%	0.555%
15	11.157	1539	1542	1545	rBV	38990	33228	1.22%	0.256%
16	11.316	1565	1569	1577	rVB	624116	595659	21.78%	4.585%
17	11.586	1610	1615	1618	rBV	36408	29506	1.08%	0.227%
18	11.692	1629	1633	1636	rVB	1245397	960006	35.11%	7.389%
19	11.827	1652	1656	1663	rBV	71513	86255	3.15%	0.664%
20	12.380	1745	1750	1752	rBV	2547275	2734664	100.00%	21.048%
21	12.404	1752	1754	1760	rVV2	2085989	1845420	67.48%	14.204%
22	12.480	1764	1767	1771	rVB	592672	480672	17.58%	3.700%
23	12.539	1771	1777	1785	rBV3	148357	276452	10.11%	2.128%
24	12.715	1804	1807	1811	rVB4	25284	28561	1.04%	0.220%
25	12.892	1834	1837	1841	rVB	292310	237393	8.68%	1.827%
26	13.127	1875	1877	1881	rVB3	34663	33389	1.22%	0.257%
27	13.204	1886	1890	1893	rBV	65455	61763	2.26%	0.475%
28	13.639	1957	1964	1969	rBV6	37737	67171	2.46%	0.517%
29	13.774	1985	1987	1992	rVB	26144	28456	1.04%	0.219%
30	13.874	2001	2004	2009	rBV	72814	61534	2.25%	0.474%
31	13.962	2015	2019	2026	rBV	599648	535487	19.58%	4.122%
32	14.398	2090	2093	2098	rBV4	34102	47065	1.72%	0.362%
33	14.492	2105	2109	2113	rBV3	28697	44045	1.61%	0.339%
34	15.027	2197	2200	2203	rVB	42519	44885	1.64%	0.345%

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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	15.386	2258	2261	2264	rBV3	36612	46009	1.68%	0.354%
36	15.427	2264	2268	2279	rVB	415867	532780	19.48%	4.101%
37	15.809	2330	2333	2337	rVB	56102	73364	2.68%	0.565%
38	16.298	2412	2416	2420	rVB3	30480	47116	1.72%	0.363%

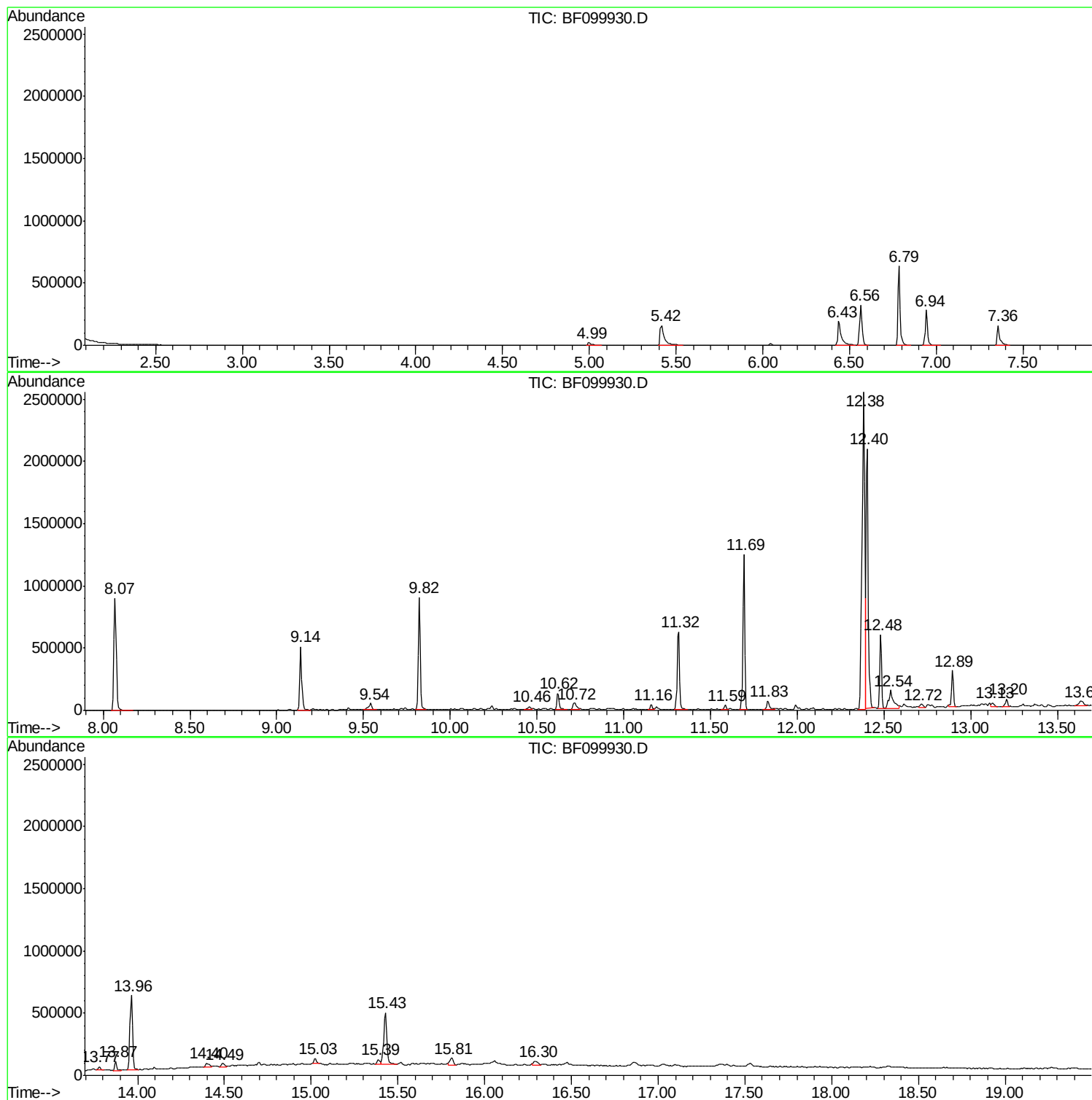
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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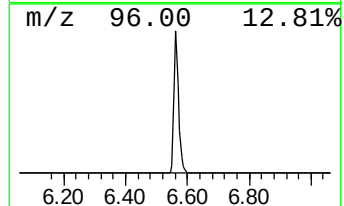
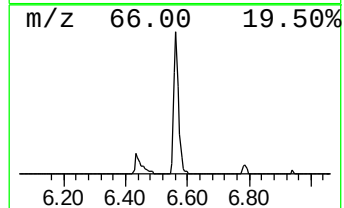
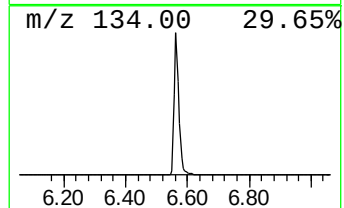
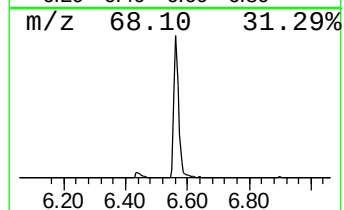
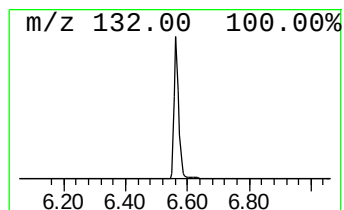
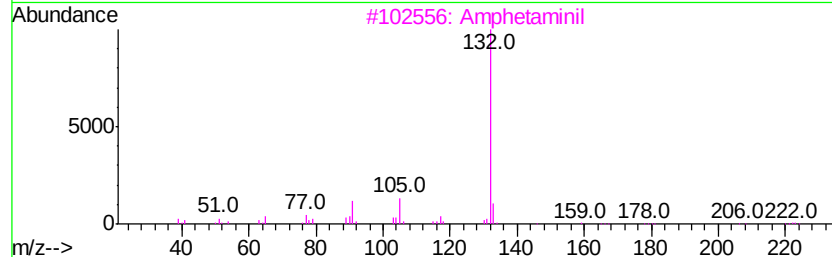
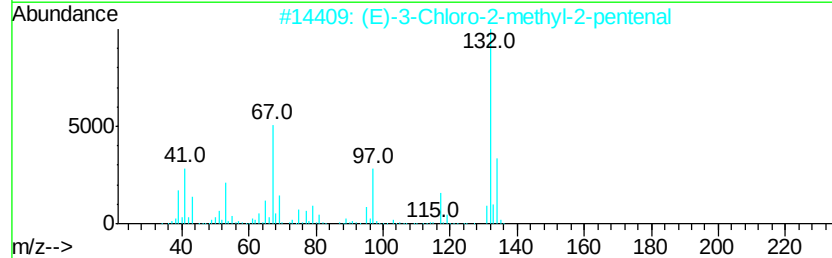
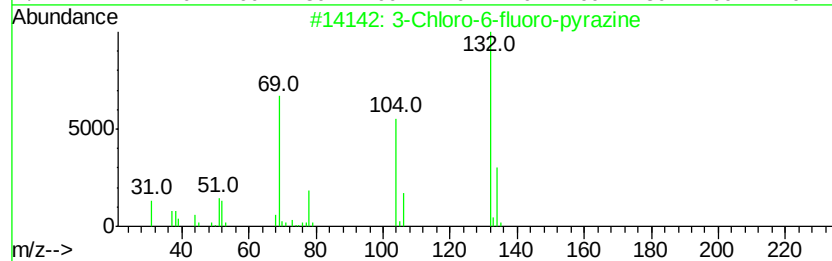
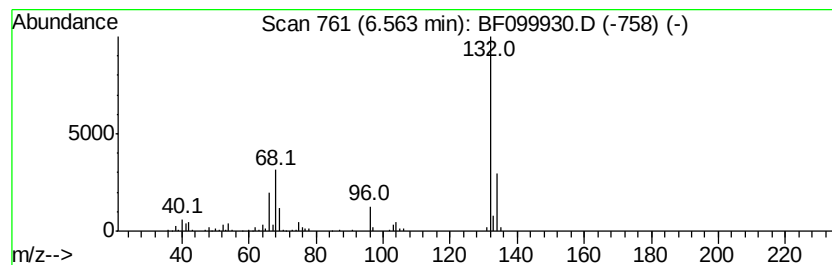
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.56 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	11.21 ng	313803	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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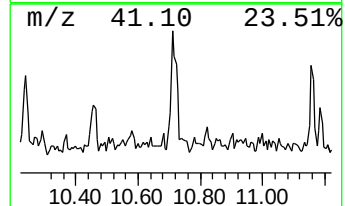
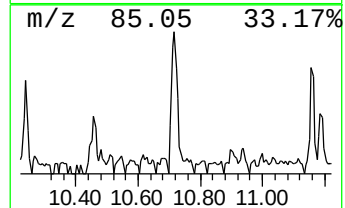
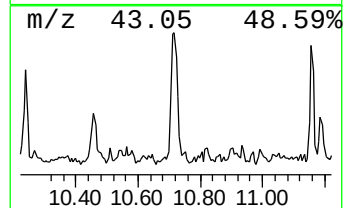
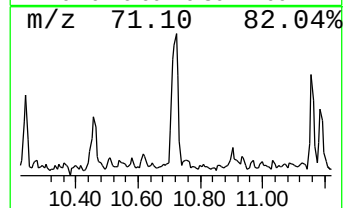
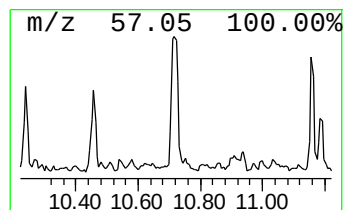
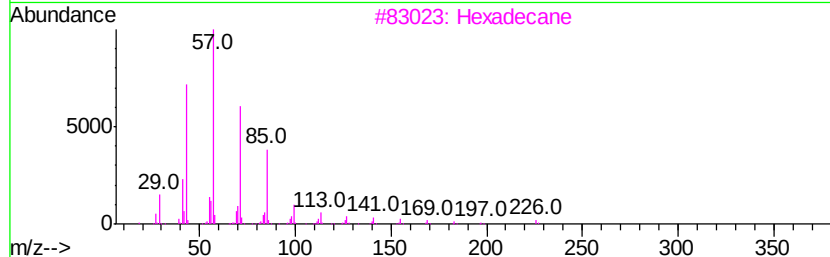
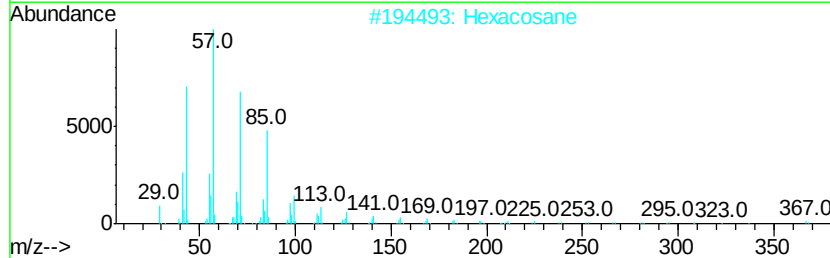
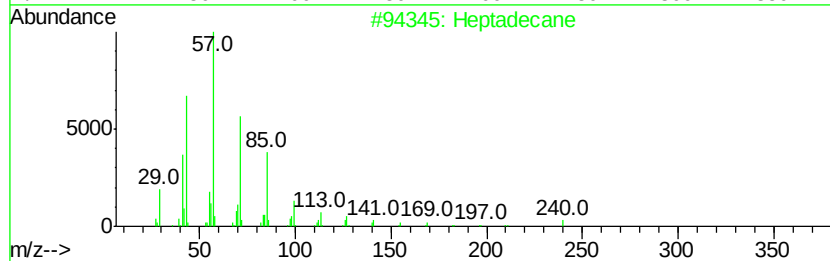
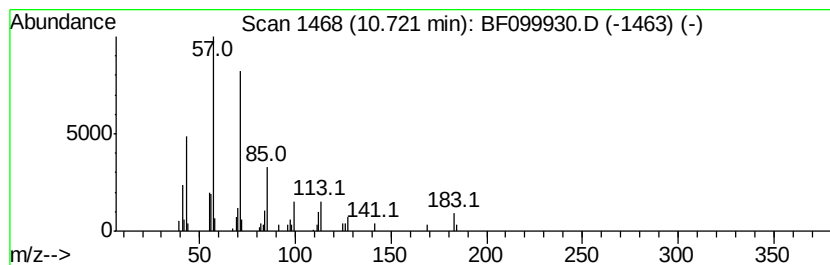
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	2.42 ng	72085	Phenanthrene-d10	11.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	87
2	Hexacosane	366 C26H54	000630-01-3	87
3	Hexadecane	226 C16H34	000544-76-3	86
4	Octacosane	394 C28H58	000630-02-4	86
5	Tetracosane	338 C24H50	000646-31-1	86



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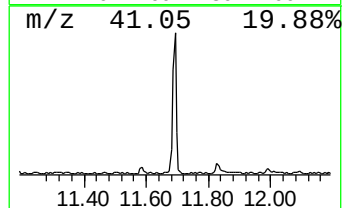
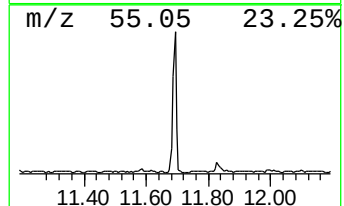
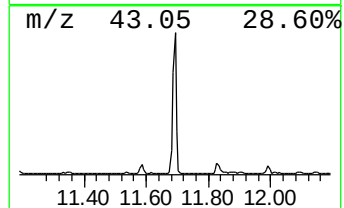
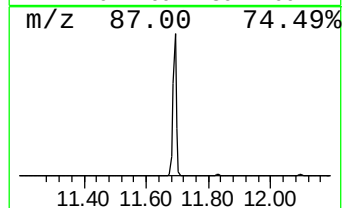
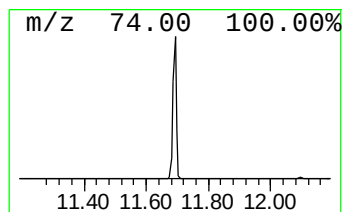
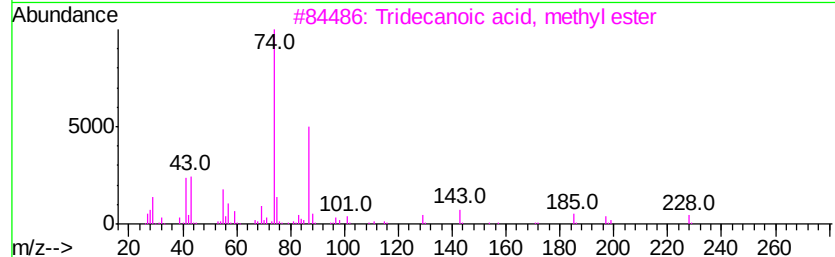
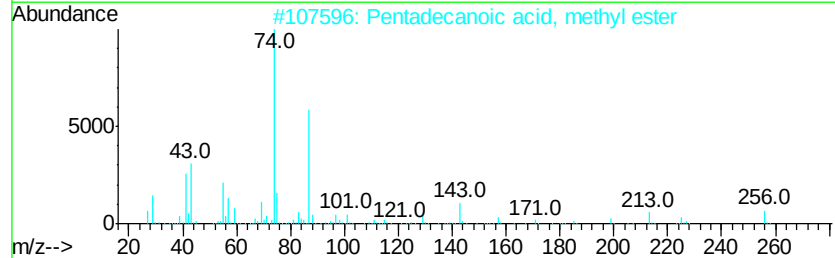
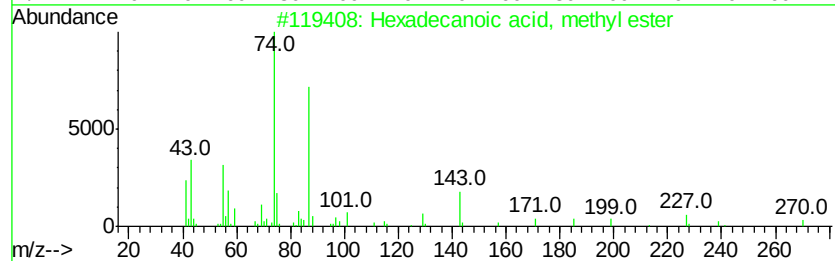
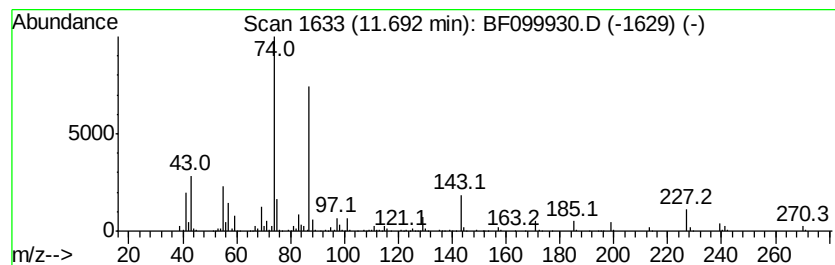
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	32.23 ng	960006	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
3		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	80
4		Methyl tetradecanoate	242	C15H30O2	000124-10-7	80
5		Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	72



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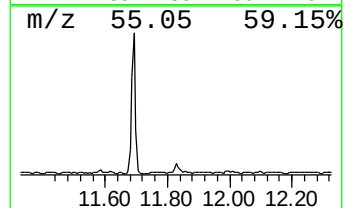
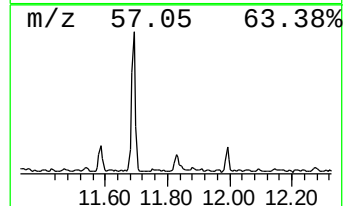
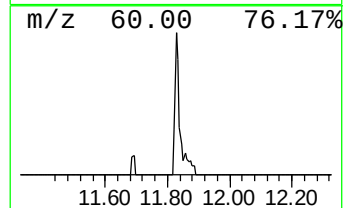
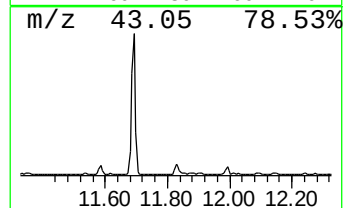
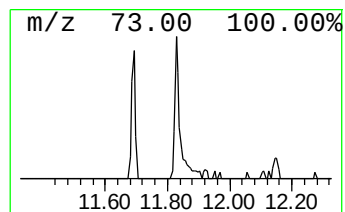
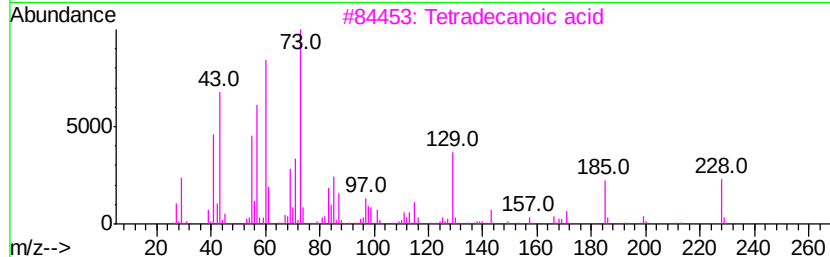
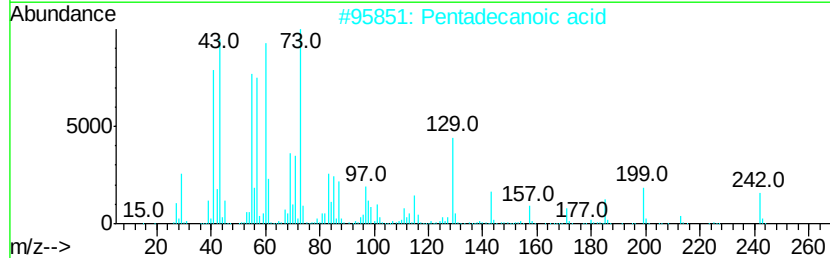
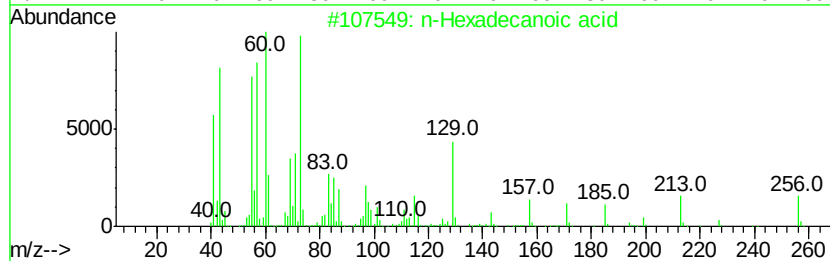
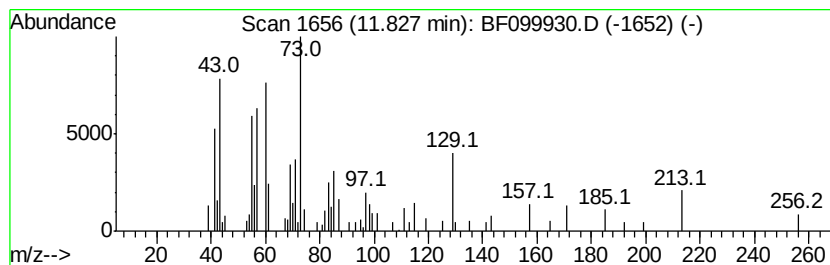
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	2.90 ng	86255	Phenanthrene-d10	11.32

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	81
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4		Tridecanoic acid	214	C13H26O2	000638-53-9	53
5		n-Decanoic acid	172	C10H20O2	000334-48-5	47



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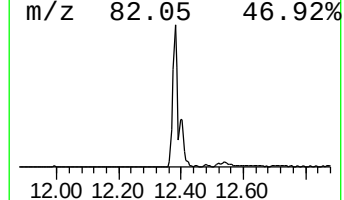
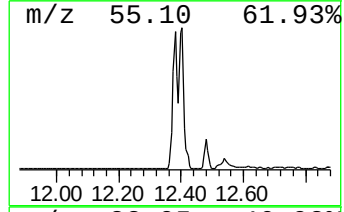
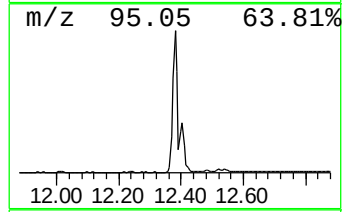
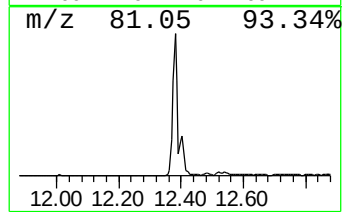
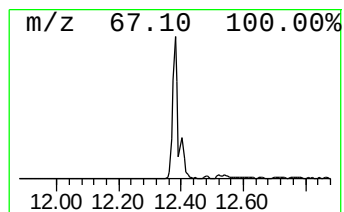
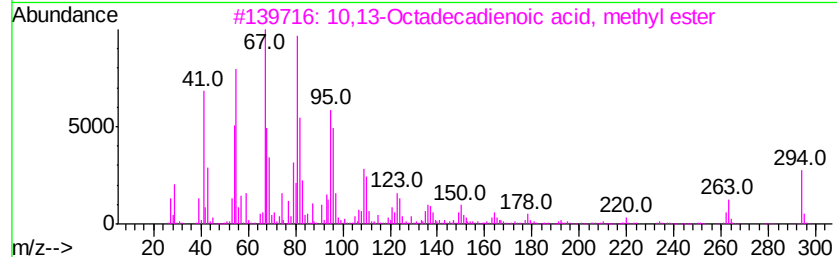
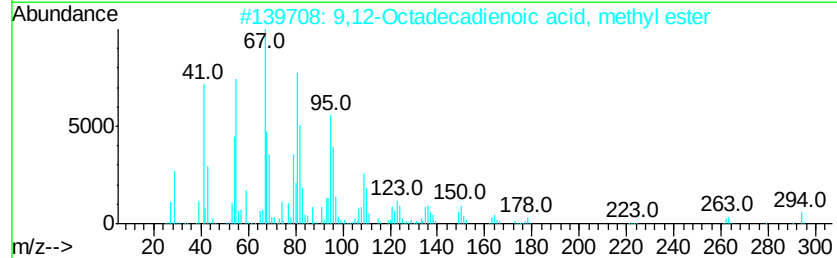
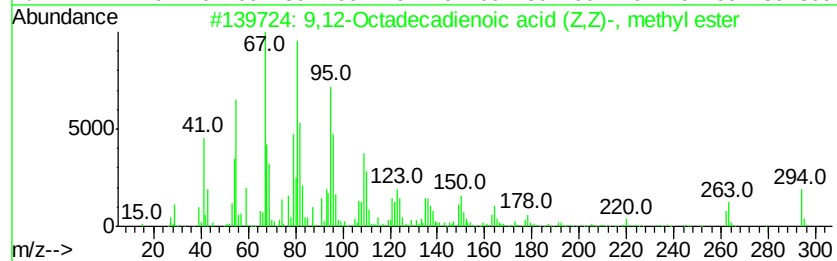
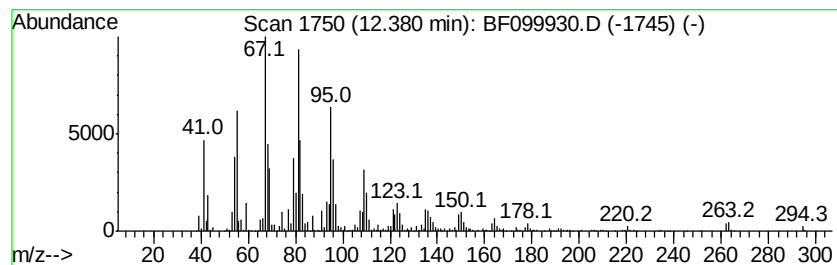
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Peak Number 6 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.38	91.82 ng	2734660	Phenanthrene-d10	11.32		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99	
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99	
3	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99	
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99	
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99	



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ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-06-102517-C

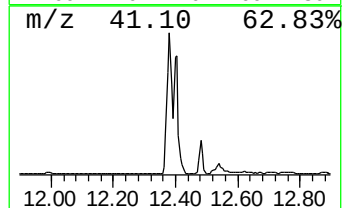
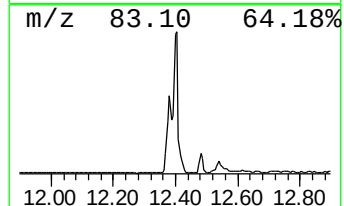
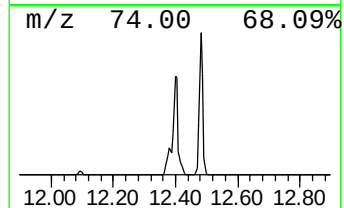
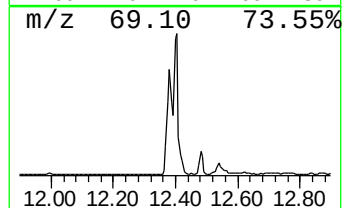
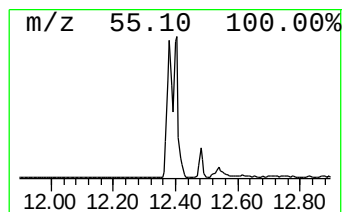
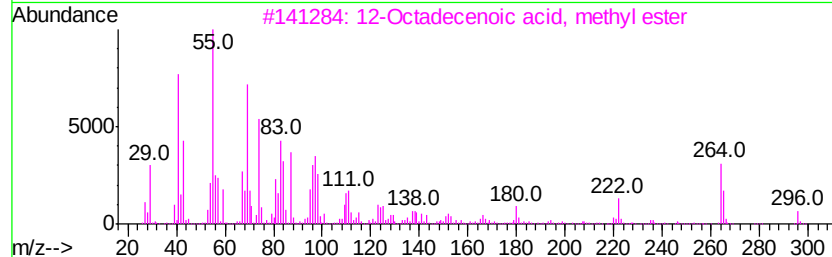
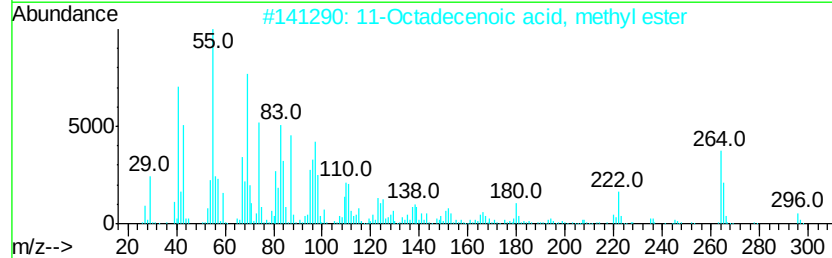
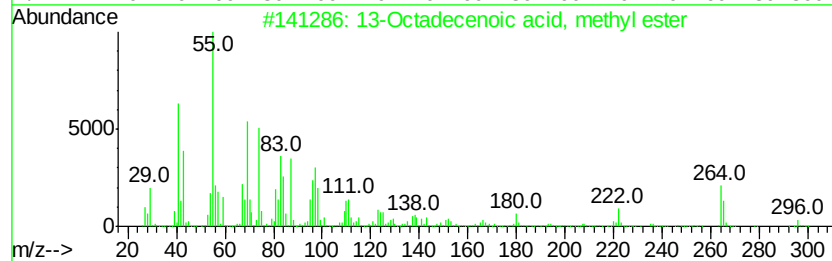
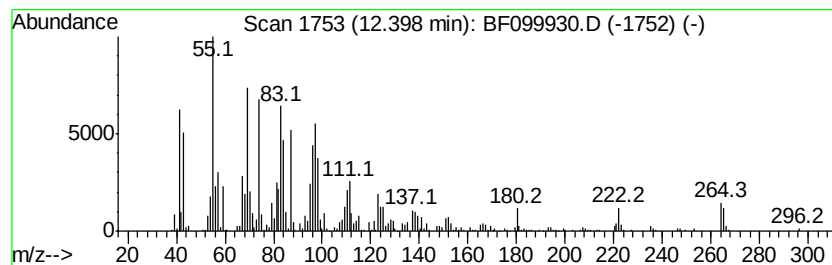
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 13-Octadecenoic acid, methyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	61.96 ng	1845420	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
2		11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
3		12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
4		11-Octadecenoic acid, methyl ester	296	C19H36O2	001937-63-9	99
5		15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099930.D
Acq On : 28 Oct 2017 21:14
Operator : SJ/JU
Sample : I6146-07 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

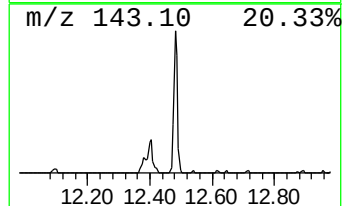
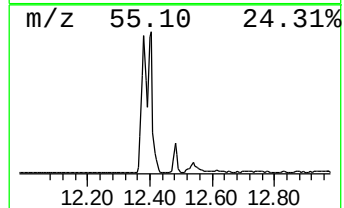
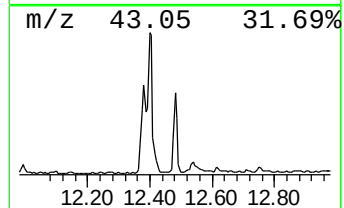
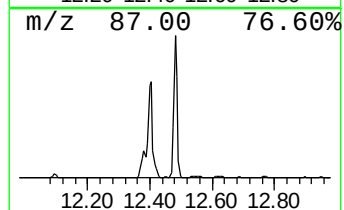
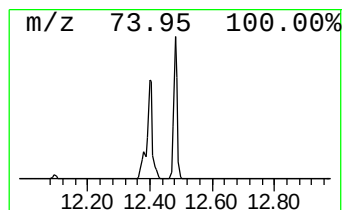
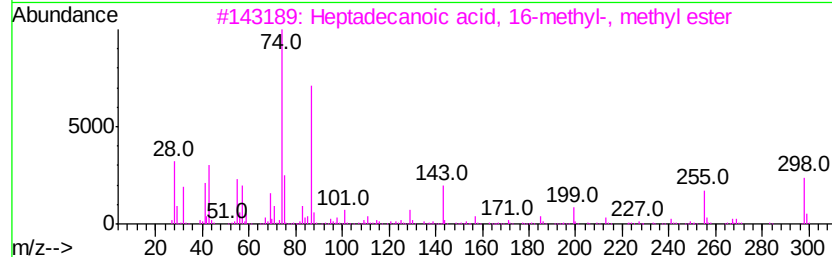
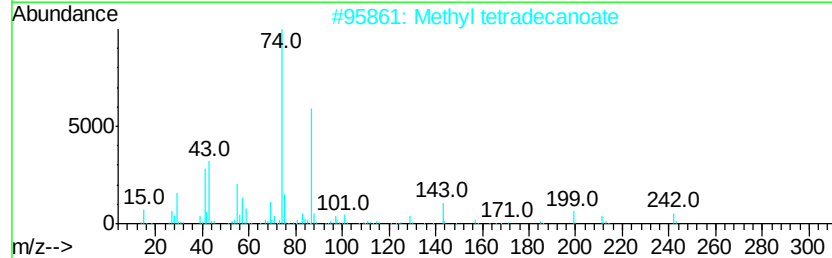
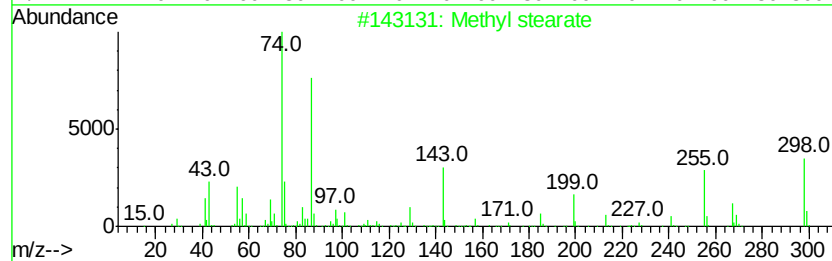
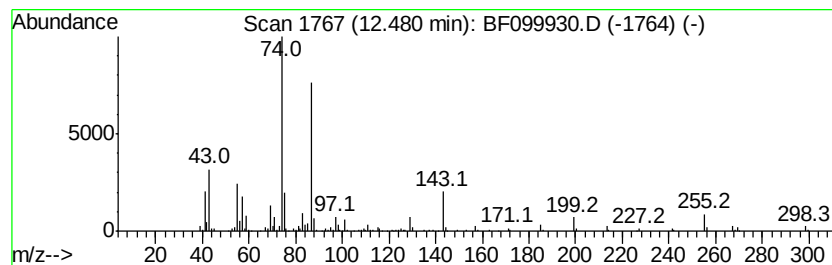
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
12.48	16.14 ng	480672	Phenanthrene-d10	11.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Methyl stearate	298 C19H38O2	000112-61-8 98
2		Methyl tetradecanoate	242 C15H30O2	000124-10-7 95
3		Heptadecanoic acid, 16-methyl-, ...	298 C19H38O2	005129-61-3 94
4		Pentadecanoic acid, 14-methyl-, ...	270 C17H34O2	005129-60-2 90
5		Pentadecanoic acid, methyl ester	256 C16H32O2	007132-64-1 90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099930.D
Acq On : 28 Oct 2017 21:14
Operator : SJ/JU
Sample : I6146-07 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

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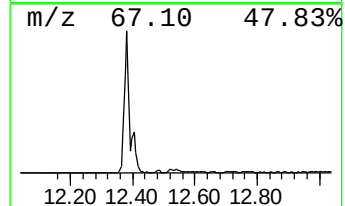
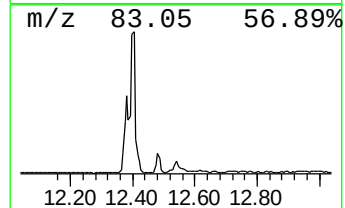
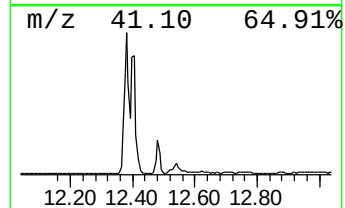
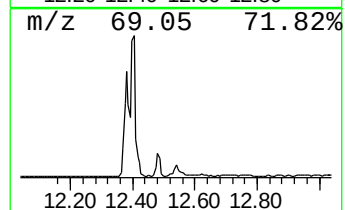
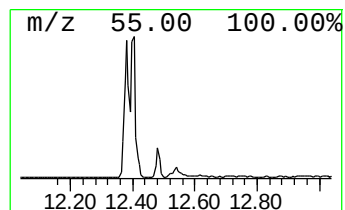
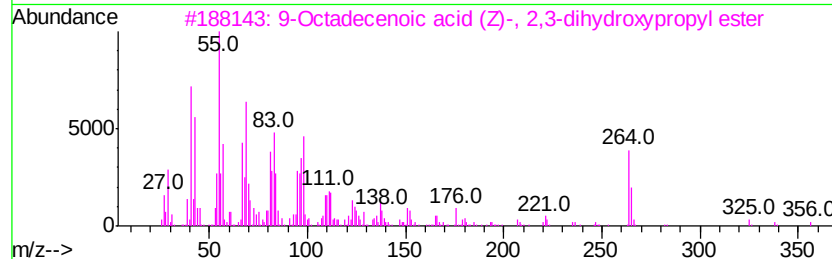
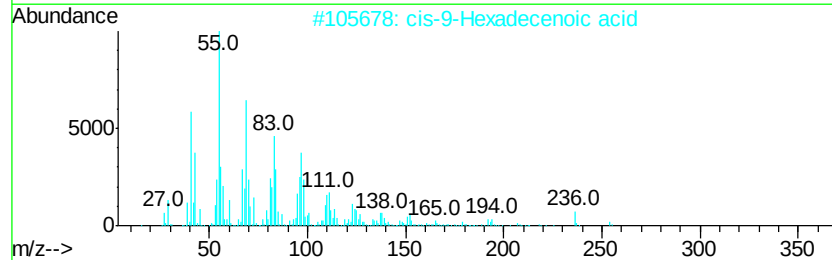
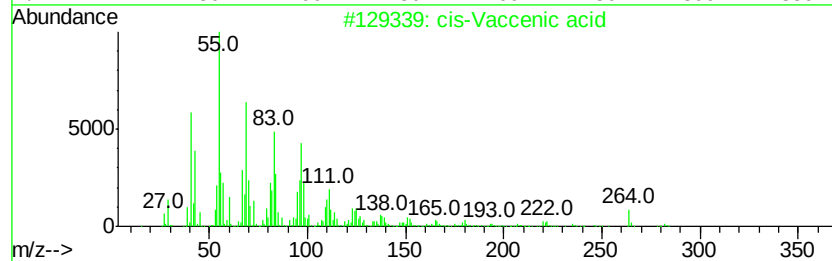
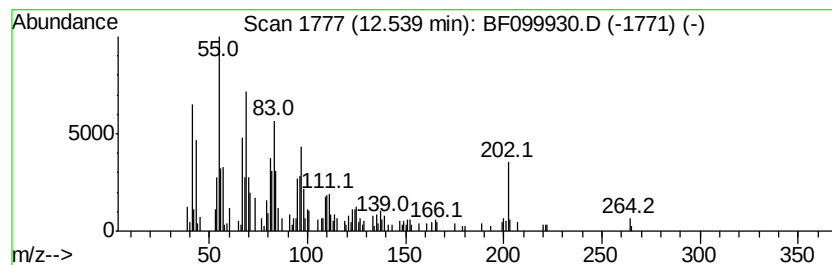
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 cis-Vaccenic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	9.28 ng	276452	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		cis-Vaccenic acid	282	C18H34O2	000506-17-2	76
2		cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	76
3		9-Octadecenoic acid (Z)-, 2,3-di...	356	C21H40O4	000111-03-5	74
4		trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	70
5		9-octadecenoic acid, 2,2,2-trifl...	364	C20H35F3O2	1000376-54-3	68



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099930.D
Acq On : 28 Oct 2017 21:14
Operator : SJ/JU
Sample : I6146-07 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

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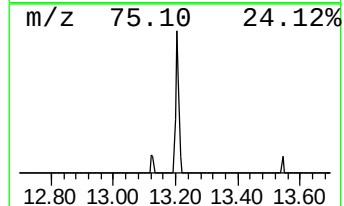
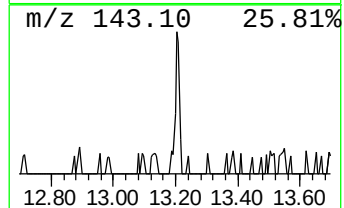
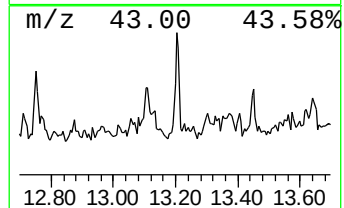
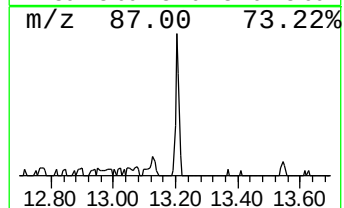
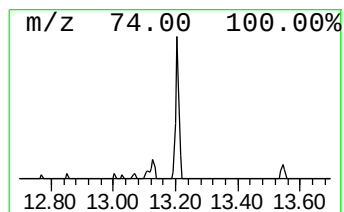
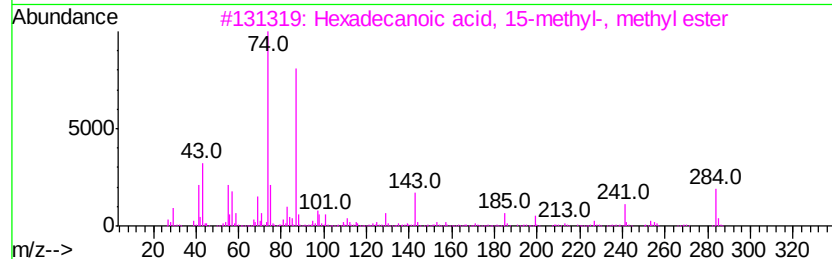
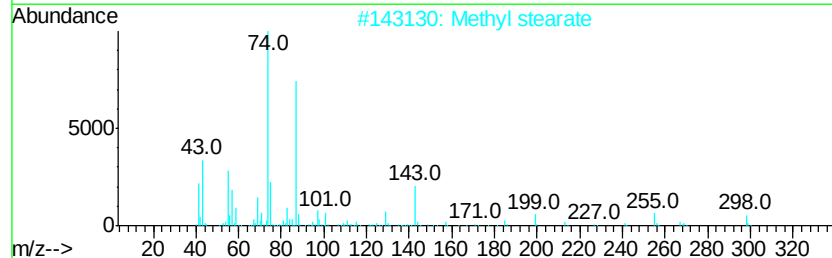
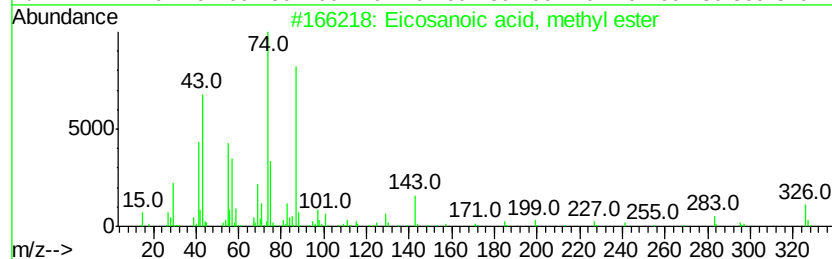
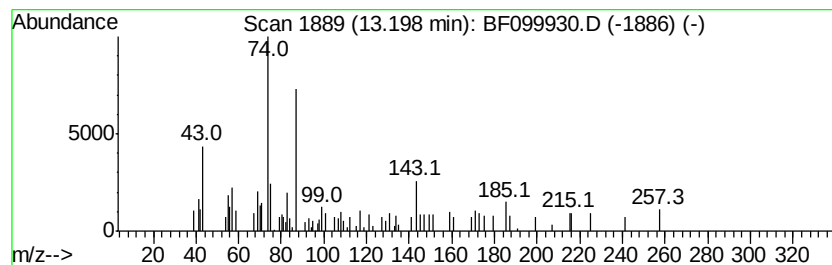
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosanoic acid, methyl ester Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.20	2.31 ng	61763	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	87
2		Methyl stearate	298	C19H38O2	000112-61-8	86
3		Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	86
4		Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	83
5		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102817\
Data File : BF099930.D
Acq On : 28 Oct 2017 21:14
Operator : SJ/JU
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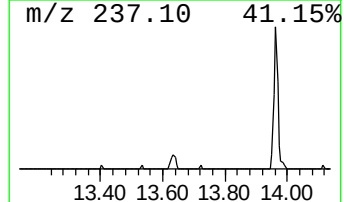
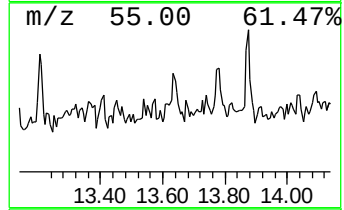
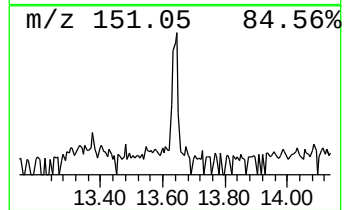
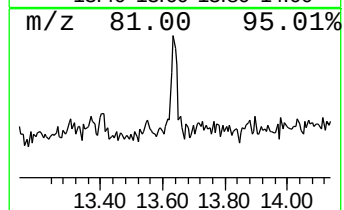
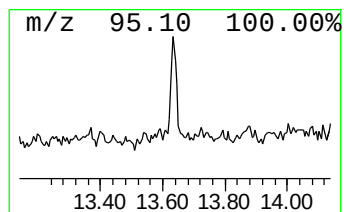
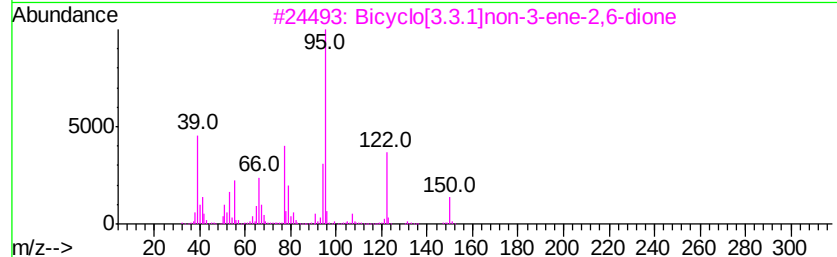
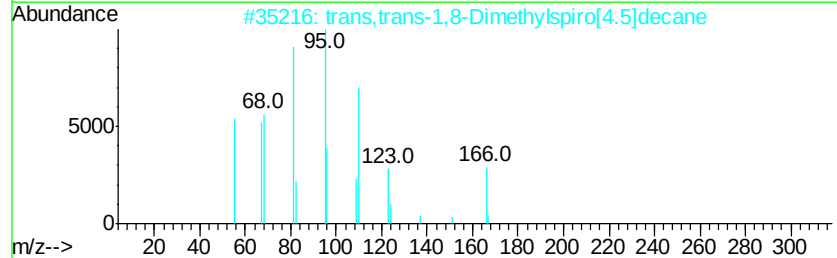
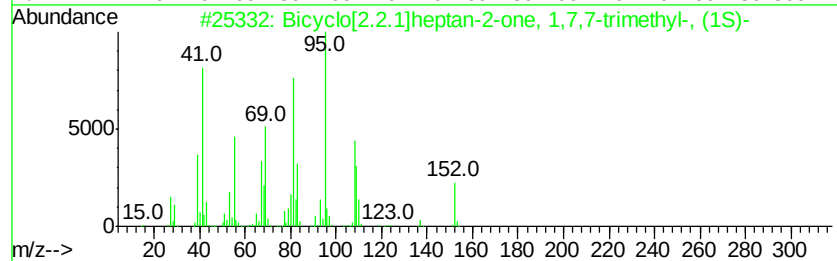
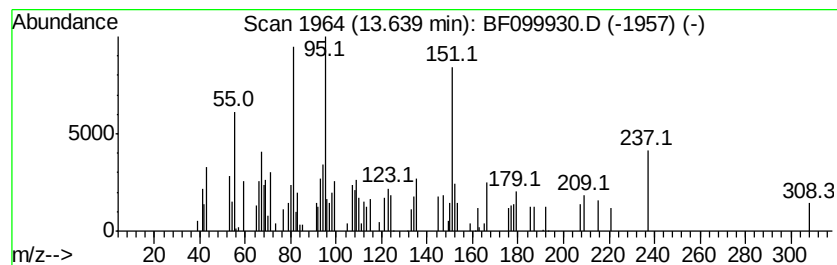
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown13.64 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	2.51 ng	67171	Chrysene-d12	13.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	38
2			trans,trans-1,8-Dimethylspiro[4....	166	C12H22	1000111-72-8	27
3			Bicyclo[3.3.1]non-3-ene-2,6-dione	150	C9H10O2	155137-46-5	25
4			3-Pyridinecarboxylic acid, 1,2-d...	139	C6H5NO3	000609-71-2	22
5			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	15



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
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Misc :
ALS Vial : 22 Sample Multiplier: 1

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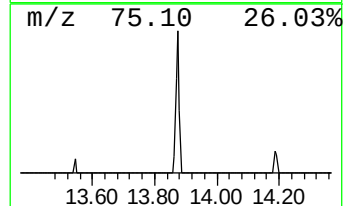
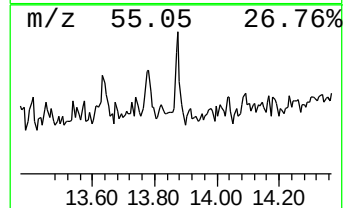
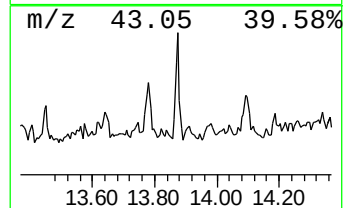
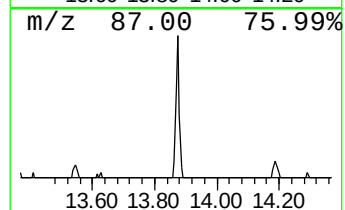
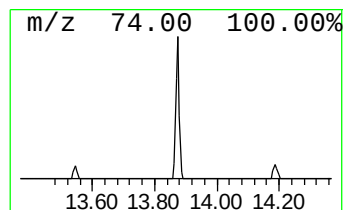
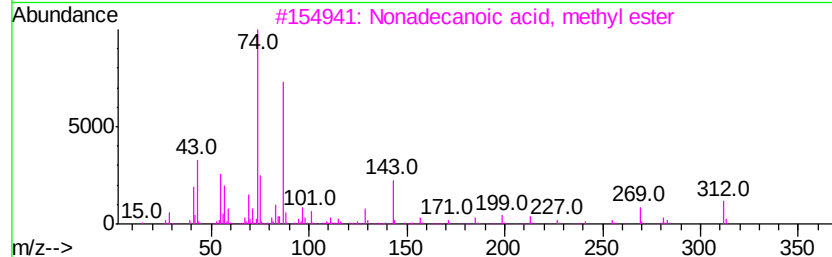
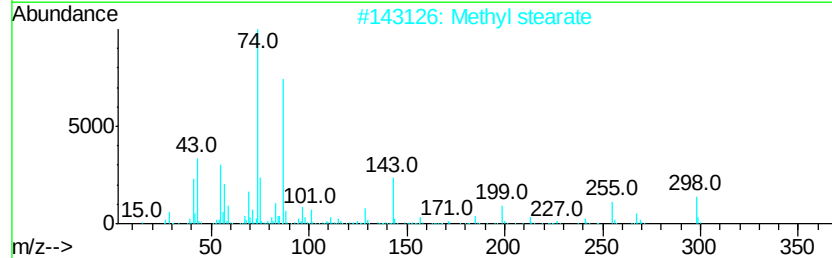
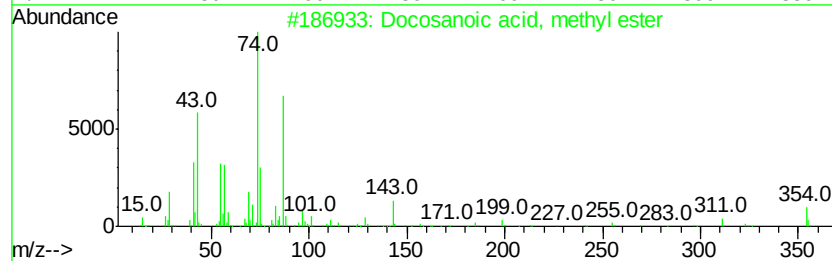
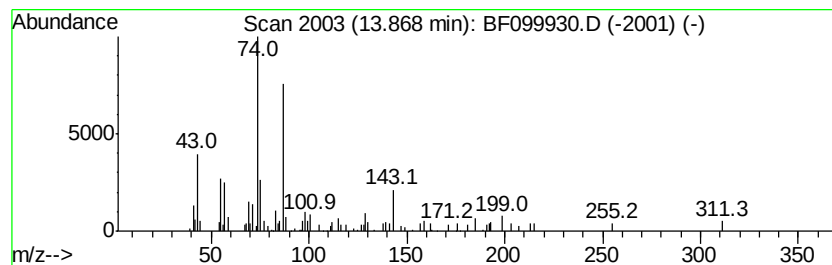
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Docosanoic acid, methyl ester Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	2.30 ng	61534	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	97
2		Methyl stearate	298	C19H38O2	000112-61-8	87
3		Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	83
4		Heneicosanoic acid, methyl ester	340	C22H44O2	006064-90-0	83
5		Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
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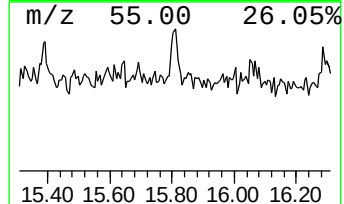
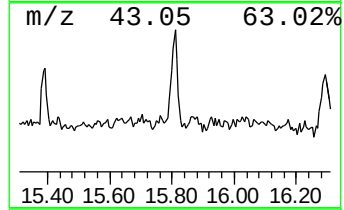
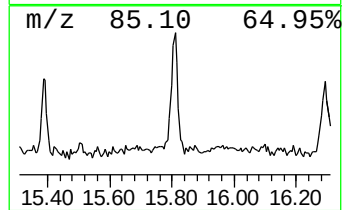
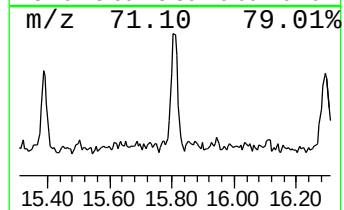
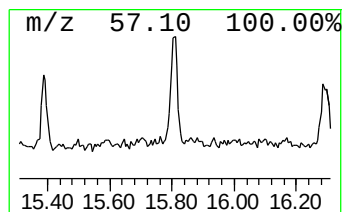
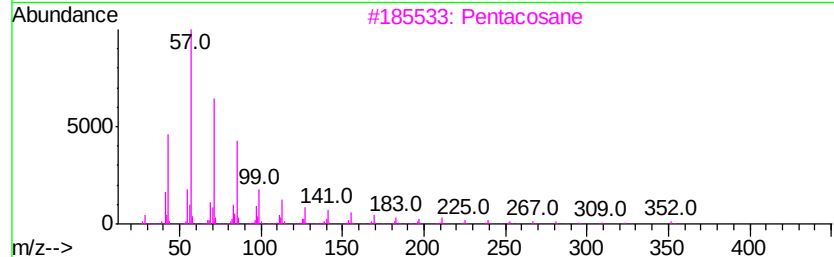
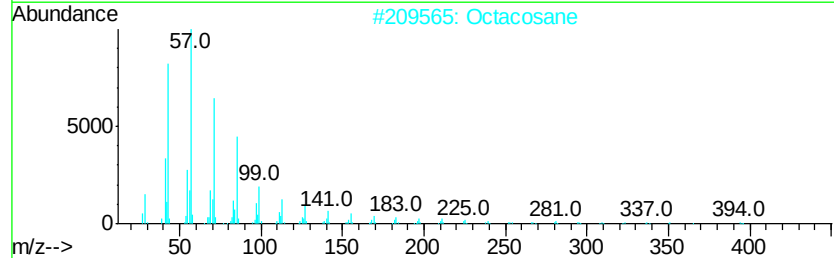
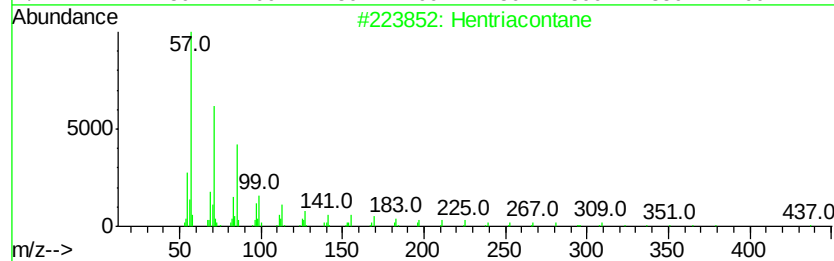
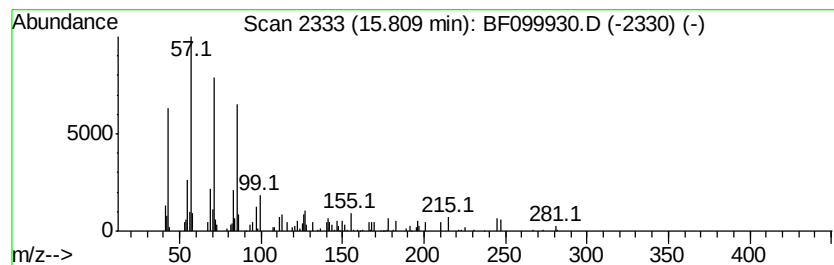
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	2.75 ng	73364	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	87
2		Octacosane	394	C28H58	000630-02-4	86
3		Pentacosane	352	C25H52	000629-99-2	86
4		Eicosane	282	C20H42	000112-95-8	86
5		Hexacosane	366	C26H54	000630-01-3	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102817\
 Data File : BF099930.D
 Acq On : 28 Oct 2017 21:14
 Operator : SJ/JU
 Sample : I6146-07 5X
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AU-06-102517-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.56	6.56	11.2	ng	313803	1	6.79	560076	20.0
Heptadecane	10.72	2.4	ng	72085	4	11.32	595659	20.0
Hexadecanoic acid...	11.69	32.2	ng	960006	4	11.32	595659	20.0
n-Hexadecanoic acid	11.83	2.9	ng	86255	4	11.32	595659	20.0
9,12-Octadecadien...	12.38	91.8	ng	2734660	4	11.32	595659	20.0
13-Octadecenoic a...	12.40	62.0	ng	1845420	4	11.32	595659	20.0
Methyl stearate	12.48	16.1	ng	480672	4	11.32	595659	20.0
cis-Vaccenic acid	12.54	9.3	ng	276452	4	11.32	595659	20.0
Eicosanoic acid, ...	13.20	2.3	ng	61763	5	13.96	535487	20.0
unknown13.64	13.64	2.5	ng	67171	5	13.96	535487	20.0
Docosanoic acid, ...	13.87	2.3	ng	61534	5	13.96	535487	20.0
Hentriacontane	15.81	2.8	ng	73364	6	15.43	532780	20.0