

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062618\
 Data File : BF106834.D
 Acq On : 26 Jun 2018 20:20
 Operator : JU/SJ
 Sample : J3251-05 2X
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SU-02-062518

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-BF061918.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	5.190	482	485	492	rBB	22884	23097	2.14%	0.352%
2	5.601	552	555	569	rBV	262266	260482	24.19%	3.966%
3	6.601	722	725	738	rBV	288284	290367	26.97%	4.421%
4	6.737	745	748	763	rVB	345802	281322	26.13%	4.284%
5	6.960	783	786	789	rBV	299124	235152	21.84%	3.581%
6	7.113	809	812	816	rBV	293018	245715	22.82%	3.741%
7	7.519	878	881	891	rBV	166728	147727	13.72%	2.249%
8	7.678	905	908	911	rBB	109327	79212	7.36%	1.206%
9	8.242	1001	1004	1009	rBV	329232	265728	24.68%	4.046%
10	9.313	1183	1186	1195	rBV	371261	324502	30.14%	4.941%
11	9.707	1248	1253	1258	rBV	31057	27158	2.52%	0.414%
12	10.001	1300	1303	1311	rVB2	322142	276149	25.64%	4.205%
13	10.795	1435	1438	1446	rBV	179004	151249	14.05%	2.303%
14	10.883	1450	1453	1459	rVB	14896	17099	1.59%	0.260%
15	11.330	1526	1529	1532	rBV	13919	11908	1.11%	0.181%
16	11.495	1553	1557	1564	rBV	353369	295757	27.47%	4.503%
17	11.695	1588	1591	1596	rBV	13499	13807	1.28%	0.210%
18	11.866	1616	1620	1623	rBV	162229	140589	13.06%	2.141%
19	12.519	1727	1731	1734	rBV	1107395	1076824	100.00%	16.397%
20	12.554	1734	1737	1739	rVV	633549	571949	53.11%	8.709%
21	12.572	1739	1740	1747	rVV2	397716	359527	33.39%	5.474%
22	12.654	1751	1754	1758	rVB	80626	69389	6.44%	1.057%
23	12.713	1761	1764	1767	rBV	13576	12157	1.13%	0.185%
24	12.895	1793	1795	1799	rVB2	19218	15980	1.48%	0.243%
25	12.942	1799	1803	1809	rBV2	18694	27920	2.59%	0.425%
26	13.007	1811	1814	1818	rBV	97893	80503	7.48%	1.226%
27	13.077	1822	1826	1829	rVV	489741	395971	36.77%	6.029%
28	13.113	1829	1832	1835	rVB2	11425	11982	1.11%	0.182%
29	13.266	1855	1858	1861	rVB3	26681	22177	2.06%	0.338%
30	13.377	1874	1877	1882	rBV	145358	127075	11.80%	1.935%
31	13.513	1897	1900	1904	rBV6	11906	17467	1.62%	0.266%
32	13.730	1935	1937	1940	rBV	59973	54066	5.02%	0.823%
33	13.954	1973	1975	1980	rBV6	15823	19833	1.84%	0.302%
34	14.077	1994	1996	2003	rVB	57347	50740	4.71%	0.773%

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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 >
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35	14.154	2005	2009	2012	rBV	333800	348019	32.32%	5.299%
36	15.695	2267	2271	2276	rVB	159180	218710	20.31%	3.330%

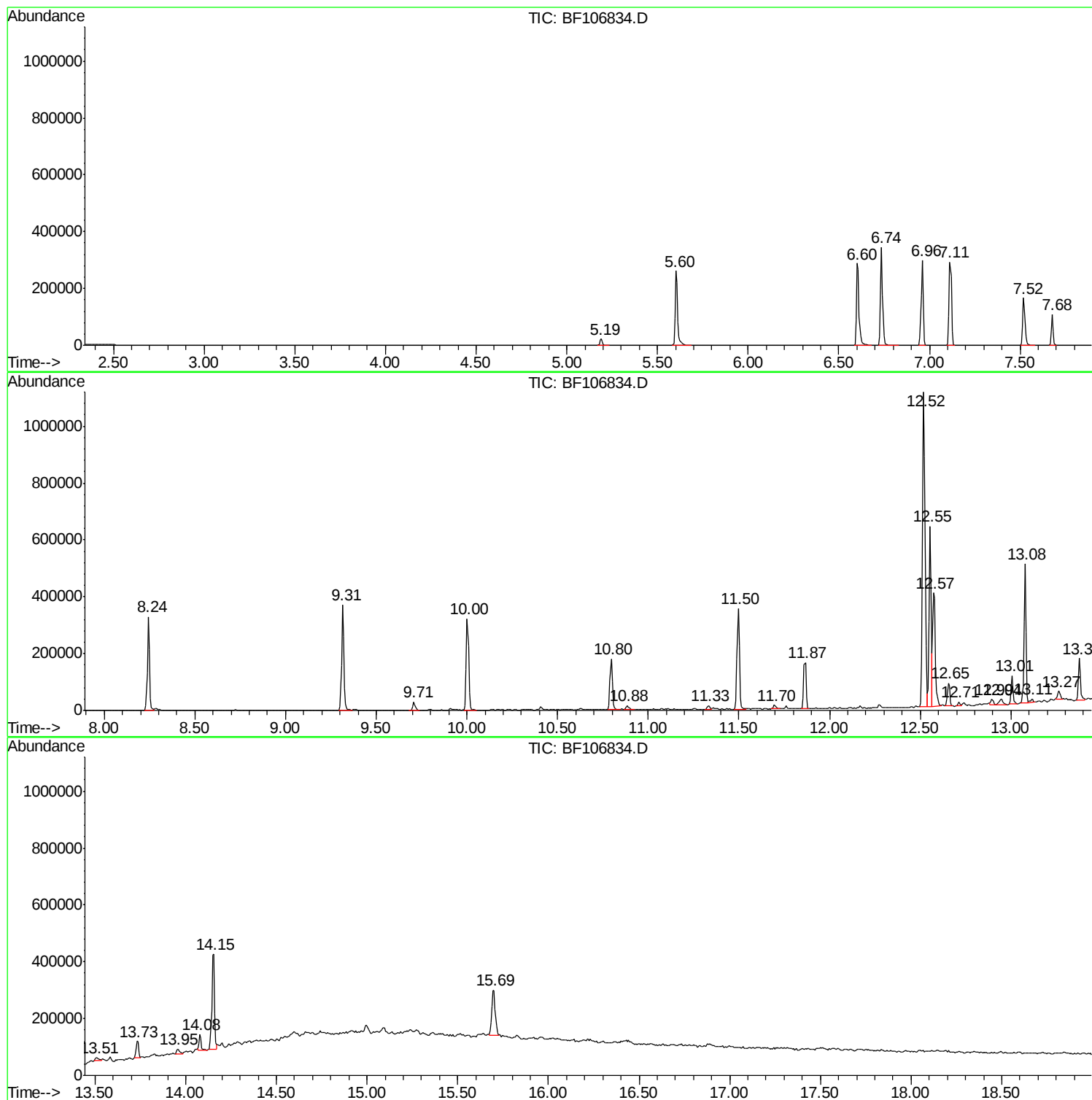
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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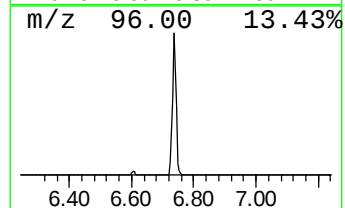
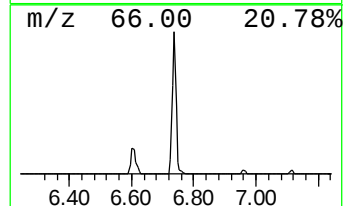
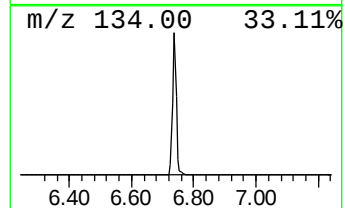
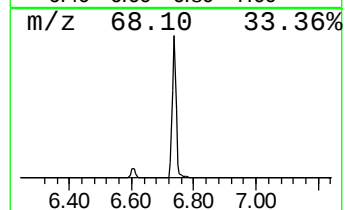
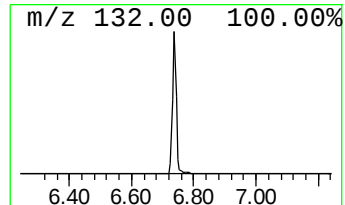
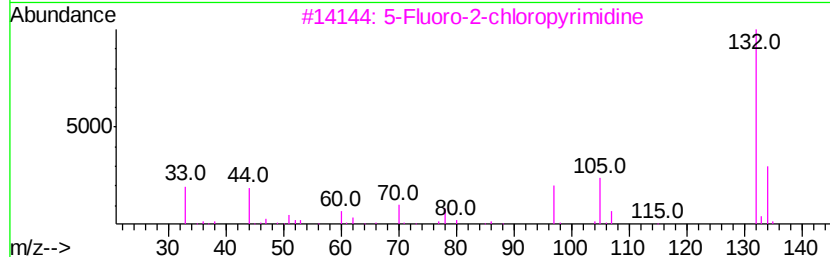
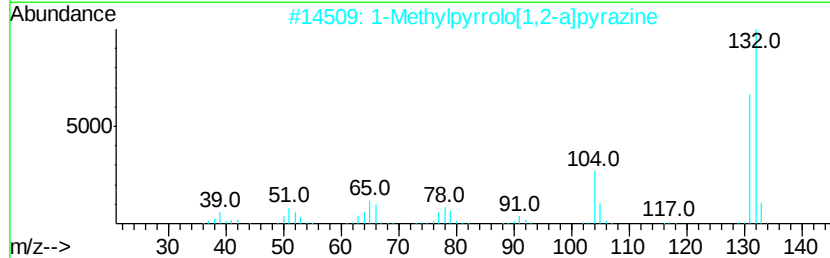
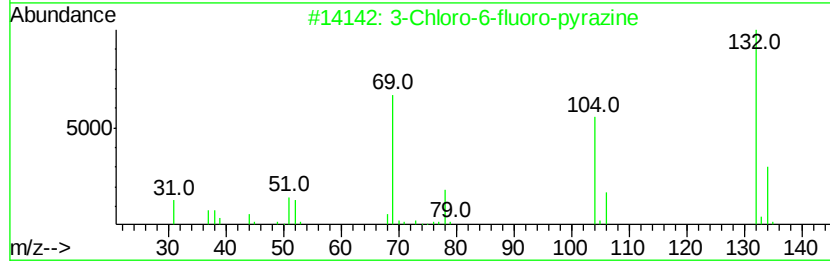
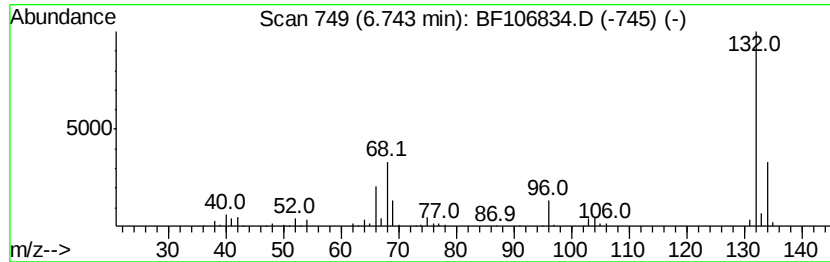
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.74 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	23.93 ng	281322	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		5-Aminoindole	132	C8H8N2	005192-03-0	9



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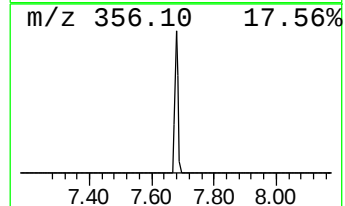
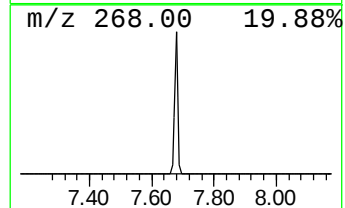
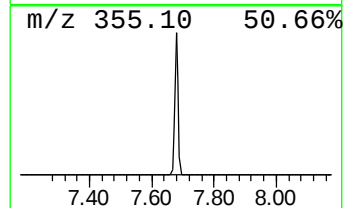
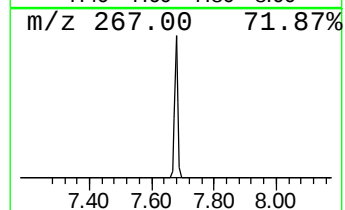
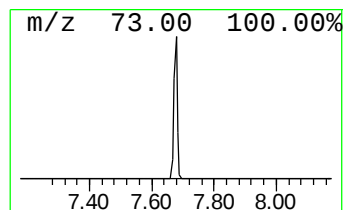
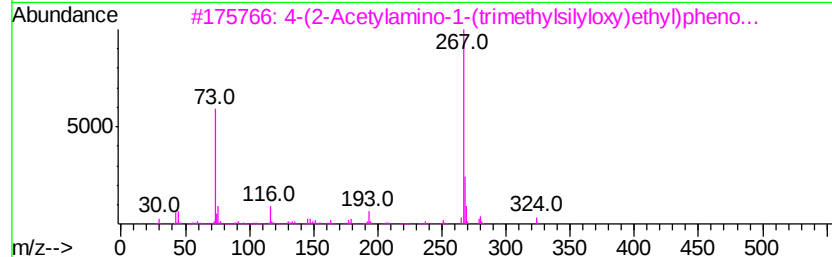
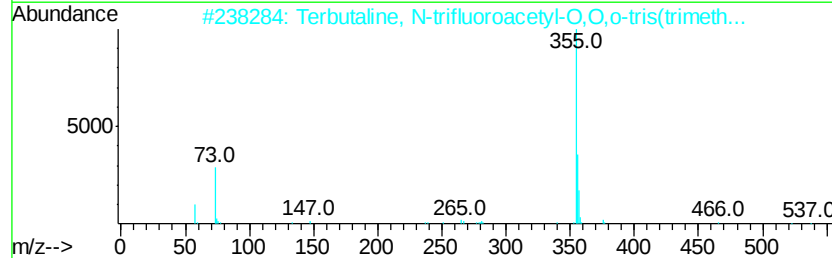
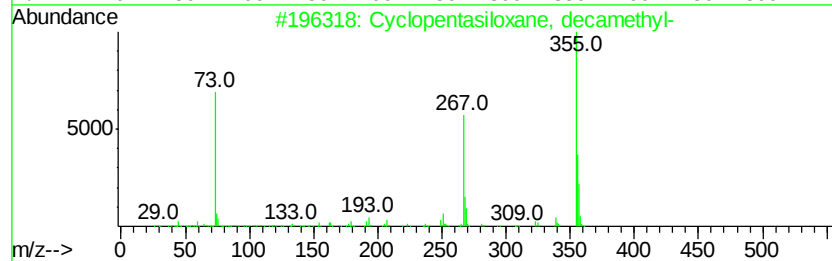
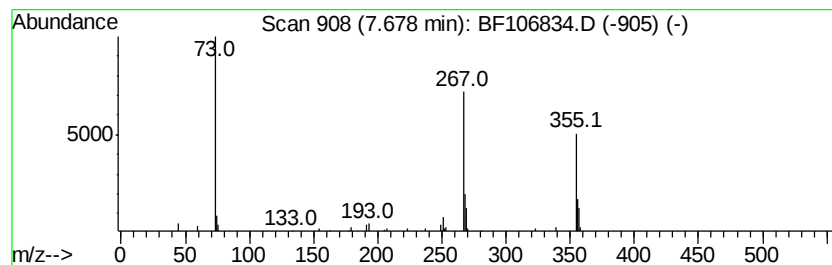
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Cyclopentasiloxane, decamet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	5.96 ng	79212	Naphthalene-d8	8.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	91
2		Terbutaline, N-trifluoroacetyl-O...	537	C23H42F3N04Si3	325836-92-8	43
3		4-(2-Acetyl-amino-1-(trimethylsil...	339	C16H29N03Si2	1000373-43-5	43
4		(-)-Epinephrine, tris(trimethyls...	399	C18H37N03Si3	1000333-51-3	38
5		Benzaldehyde, 2,5-bis[(trimethyl...	282	C13H22O3Si2	056114-69-3	38



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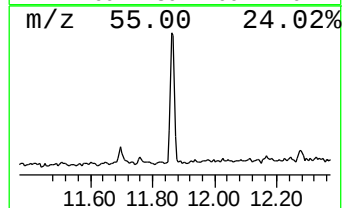
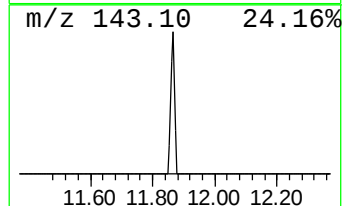
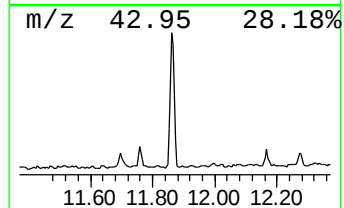
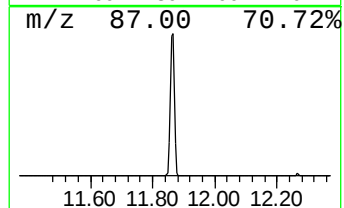
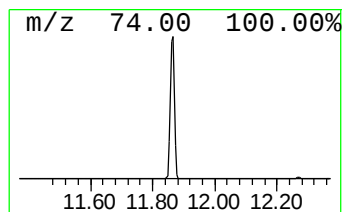
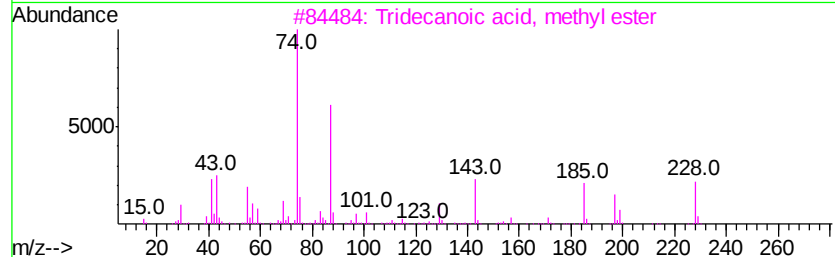
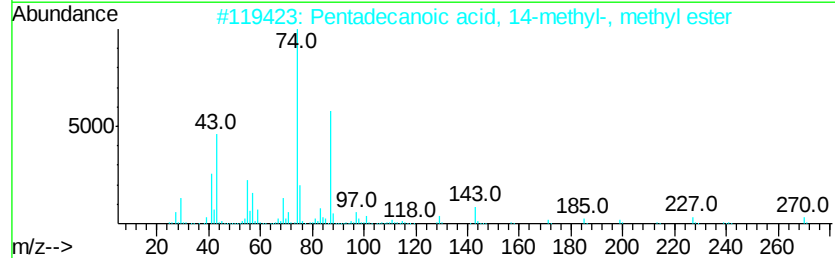
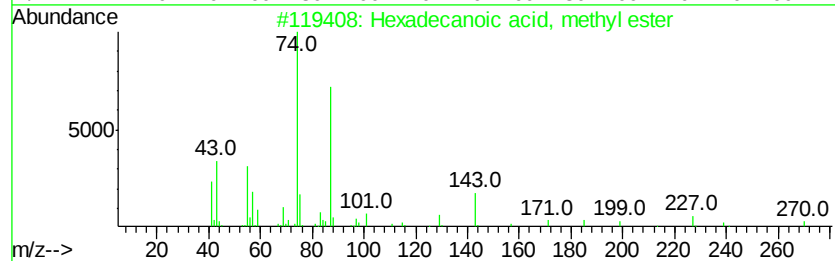
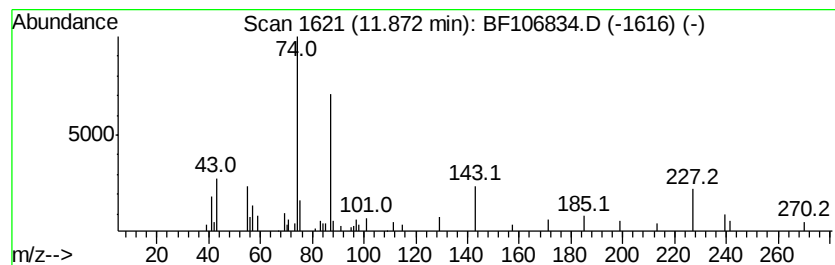
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Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	9.51 ng	140589	Phenanthrene-d10	11.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	83
5			Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	80



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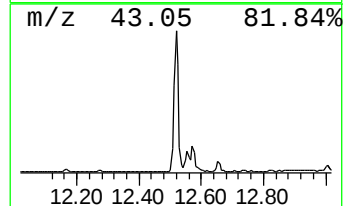
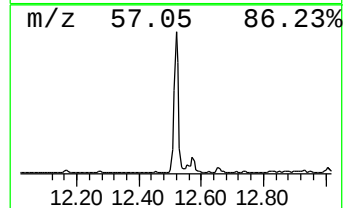
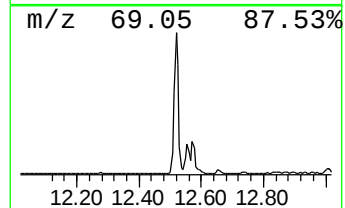
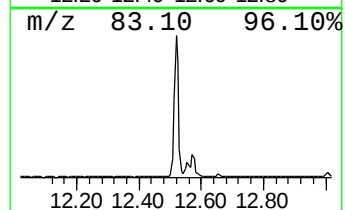
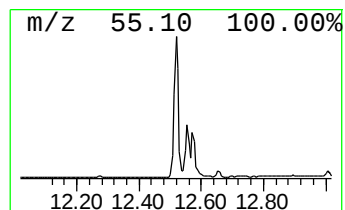
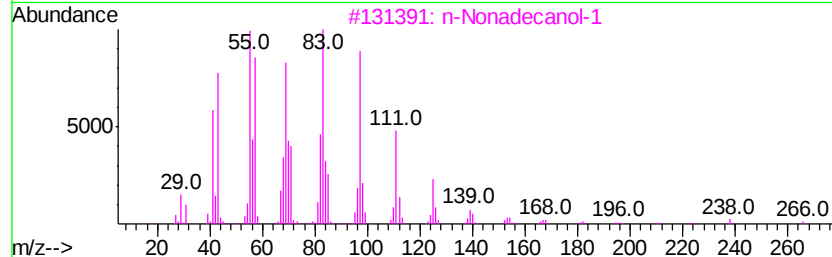
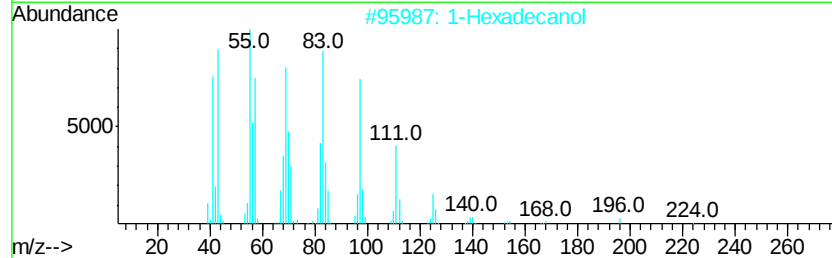
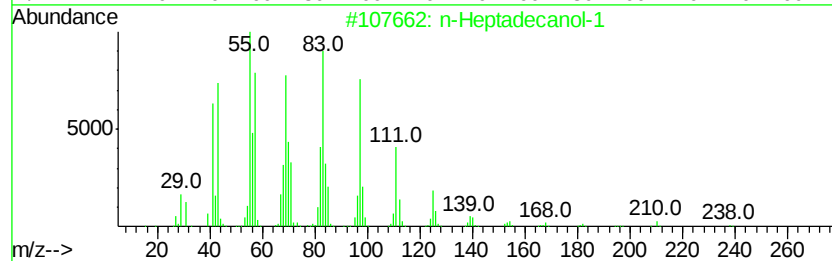
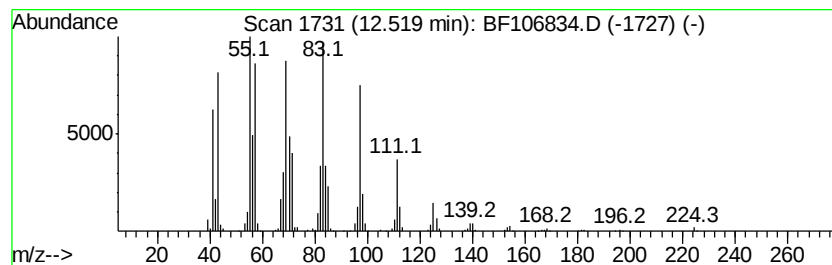
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Peak Number 5 n-Heptadecanol-1 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	72.82 ng	1076820	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Heptadecanol-1	256	C17H36O	001454-85-9	95
2		1-Hexadecanol	242	C16H34O	036653-82-4	93
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4		9-Octadecene, (E)-	252	C18H36	007206-25-9	91
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	91



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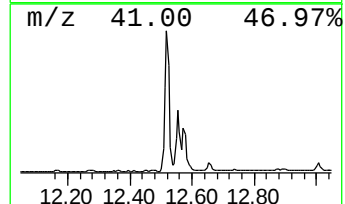
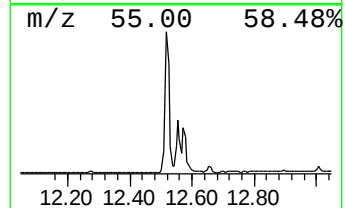
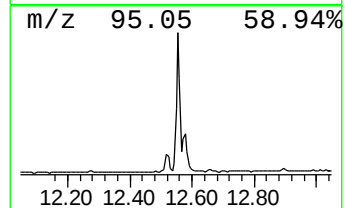
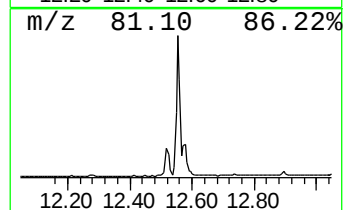
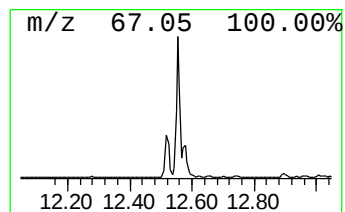
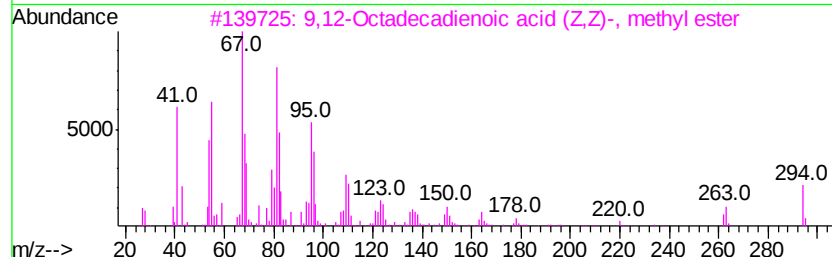
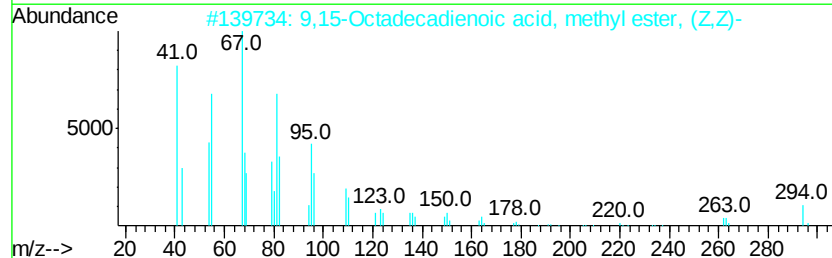
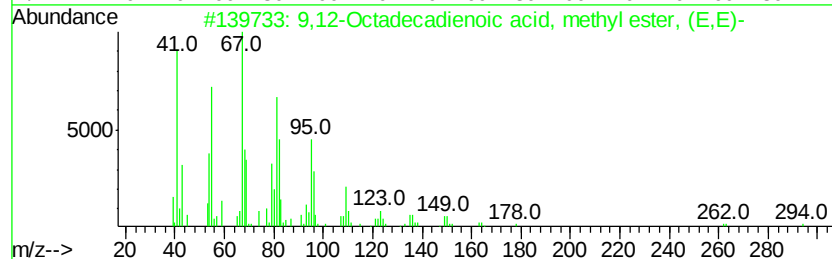
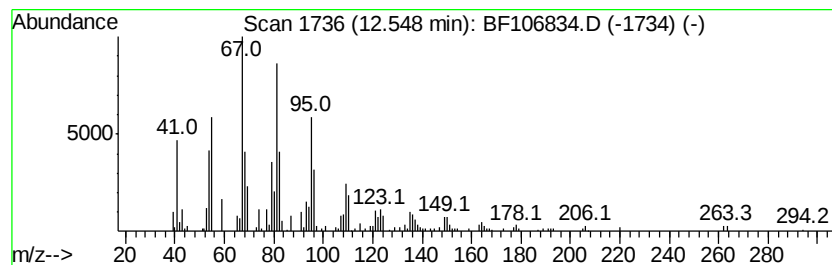
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Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.55	38.68 ng	571949	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	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	97	
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	97	
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	96	
5	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	95	



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062618\
Data File : BF106834.D
Acq On : 26 Jun 2018 20:20
Operator : JU/SJ
Sample : J3251-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-02-062518

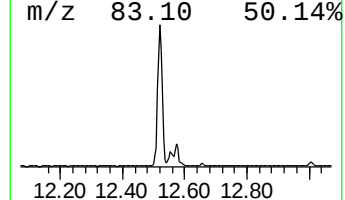
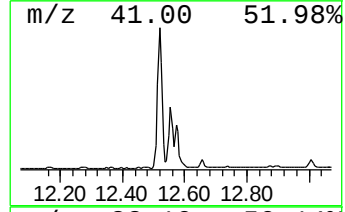
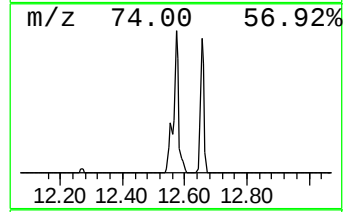
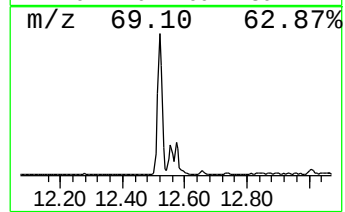
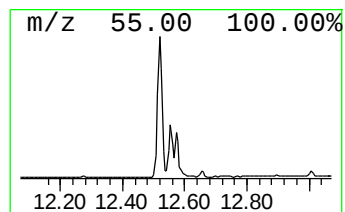
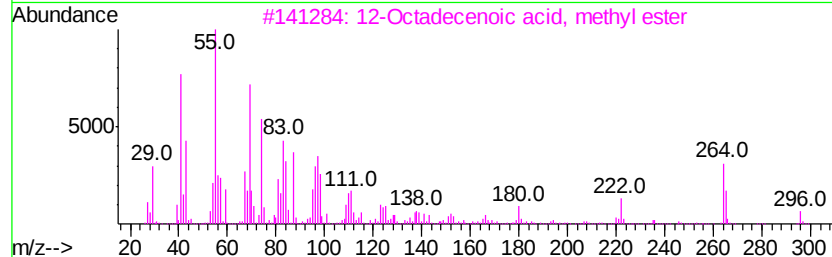
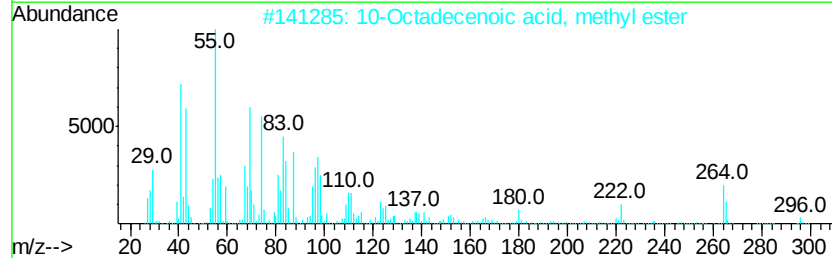
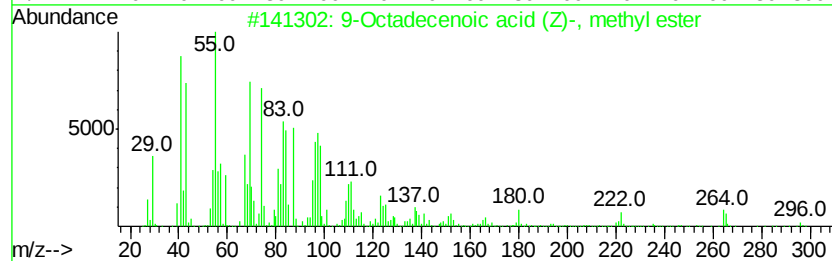
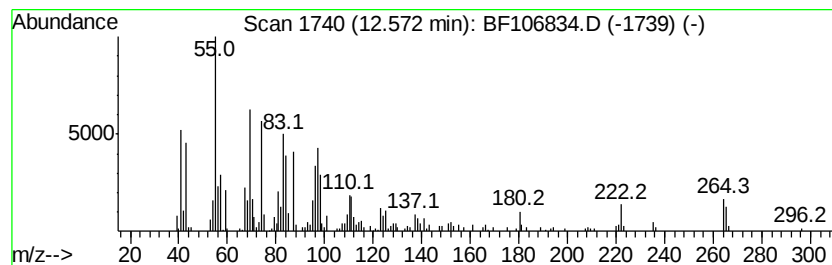
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	24.31 ng	359527	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
3		12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
4		16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
5		11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062618\
Data File : BF106834.D
Acq On : 26 Jun 2018 20:20
Operator : JU/SJ
Sample : J3251-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-02-062518

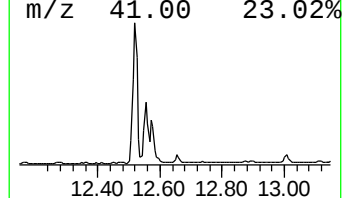
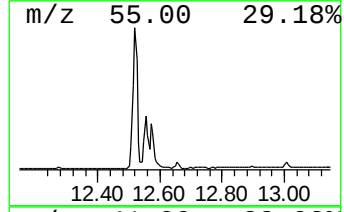
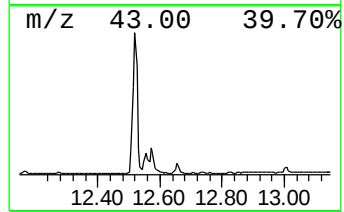
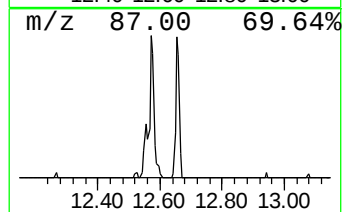
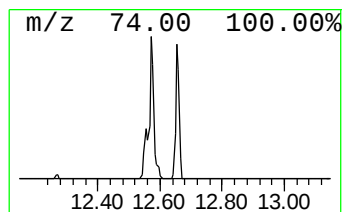
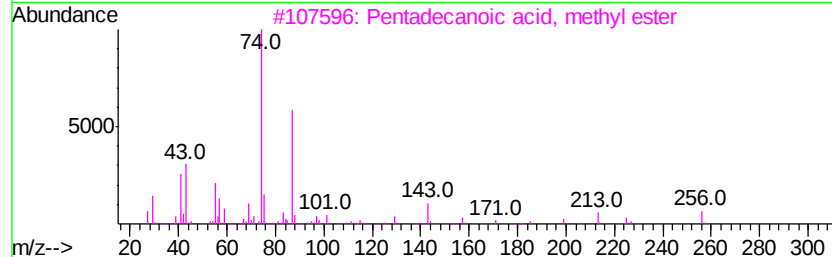
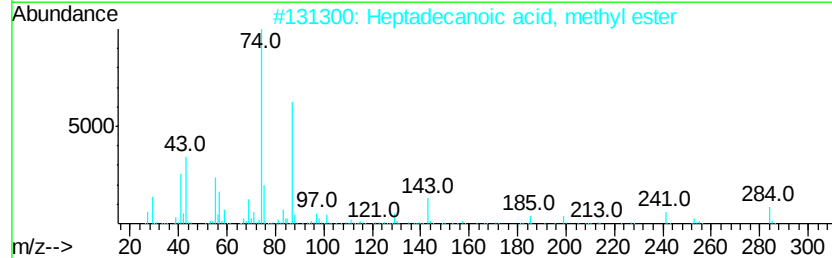
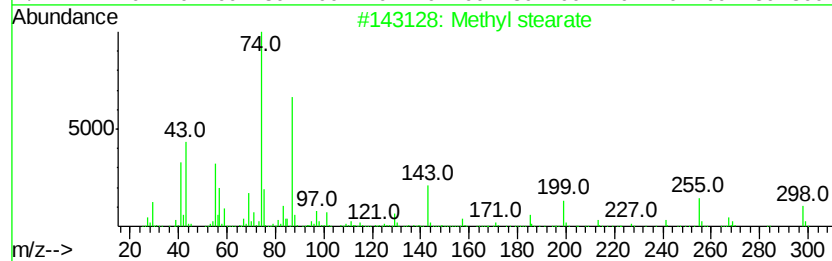
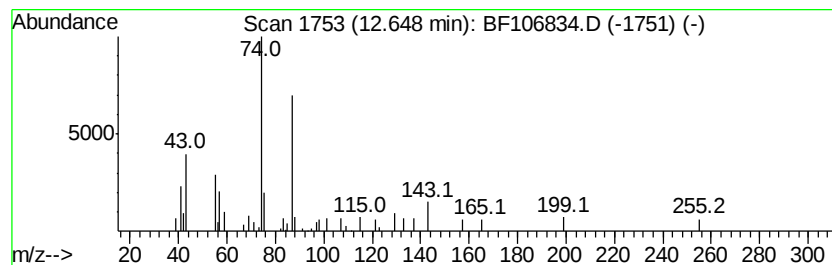
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methyl stearate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	4.69 ng	69389	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methyl stearate	298	C19H38O2	000112-61-8	94
2		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	87
3		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
4		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
5		Methyl 13-methyltetradecanoate	256	C16H32O2	1000336-31-4	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062618\
Data File : BF106834.D
Acq On : 26 Jun 2018 20:20
Operator : JU/SJ
Sample : J3251-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SU-02-062518

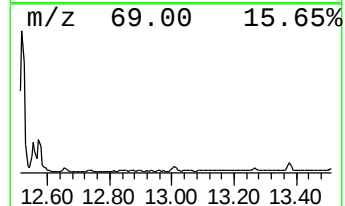
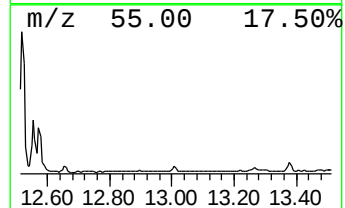
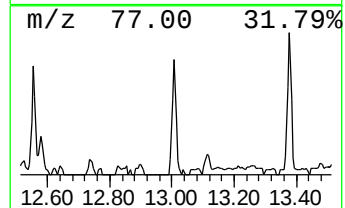
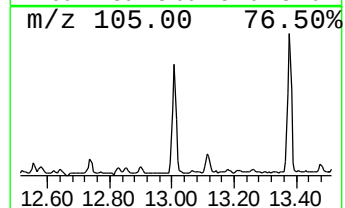
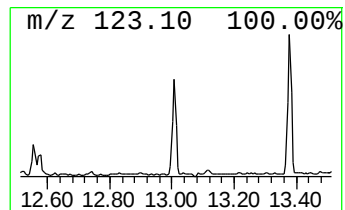
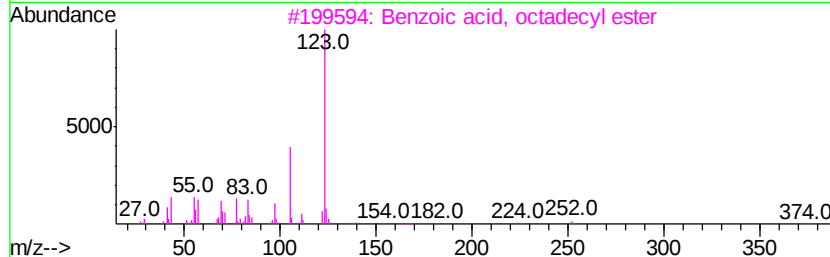
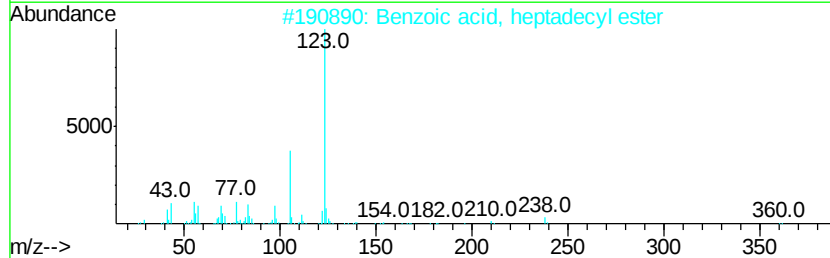
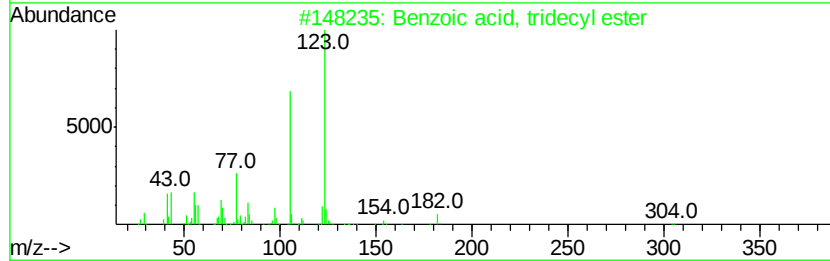
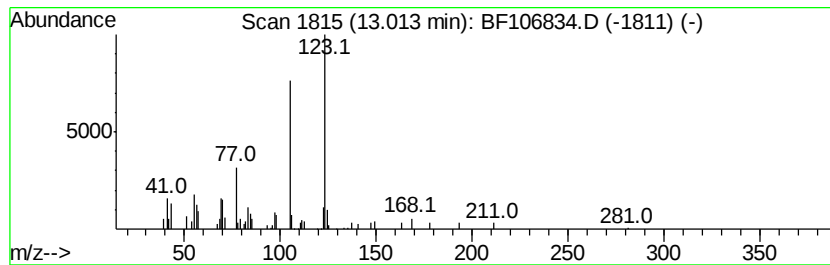
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzoic acid, tridecyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.01	4.63 ng	80503	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, tridecyl ester	304	C20H32O2	1000340-22-6	91
2		Benzoic acid, heptadecyl ester	360	C24H40O2	1000340-23-0	87
3		Benzoic acid, octadecyl ester	374	C25H42O2	1000340-23-1	87
4		Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	83
5		Benzoic acid, eicosyl ester	402	C27H46O2	1000340-23-3	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062618\
Data File : BF106834.D
Acq On : 26 Jun 2018 20:20
Operator : JU/SJ
Sample : J3251-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-02-062518

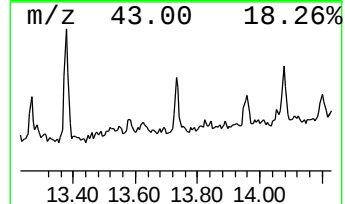
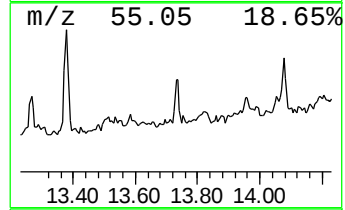
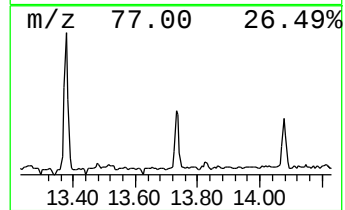
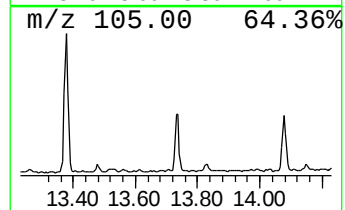
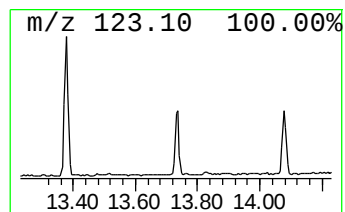
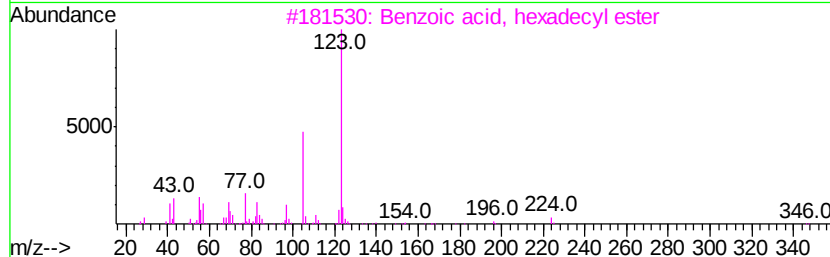
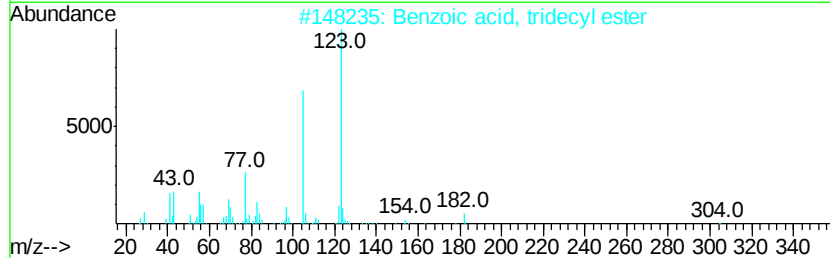
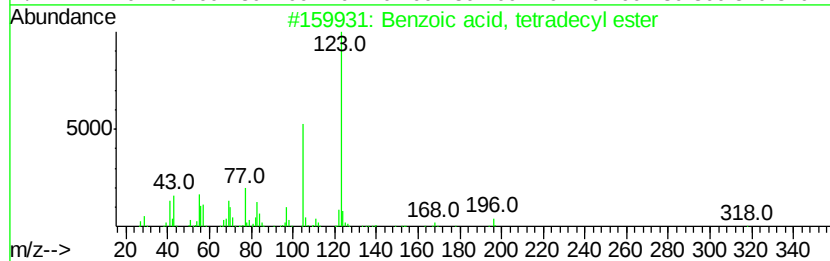
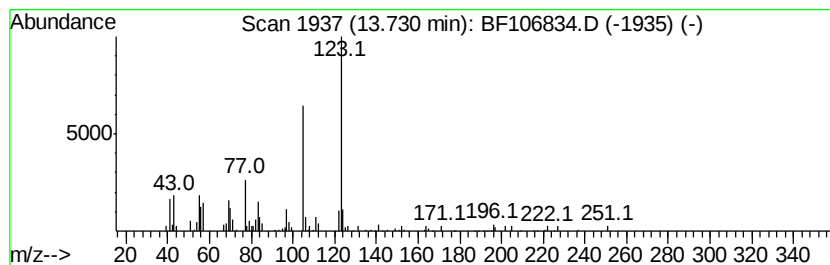
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzoic acid, tetradecyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	3.11 ng	54066	Chrysene-d12	14.15

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	87
2			Benzoic acid, tridecyl ester	304	C20H32O2	1000340-22-6	87
3			Benzoic acid, hexadecyl ester	346	C23H38O2	1000340-22-9	86
4			Benzoic acid, pentadecyl ester	332	C22H36O2	1000340-22-8	86
5			Benzoic acid, octadecyl ester	374	C25H42O2	1000340-23-1	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062618\
Data File : BF106834.D
Acq On : 26 Jun 2018 20:20
Operator : JU/SJ
Sample : J3251-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SU-02-062518

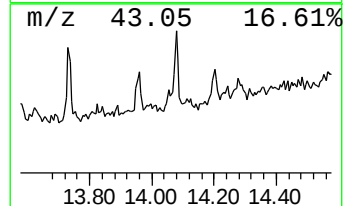
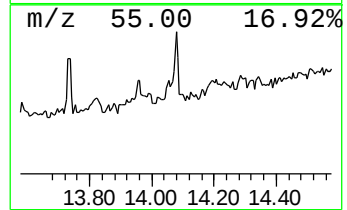
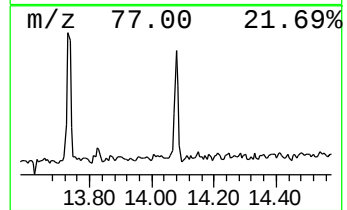
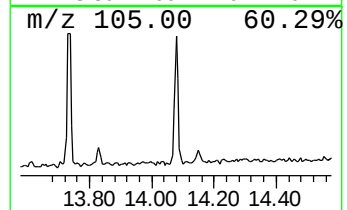
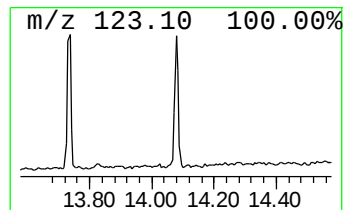
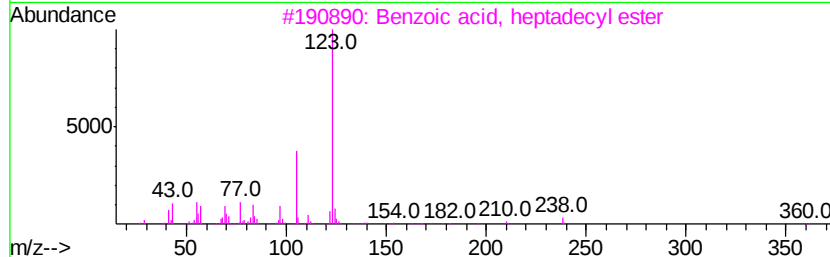
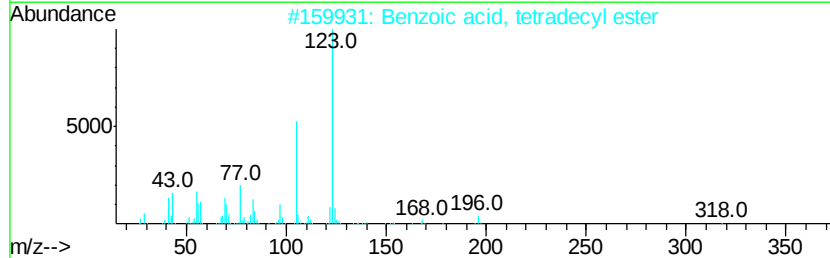
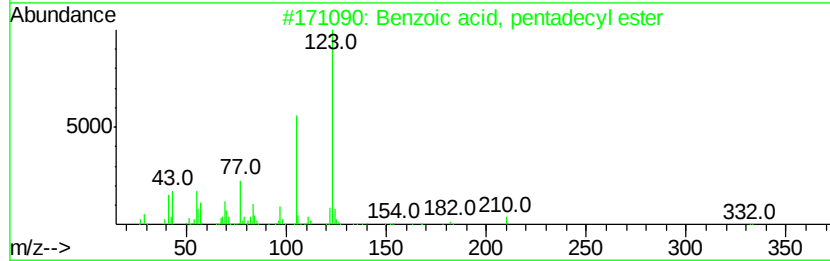
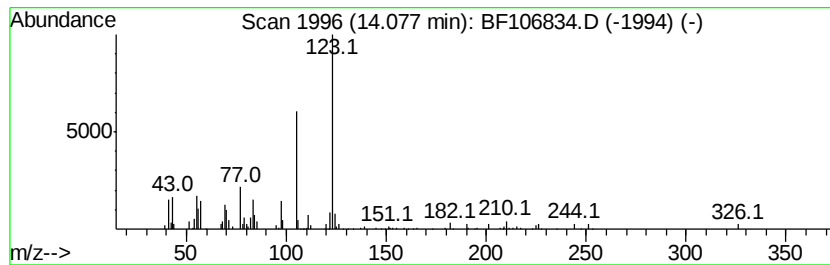
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benzoic acid, pentadecyl ester Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.08	2.92 ng	50740	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, pentadecyl ester	332	C22H36O2	1000340-22-8	91
2		Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	87
3		Benzoic acid, heptadecyl ester	360	C24H40O2	1000340-23-0	80
4		Benzoic acid, octadecyl ester	374	C25H42O2	1000340-23-1	72
5		Benzoic acid, hexadecyl ester	346	C23H38O2	1000340-22-9	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062618\
Data File : BF106834.D
Acq On : 26 Jun 2018 20:20
Operator : JU/SJ
Sample : J3251-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-02-062518

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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
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Cyclopentasiloxan...	7.68	6.0	ng	79212	2	8.24	265728	20.0
Hexadecanoic acid...	11.87	9.5	ng	140589	4	11.50	295757	20.0
n-Heptadecanol-1	12.52	72.8	ng	1076820	4	11.50	295757	20.0
9,12-Octadecadien...	12.55	38.7	ng	571949	4	11.50	295757	20.0
9-Octadecenoic ac...	12.57	24.3	ng	359527	4	11.50	295757	20.0
Methyl stearate	12.65	4.7	ng	69389	4	11.50	295757	20.0
Benzoic acid, tri...	13.01	4.6	ng	80503	5	14.15	348019	20.0
Benzoic acid, tet...	13.73	3.1	ng	54066	5	14.15	348019	20.0
Benzoic acid, pen...	14.08	2.9	ng	50740	5	14.15	348019	20.0