

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061118\
 Data File : BF106299.D
 Acq On : 11 Jun 2018 17:21
 Operator : JU/SJ
 Sample : J3240-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-02-060718

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-BF061118.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	4.113	298	302	310	rVB	57292	65784	1.33%	0.130%
2	5.207	482	488	498	rVB	317439	414975	8.40%	0.817%
3	5.590	547	553	556	rBV	4164249	4214129	85.25%	8.301%
4	6.584	716	722	726	rBV	3743258	4473005	90.49%	8.811%
5	6.737	743	748	751	rBV	4323627	4309609	87.19%	8.489%
6	6.966	784	787	791	rVB	1522958	1274058	25.77%	2.510%
7	7.125	810	814	817	rBV	3715410	3163319	64.00%	6.231%
8	7.531	877	883	886	rBV	2854664	2857063	57.80%	5.628%
9	8.248	1001	1005	1009	rBV	1900125	1634527	33.07%	3.220%
10	9.325	1183	1188	1191	rBV	4973828	4486294	90.76%	8.837%
11	9.713	1251	1254	1257	rBV	896212	740812	14.99%	1.459%
12	9.925	1283	1290	1293	rVB2	119812	123862	2.51%	0.244%
13	10.007	1300	1304	1308	rBV2	2087486	1882659	38.09%	3.708%
14	10.425	1373	1375	1378	rVB	172551	136809	2.77%	0.269%
15	10.648	1408	1413	1415	rBV	46428	53552	1.08%	0.105%
16	10.795	1434	1438	1442	rBV	3224578	3241979	65.59%	6.386%
17	10.901	1453	1456	1462	rBV	157398	152032	3.08%	0.299%
18	11.348	1529	1532	1535	rBV	82241	63895	1.29%	0.126%
19	11.501	1554	1558	1561	rBV	2219528	2009785	40.66%	3.959%
20	11.877	1619	1622	1626	rVB	1008805	790418	15.99%	1.557%
21	12.013	1638	1645	1659	rBV2	377914	435763	8.82%	0.858%
22	12.571	1736	1740	1741	rBV	2210195	2100926	42.50%	4.138%
23	12.589	1741	1743	1750	rVV2	3071745	2748105	55.60%	5.413%
24	12.671	1754	1757	1760	rVV	595514	459606	9.30%	0.905%
25	12.795	1775	1778	1784	rBV	104867	104690	2.12%	0.206%
26	13.089	1823	1828	1831	rBV	4955500	4943023	100.00%	9.736%
27	13.324	1862	1868	1874	rVB2	94979	126281	2.55%	0.249%
28	13.507	1896	1899	1904	rBV	206176	189921	3.84%	0.374%
29	13.971	1974	1978	1986	rBV	239207	250440	5.07%	0.493%
30	14.148	2004	2008	2012	rBV	2013034	1790101	36.21%	3.526%
31	15.024	2153	2157	2164	rVB	202533	201643	4.08%	0.397%
32	15.301	2200	2204	2212	rBV2	36263	51727	1.05%	0.102%
33	15.689	2264	2270	2280	rVB	954292	1278140	25.86%	2.518%

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-02-060718

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-BF061118.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

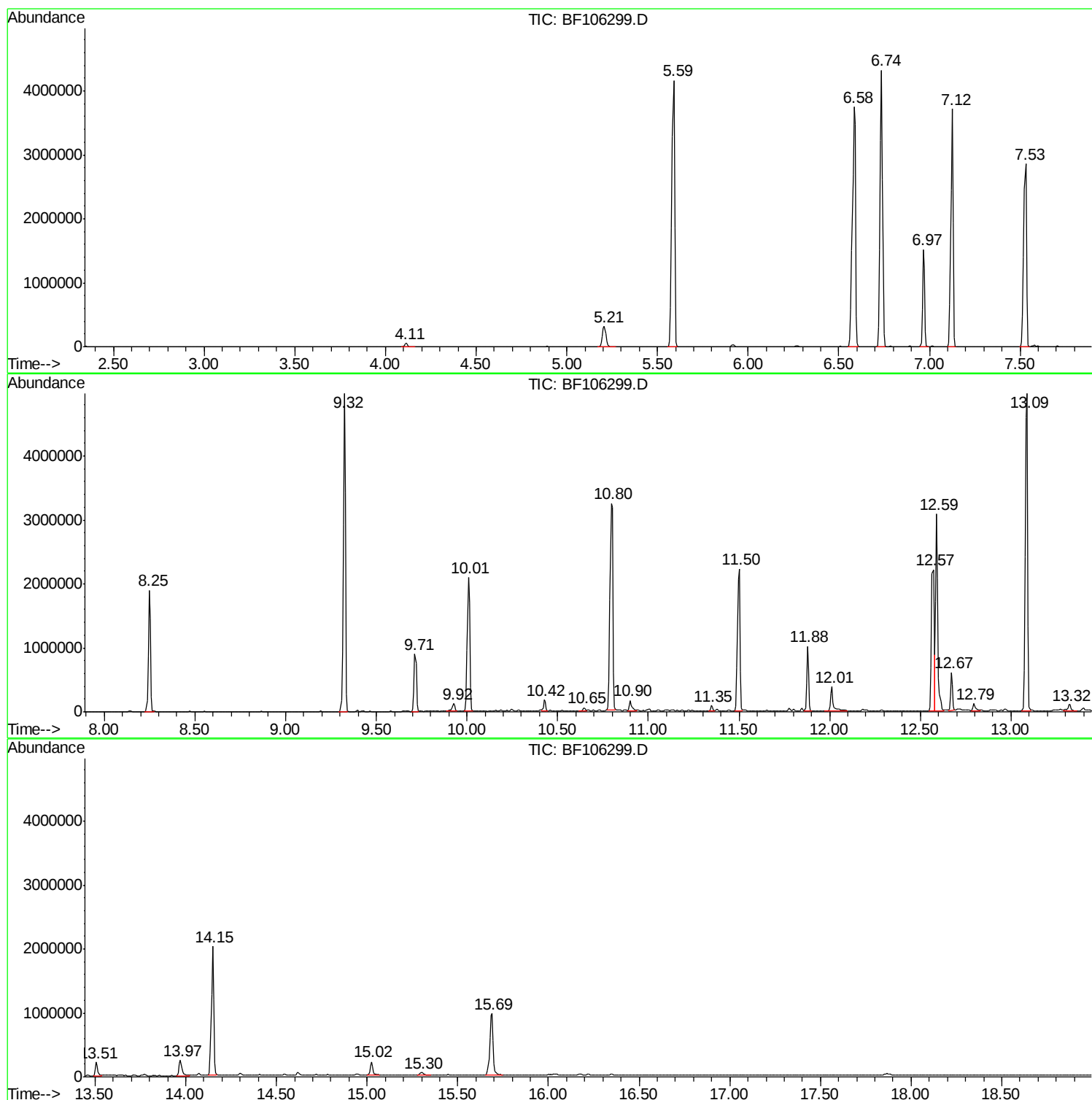
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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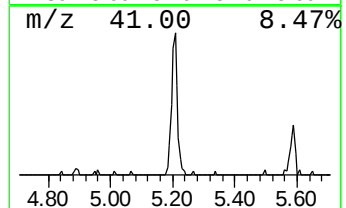
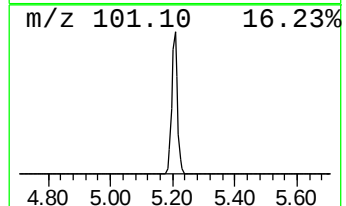
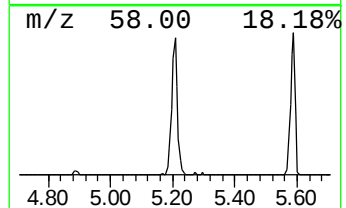
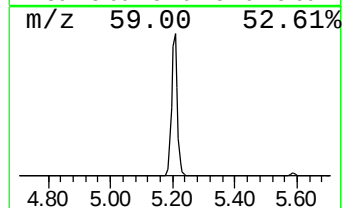
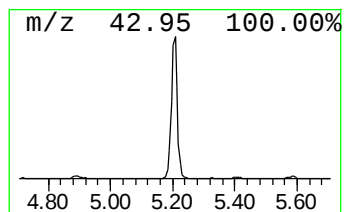
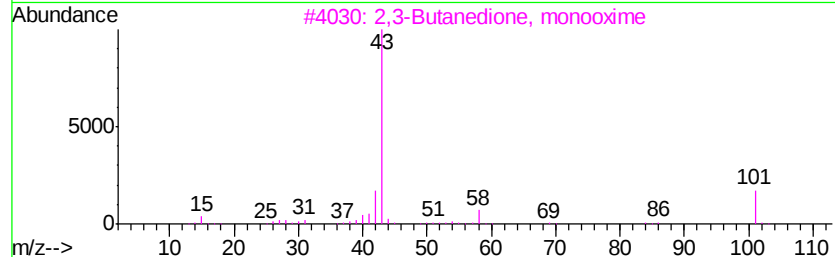
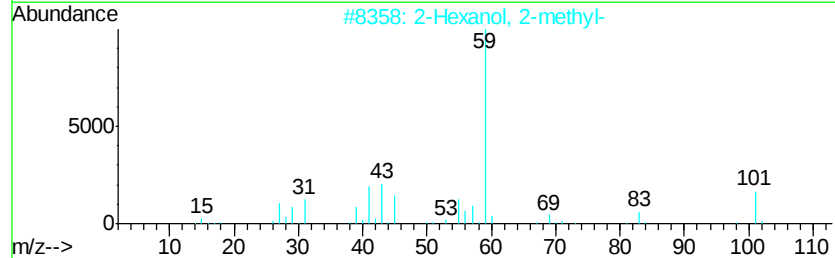
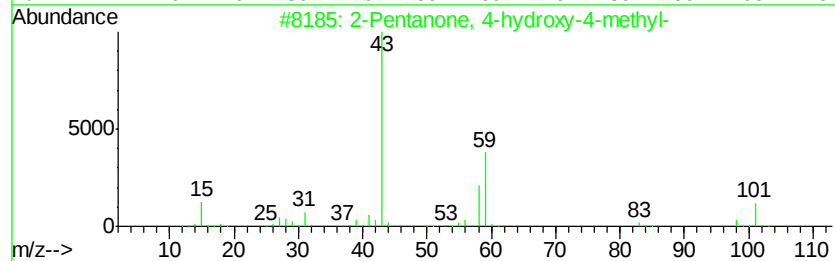
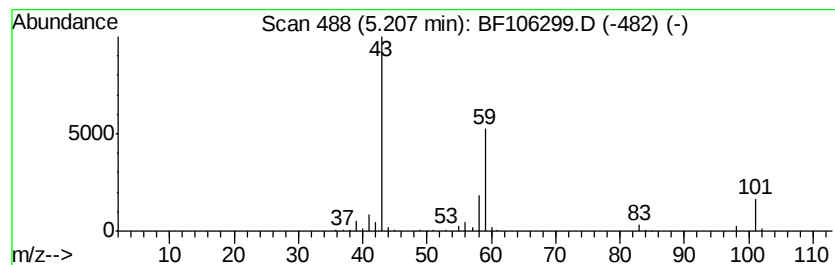
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	6.51 ng	414975	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17



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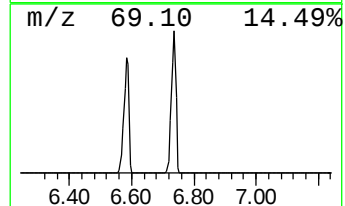
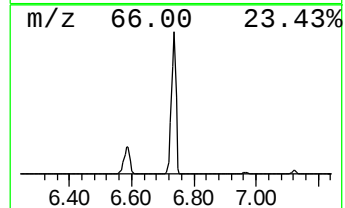
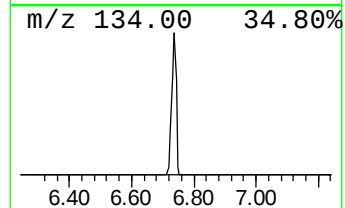
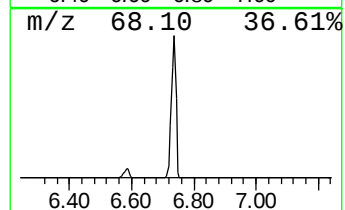
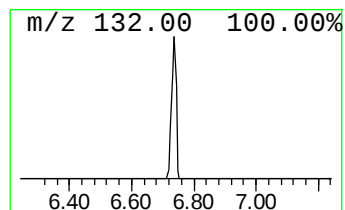
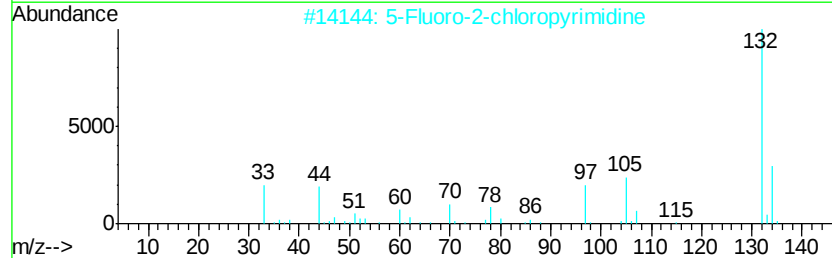
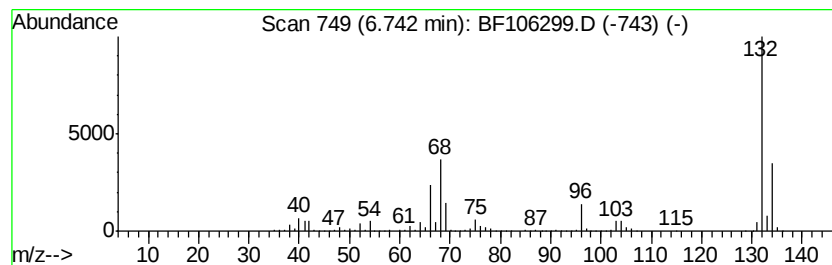
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	67.65 ng	4309610	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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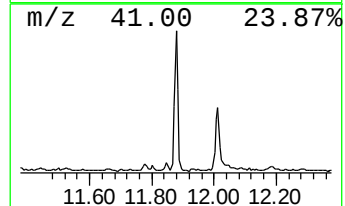
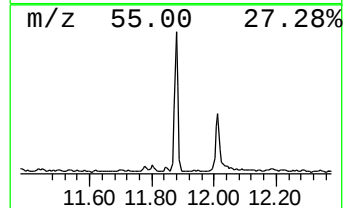
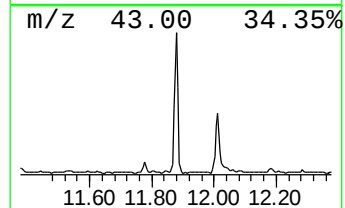
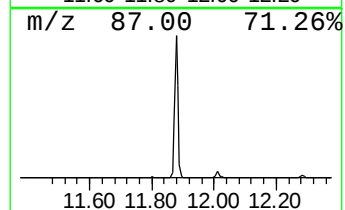
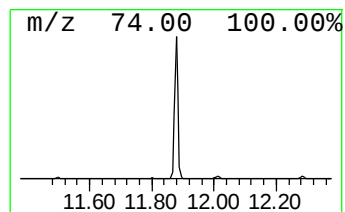
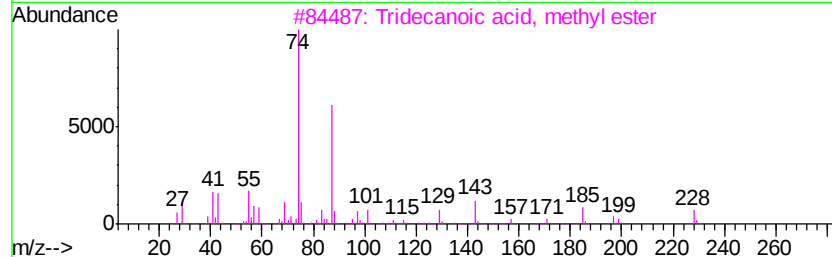
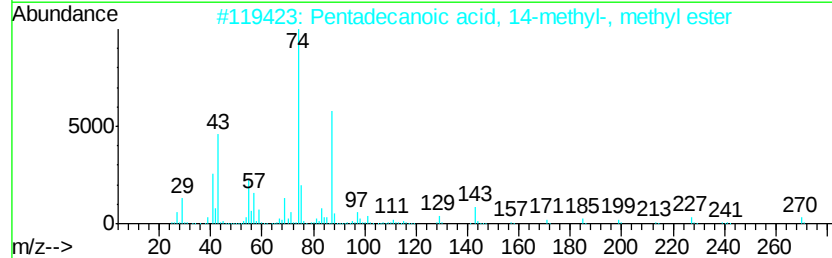
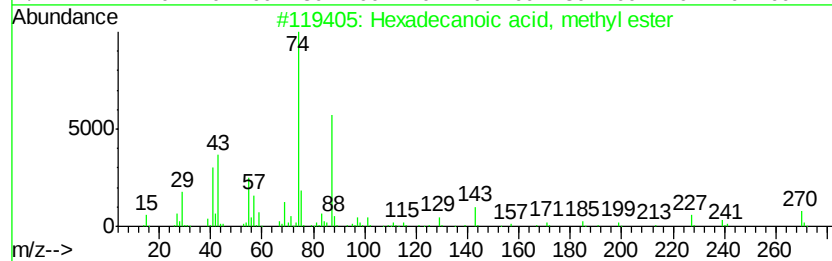
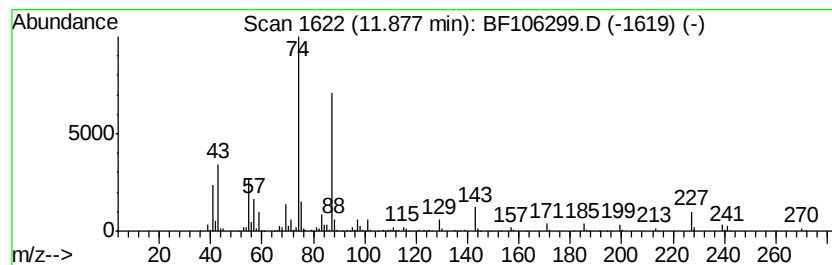
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	7.87 ng	790418	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4		Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
5		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



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ALS Vial : 6 Sample Multiplier: 1

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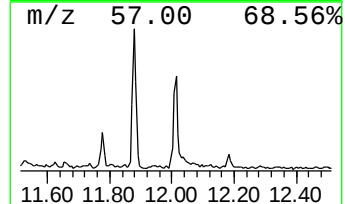
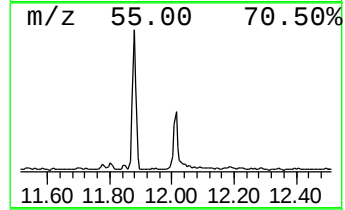
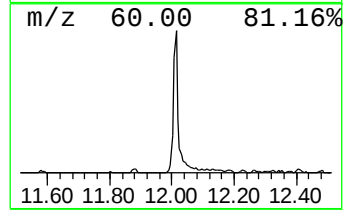
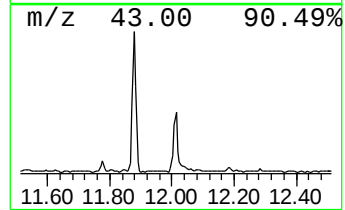
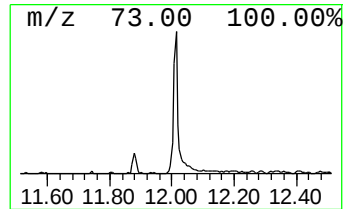
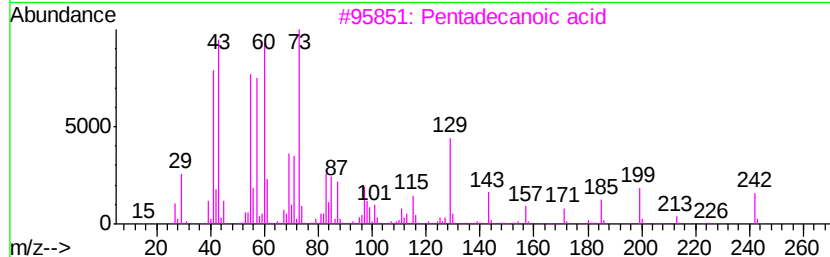
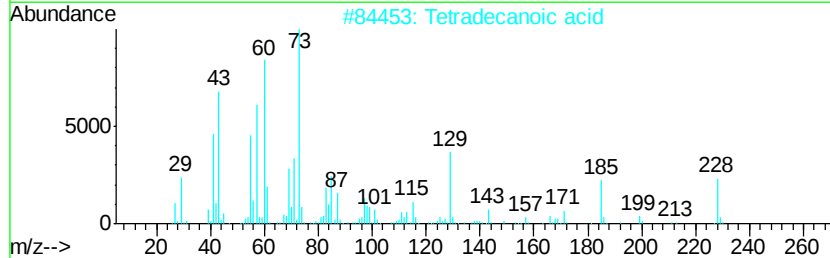
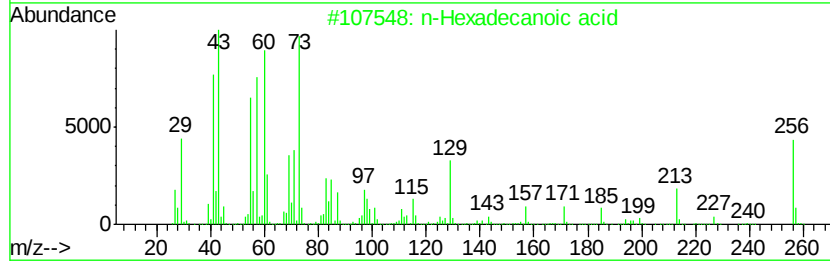
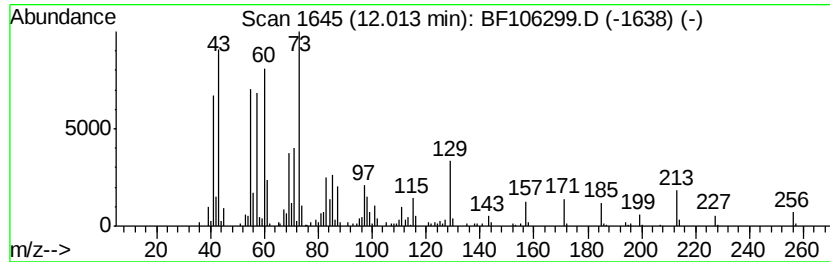
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	4.34 ng	435763	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tridecanoic acid	214	C13H26O2	000638-53-9	76
5		Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	30



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ALS Vial : 6 Sample Multiplier: 1

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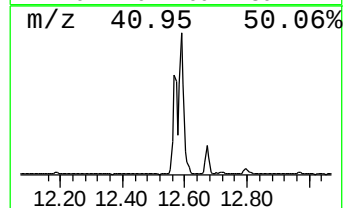
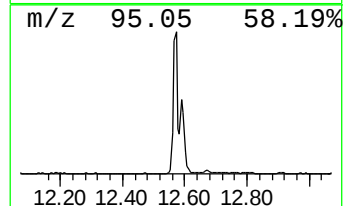
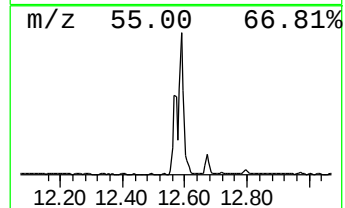
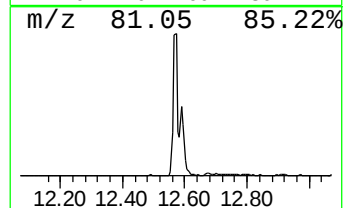
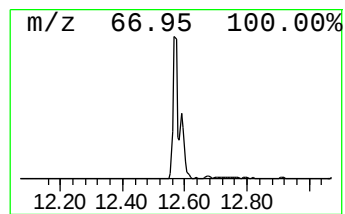
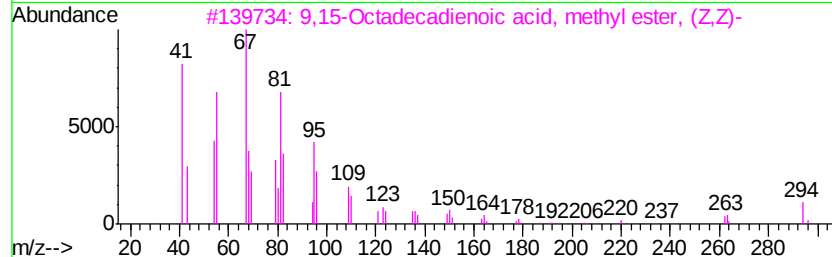
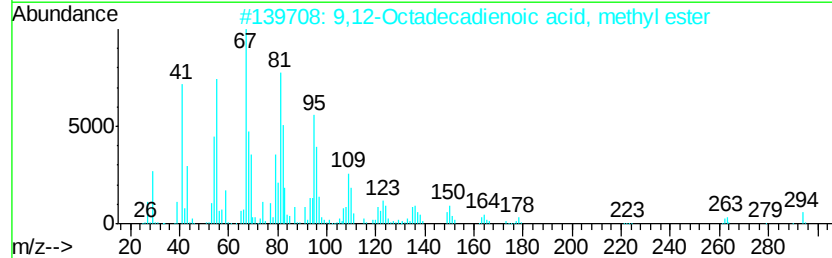
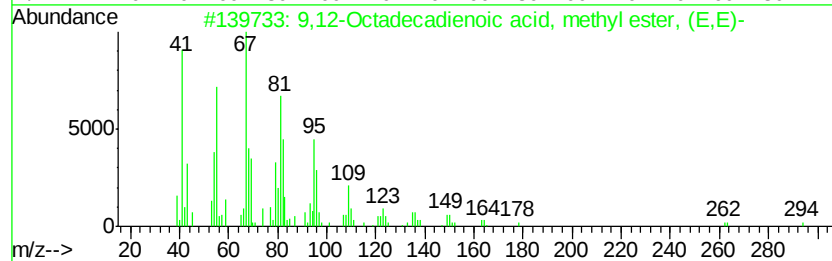
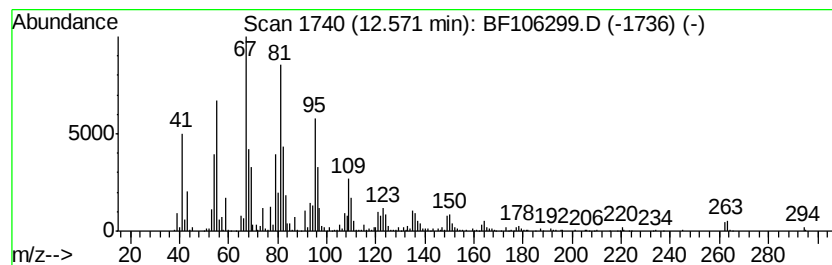
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	20.91 ng	2100930	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3		9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
5		Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	98



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ClientSampleId :
BU-02-060718

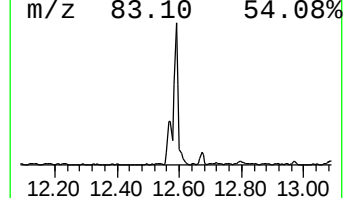
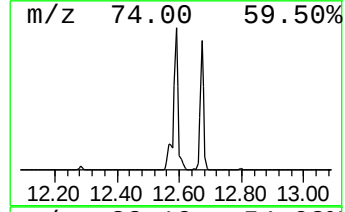
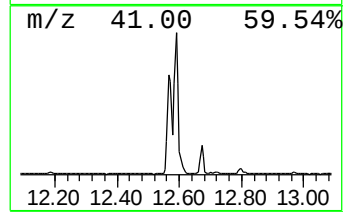
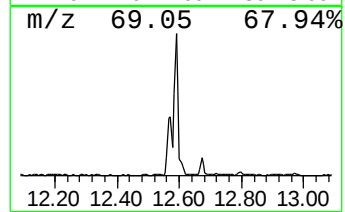
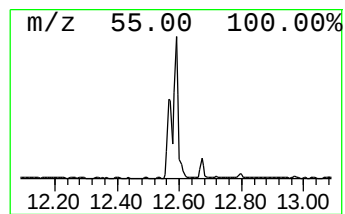
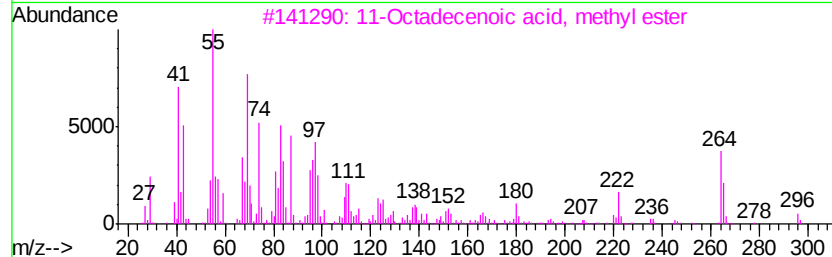
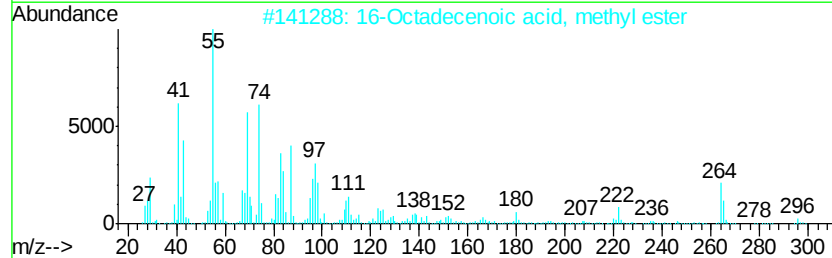
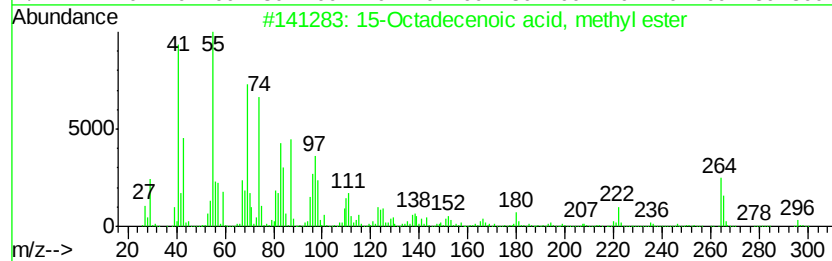
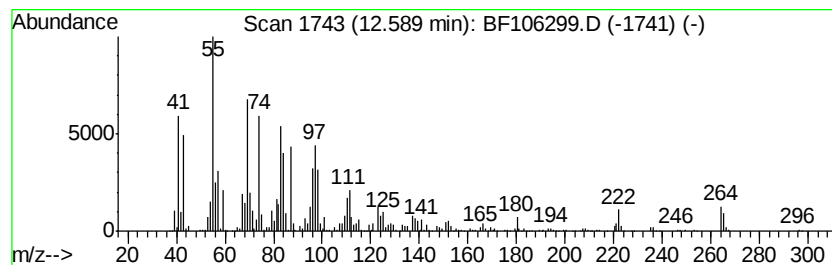
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 15-Octadecenoic acid, methy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	27.35 ng	2748110	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	98	
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	97	
3	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	95	
4	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	94	
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94	



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061118\
Data File : BF106299.D
Acq On : 11 Jun 2018 17:21
Operator : JU/SJ
Sample : J3240-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-02-060718

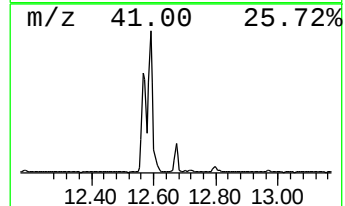
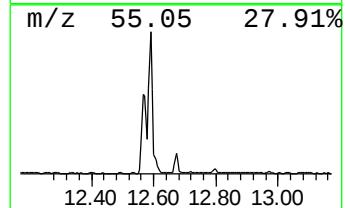
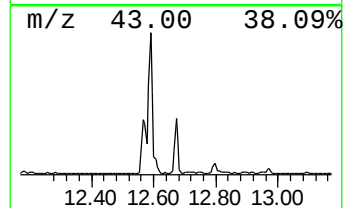
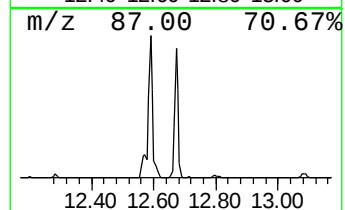
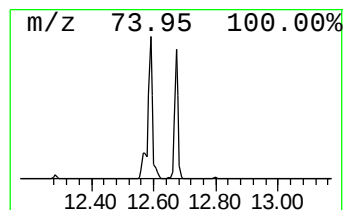
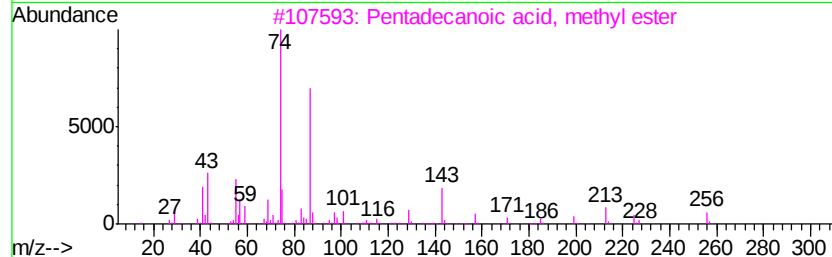
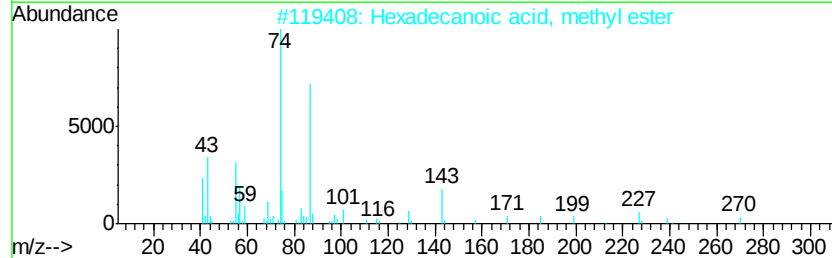
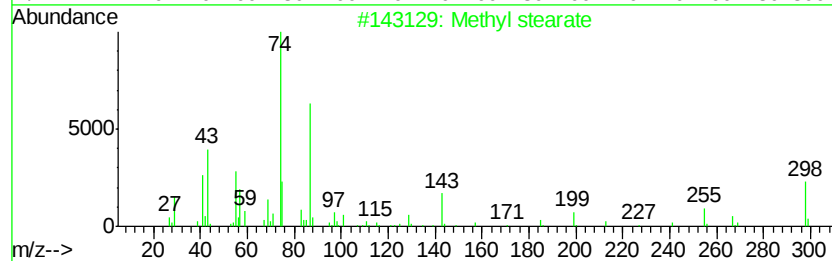
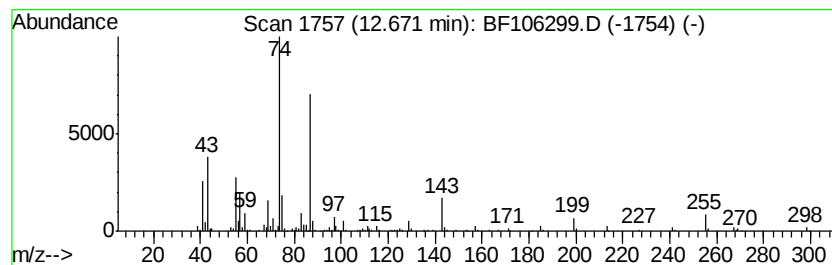
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	4.57 ng	459606	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methyl stearate	298	C19H38O2	000112-61-8	97
2		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	94
3		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	91
4		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
5		Methyl tetradecanoate	242	C15H30O2	000124-10-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061118\
Data File : BF106299.D
Acq On : 11 Jun 2018 17:21
Operator : JU/SJ
Sample : J3240-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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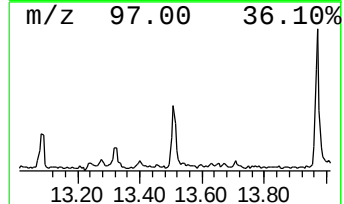
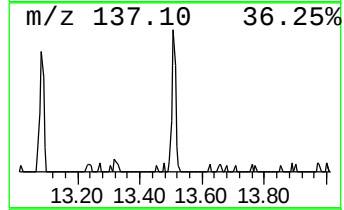
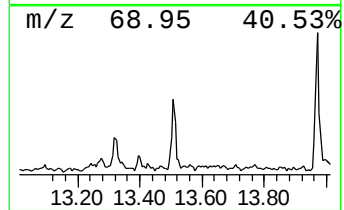
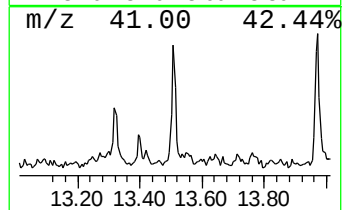
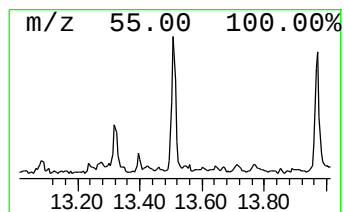
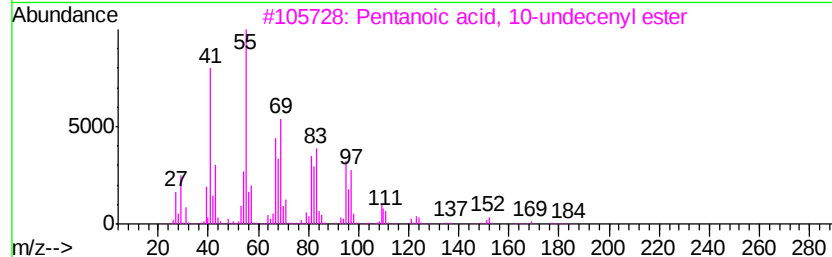
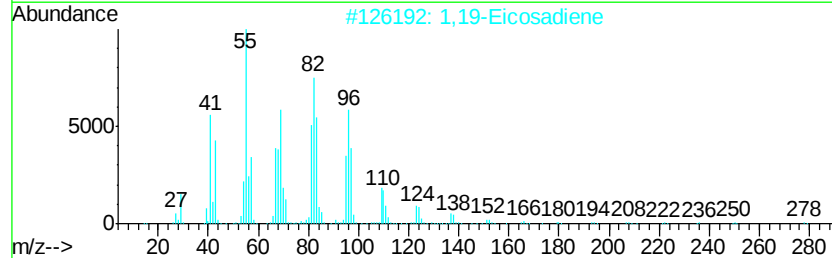
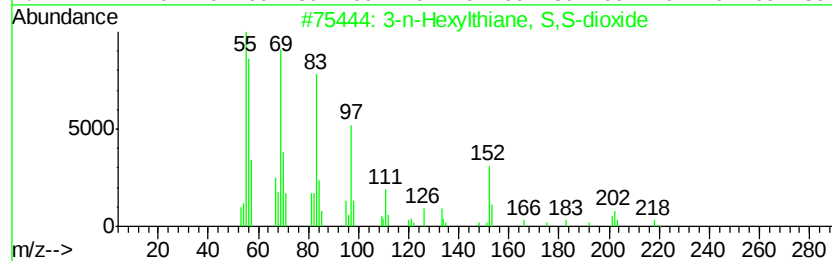
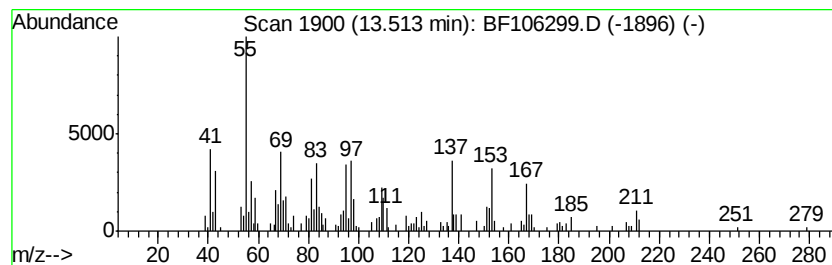
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.51 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	2.12 ng	189921	Chrysene-d12	14.15

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-n-Hexylthiane, S,S-dioxide	218	C11H22O2S	061639-18-7	22
2			1,19-Eicosadiene	278	C20H38	014811-95-1	16
3			Pentanoic acid, 10-undecenyl ester	254	C16H30O2	1000159-93-4	16
4			Fumaric acid, di(2-methylallyl) ...	224	C12H16O4	1000330-55-8	14
5			Cyclopentanecarboxylic acid, 1-(...	210	C12H18O3	112825-89-5	14



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061118\
Data File : BF106299.D
Acq On : 11 Jun 2018 17:21
Operator : JU/SJ
Sample : J3240-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-02-060718

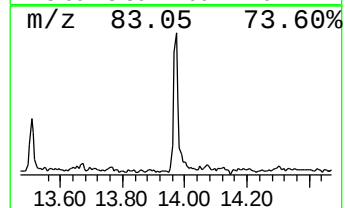
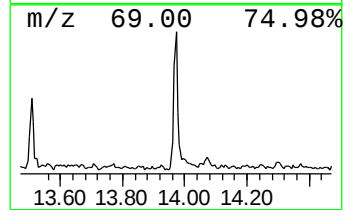
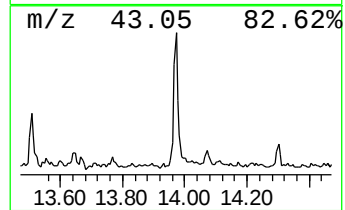
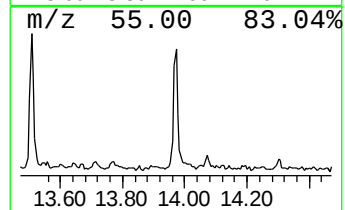
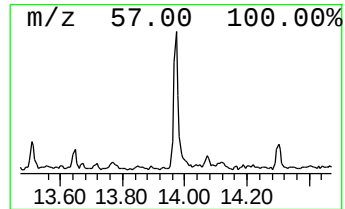
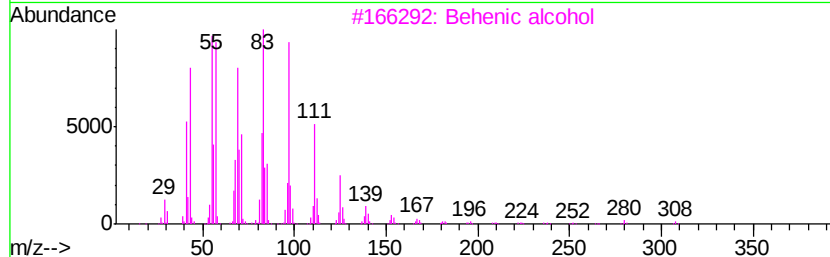
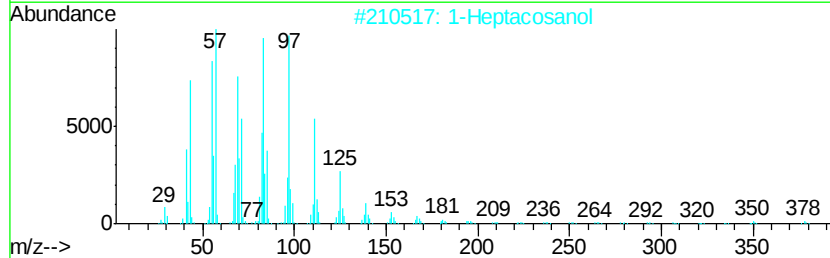
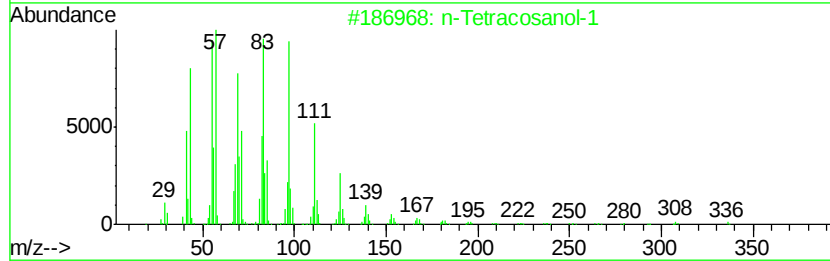
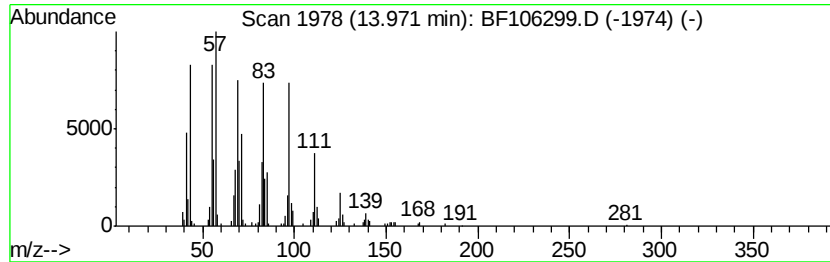
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Tetracosanol-1 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	2.80 ng	250440	Chrysene-d12	14.15

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2			1-Heptacosanol	396	C27H56O	002004-39-9	91
3			Behenic alcohol	326	C22H46O	000661-19-8	91
4			Heptadecyl heptafluorobutyrte	452	C21H35F7O2	959085-66-6	91
5			Octacosanol	410	C28H58O	000557-61-9	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061118\
Data File : BF106299.D
Acq On : 11 Jun 2018 17:21
Operator : JU/SJ
Sample : J3240-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BU-02-060718

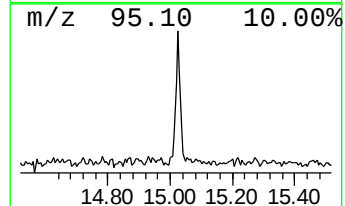
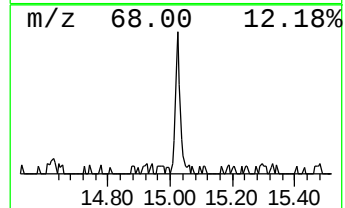
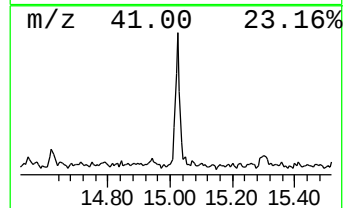
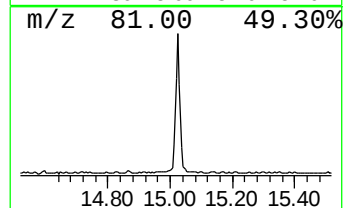
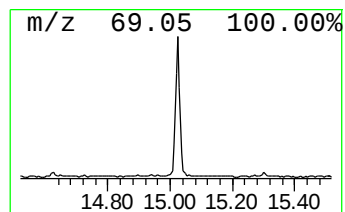
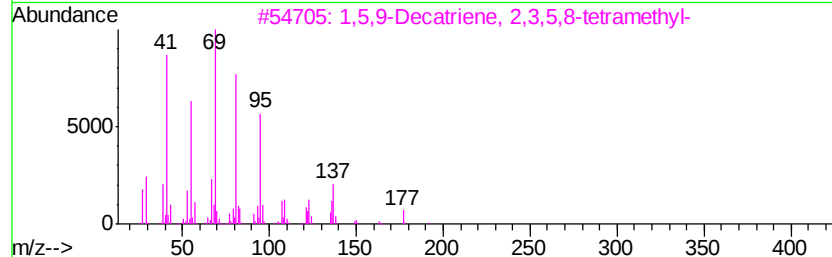
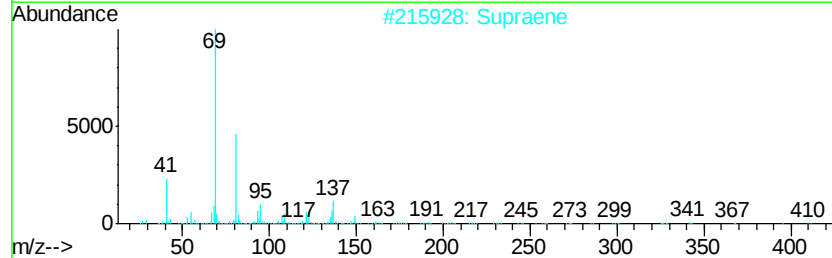
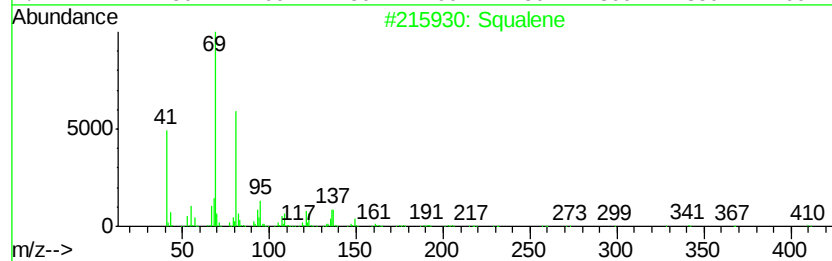
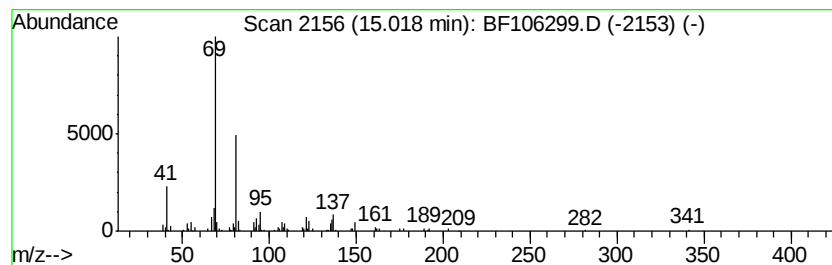
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	3.16 ng	201643	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	83
3		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	80
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5		1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061118\
Data File : BF106299.D
Acq On : 11 Jun 2018 17:21
Operator : JU/SJ
Sample : J3240-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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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unknown6.74	6.74	67.7	ng	4309610	1	6.97	1274060	20.0
Hexadecanoic acid...	11.88	7.9	ng	790418	4	11.50	2009790	20.0
n-Hexadecanoic acid	12.01	4.3	ng	435763	4	11.50	2009790	20.0
9,12-Octadecadien...	12.57	20.9	ng	2100930	4	11.50	2009790	20.0
15-Octadecenoic a...	12.59	27.4	ng	2748110	4	11.50	2009790	20.0
Methyl stearate	12.67	4.6	ng	459606	4	11.50	2009790	20.0
unknown13.51	13.51	2.1	ng	189921	5	14.15	1790100	20.0
n-Tetracosanol-1	13.97	2.8	ng	250440	5	14.15	1790100	20.0
Squalene	15.02	3.2	ng	201643	6	15.69	1278140	20.0