

Data Path : Z:\HPCHEM1\BNA F\Data\BF071417\
 Data File : BF096766.D
 Acq On : 14 Jul 2017 10:50
 Operator : SJ/JU
 Sample : I4113-05
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-6(11.0-11.5)

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-BF071317.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	4.810	476	480	489	rVB	94420	122440	4.80%	0.675%
2	5.239	549	553	557	rBV	1644694	1560190	61.21%	8.601%
3	6.281	725	730	738	rBV	1479440	1443688	56.63%	7.959%
4	6.404	747	751	754	rBV	1706166	1523578	59.77%	8.399%
5	6.634	787	790	794	rBV	650879	583950	22.91%	3.219%
6	6.792	813	817	820	rBV	1535859	1292094	50.69%	7.123%
7	7.198	881	886	889	rBV	1103120	960834	37.69%	5.297%
8	7.916	1004	1008	1012	rBV	882628	808261	31.71%	4.456%
9	8.998	1187	1192	1195	rBV	1751847	1593441	62.51%	8.784%
10	9.392	1255	1259	1262	rBV	72164	63257	2.48%	0.349%
11	9.669	1302	1306	1310	rBV	990275	854744	33.53%	4.712%
12	9.886	1335	1343	1350	rBV	54862	98098	3.85%	0.541%
13	10.451	1436	1439	1443	rBV	759696	645677	25.33%	3.559%
14	10.586	1459	1462	1469	rBV2	24267	31991	1.25%	0.176%
15	10.833	1499	1504	1509	rBV4	33053	43462	1.70%	0.240%
16	11.145	1553	1557	1561	rVB	972869	809566	31.76%	4.463%
17	11.557	1623	1627	1630	rBV	33484	38538	1.51%	0.212%
18	11.639	1632	1641	1645	rBV5	37972	93930	3.68%	0.518%
19	11.698	1645	1651	1659	rVB	438286	545511	21.40%	3.007%
20	12.021	1702	1706	1709	rBV5	24235	35355	1.39%	0.195%
21	12.257	1740	1746	1750	rBV9	17286	43255	1.70%	0.238%
22	12.351	1755	1762	1765	rBV	104037	161473	6.33%	0.890%
23	12.480	1776	1784	1795	rBV	483826	779657	30.59%	4.298%
24	12.739	1822	1828	1831	rBV	2444783	2549114	100.00%	14.052%
25	13.274	1914	1919	1927	rVB4	46231	114898	4.51%	0.633%
26	13.639	1978	1981	1987	rBV	118492	127174	4.99%	0.701%
27	13.774	2000	2004	2010	rVB	686212	605193	23.74%	3.336%
28	15.156	2235	2239	2244	rVB	393599	458499	17.99%	2.528%
29	15.892	2360	2364	2373	rVB9	70854	152139	5.97%	0.839%

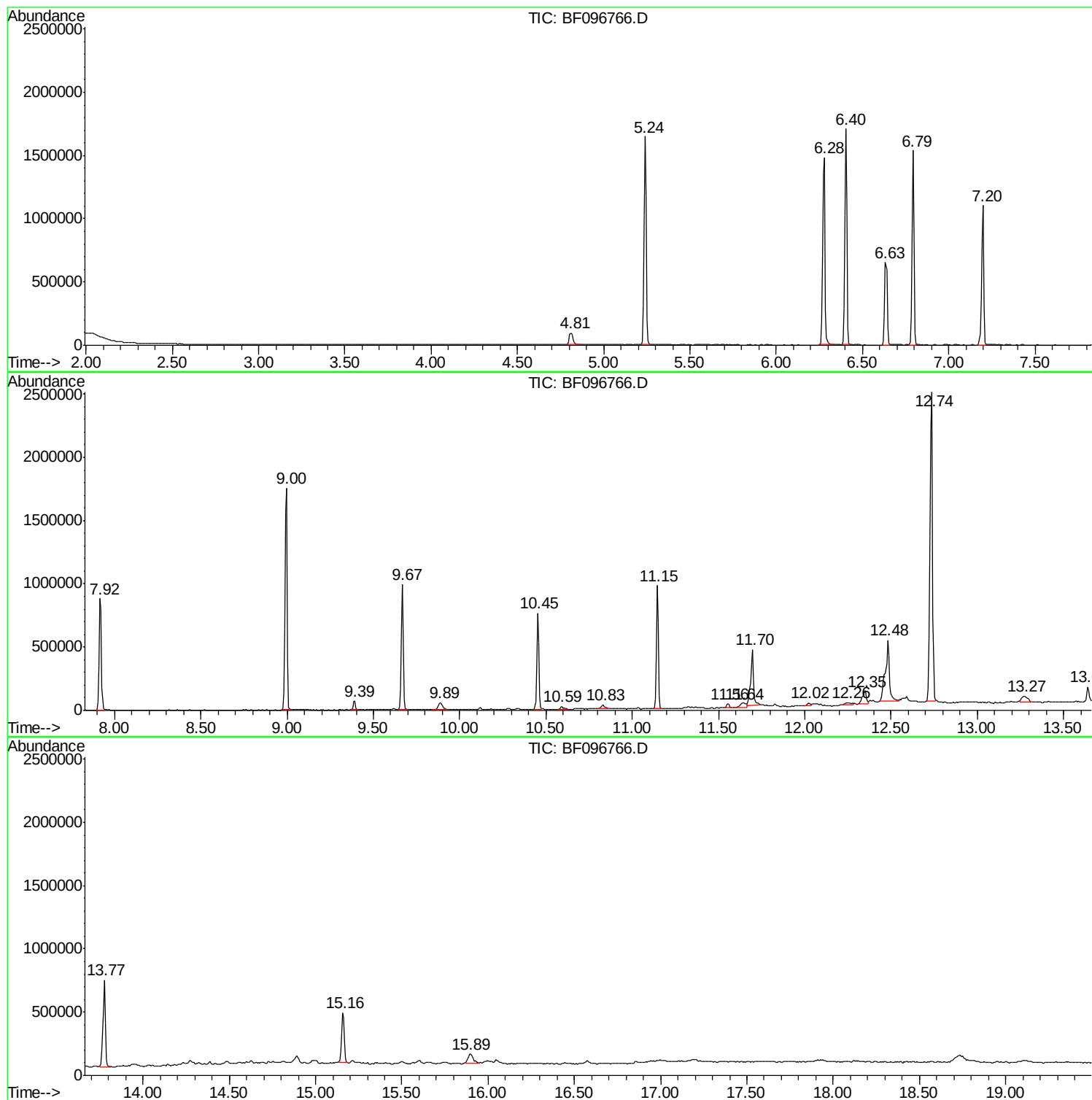
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ClientSampleId :
SB-6(11.0-11.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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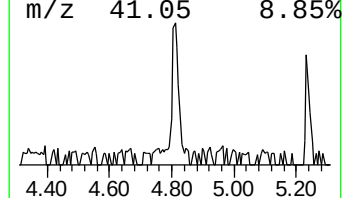
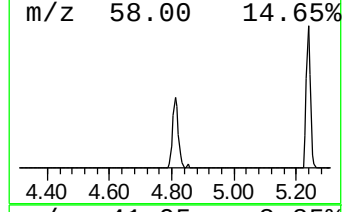
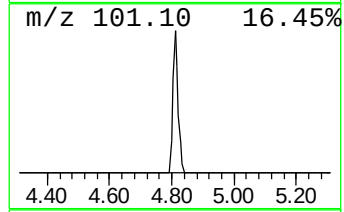
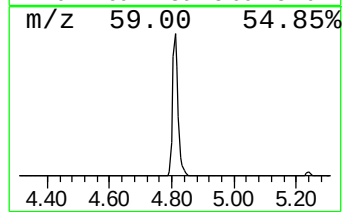
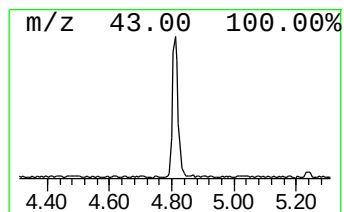
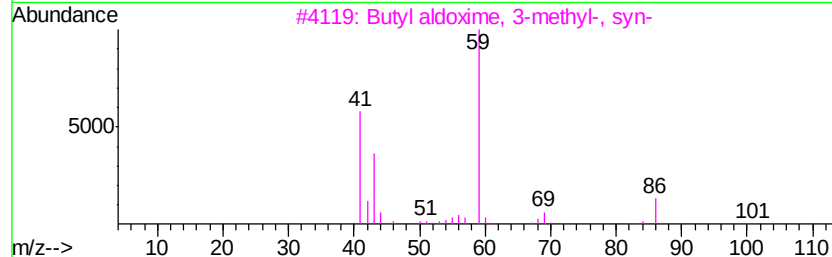
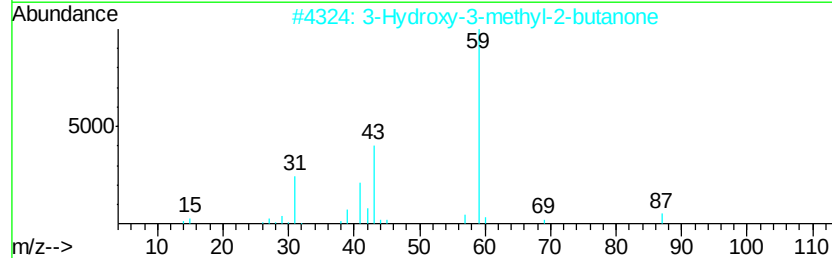
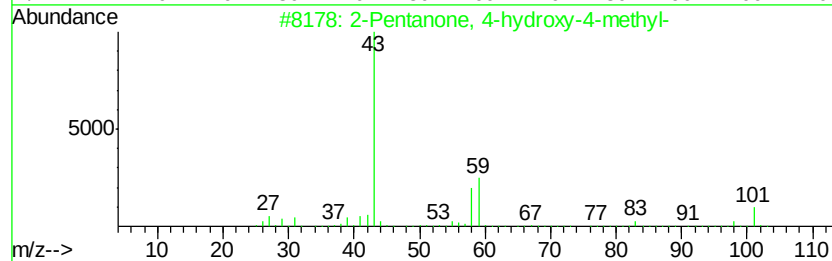
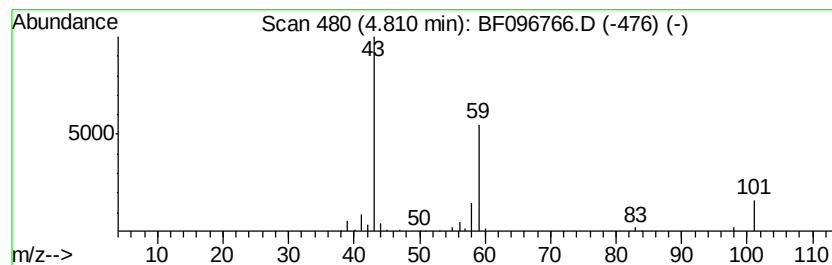
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	4.19 ng	122440	1,4-Dichlorobenzene-d4	6.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
4			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9
5			3-Heptanol	116	C7H16O	000589-82-2	9



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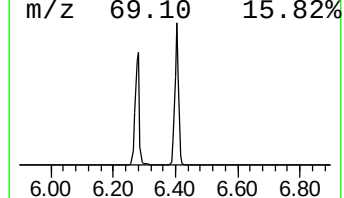
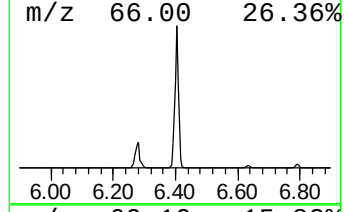
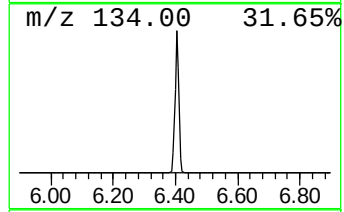
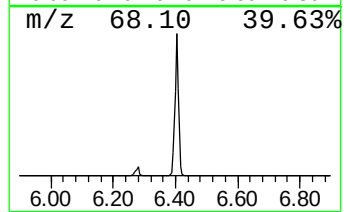
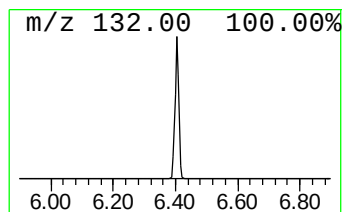
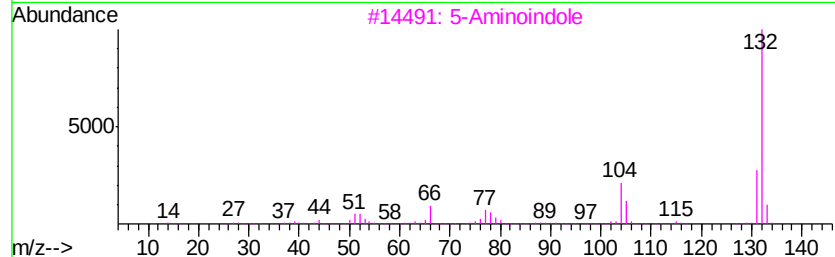
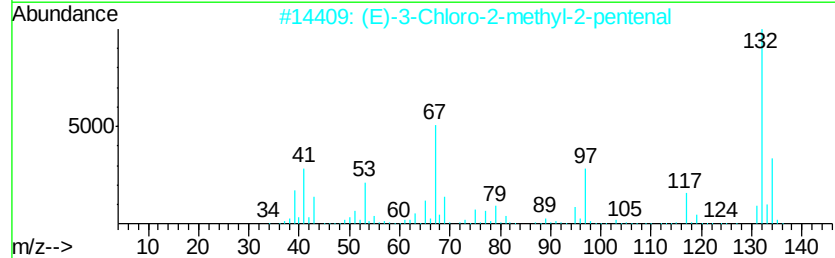
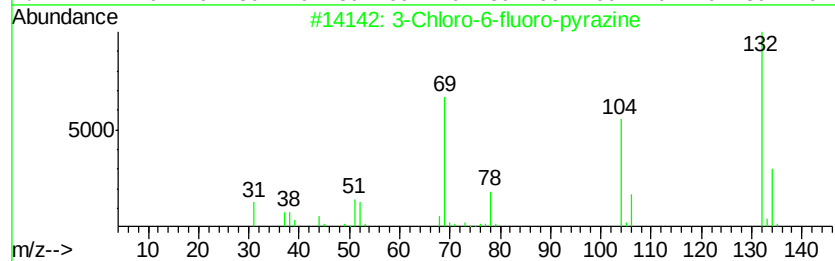
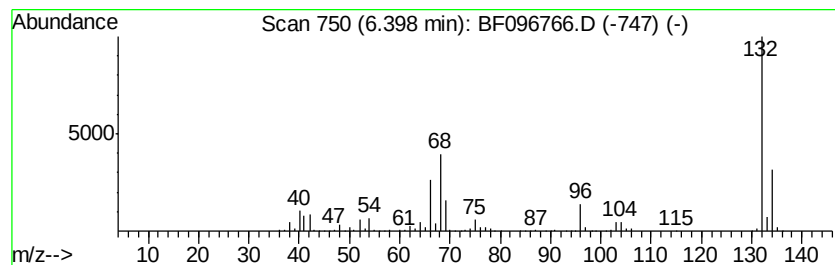
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Peak Number 2 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	52.18 ng	1523580	1,4-Dichlorobenzene-d4	6.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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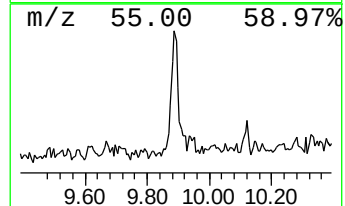
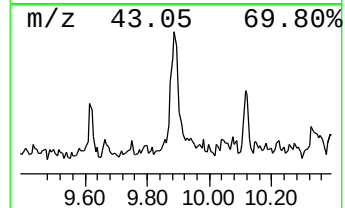
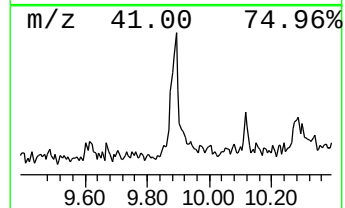
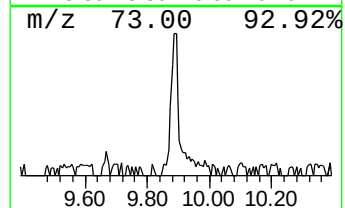
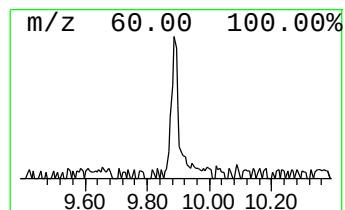
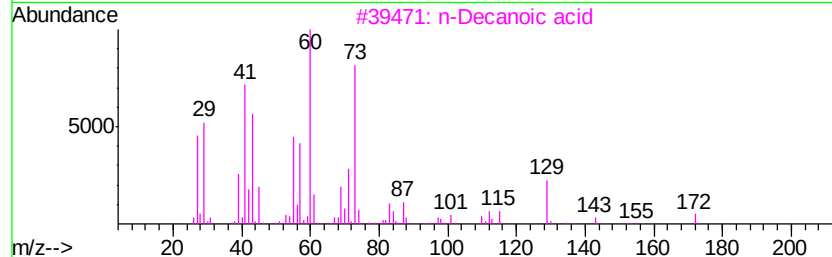
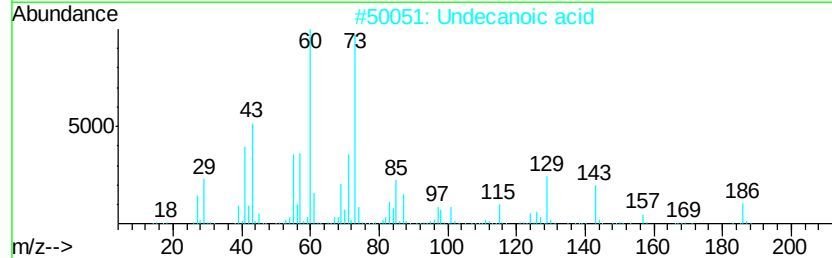
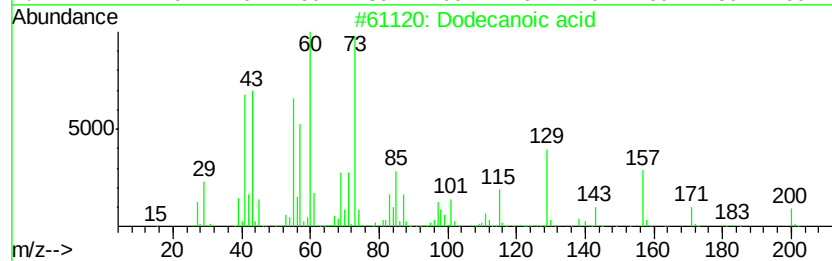
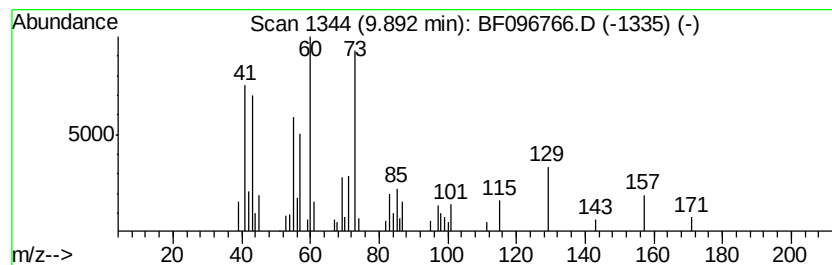
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Peak Number 4 Dodecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.89	2.30 ng	98098	Acenaphthene-d10	9.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid		200	C12H24O2	000143-07-7	96
2	Undecanoic acid		186	C11H22O2	000112-37-8	59
3	n-Decanoic acid		172	C10H20O2	000334-48-5	50
4	Octanoic acid, silver(1+) salt		250	C8H15AgO2	024927-67-1	47
5	d-Glucohexodialdose		178	C6H10O6	1000149-19-1	47



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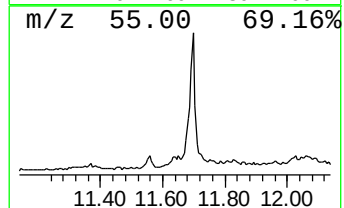
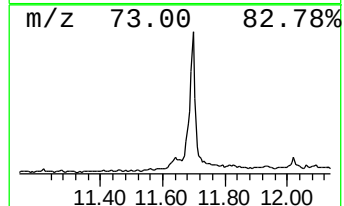
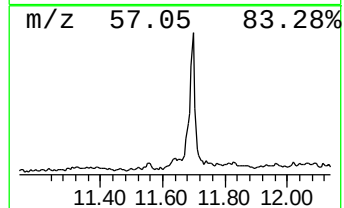
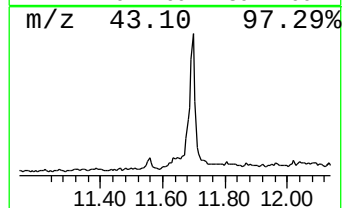
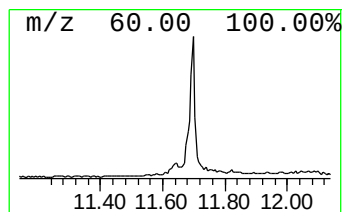
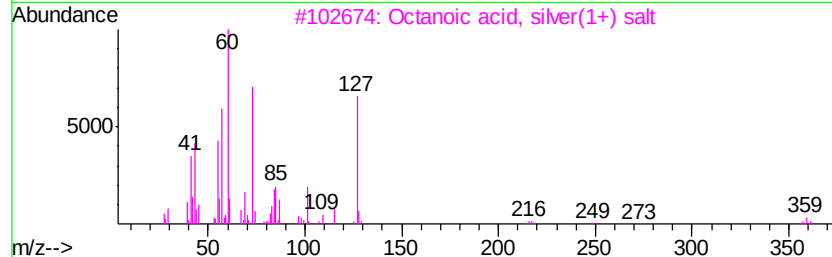
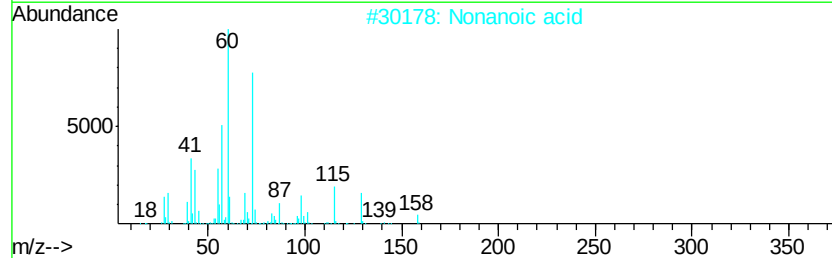
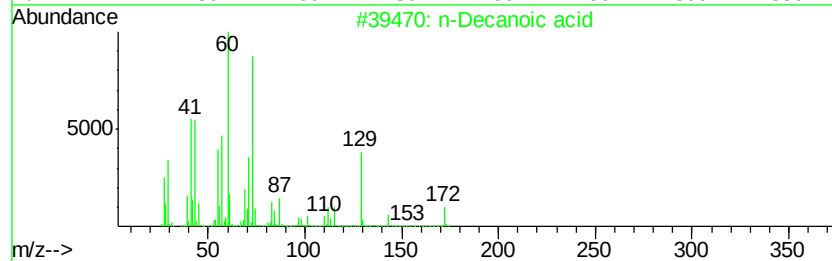
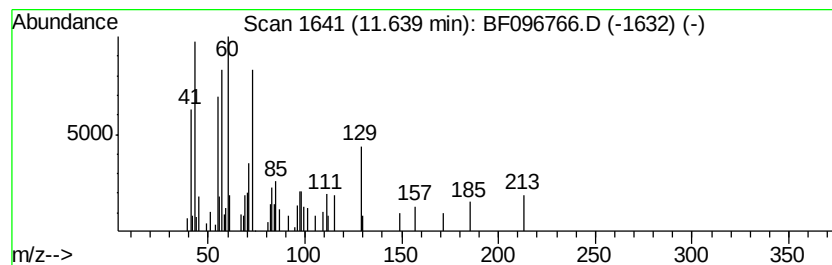
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown11.64 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.64	2.32 ng	93930	Phenanthrene-d10	11.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Decanoic acid	172	C10H20O2	000334-48-5	47
2		Nonanoic acid	158	C9H18O2	000112-05-0	43
3		Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	38
4		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	35
5		Undecanoic acid, 10-bromo-	264	C11H21BrO2	018294-93-4	35



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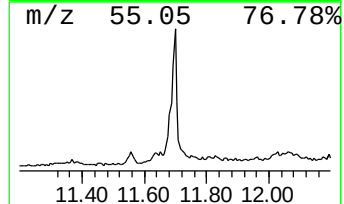
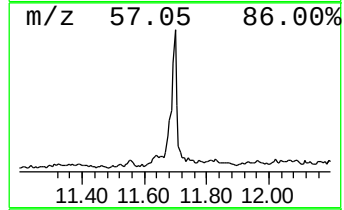
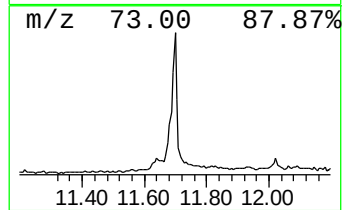
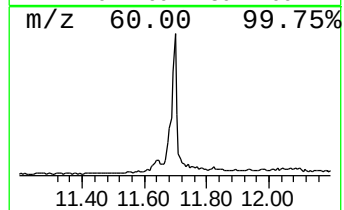
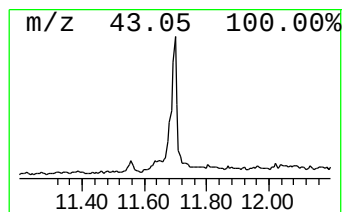
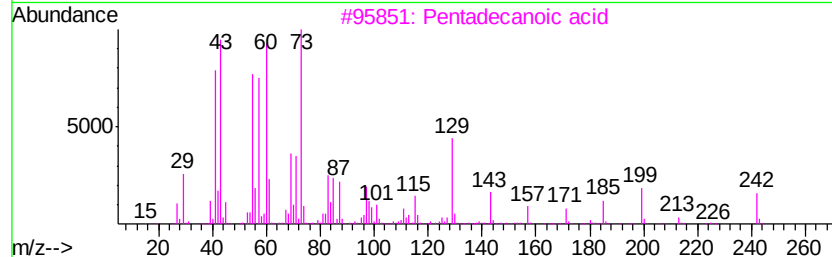
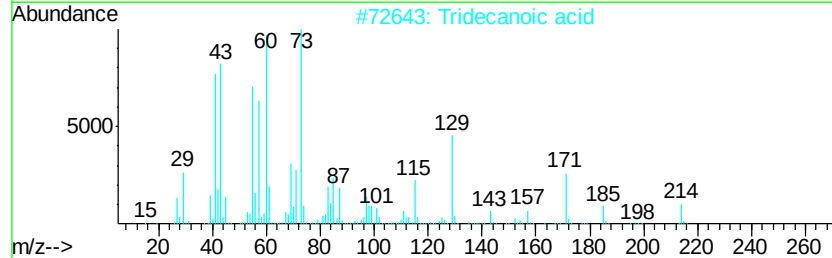
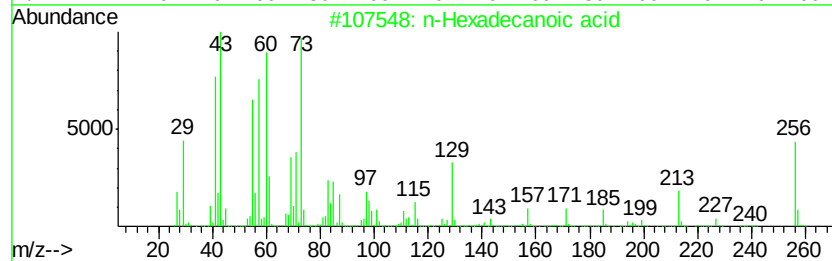
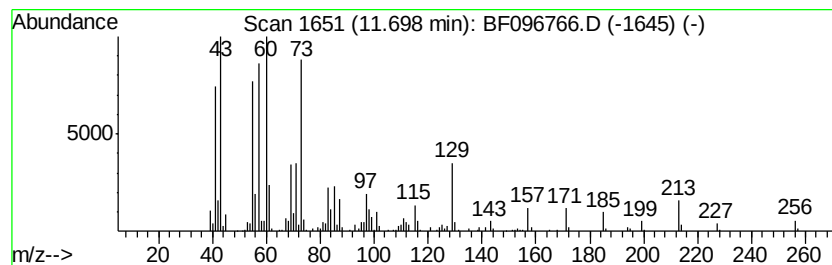
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	13.48 ng	545511	Phenanthrene-d10	11.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	47



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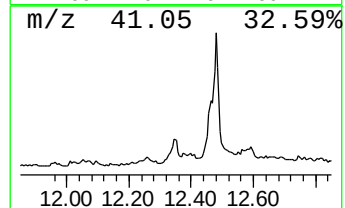
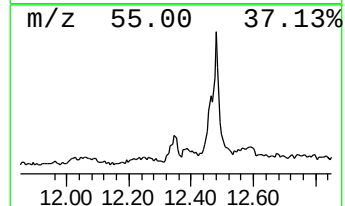
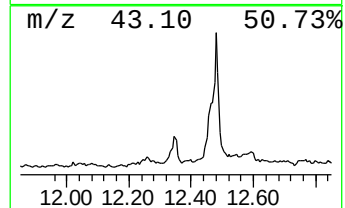
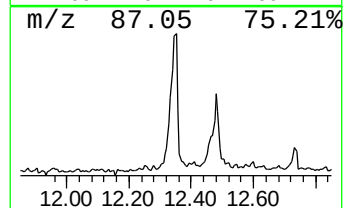
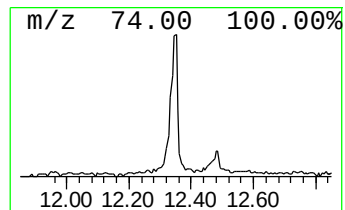
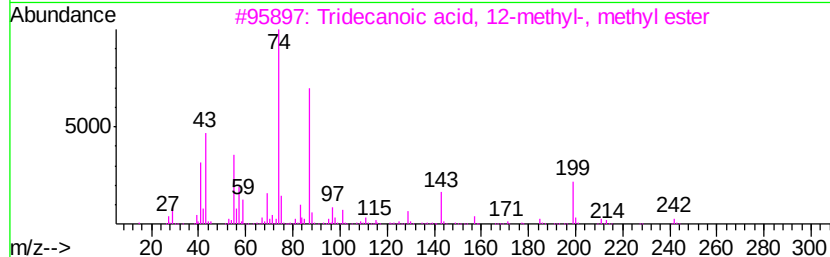
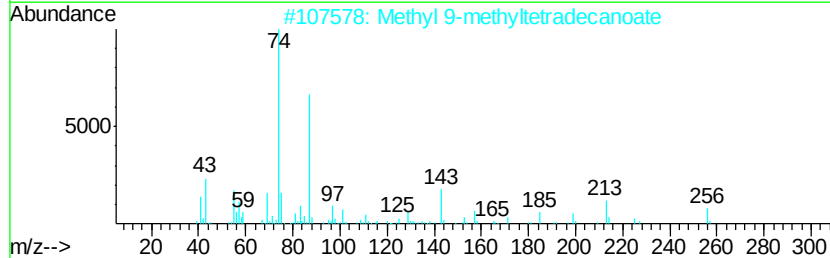
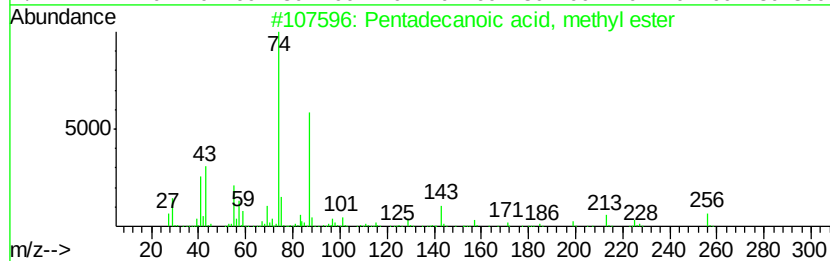
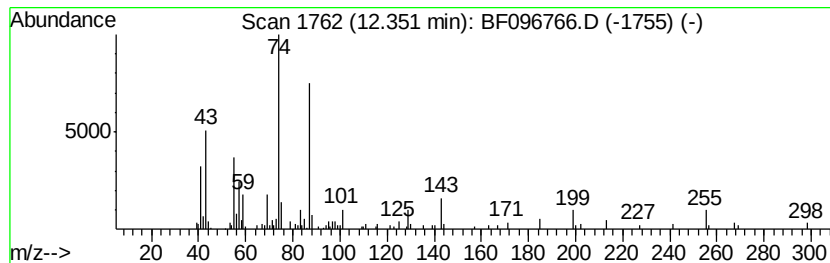
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecanoic acid, methyl ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.35	3.99 ng	161473	Phenanthrene-d10	11.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
2		Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	87
3		Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	86
4		Methyl stearate	298	C19H38O2	000112-61-8	78
5		Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	72



Data Path : Z:\HPCHEM1\BNA F\Data\BF071417\
Data File : BF096766.D
Acq On : 14 Jul 2017 10:50
Operator : SJ/JU
Sample : I4113-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-6(11.0-11.5)

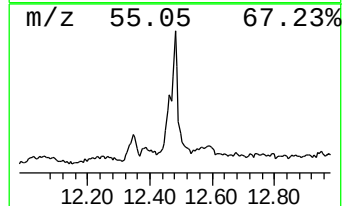
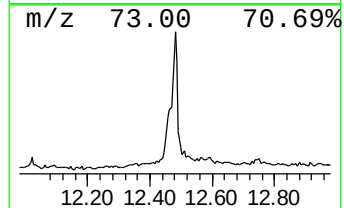
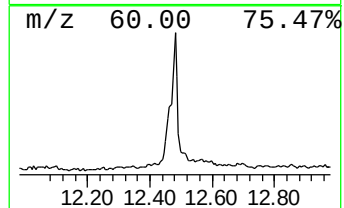
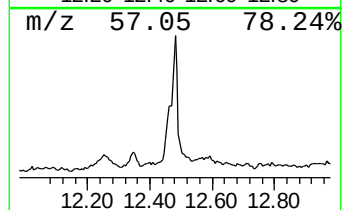
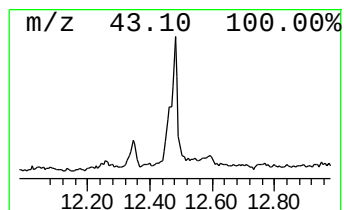
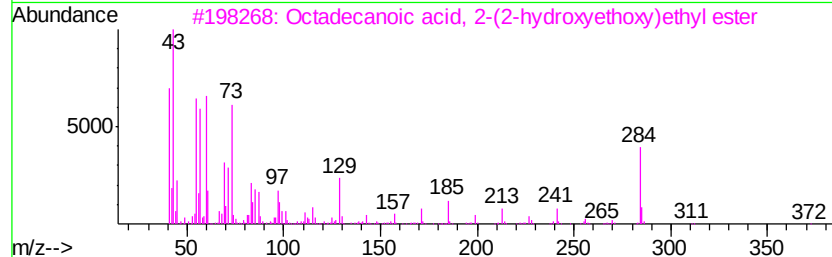
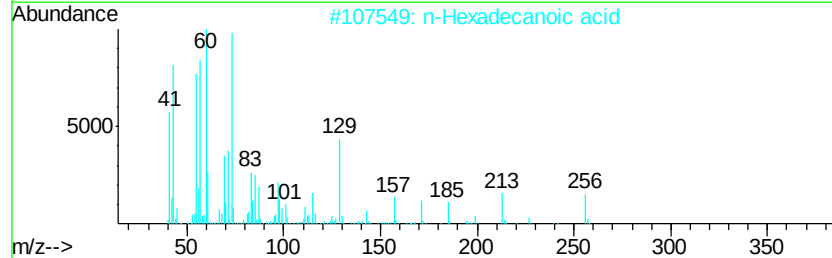
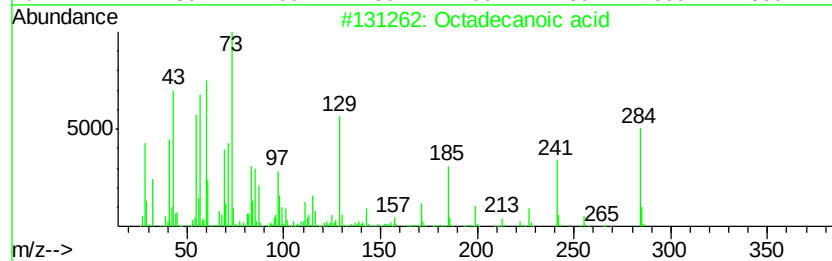
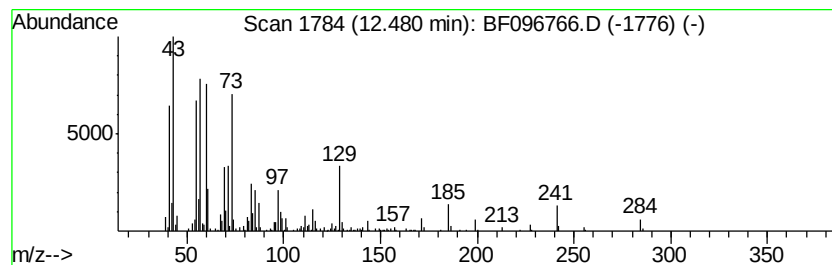
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	25.77 ng	779657	Chrysene-d12	13.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	91
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	55



Data Path : Z:\HPCHEM1\BNA F\Data\BF071417\
Data File : BF096766.D
Acq On : 14 Jul 2017 10:50
Operator : SJ/JU
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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-6(11.0-11.5)

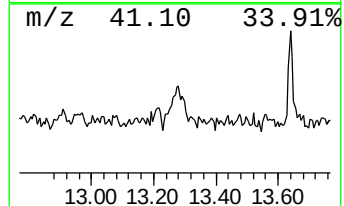
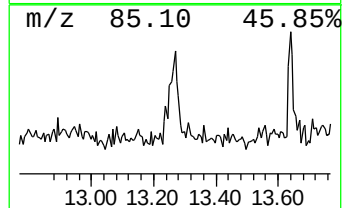
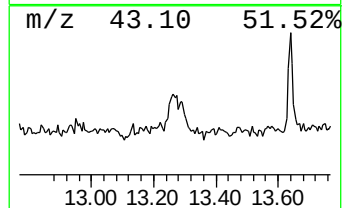
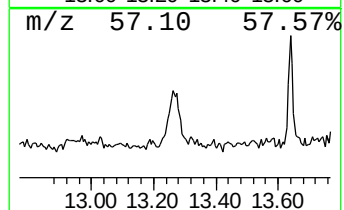
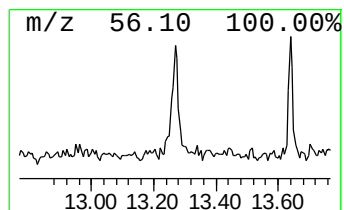
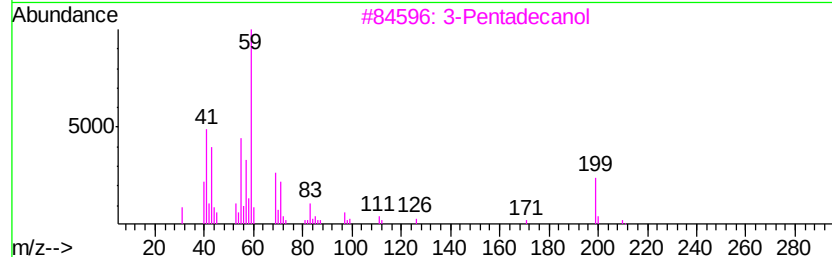
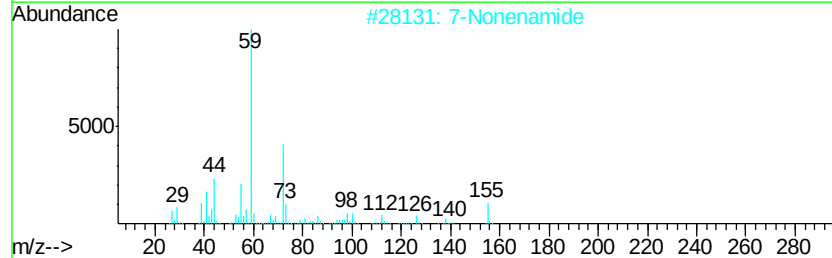
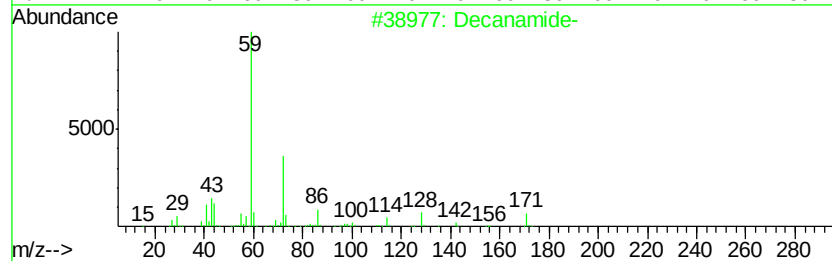
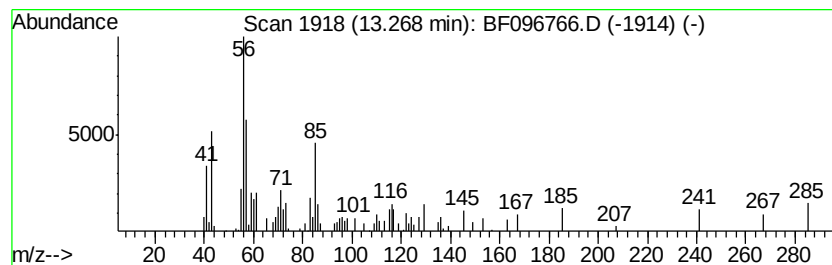
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.27 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.27	3.80 ng	114898	Chrysene-d12	13.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decanamide-	171	C10H21NO	002319-29-1	27
2		7-Nonenamide	155	C9H17NO	090949-53-4	27
3		3-Pentadecanol	228	C15H32O	053346-71-7	22
4		tert-Butyl N-hydroxycarbamate	133	C5H11NO3	036016-38-3	22
5		Acetic acid, ethoxy-	104	C4H8O3	000627-03-2	22



Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
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Acq On : 14 Jul 2017 10:50
Operator : SJ/JU
Sample : I4113-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

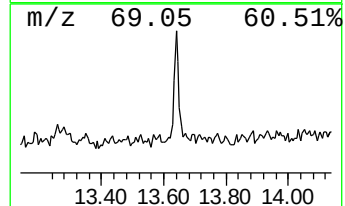
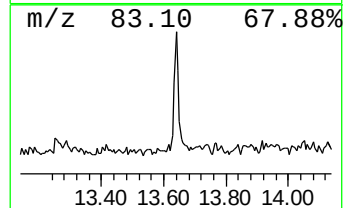
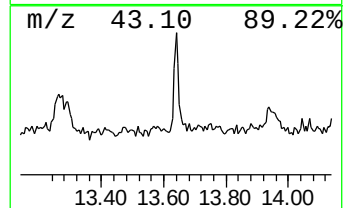
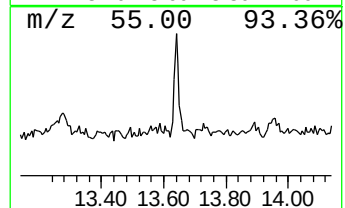
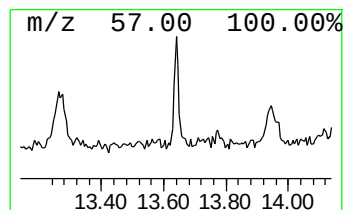
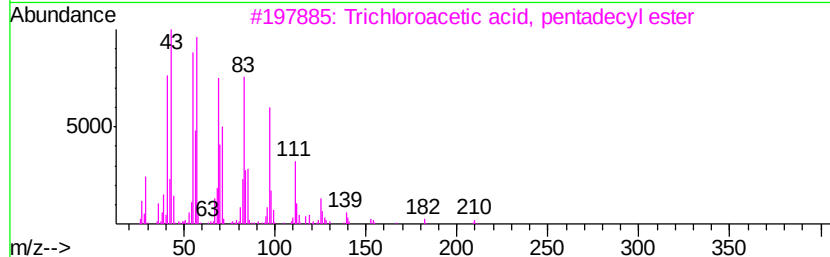
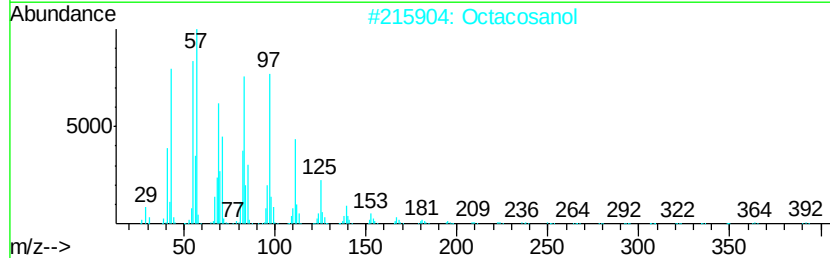
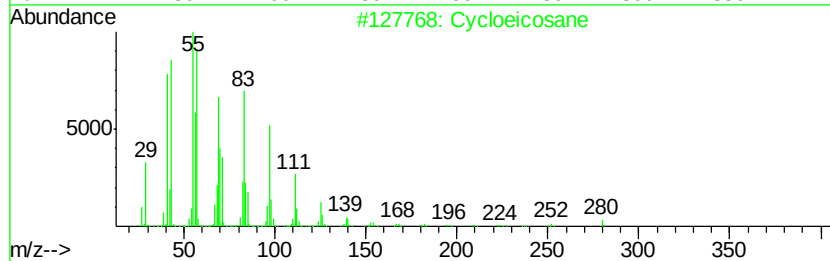
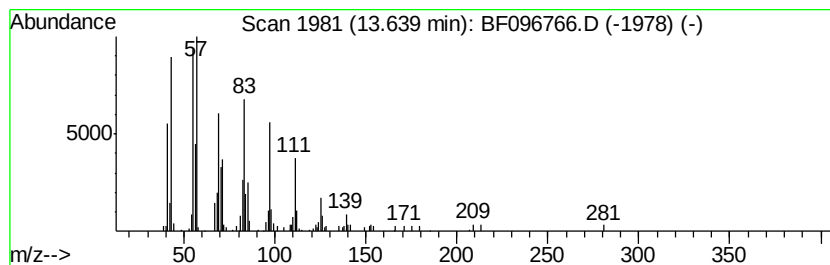
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cycloeicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	4.20 ng	127174	Chrysene-d12	13.77
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cycloeicosane	280 C20H40	000296-56-0 91
2		Octacosanol	410 C28H58O	000557-61-9 91
3		Trichloroacetic acid, pentadecyl...	372 C17H31Cl3O2	074339-53-0 91
4		Carbonic acid, heptadecyl isobut...	356 C22H44O3	1000314-61-4 91
5		1-Hexadecanol	242 C16H34O	036653-82-4 91



Data Path : Z:\HPCHEM1\BNA F\Data\BF071417\
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Sample : I4113-05
Misc :
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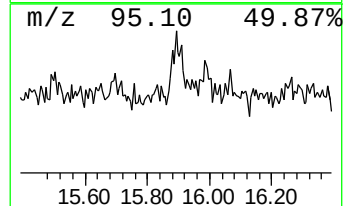
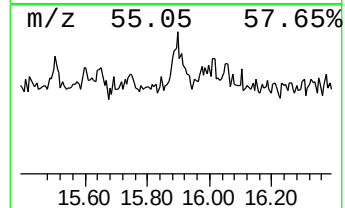
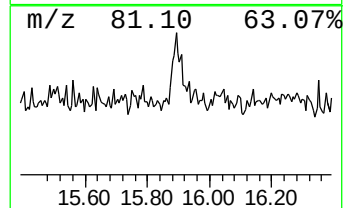
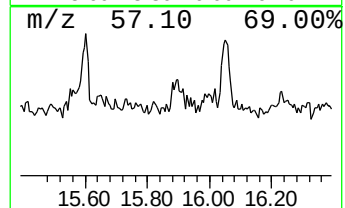
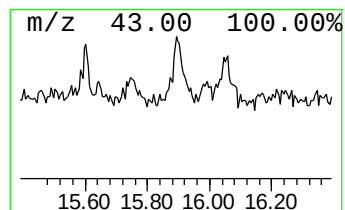
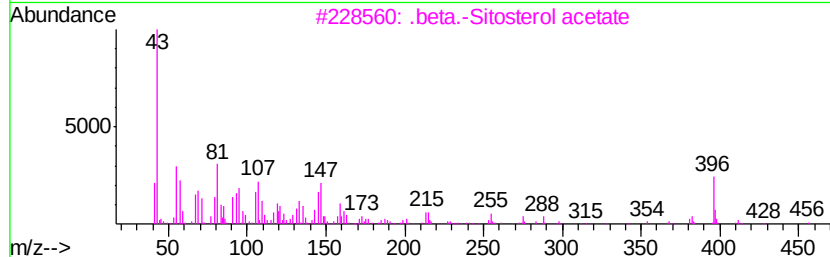
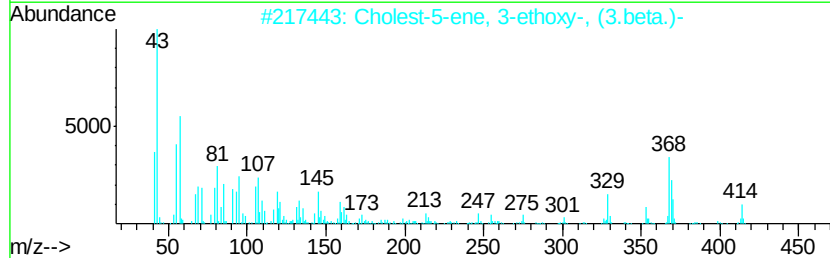
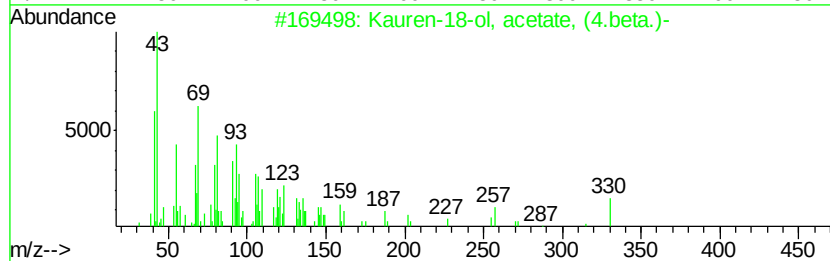
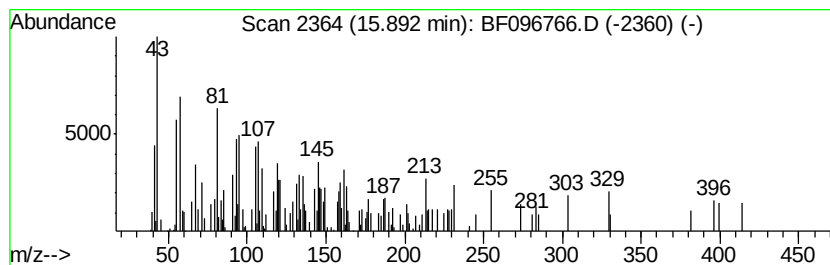
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Kauren-18-ol, acetate, (4.b... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	6.64 ng	152139	Perylene-d12	15.16
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Kauren-18-ol, acetate, (4.beta.)-	330 C22H34O2	072150-74-4 50
2		Cholest-5-ene, 3-ethoxy-, (3.bet...	414 C29H50O	000986-19-6 38
3		.beta.-Sitosterol acetate	456 C31H52O2	000915-05-9 38
4		5.beta.-Cholan-24-oic acid, 3-oxo-	374 C24H38O3	001553-56-6 35
5		5-Cholene, 3,24-dihydroxy-	360 C24H40O2	1000251-69-2 35



Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
Data File : BF096766.D
Acq On : 14 Jul 2017 10:50
Operator : SJ/JU
Sample : I4113-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-6(11.0-11.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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unknown6.40	6.40	52.2	ng	1523580	1	6.63	583950	20.0
Dodecanoic acid	9.89	2.3	ng	98098	3	9.67	854744	20.0
unknown11.64	11.64	2.3	ng	93930	4	11.15	809566	20.0
n-Hexadecanoic acid	11.70	13.5	ng	545511	4	11.15	809566	20.0
Pentadecanoic aci...	12.35	4.0	ng	161473	4	11.15	809566	20.0
Octadecanoic acid	12.48	25.8	ng	779657	5	13.77	605193	20.0
unknown13.27	13.27	3.8	ng	114898	5	13.77	605193	20.0
Cycloeicosane	13.64	4.2	ng	127174	5	13.77	605193	20.0
Kauren-18-ol, ace...	15.89	6.6	ng	152139	6	15.16	458499	20.0