

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
 Data File : BF107944.D
 Acq On : 3 Aug 2018 18:11
 Operator : JU/SJ
 Sample : J4316-09
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OW-2-4

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-BF073018.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	5.178	480	483	495	rBV	137445	226610	5.75%	0.784%
2	5.601	551	555	577	rBV	273599	1091000	27.66%	3.774%
3	6.607	722	726	743	rBV	217843	836658	21.21%	2.894%
4	6.725	743	746	760	rBV	1703136	2719087	68.94%	9.406%
5	6.954	781	785	791	rBV	344577	604781	15.33%	2.092%
6	7.001	791	793	800	rVB2	142346	239051	6.06%	0.827%
7	7.101	807	810	834	rVB	2034153	2824157	71.60%	9.770%
8	7.337	847	850	854	rBV	43296	53411	1.35%	0.185%
9	7.519	878	881	895	rBV	1127805	2119373	53.73%	7.332%
10	7.678	905	908	915	rVB2	91975	137060	3.47%	0.474%
11	7.760	919	922	927	rVB	63279	67670	1.72%	0.234%
12	8.101	977	980	983	rVB	51908	58563	1.48%	0.203%
13	8.142	983	987	994	rBV8	26165	58555	1.48%	0.203%
14	8.231	998	1002	1011	rBV	720544	1260989	31.97%	4.362%
15	8.325	1016	1018	1021	rVV4	61522	76492	1.94%	0.265%
16	8.360	1021	1024	1028	rVV2	62024	85547	2.17%	0.296%
17	8.442	1028	1038	1042	rVV3	67095	230863	5.85%	0.799%
18	8.525	1049	1052	1056	rBV	57776	73640	1.87%	0.255%
19	8.707	1081	1083	1089	rVB6	49571	70696	1.79%	0.245%
20	8.766	1090	1093	1097	rVV2	32809	42022	1.07%	0.145%
21	8.872	1108	1111	1115	rBV2	105986	116958	2.97%	0.405%
22	8.931	1115	1121	1124	rBV2	148299	251136	6.37%	0.869%
23	9.172	1159	1162	1170	rBV4	155336	235761	5.98%	0.816%
24	9.254	1170	1176	1179	rBV2	115869	179604	4.55%	0.621%
25	9.307	1180	1185	1193	rBV	3301991	3944371	100.00%	13.645%
26	9.701	1249	1252	1258	rVB	225615	235890	5.98%	0.816%
27	9.989	1294	1301	1309	rBV3	1318381	1822550	46.21%	6.305%
28	10.789	1434	1437	1448	rBV	1600440	2231188	56.57%	7.718%
29	11.348	1529	1532	1537	rBV	270520	286806	7.27%	0.992%
30	11.489	1553	1556	1566	rVB	729756	916766	23.24%	3.171%
31	12.001	1641	1643	1651	rVB2	313552	366925	9.30%	1.269%
32	12.736	1766	1768	1773	rVB	320347	263257	6.67%	0.911%
33	12.783	1774	1776	1781	rVB	247973	265332	6.73%	0.918%
34	13.071	1821	1825	1839	rVB	2443871	2898634	73.49%	10.027%

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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 >
Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.948	1972	1974	1979	rVB2	151312	172606	4.38%	0.597%
36	14.142	2004	2007	2020	rVB	576405	765584	19.41%	2.648%
37	14.965	2144	2147	2152	rVB	101517	110877	2.81%	0.384%
38	15.236	2190	2193	2197	rVB	75248	94133	2.39%	0.326%
39	15.677	2263	2268	2279	rVB	419988	787770	19.97%	2.725%
40	16.089	2335	2338	2345	rVB	53715	85090	2.16%	0.294%

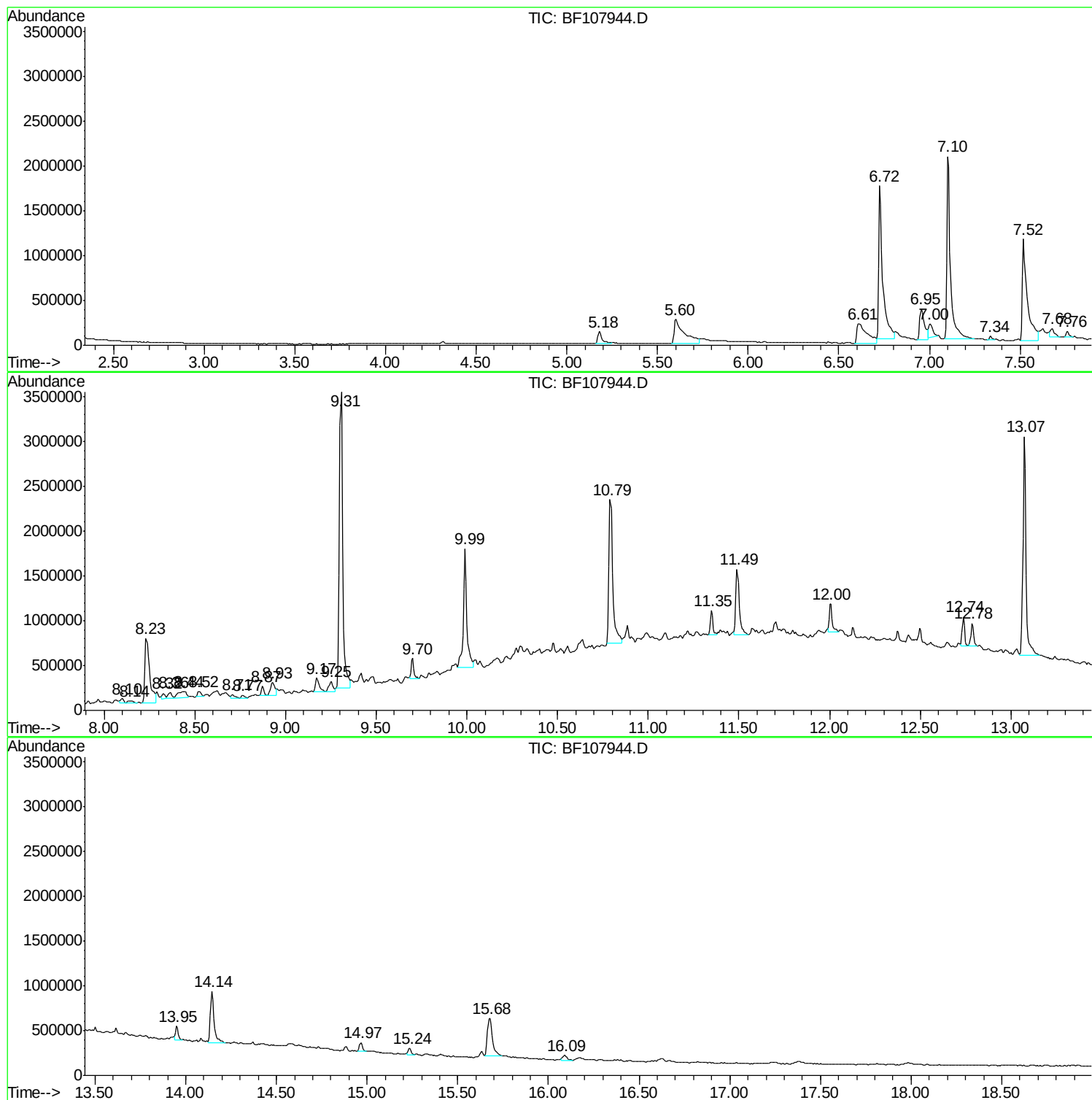
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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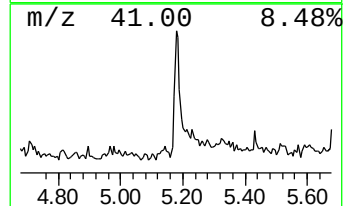
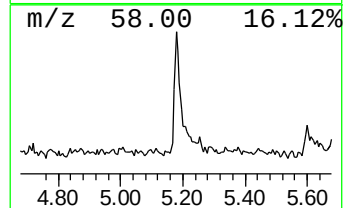
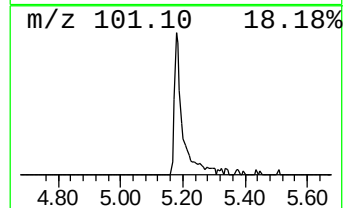
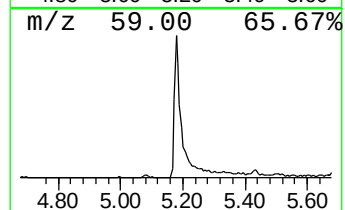
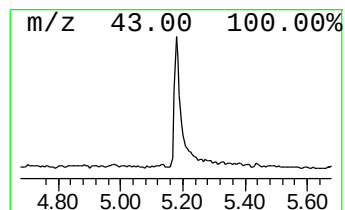
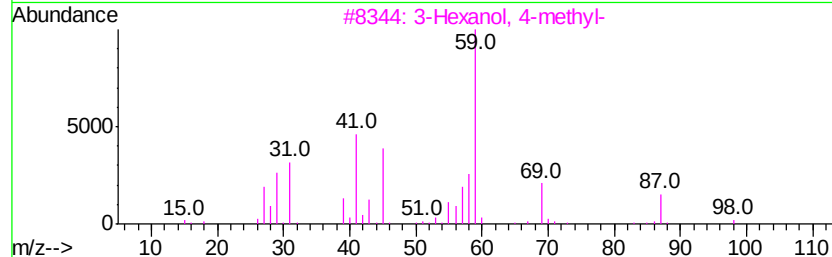
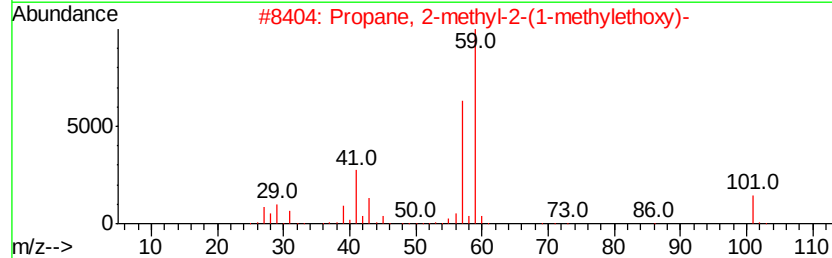
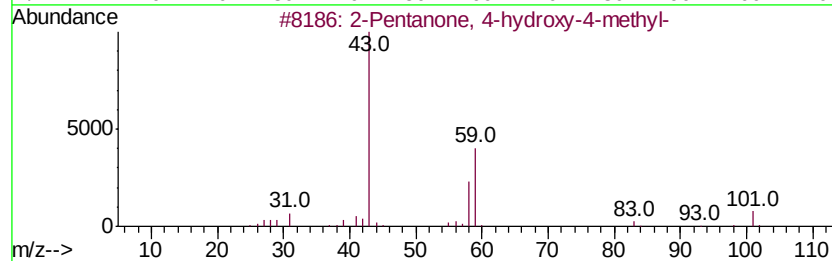
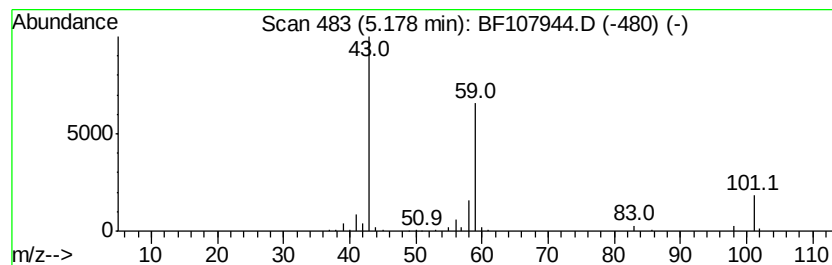
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	7.49 ng	226610	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	42
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		1,2-Butanediol	90	C4H10O2	000584-03-2	25



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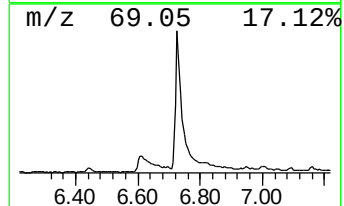
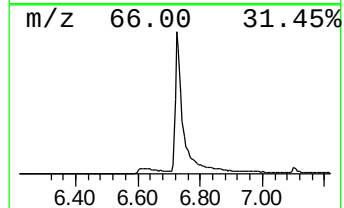
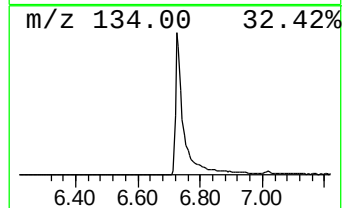
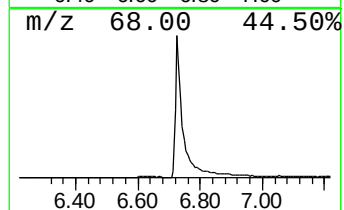
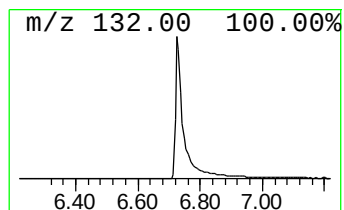
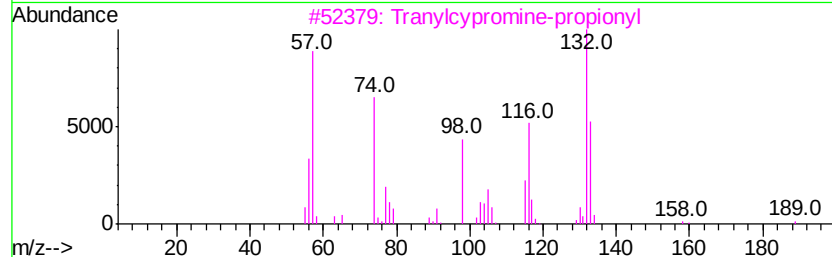
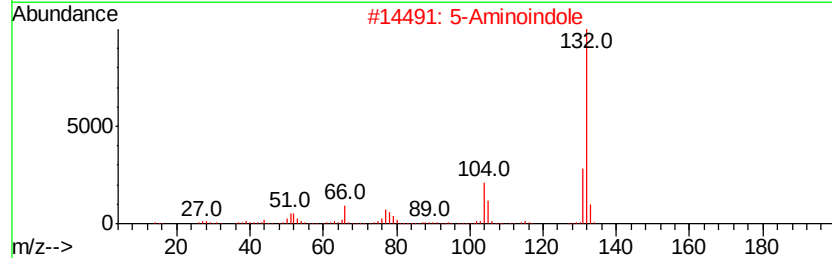
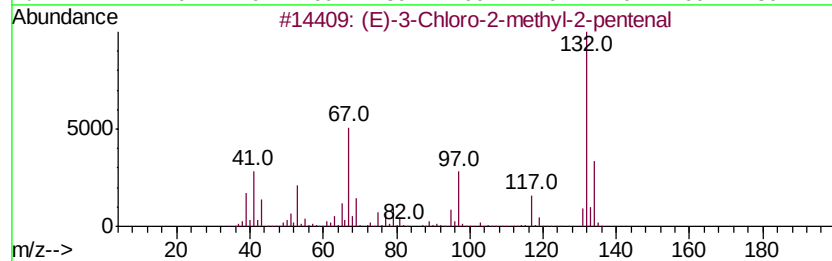
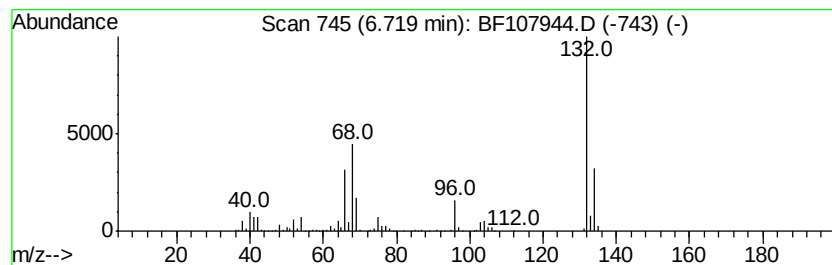
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.72 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	89.92 ng	2719090	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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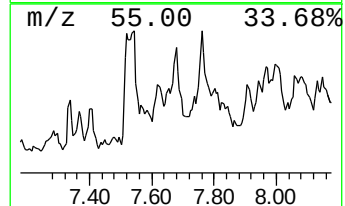
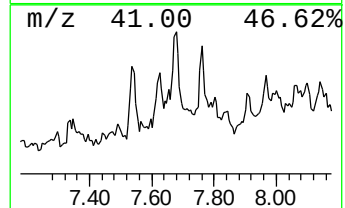
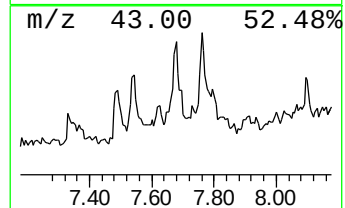
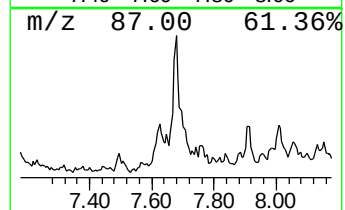
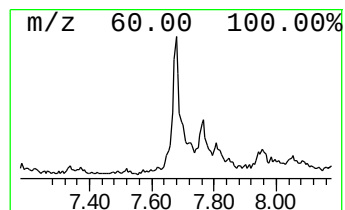
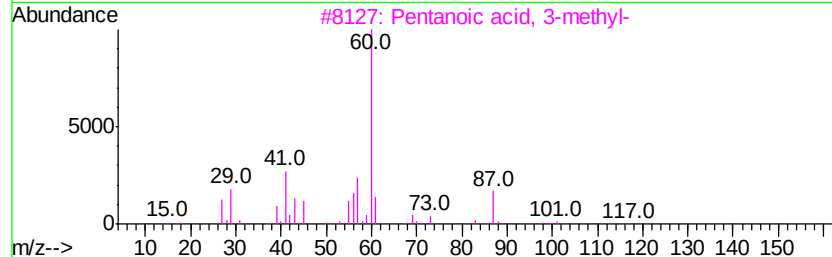
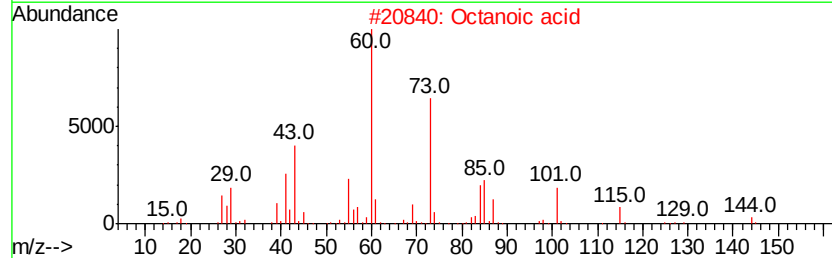
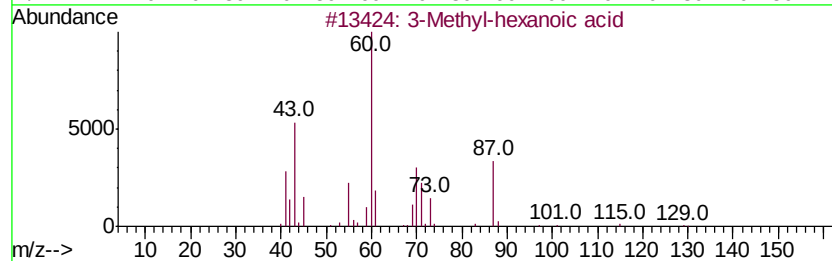
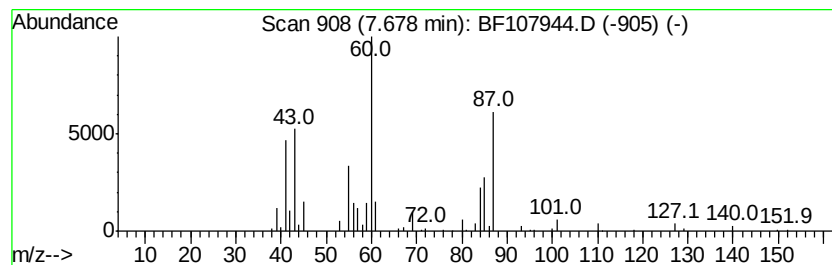
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.68 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	2.17 ng	137060	Naphthalene-d8	8.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	47	
2	Octanoic acid	144	C8H16O2	000124-07-2	42	
3	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	33	
4	Hexanoic acid	116	C6H12O2	000142-62-1	32	
5	2-Butenoic acid, 4-hydroxy-, met...	116	C5H8O3	004508-99-0	27	



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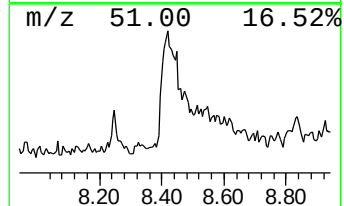
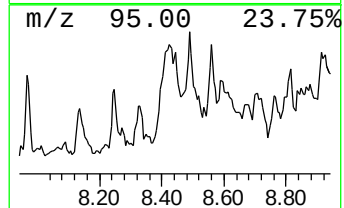
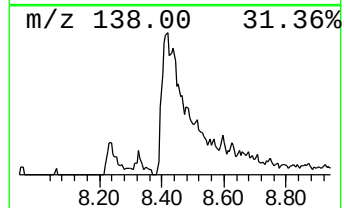
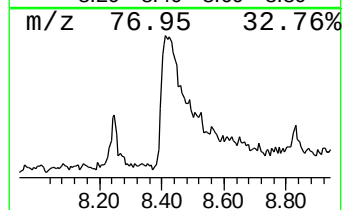
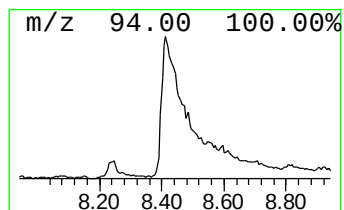
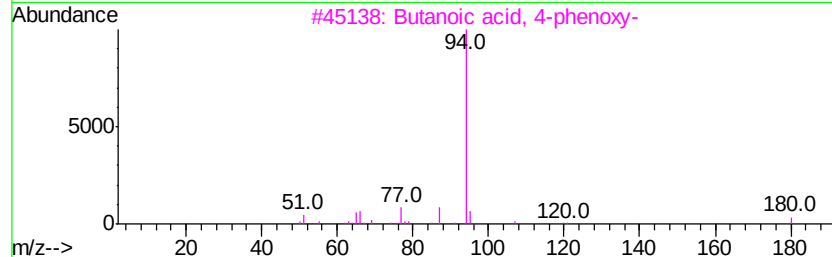
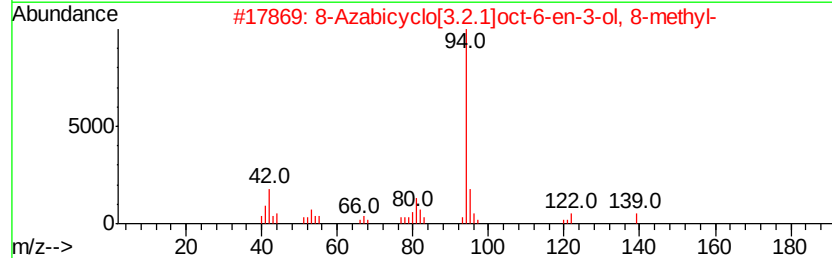
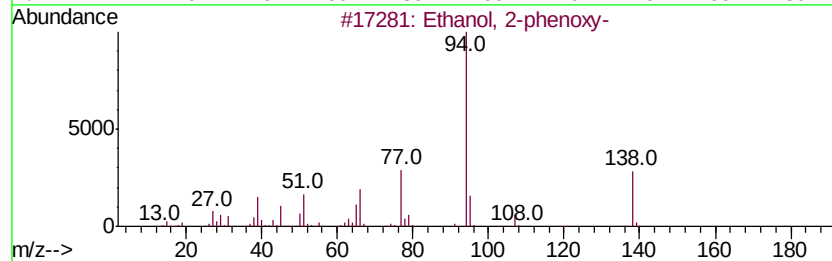
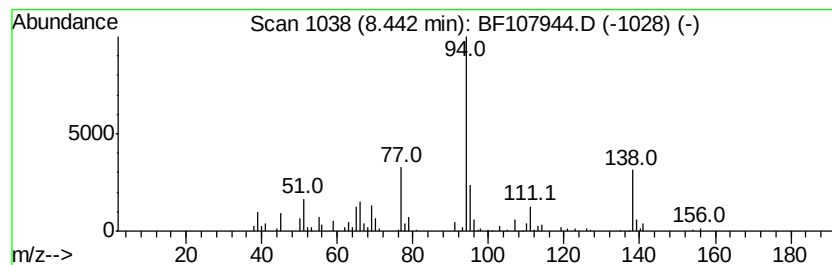
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 2-phenoxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.44	3.66 ng	230863	Naphthalene-d8	8.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	94
2		8-Azabicyclo[3.2.1]oct-6-en-3-ol...	139	C8H13NO	054725-49-4	47
3		Butanoic acid, 4-phenoxy-	180	C10H12O3	006303-58-8	47
4		Phenol	94	C6H6O	000108-95-2	46
5		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	40



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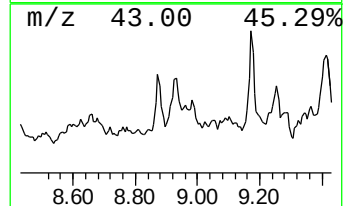
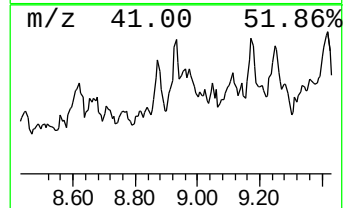
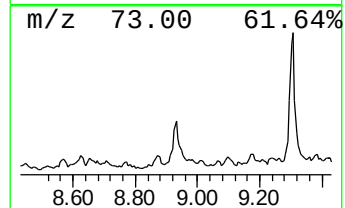
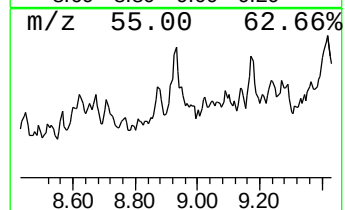
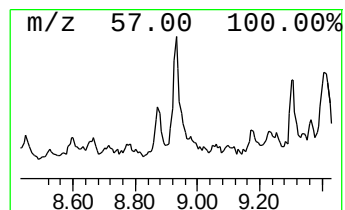
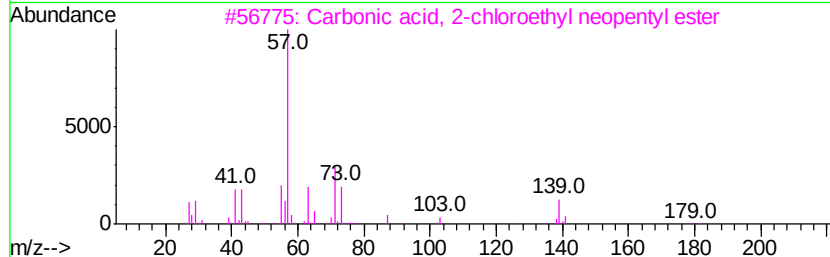
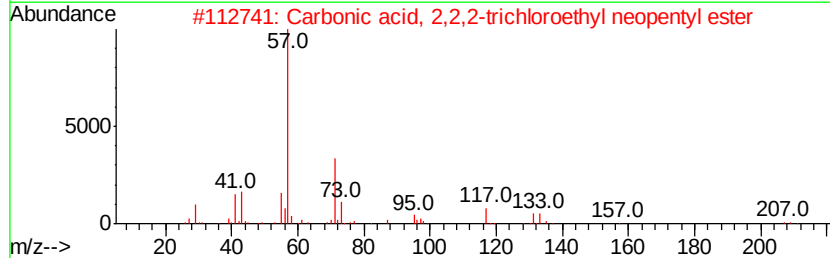
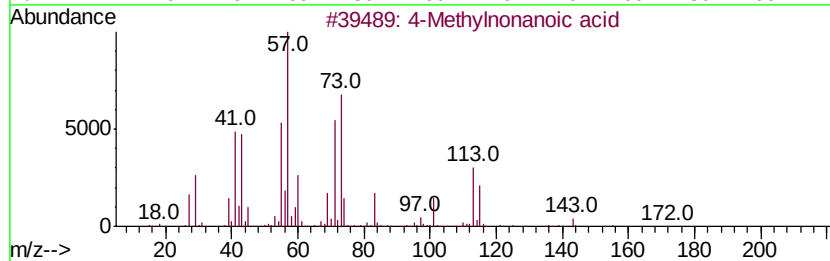
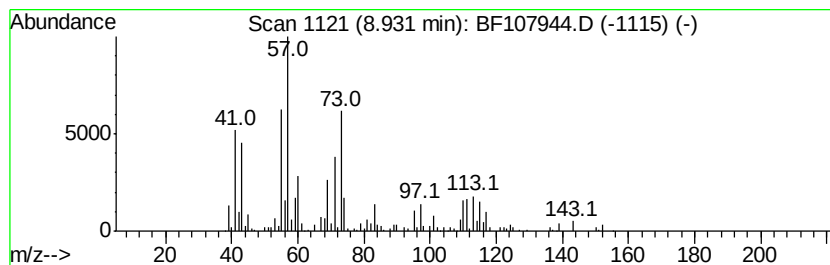
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Peak Number 6 unknown8.93 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.93	3.98 ng	251136	Napthalene-d8	8.23

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methylnonanoic acid	172	C10H20O2	045019-28-1	47
2			Carbonic acid, 2,2,2-trichloroet...	262	C8H13Cl3O3	1000357-89-3	38
3			Carbonic acid, 2-chloroethyl neo...	194	C8H15ClO3	1000357-87-7	25
4			Sulfurous acid, 2-ethylhexyl iso...	250	C12H26O3S	1000309-18-7	22
5			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	16



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107944.D
Acq On : 3 Aug 2018 18:11
Operator : JU/SJ
Sample : J4316-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OW-2-4

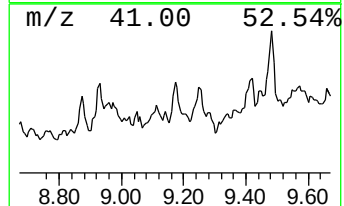
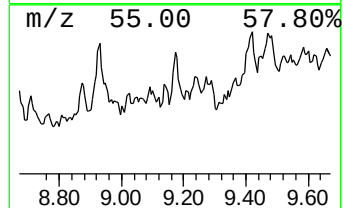
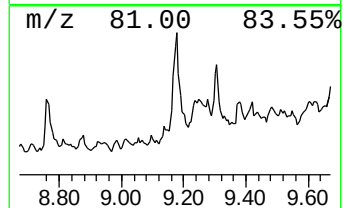
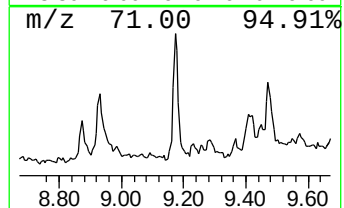
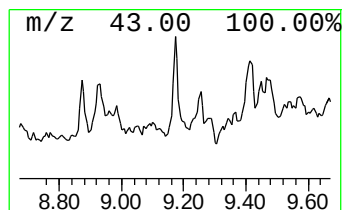
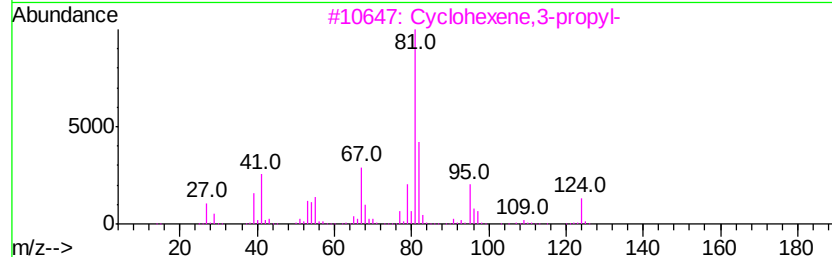
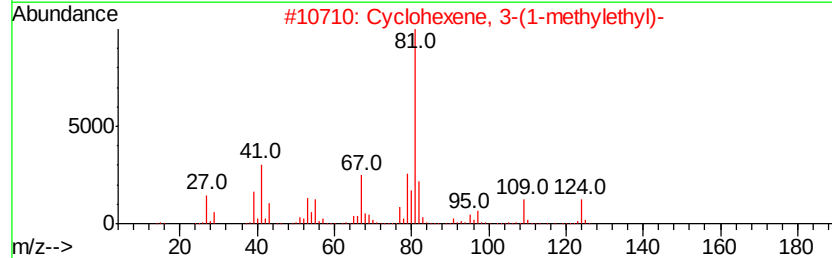
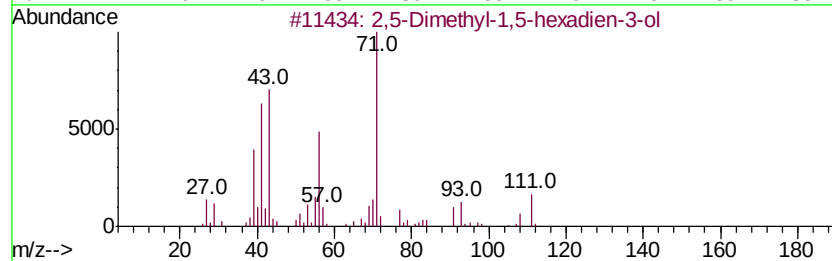
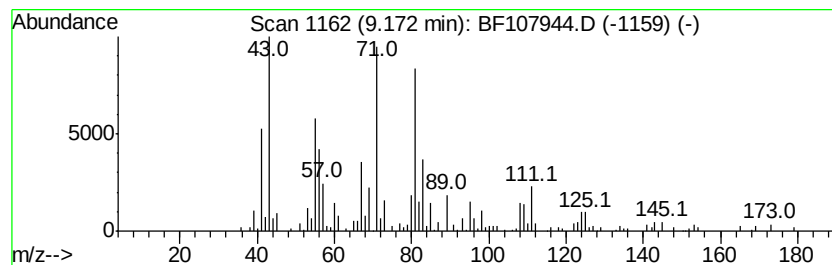
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown9.17 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.17	2.59 ng	235761	Acenaphthene-d10	9.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,5-Dimethyl-1,5-hexadien-3-ol	126	C8H14O	017123-63-6	43
2		Cyclohexene, 3-(1-methylethyl)-	124	C9H16	003983-08-2	25
3		Cyclohexene, 3-propyl-	124	C9H16	003983-06-0	22
4		3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	22
5		Bicyclo[2.2.2]oct-5-en-2-yl dimet...	151	C10H17N	033162-94-6	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107944.D
Acq On : 3 Aug 2018 18:11
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Sample : J4316-09
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ClientSampleId :
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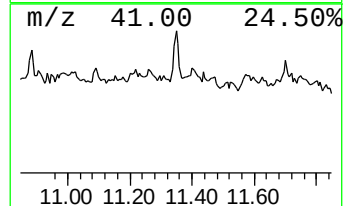
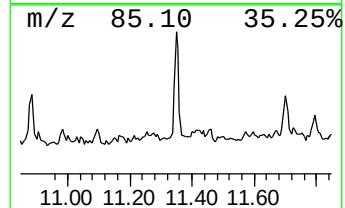
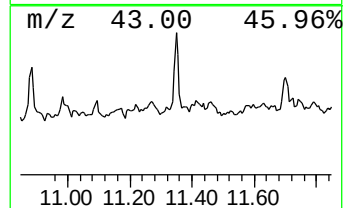
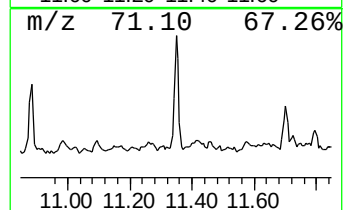
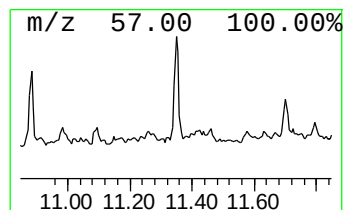
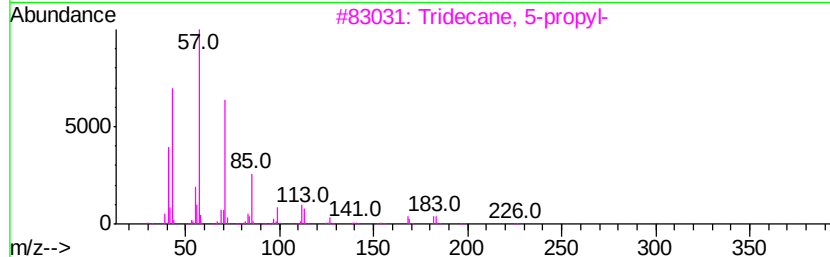
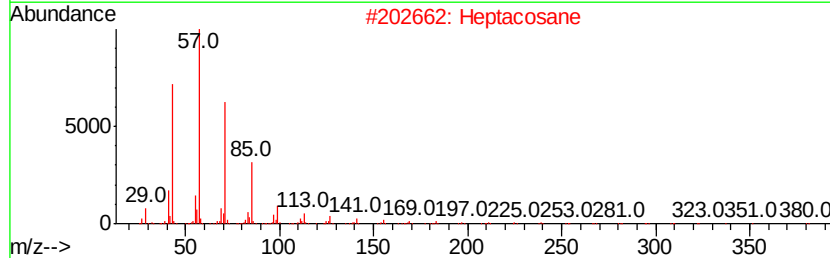
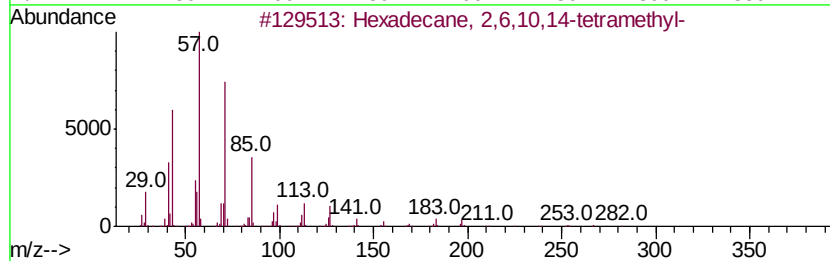
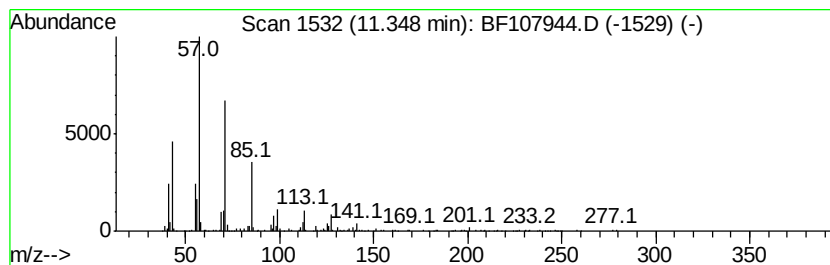
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane, 2,6,10,14-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.35	6.26 ng	286806	Phenanthrene-d10	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
2		Heptacosane	380	C27H56	000593-49-7	83
3		Tridecane, 5-propyl-	226	C16H34	055045-11-9	74
4		Nonadecane	268	C19H40	000629-92-5	64
5		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107944.D
Acq On : 3 Aug 2018 18:11
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Sample : J4316-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

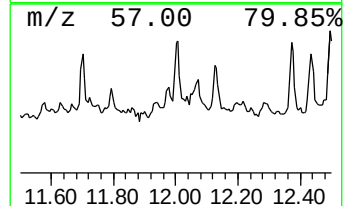
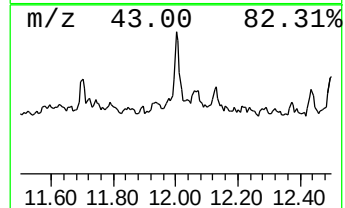
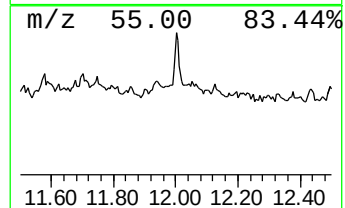
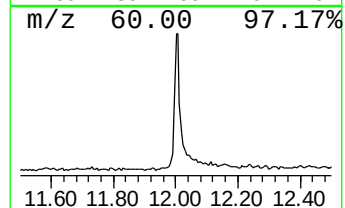
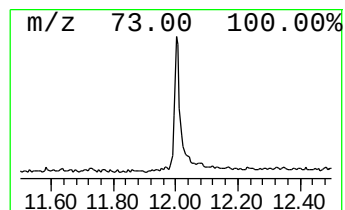
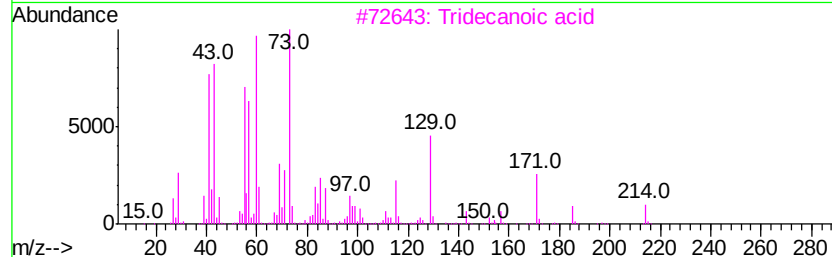
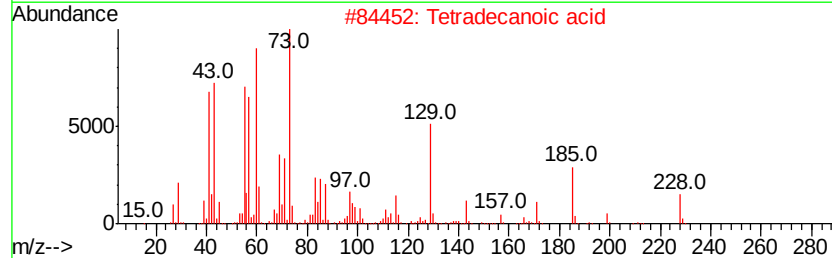
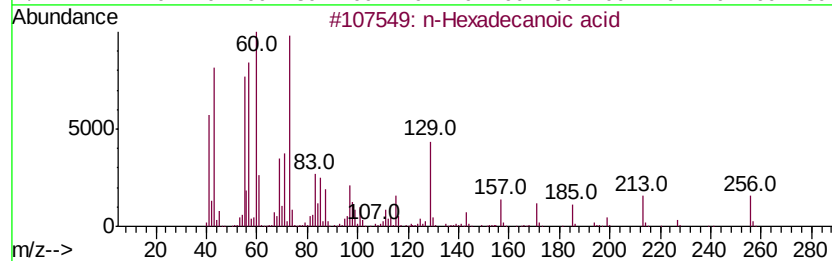
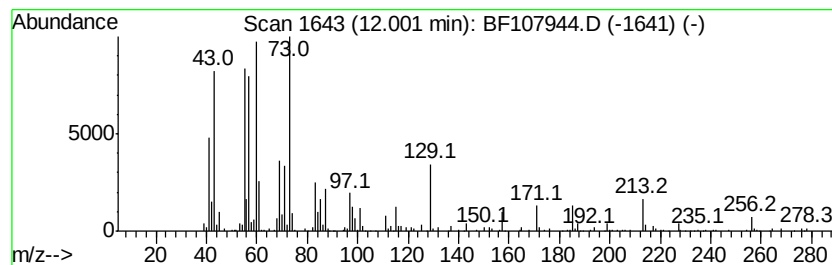
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.00	8.00 ng	366925	Phenanthrene-d10	11.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107944.D
Acq On : 3 Aug 2018 18:11
Operator : JU/SJ
Sample : J4316-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

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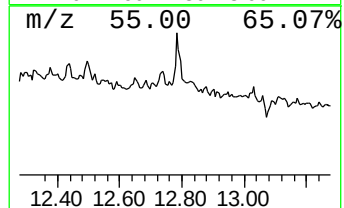
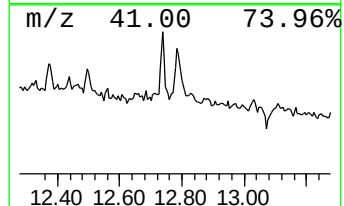
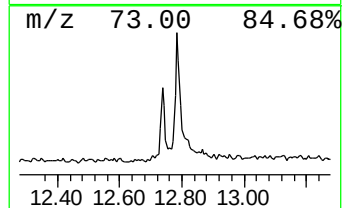
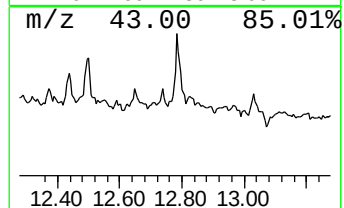
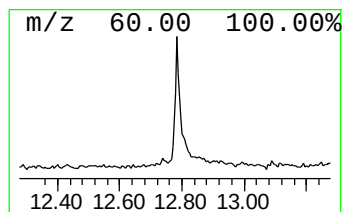
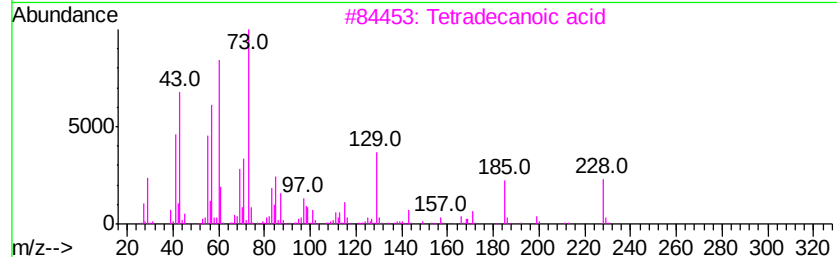
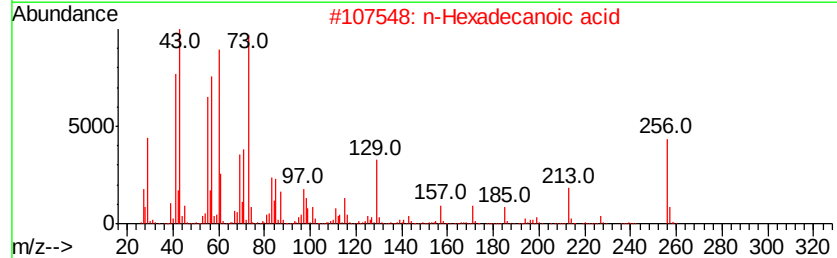
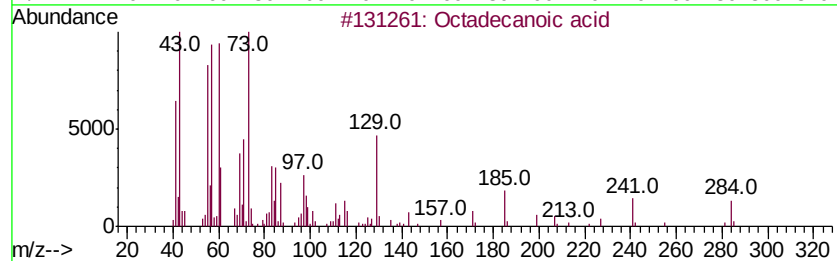
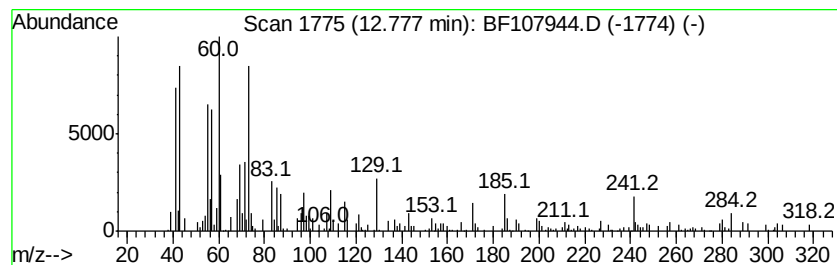
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	5.79 ng	265332	Phenanthrene-d10	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5		Tridecanoic acid	214	C13H26O2	000638-53-9	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
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Sample : J4316-09
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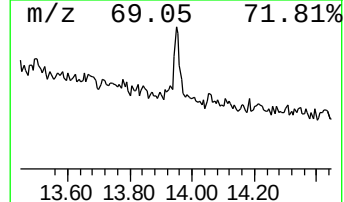
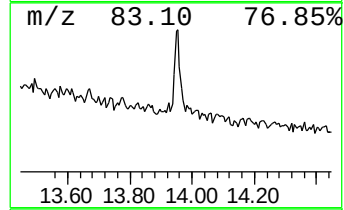
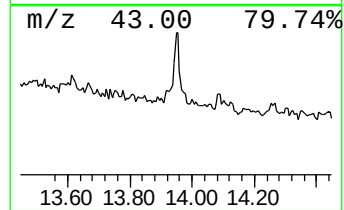
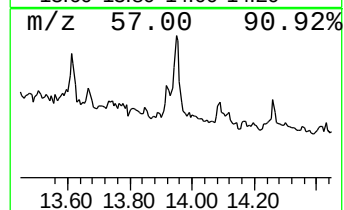
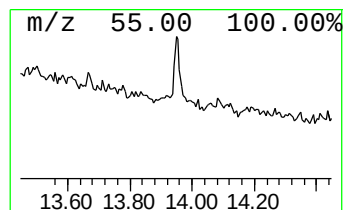
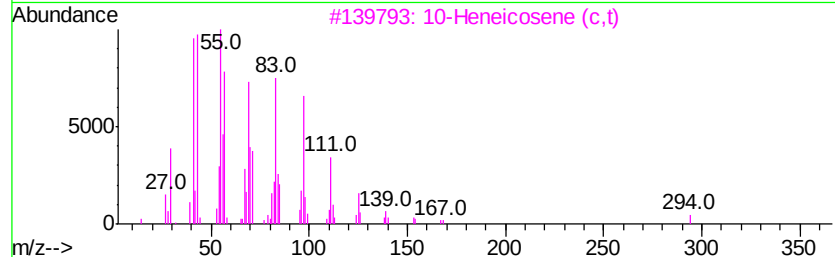
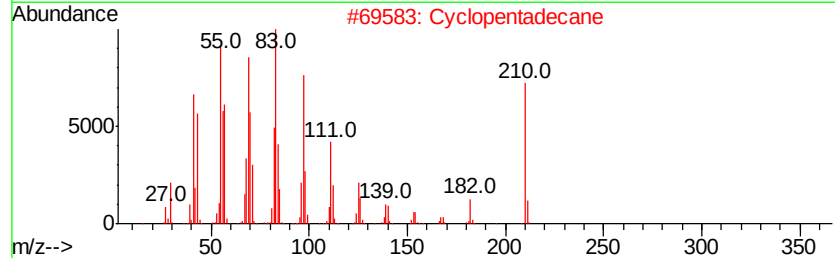
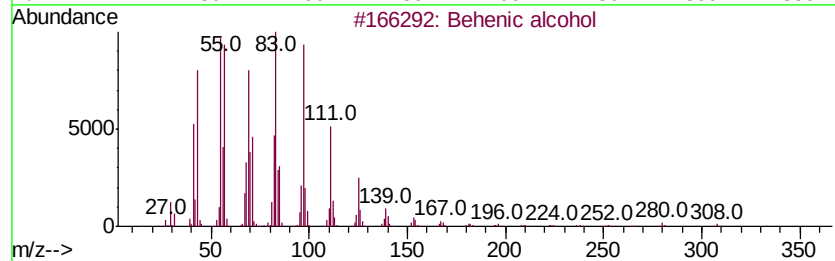
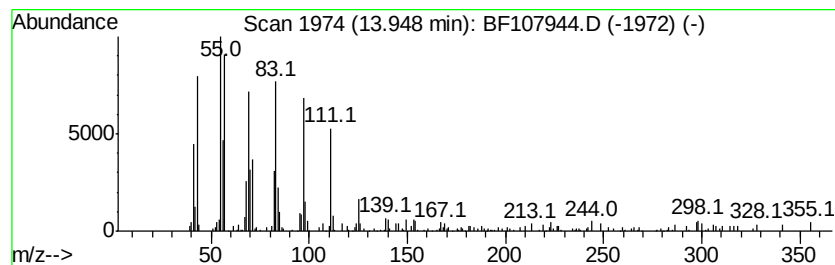
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Behenic alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.95	4.51 ng	172606	Chrysene-d12	14.14	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	72
2	Cyclopentadecane	210	C15H30	000295-48-7	72
3	10-Heneicosene (c,t)	294	C21H42	095008-11-0	72
4	1-Eicosanol	298	C20H42O	000629-96-9	72
5	Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107944.D
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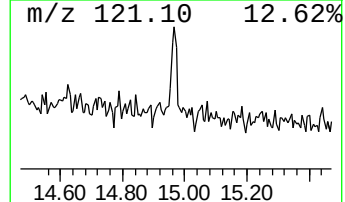
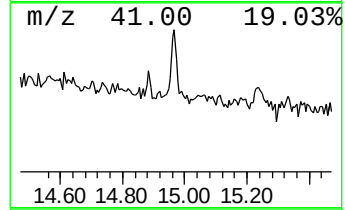
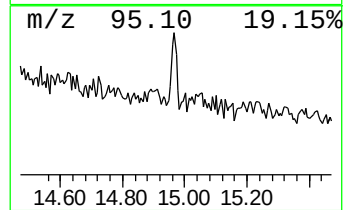
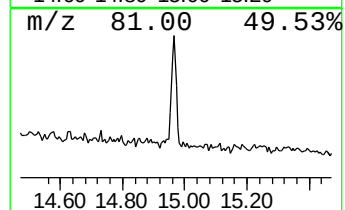
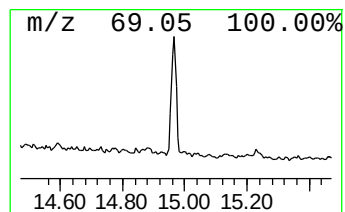
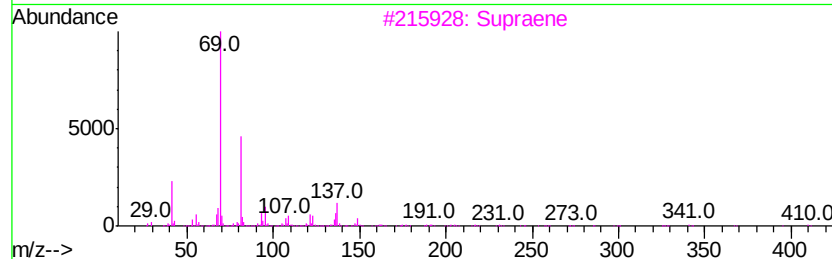
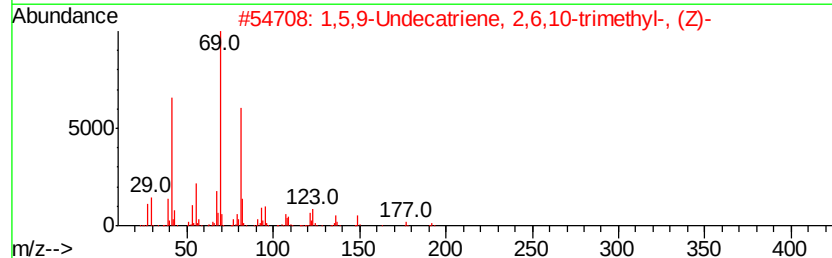
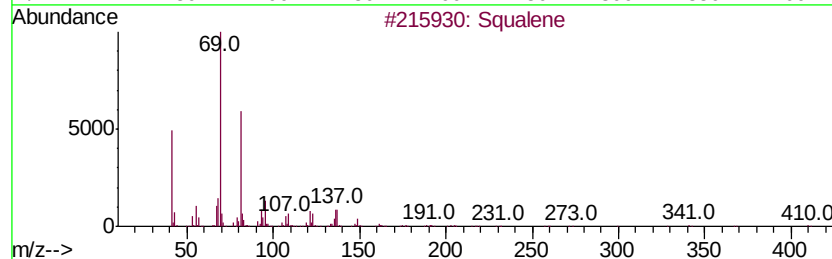
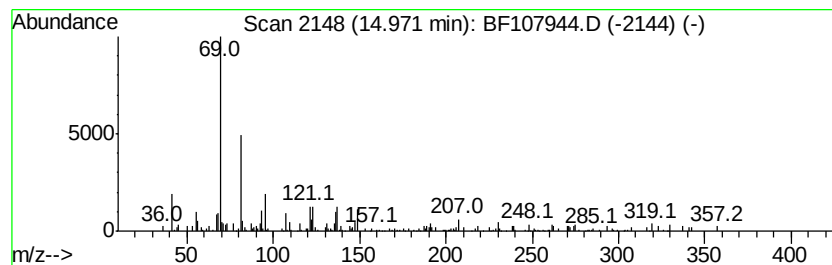
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Squalene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	2.81 ng	110877	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	86
2		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	81
3		Supraene	410	C30H50	007683-64-9	72
4		trans-Farnesol	222	C15H26O	000106-28-5	53
5		4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
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ALS Vial : 11 Sample Multiplier: 1

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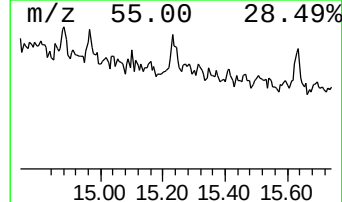
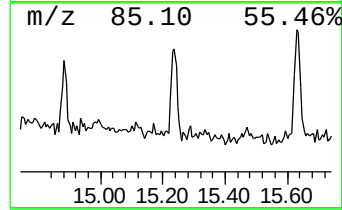
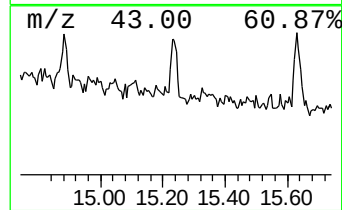
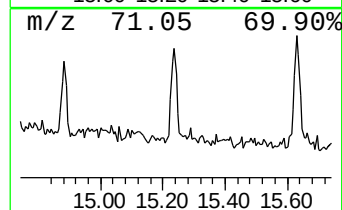
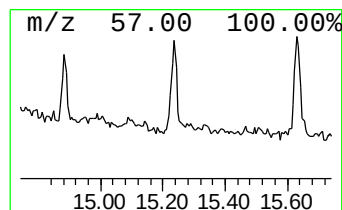
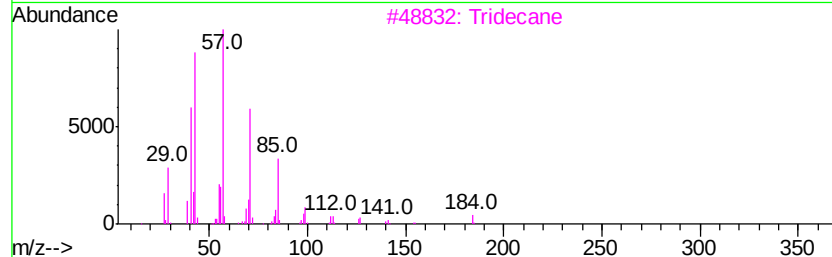
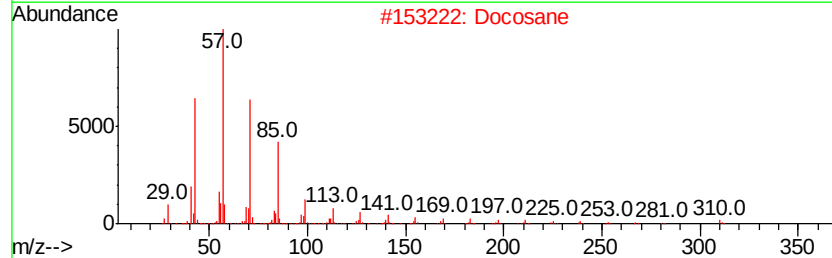
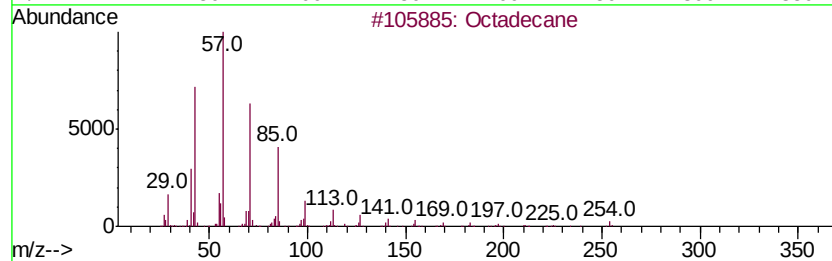
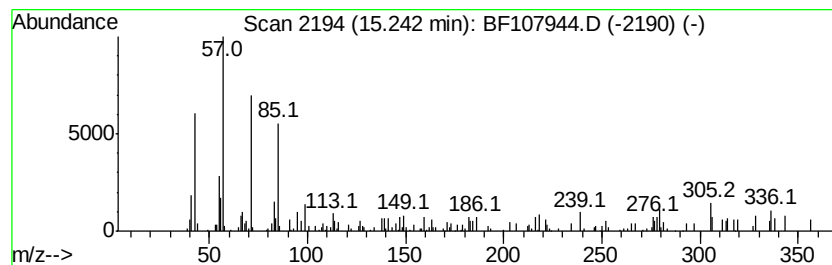
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Octadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	2.39 ng	94133	Perylene-d12	15.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	92
2			Docosane	310	C22H46	000629-97-0	53
3			Tridecane	184	C13H28	000629-50-5	53
4			Heneicosane	296	C21H44	000629-94-7	53
5			Pentacosane	352	C25H52	000629-99-2	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107944.D
Acq On : 3 Aug 2018 18:11
Operator : JU/SJ
Sample : J4316-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OW-2-4

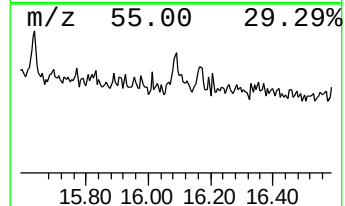
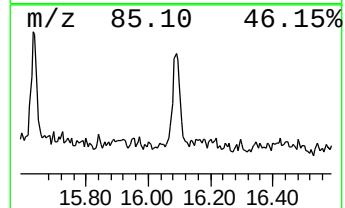
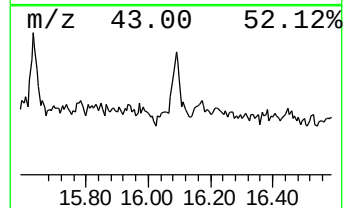
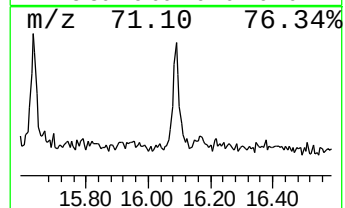
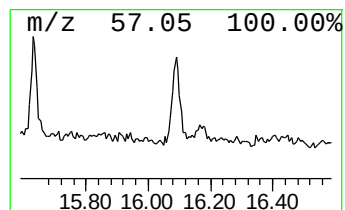
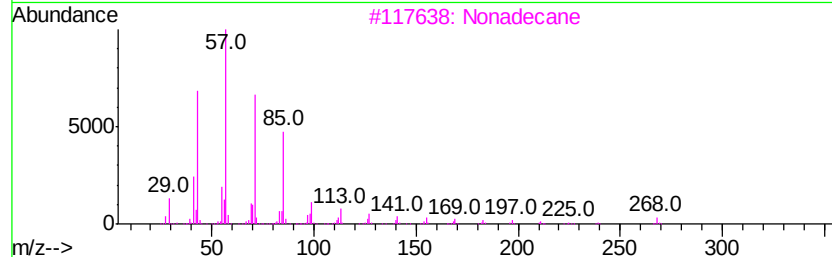
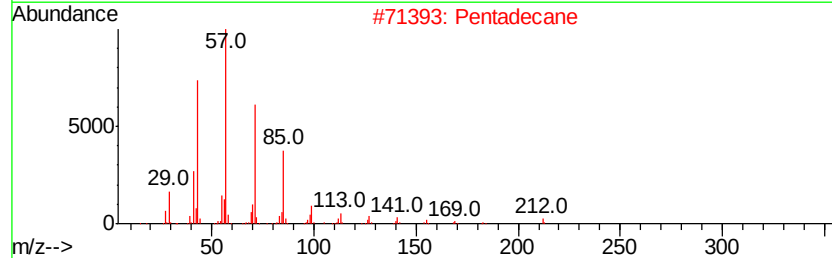
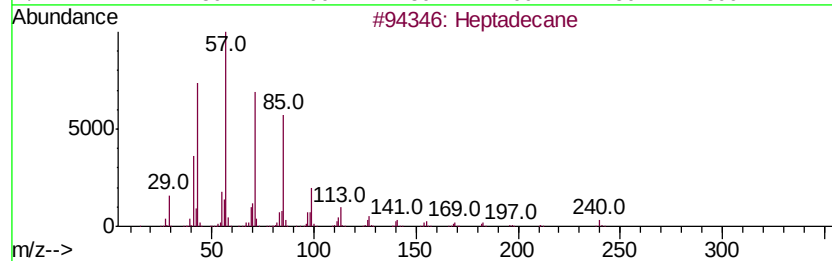
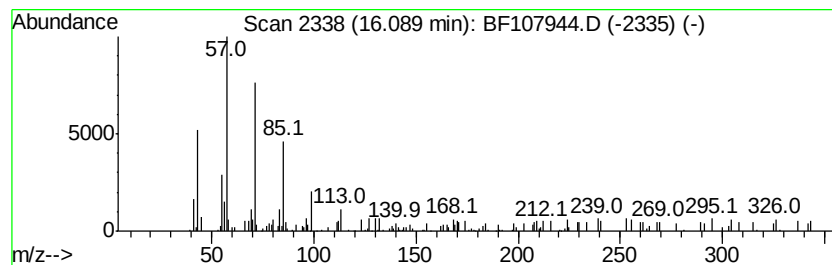
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Heptadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	2.16 ng	85090	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	90
2		Pentadecane	212	C15H32	000629-62-9	76
3		Nonadecane	268	C19H40	000629-92-5	76
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72
5		Tetradecane	198	C14H30	000629-59-4	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080318\
Data File : BF107944.D
Acq On : 3 Aug 2018 18:11
Operator : JU/SJ
Sample : J4316-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OW-2-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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
2-Pentanone, 4-hy...	5.18	7.5	ng	226610	1	6.95	604781	20.0
unknown6.72	6.72	89.9	ng	2719090	1	6.95	604781	20.0
unknown7.68	7.68	2.2	ng	137060	2	8.23	1260990	20.0
Ethanol, 2-phenoxy-	8.44	3.7	ng	230863	2	8.23	1260990	20.0
unknown8.93	8.93	4.0	ng	251136	2	8.23	1260990	20.0
unknown9.17	9.17	2.6	ng	235761	3	9.99	1822550	20.0
Hexadecane, 2,6,1...	11.35	6.3	ng	286806	4	11.49	916766	20.0
n-Hexadecanoic acid	12.00	8.0	ng	366925	4	11.49	916766	20.0
unknown12.74	12.74	5.7	ng	263257	4	11.49	916766	20.0
Octadecanoic acid	12.78	5.8	ng	265332	4	11.49	916766	20.0
Behenic alcohol	13.95	4.5	ng	172606	5	14.14	765584	20.0
Squalene	14.97	2.8	ng	110877	6	15.68	787770	20.0
Octadecane	15.24	2.4	ng	94133	6	15.68	787770	20.0
Heptadecane	16.09	2.2	ng	85090	6	15.68	787770	20.0