

Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
 Data File : BF103379.D
 Acq On : 2 Mar 2018 21:29
 Operator : SJ/JU
 Sample : J1721-11
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-50

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-BF022218.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	2.134	3	8	19	rVB	260282	378070	9.21%	1.018%
2	2.469	46	65	81	rVB	224788	652917	15.90%	1.758%
3	5.116	512	515	531	rVB	104081	152635	3.72%	0.411%
4	5.504	577	581	600	rBV	3692064	4078577	99.35%	10.983%
5	6.516	748	753	770	rBV	3293542	4105245	100.00%	11.054%
6	6.651	771	776	779	rBV	3802953	3756552	91.51%	10.116%
7	6.875	811	814	821	rBV	1191569	1017551	24.79%	2.740%
8	7.033	837	841	844	rBV	3162775	2848736	69.39%	7.671%
9	7.445	906	911	914	rBV	2631512	2610239	63.58%	7.029%
10	8.157	1029	1032	1043	rBV	1298362	1388337	33.82%	3.738%
11	9.233	1211	1215	1224	rBV	3694422	3544719	86.35%	9.545%
12	9.298	1224	1226	1230	rVB	85601	80546	1.96%	0.217%
13	9.627	1276	1282	1289	rBV	314664	390408	9.51%	1.051%
14	9.780	1304	1308	1312	rBV	55351	77284	1.88%	0.208%
15	9.833	1313	1317	1320	rVB	185393	160260	3.90%	0.432%
16	9.916	1327	1331	1335	rBV2	1346514	1245829	30.35%	3.355%
17	10.121	1363	1366	1369	rBV2	39033	42673	1.04%	0.115%
18	10.151	1369	1371	1375	rVB3	46138	46074	1.12%	0.124%
19	10.333	1399	1402	1405	rVB	189405	164413	4.00%	0.443%
20	10.551	1435	1439	1441	rBV	54411	57763	1.41%	0.156%
21	10.716	1462	1467	1475	rBV	1631739	1802178	43.90%	4.853%
22	10.804	1479	1482	1492	rVB	157246	210069	5.12%	0.566%
23	10.951	1504	1507	1513	rVB4	30220	42965	1.05%	0.116%
24	11.257	1556	1559	1562	rBV	97554	98489	2.40%	0.265%
25	11.410	1581	1585	1587	rBV	1063787	956352	23.30%	2.575%
26	11.433	1587	1589	1594	rVV	385442	341674	8.32%	0.920%
27	11.486	1596	1598	1603	rVB	88257	84431	2.06%	0.227%
28	11.651	1621	1626	1628	rBV2	36396	48963	1.19%	0.132%
29	11.921	1668	1672	1680	rBV3	268322	405220	9.87%	1.091%
30	12.027	1687	1690	1692	rBV2	87554	84058	2.05%	0.226%
31	12.245	1724	1727	1731	rVB5	45825	46696	1.14%	0.126%
32	12.463	1761	1764	1769	rBV2	51156	88035	2.14%	0.237%
33	12.627	1789	1792	1795	rBV	566963	510096	12.43%	1.374%
34	12.710	1804	1806	1811	rBV3	46332	59313	1.44%	0.160%

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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	12.798	1818	1821	1825	rVB	475042	399388	9.73%	1.075%
36	12.862	1825	1832	1837	rBV	523890	678923	16.54%	1.828%
37	12.998	1850	1855	1858	rBV	1955223	1956551	47.66%	5.269%
38	13.186	1885	1887	1890	rVB	69417	59210	1.44%	0.159%
39	13.462	1931	1934	1936	rVB	88446	67371	1.64%	0.181%
40	13.504	1938	1941	1945	rVB2	316418	274037	6.68%	0.738%
41	13.874	2001	2004	2009	rBV3	493095	508912	12.40%	1.370%
42	14.062	2032	2036	2039	rBV2	822046	984861	23.99%	2.652%
43	14.086	2039	2040	2048	rVB	247145	216383	5.27%	0.583%
44	15.574	2290	2293	2298	rVB2	337342	413446	10.07%	1.113%

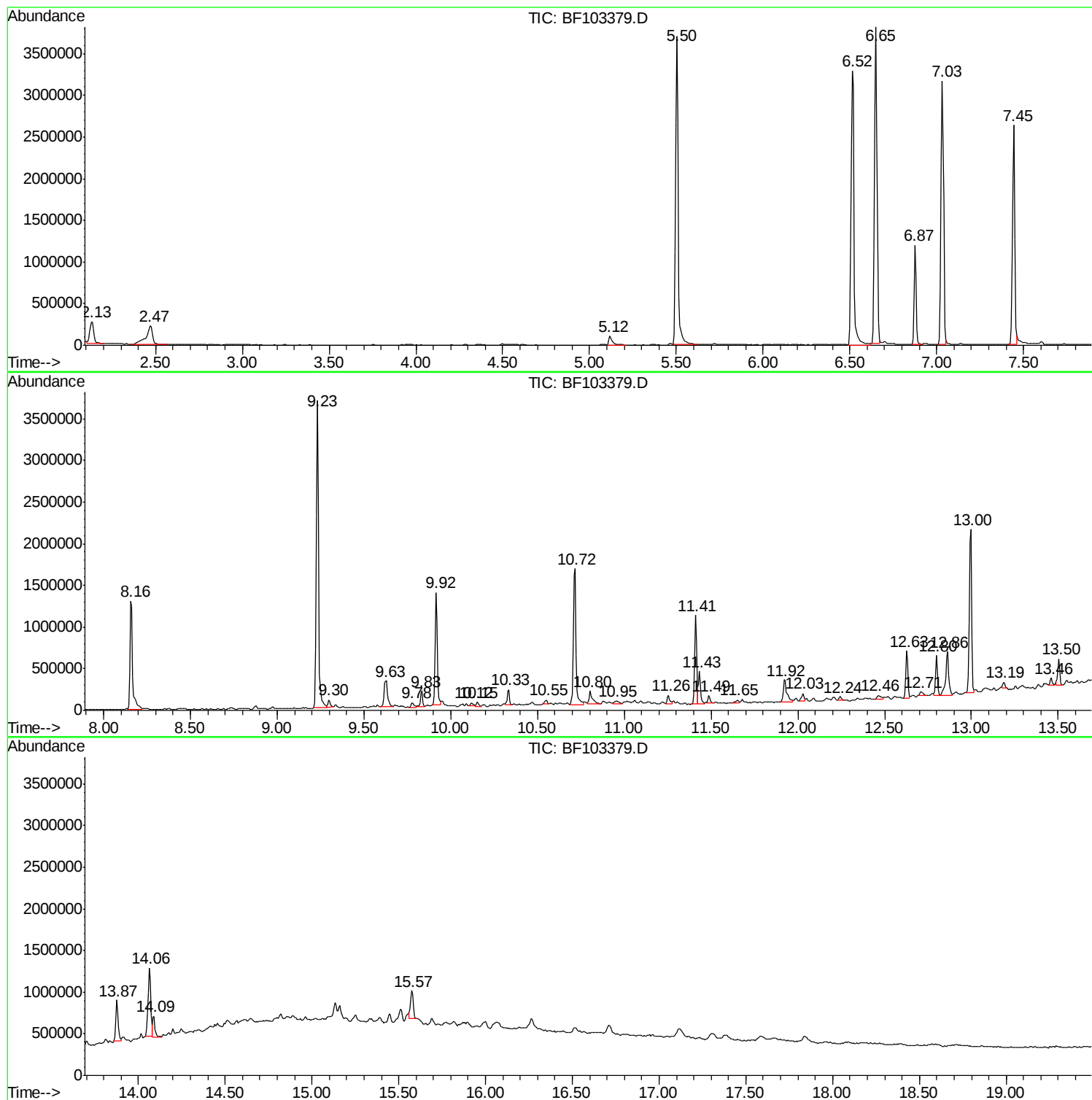
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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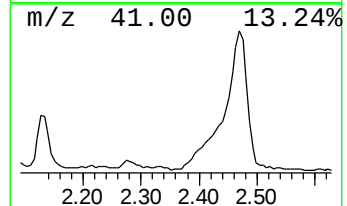
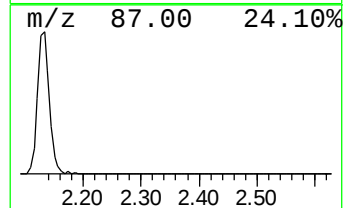
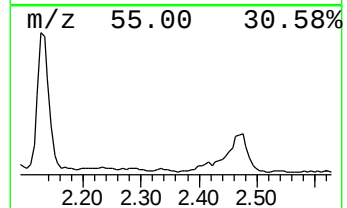
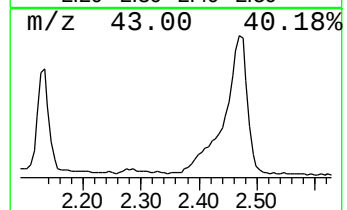
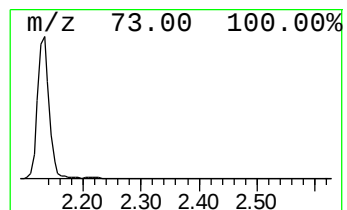
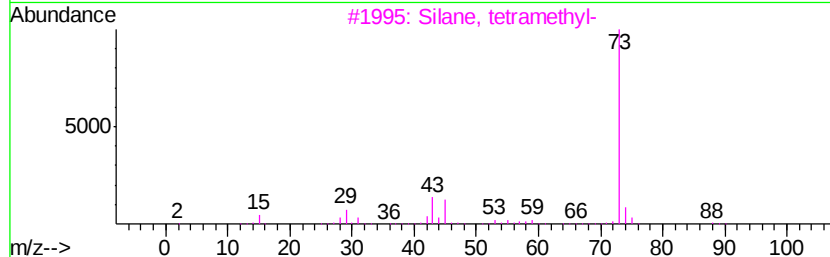
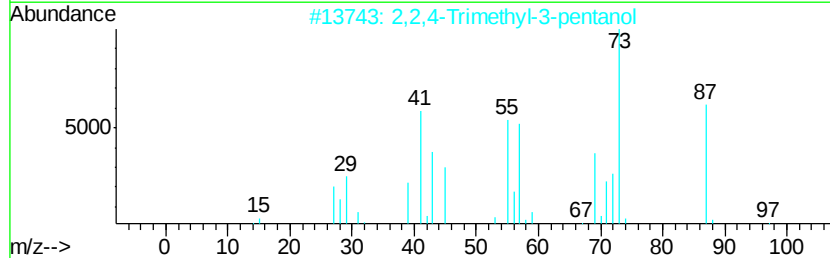
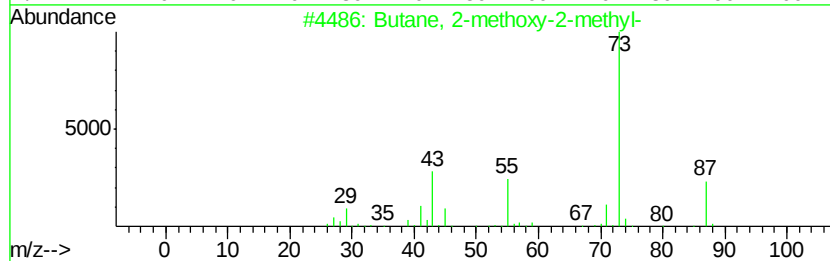
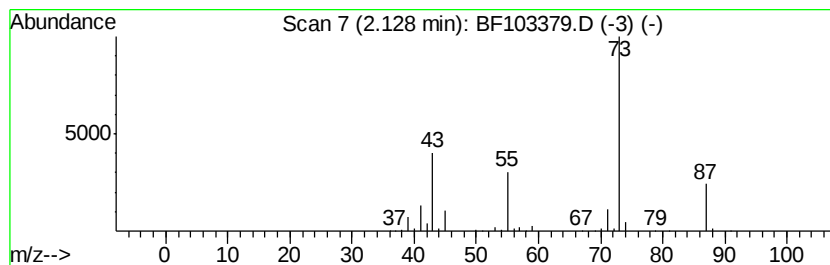
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	7.43 ng	378070	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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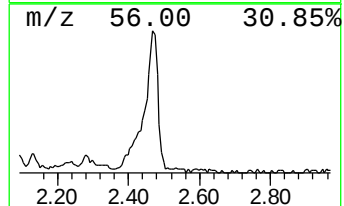
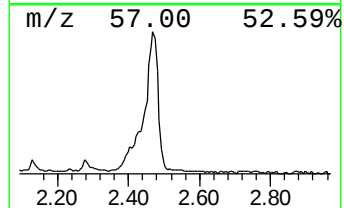
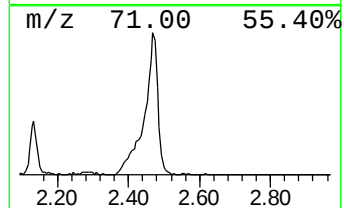
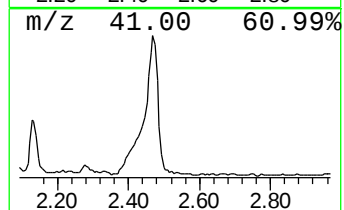
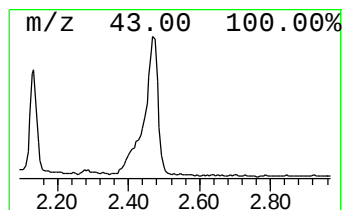
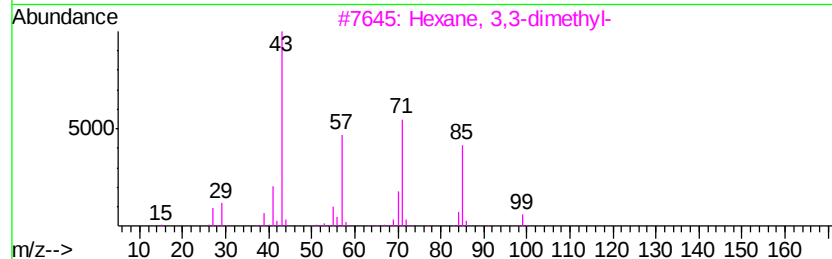
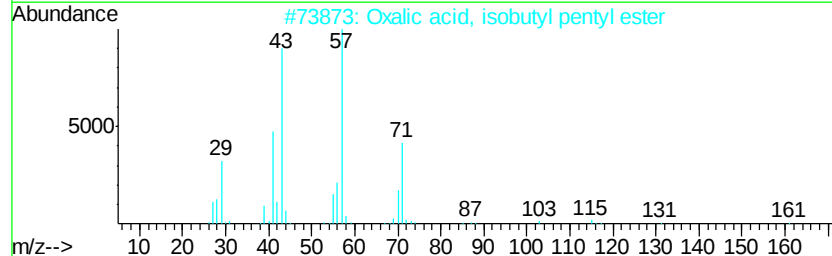
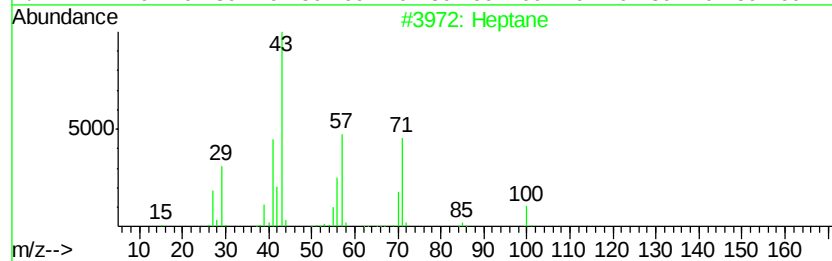
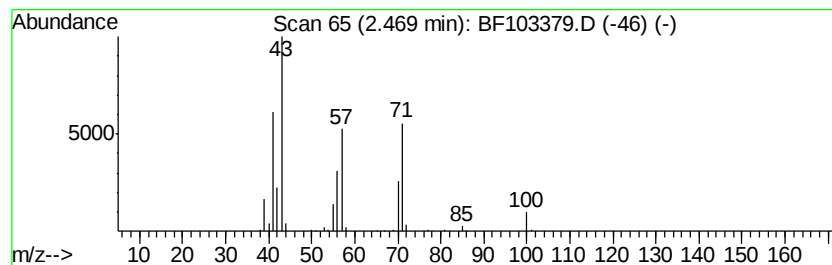
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Heptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.47	12.83 ng	652917	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane	100	C7H16	000142-82-5	90
2		Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	59
3		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	50
4		Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	40
5		Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40



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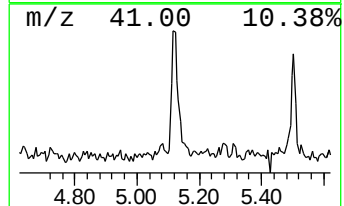
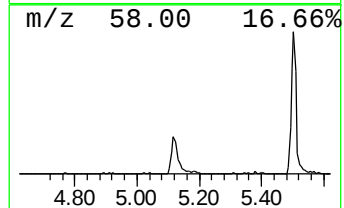
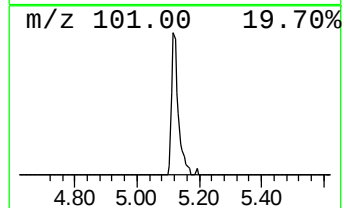
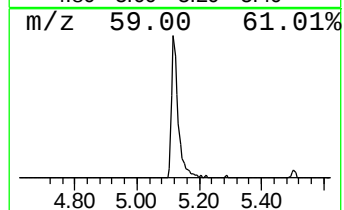
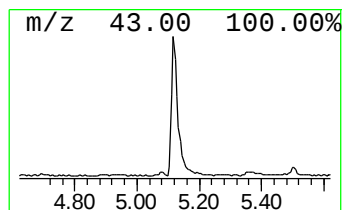
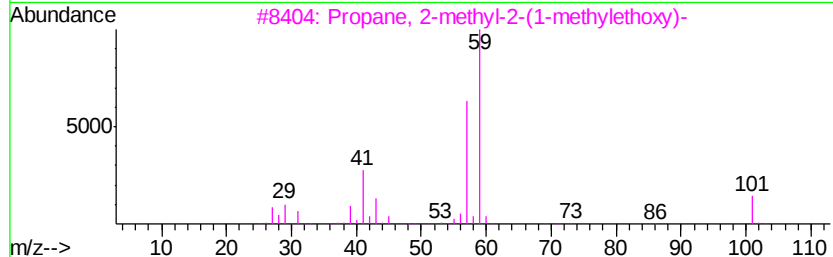
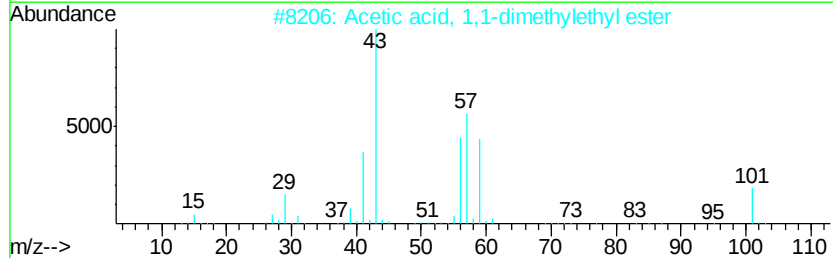
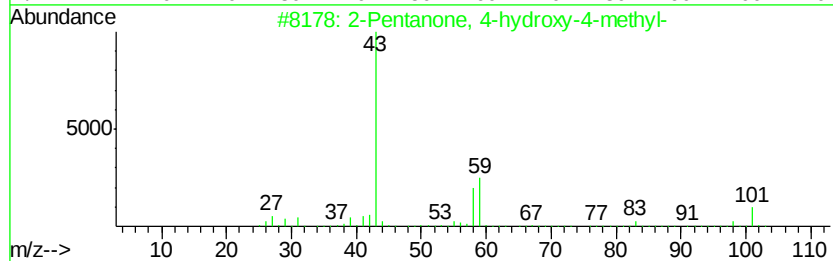
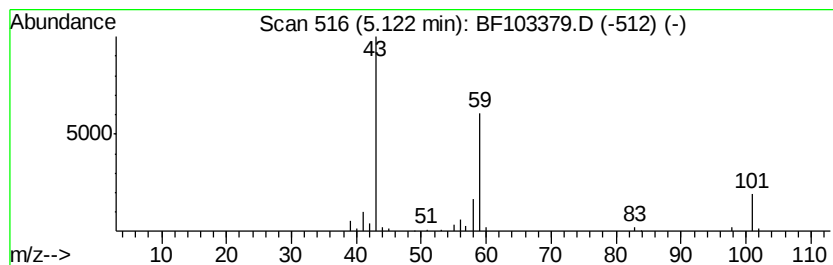
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.00 ng	152635	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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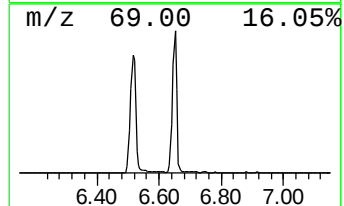
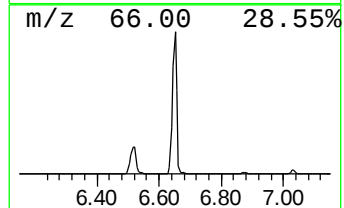
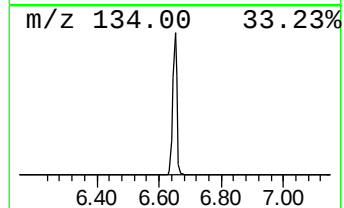
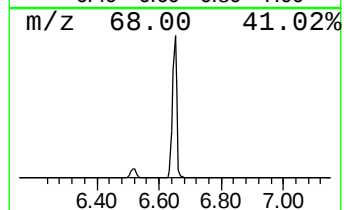
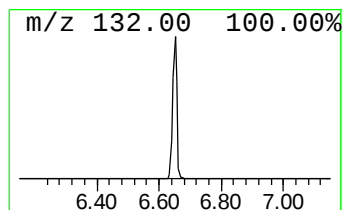
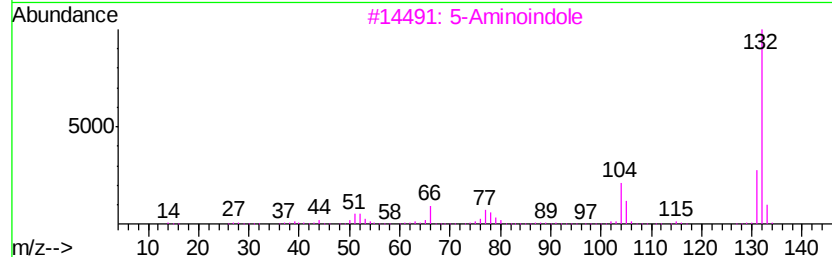
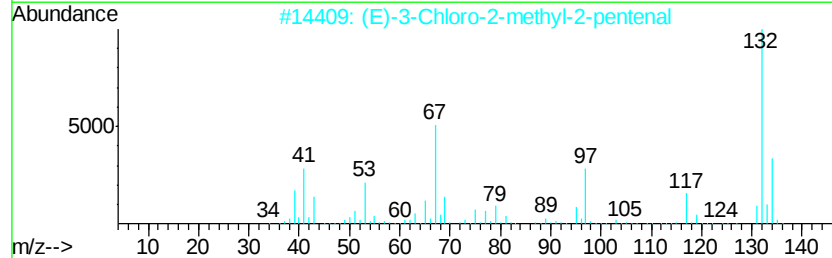
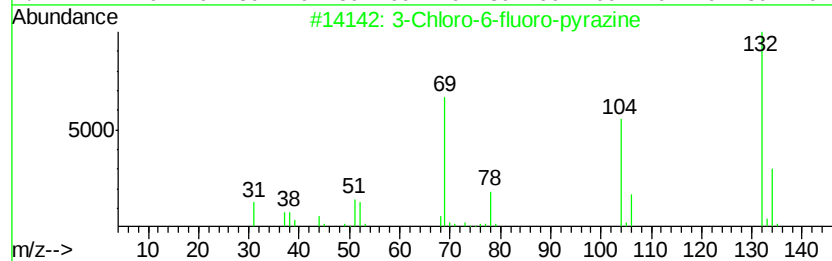
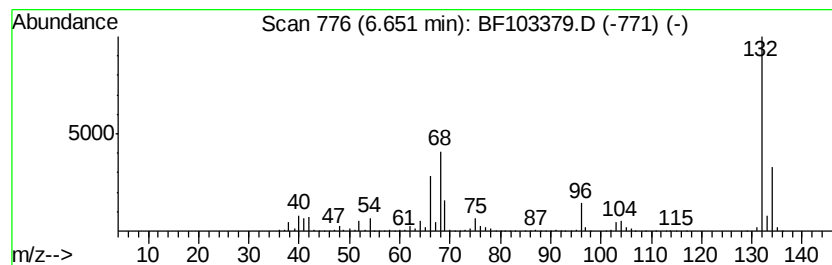
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	73.84 ng	3756550	1,4-Dichlorobenzene-d4	6.87

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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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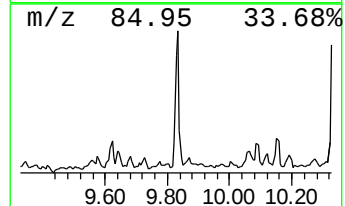
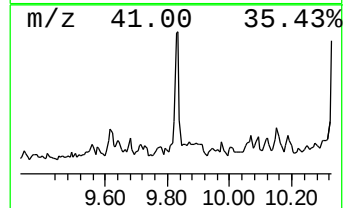
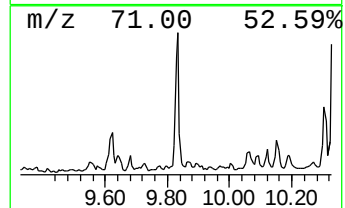
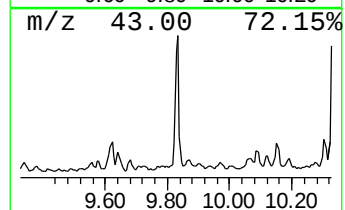
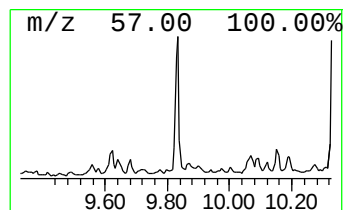
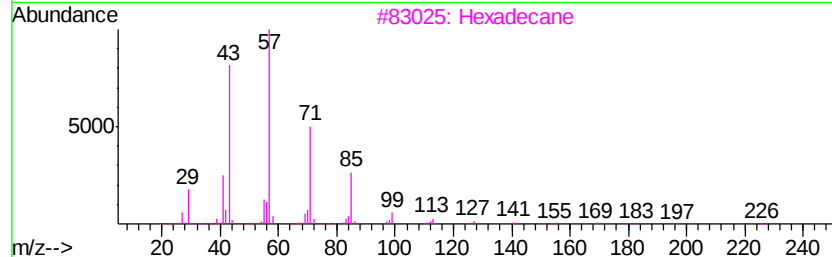
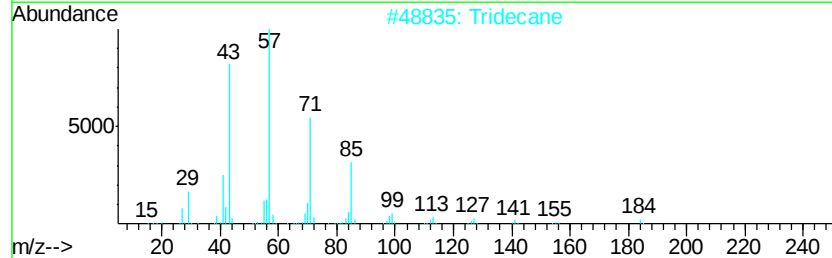
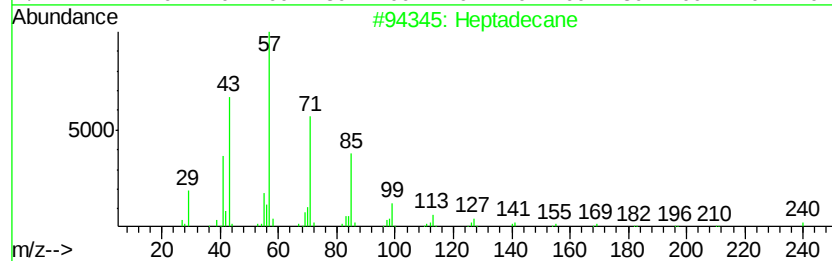
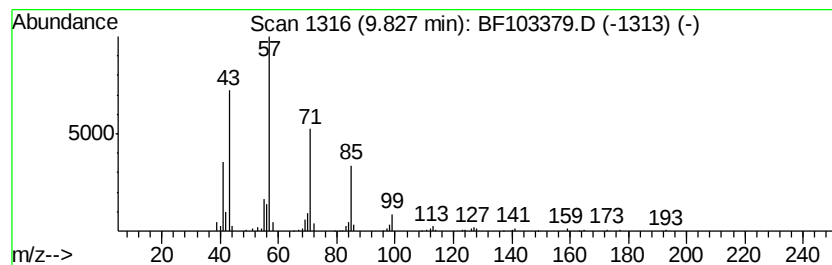
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	2.57 ng	160260	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	90
2	Tridecane	184 C13H28	000629-50-5	90
3	Hexadecane	226 C16H34	000544-76-3	90
4	Tetratetracontane	619 C44H90	007098-22-8	83
5	Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2	80



Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
Data File : BF103379.D
Acq On : 2 Mar 2018 21:29
Operator : SJ/JU
Sample : J1721-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

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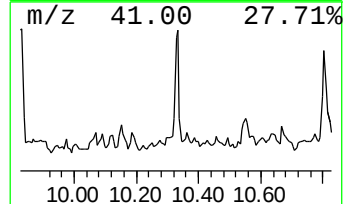
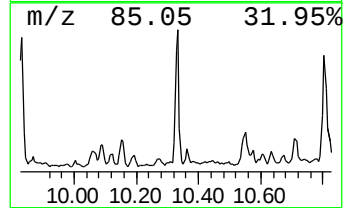
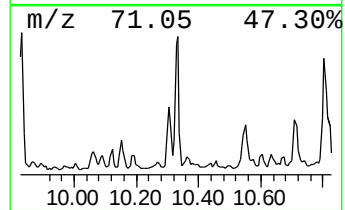
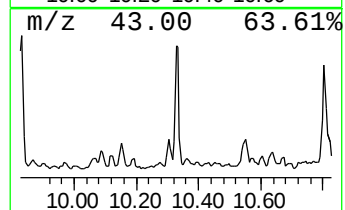
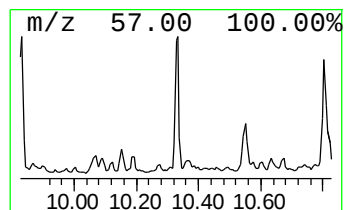
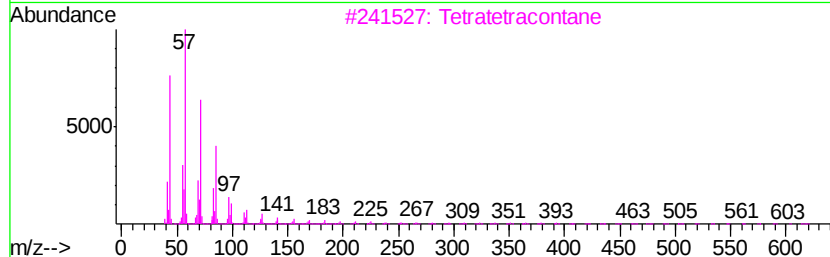
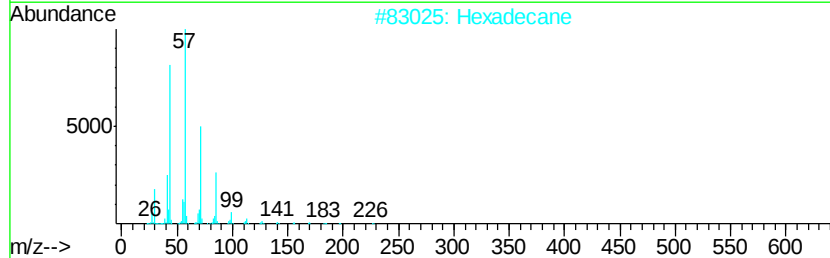
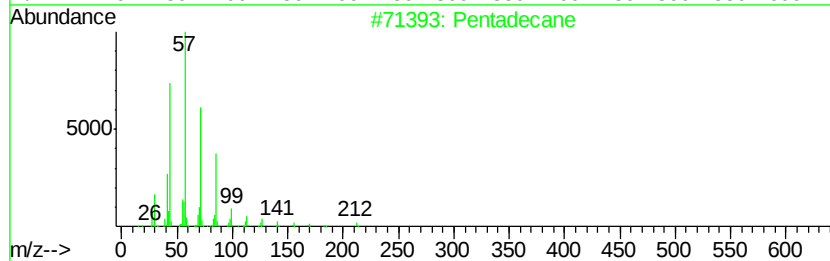
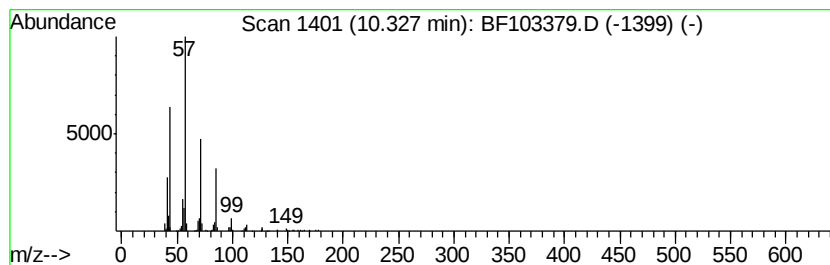
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	2.64 ng	164413	Acenaphthene-d10	9.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	90
2	Hexadecane		226	C16H34	000544-76-3	90
3	Tetratetracontane		619	C44H90	007098-22-8	90
4	Tetradecane		198	C14H30	000629-59-4	86
5	Tridecane		184	C13H28	000629-50-5	83



Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
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Sample : J1721-11
Misc :
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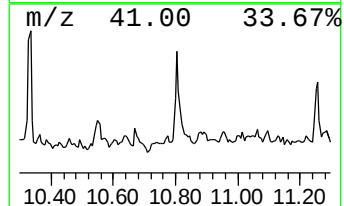
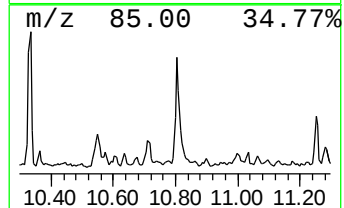
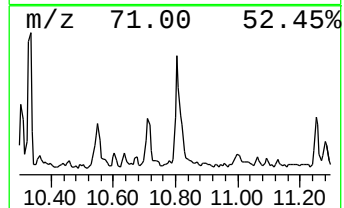
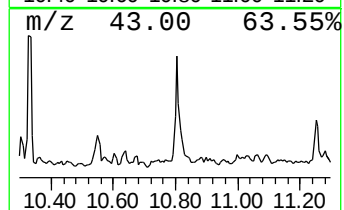
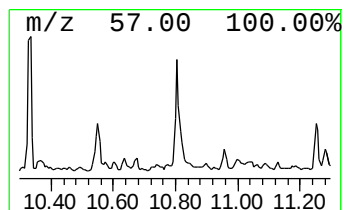
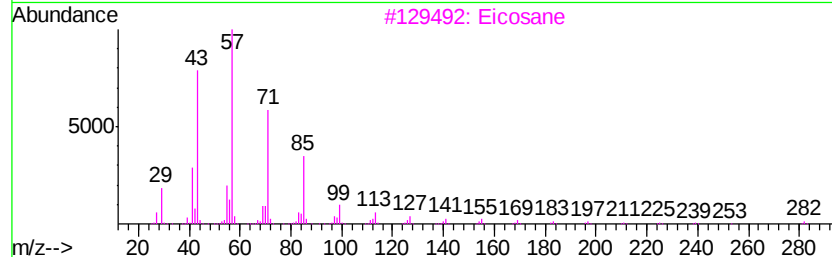
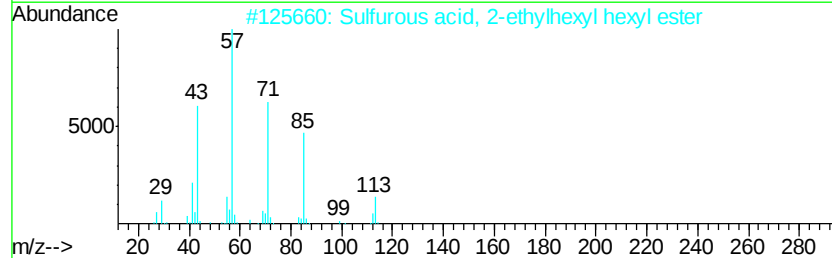
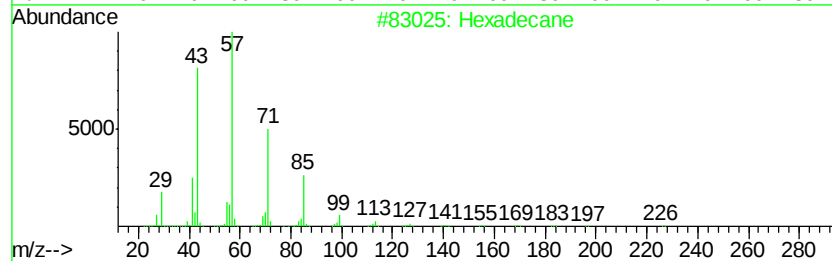
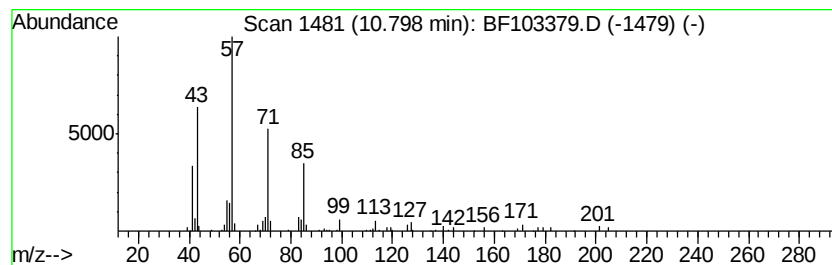
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.80	4.39 ng	210069	Phenanthrene-d10	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	86
3	Eicosane	282	C20H42	000112-95-8	78
4	Tridecane, 5-propyl-	226	C16H34	055045-11-9	72
5	Bacchotricuneatin c	342	C20H22O5	066563-30-2	68



Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
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Acq On : 2 Mar 2018 21:29
Operator : SJ/JU
Sample : J1721-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

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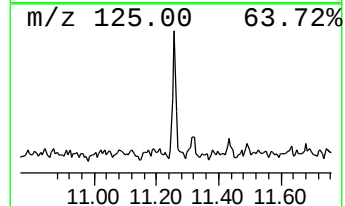
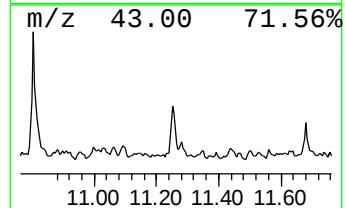
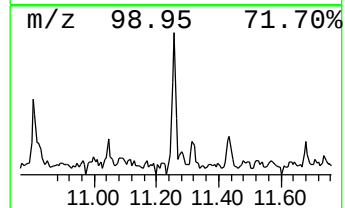
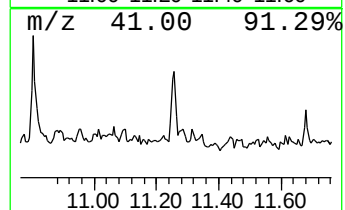
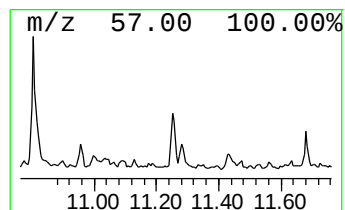
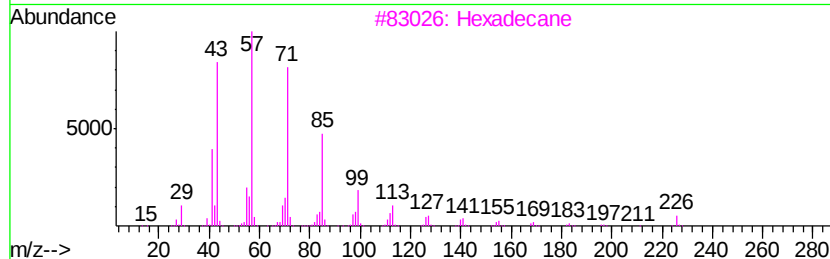
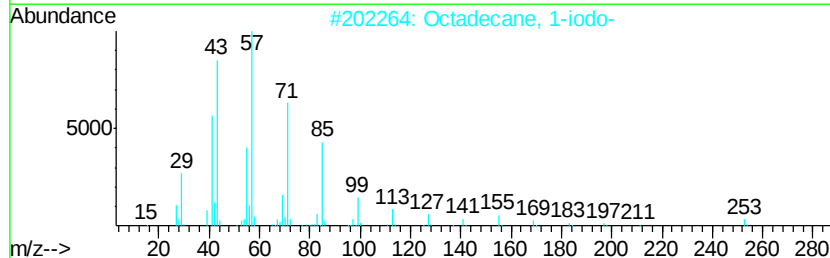
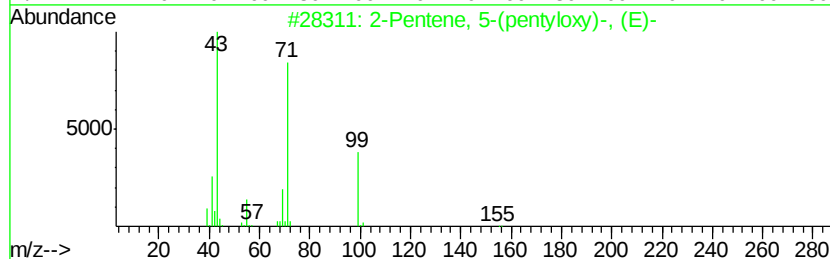
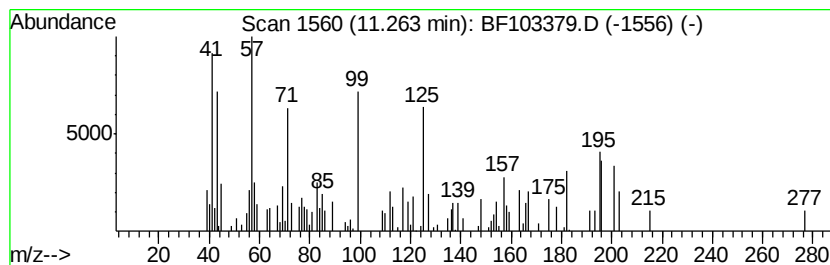
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown11.26 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.26	2.06 ng	98489	Phenanthrene-d10	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 5-(pentvloxv)-, (E)-	156	C10H200	056052-85-8	27	
2	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	25	
3	Hexadecane	226	C16H34	000544-76-3	25	
4	Heneicosane	296	C21H44	000629-94-7	25	
5	Heptadecane	240	C17H36	000629-78-7	25	



Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
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Sample : J1721-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

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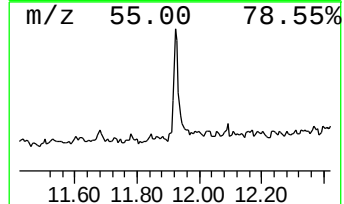
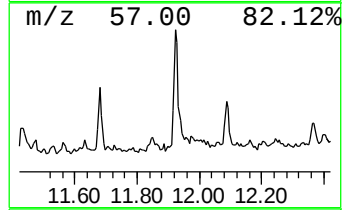
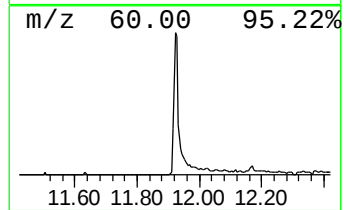
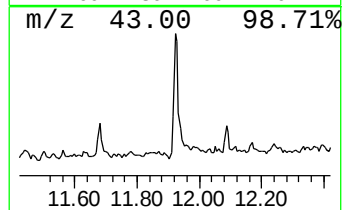
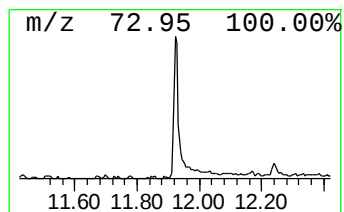
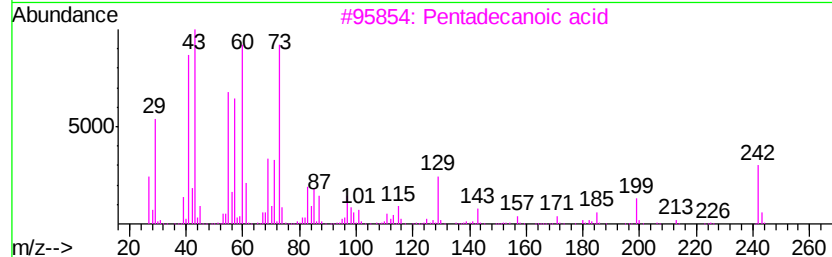
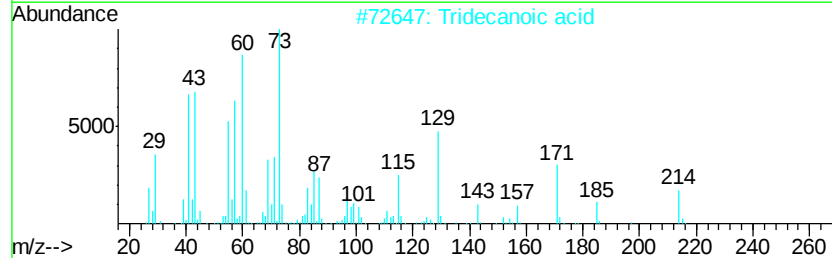
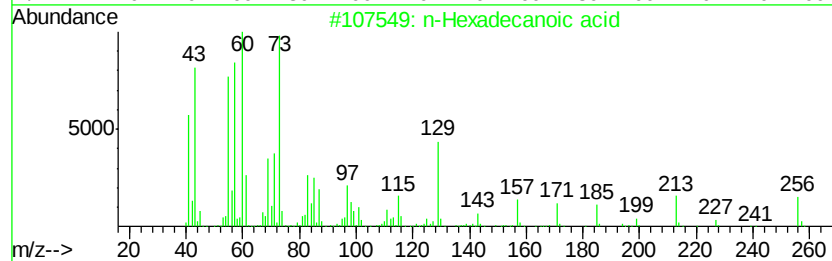
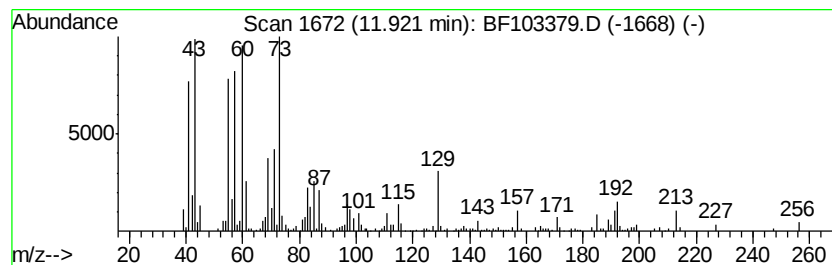
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	8.47 ng	405220	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	72



Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
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ALS Vial : 15 Sample Multiplier: 1

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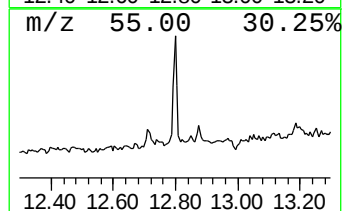
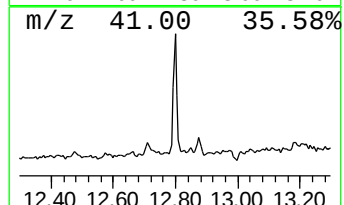
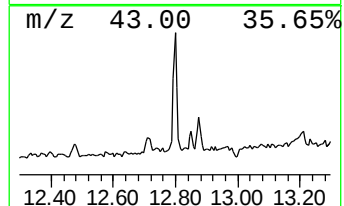
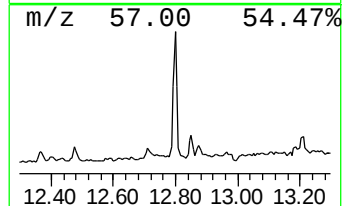
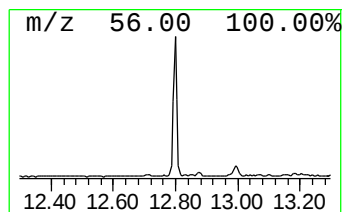
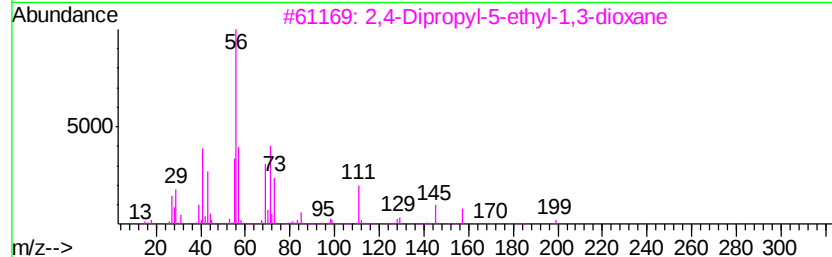
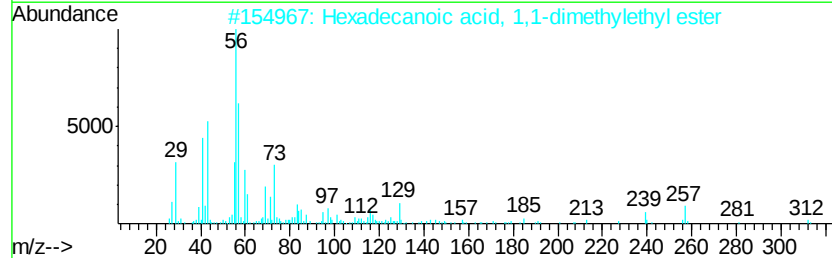
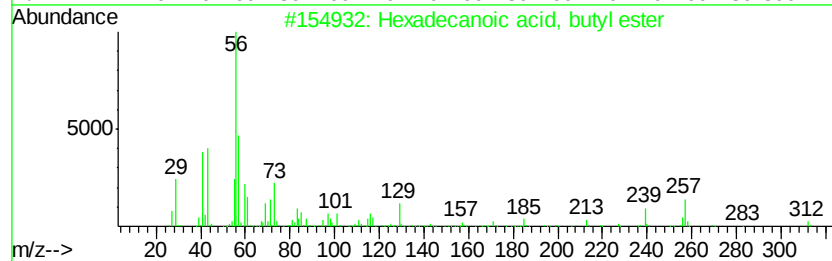
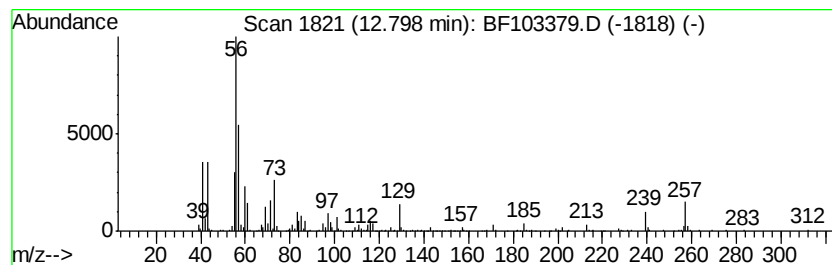
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	8.11 ng	399388	Chrysene-d12	14.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	93
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
3			2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	38
4			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
5			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38



Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
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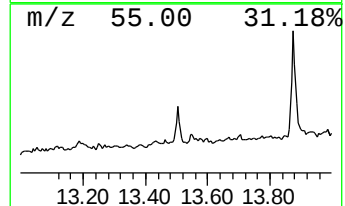
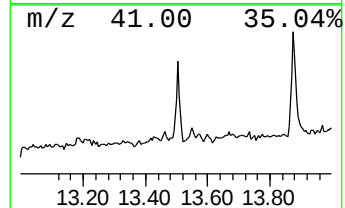
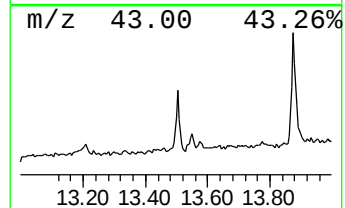
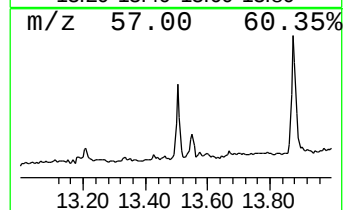
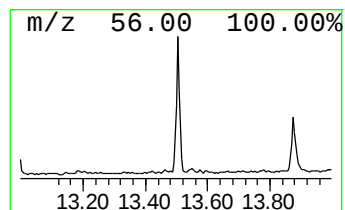
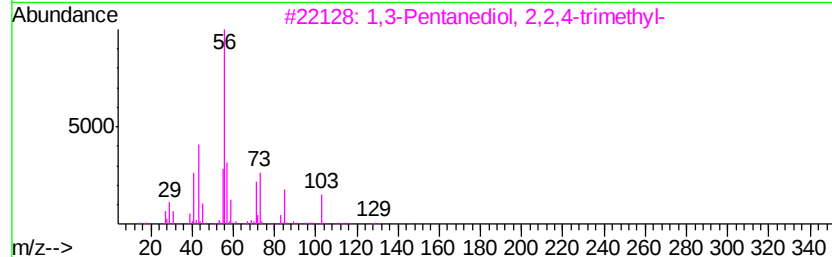
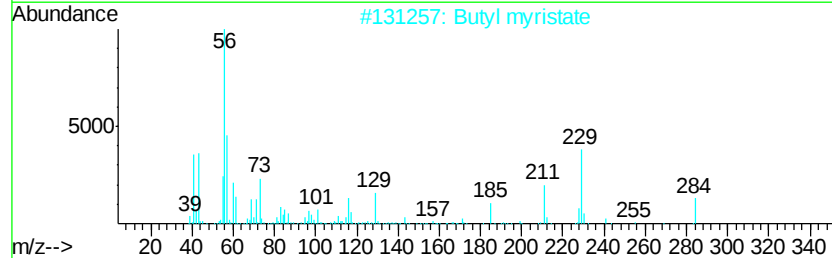
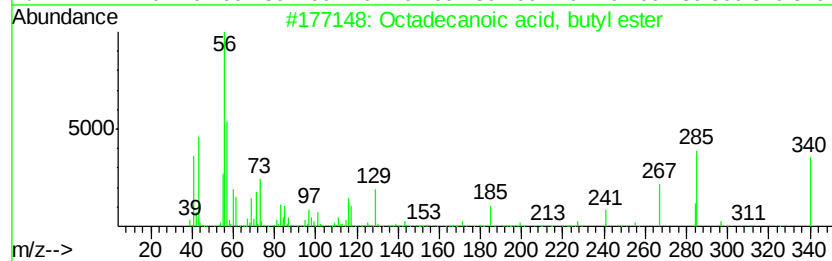
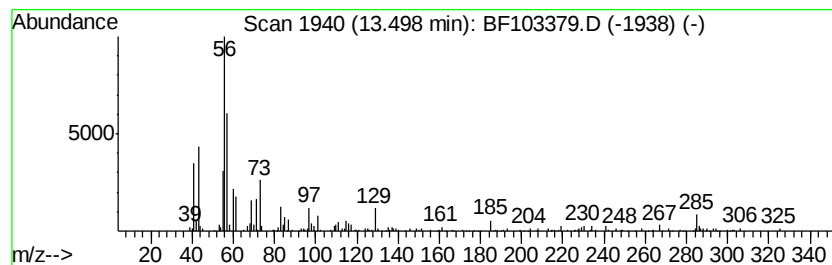
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	5.56 ng	274037	Chrysene-d12	14.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2			Butyl myristate	284	C18H36O2	000110-36-1	86
3			1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	47
4			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	43
5			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38



Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
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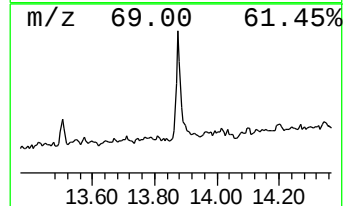
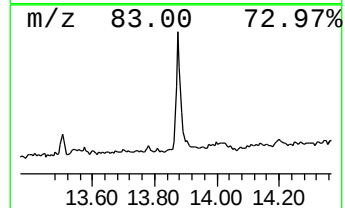
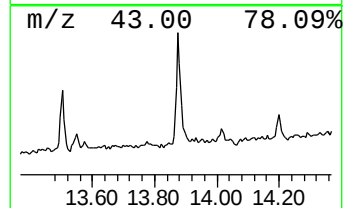
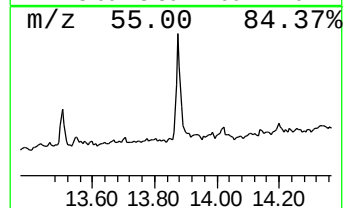
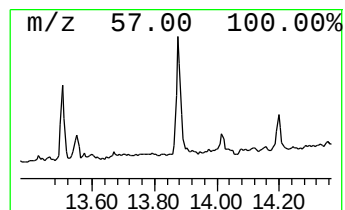
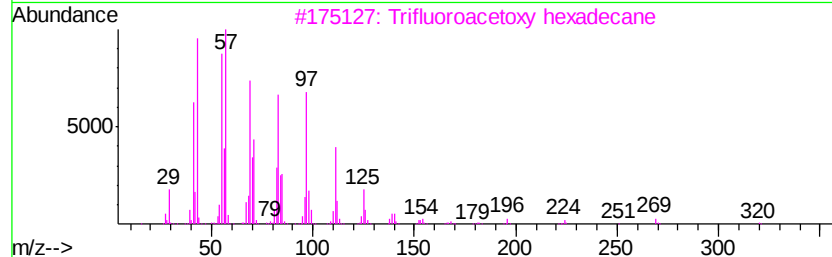
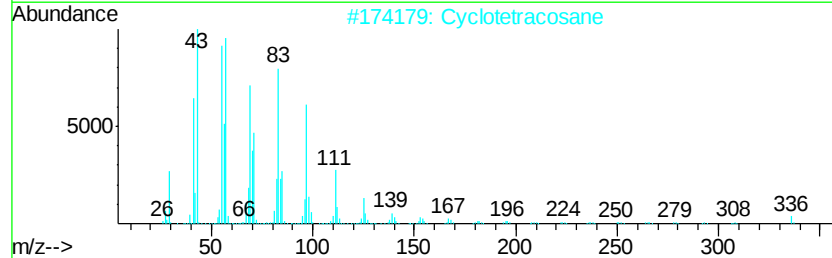
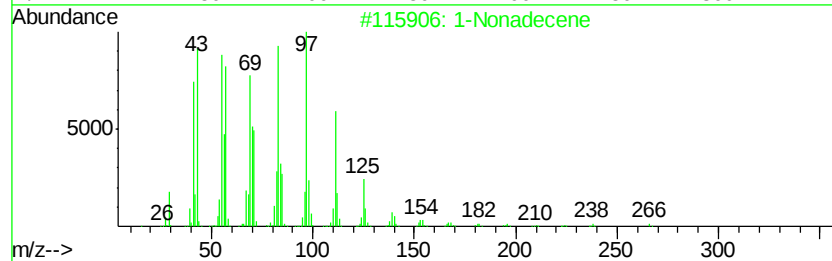
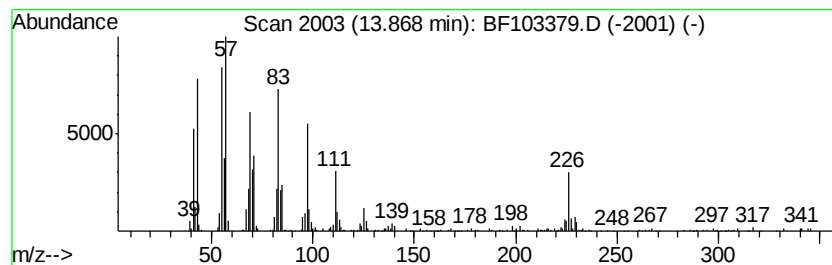
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BNA_F
ClientSampleId :
SP-50

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	10.33 ng	508912	Chrysene-d12	14.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Nonadecene	266 C19H38	018435-45-5	97
2	Cyclotetracosane	336 C24H48	000297-03-0	93
3	Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3	90
4	Pentafluoropropionic acid, hexad...	388 C19H33F5O2	006222-07-7	90
5	Heptadecyl trifluoroacetate	352 C19H35F3O2	1000351-87-0	90



Data Path : Z:\HPCHEM1\BNA_F\Data\BF030218\
Data File : BF103379.D
Acq On : 2 Mar 2018 21:29
Operator : SJ/JU
Sample : J1721-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-50

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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
Butane, 2-methoxy...	2.13	7.4	ng	378070	1	6.87	1017550	20.0
Heptane	2.47	12.8	ng	652917	1	6.87	1017550	20.0
2-Pentanone, 4-hy...	5.12	3.0	ng	152635	1	6.87	1017550	20.0
unknown6.65	6.65	73.8	ng	3756550	1	6.87	1017550	20.0
Heptadecane	9.83	2.6	ng	160260	3	9.92	1245830	20.0
Pentadecane	10.33	2.6	ng	164413	3	9.92	1245830	20.0
Hexadecane	10.80	4.4	ng	210069	4	11.41	956352	20.0
unknown11.26	11.26	2.1	ng	98489	4	11.41	956352	20.0
n-Hexadecanoic acid	11.92	8.5	ng	405220	4	11.41	956352	20.0
Hexadecanoic acid...	12.80	8.1	ng	399388	5	14.06	984861	20.0
Octadecanoic acid...	13.50	5.6	ng	274037	5	14.06	984861	20.0
1-Nonadecene	13.87	10.3	ng	508912	5	14.06	984861	20.0