

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
 Data File : BF097434.D
 Acq On : 7 Aug 2017 17:34
 Operator : SJ/JU
 Sample : I4642-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-03-080417

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-BF072517.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	4.534	464	467	481	rBV2	127852	212908	10.75%	1.110%
2	5.004	544	547	567	rBV	1598411	1980774	100.00%	10.331%
3	6.081	727	730	744	rBV	1530626	1816252	91.69%	9.473%
4	6.186	744	748	758	rVB	1843623	1860732	93.94%	9.705%
5	6.410	783	786	798	rBV	594172	532843	26.90%	2.779%
6	6.563	809	812	823	rBV	1336562	1336832	67.49%	6.972%
7	6.981	880	883	899	rBV	1130168	1171433	59.14%	6.110%
8	7.692	1001	1004	1012	rBV	854132	726554	36.68%	3.789%
9	8.769	1183	1187	1191	rBV	1657510	1623044	81.94%	8.465%
10	9.175	1253	1256	1263	rBV	189822	160584	8.11%	0.838%
11	9.298	1272	1277	1282	rBV	30957	31269	1.58%	0.163%
12	9.439	1297	1301	1305	rBV	688807	670790	33.87%	3.499%
13	9.892	1375	1378	1381	rVB	31997	24558	1.24%	0.128%
14	10.110	1409	1415	1419	rBV3	18249	26833	1.35%	0.140%
15	10.222	1431	1434	1443	rBV	834330	839487	42.38%	4.378%
16	10.363	1455	1458	1466	rBV	56439	70630	3.57%	0.368%
17	10.810	1530	1534	1536	rBV	27585	27935	1.41%	0.146%
18	10.910	1547	1551	1554	rBV	674539	589349	29.75%	3.074%
19	10.933	1554	1555	1559	rVV	38807	22305	1.13%	0.116%
20	10.986	1562	1564	1569	rVB	38062	37414	1.89%	0.195%
21	11.327	1619	1622	1626	rBV	230167	197872	9.99%	1.032%
22	11.468	1643	1646	1649	rBV	108219	93714	4.73%	0.489%
23	11.521	1652	1655	1657	rBV	25043	22451	1.13%	0.117%
24	11.957	1727	1729	1732	rBV	35838	34027	1.72%	0.177%
25	12.004	1733	1737	1740	rVV	691396	770146	38.88%	4.017%
26	12.027	1740	1741	1748	rVB	531902	426348	21.52%	2.224%
27	12.116	1752	1756	1760	rVB	295416	260931	13.17%	1.361%
28	12.180	1760	1767	1771	rBV9	22962	57923	2.92%	0.302%
29	12.245	1775	1778	1784	rBV5	27869	51247	2.59%	0.267%
30	12.339	1789	1794	1798	rBV	195342	194017	9.80%	1.012%
31	12.492	1816	1820	1823	rVV	1025837	953833	48.15%	4.975%
32	12.563	1827	1832	1838	rBV3	31827	60531	3.06%	0.316%
33	12.645	1843	1846	1849	rBV3	31265	41377	2.09%	0.216%
34	12.668	1849	1850	1854	rVB	33172	27231	1.37%	0.142%

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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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35	12.739	1858	1862	1865	rBV2	34149	43444	2.19%	0.227%
36	12.774	1865	1868	1872	rVB	58485	66686	3.37%	0.348%
37	12.833	1875	1878	1881	rBV4	20163	25644	1.29%	0.134%
38	12.863	1881	1883	1886	rVB	28876	23887	1.21%	0.125%
39	12.892	1886	1888	1890	rBV2	30213	23069	1.16%	0.120%
40	13.045	1911	1914	1916	rBV3	22789	25870	1.31%	0.135%
41	13.186	1935	1938	1941	rVB	31645	29905	1.51%	0.156%
42	13.398	1971	1974	1975	rBV	26901	23957	1.21%	0.125%
43	13.415	1975	1977	1986	rVB4	89059	140624	7.10%	0.733%
44	13.533	1990	1997	2000	rBV2	623694	728297	36.77%	3.799%
45	13.557	2000	2001	2009	rVB	133067	110162	5.56%	0.575%
46	13.921	2061	2063	2066	rVB	41371	31602	1.60%	0.165%
47	13.957	2067	2069	2072	rVB2	35186	31912	1.61%	0.166%
48	14.527	2163	2166	2173	rBV	141547	224555	11.34%	1.171%
49	14.774	2205	2208	2213	rVB	72556	79885	4.03%	0.417%
50	14.821	2213	2216	2220	rBV	107821	116399	5.88%	0.607%
51	14.874	2221	2225	2228	rBV	350343	385962	19.49%	2.013%
52	16.203	2449	2451	2454	rBV4	44109	40663	2.05%	0.212%
53	17.809	2721	2724	2725	rBV3	27652	34039	1.72%	0.178%
54	18.368	2816	2819	2820	rBV3	31069	32207	1.63%	0.168%

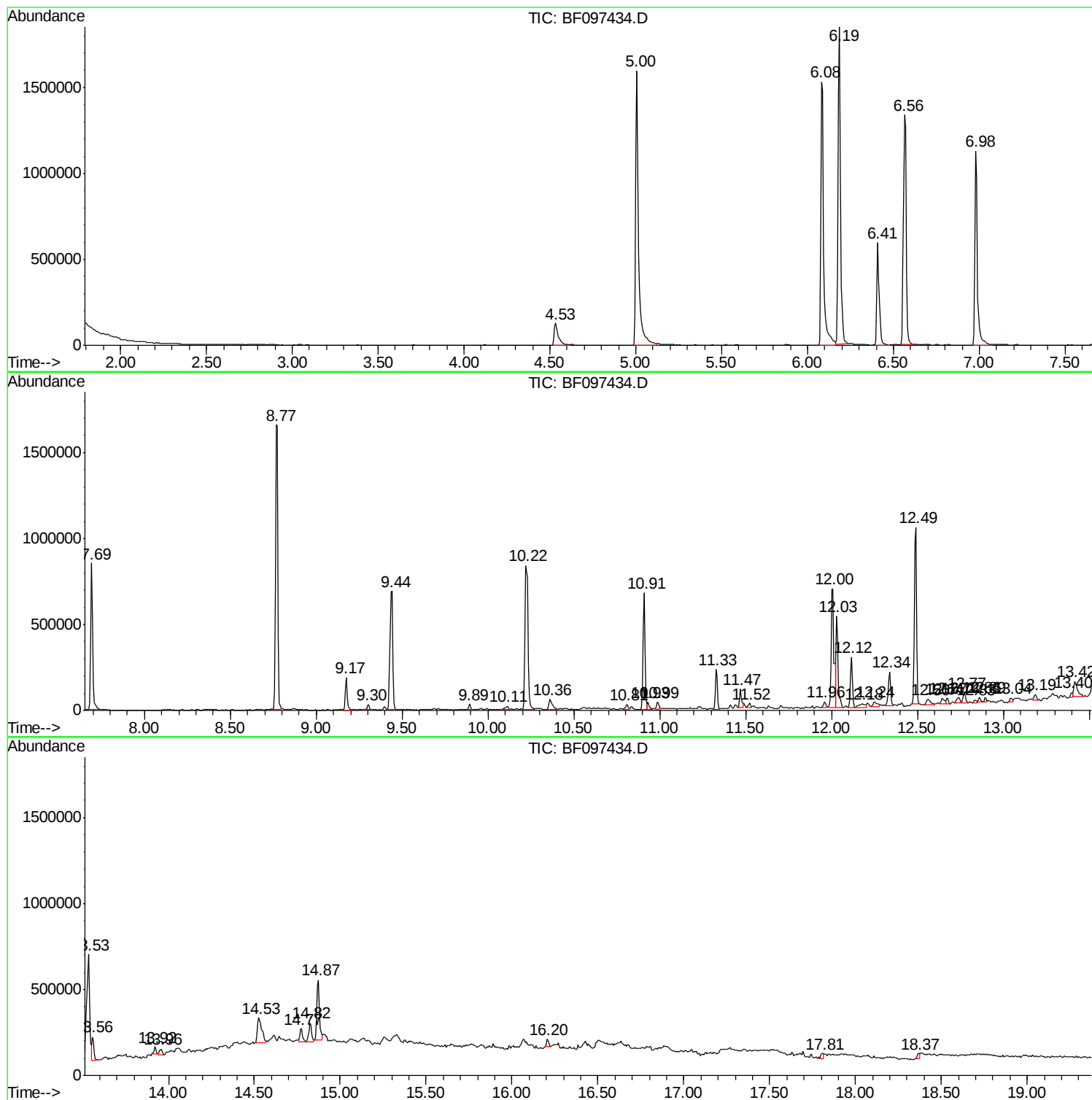
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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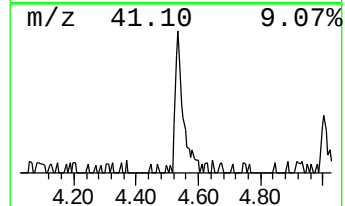
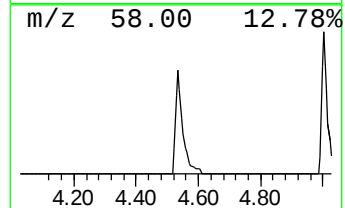
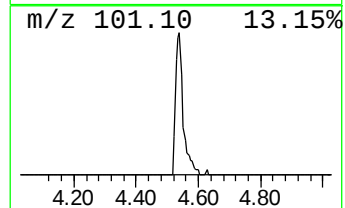
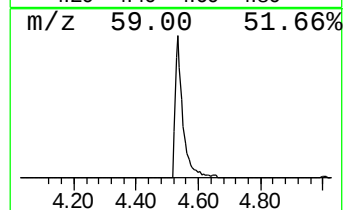
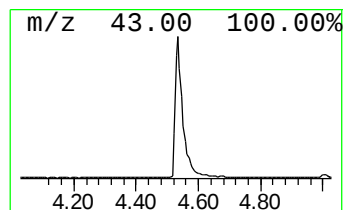
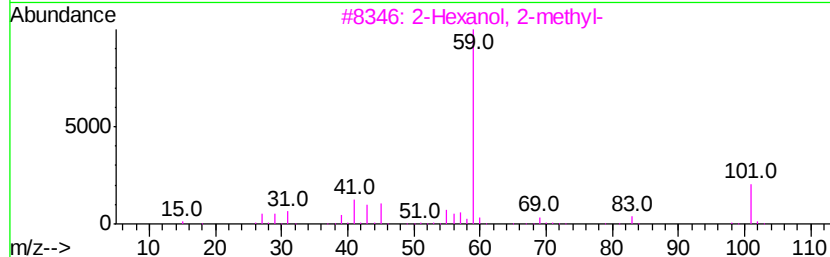
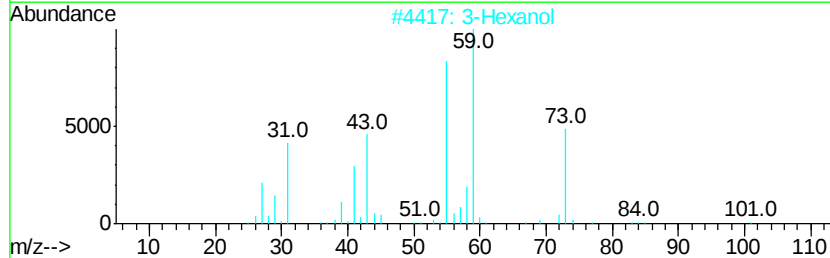
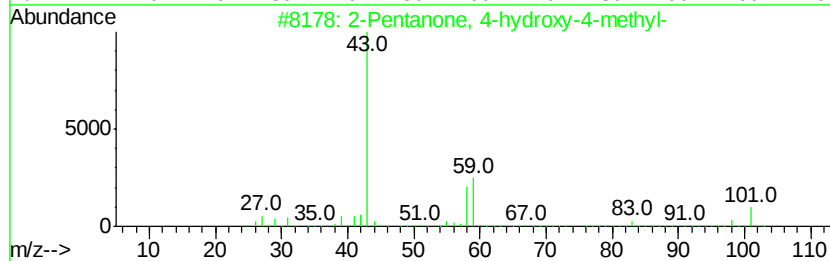
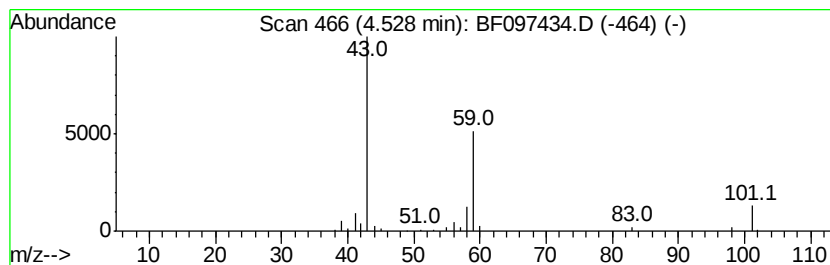
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	7.99 ng	212908	1,4-Dichlorobenzene-d4	6.41

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	3-Hexanol	102	C6H14O	000623-37-0	33		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9		
5	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	9		



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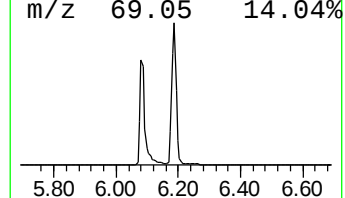
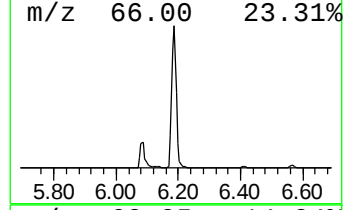
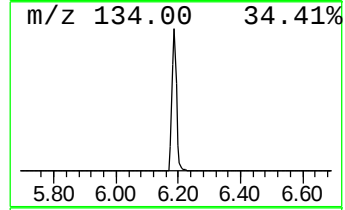
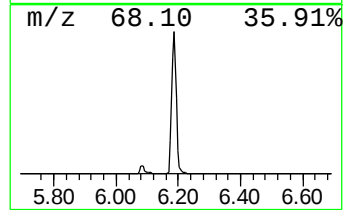
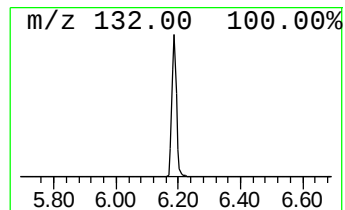
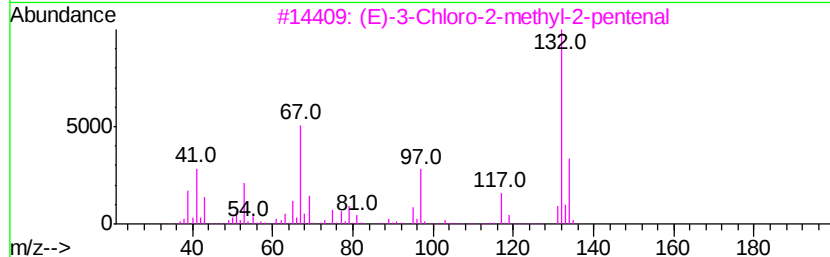
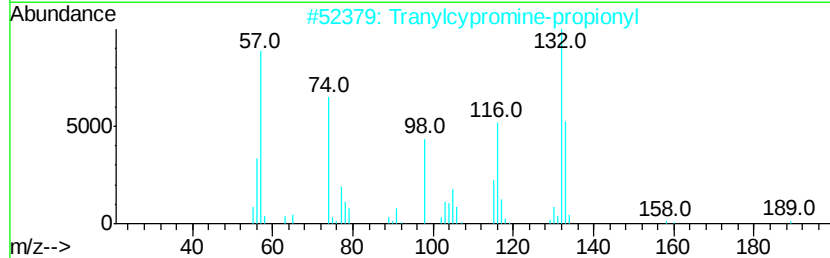
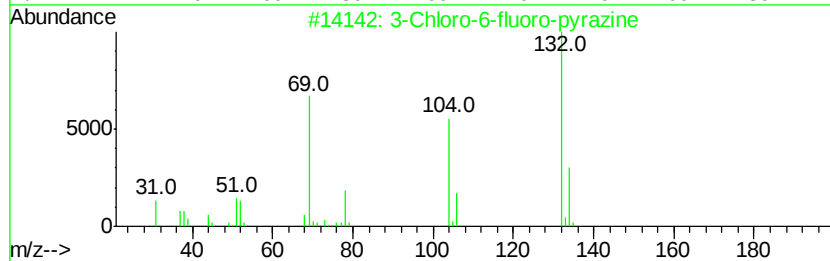
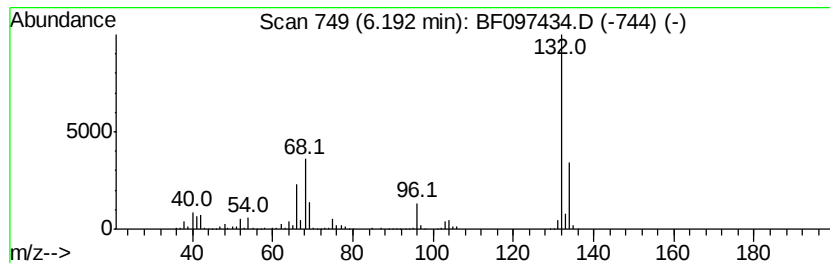
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.19	69.84 ng	1860730	1,4-Dichlorobenzene-d4	6.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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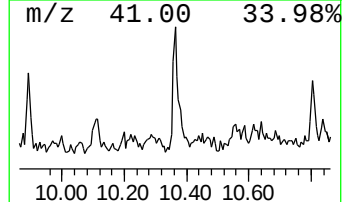
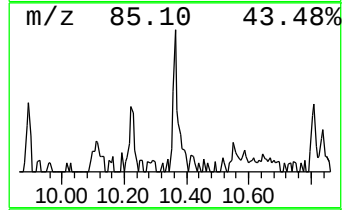
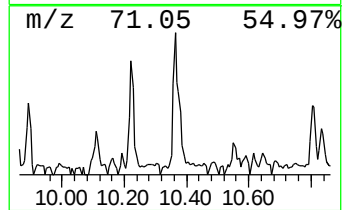
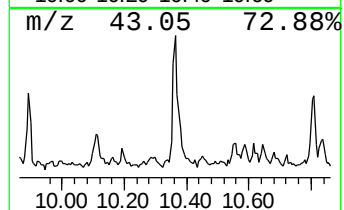
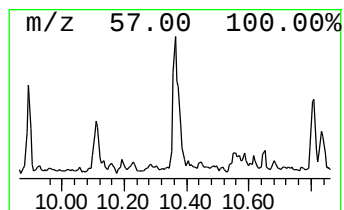
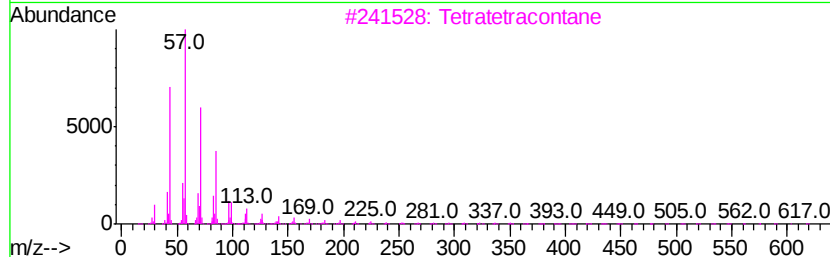
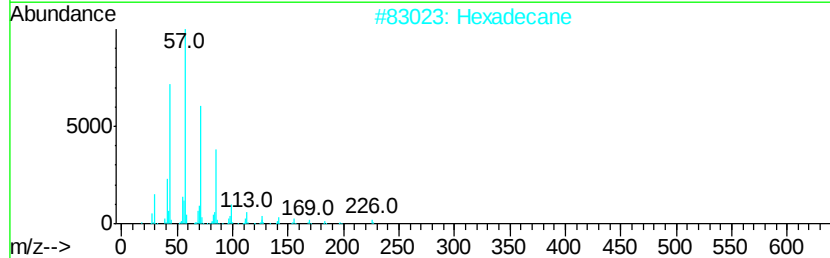
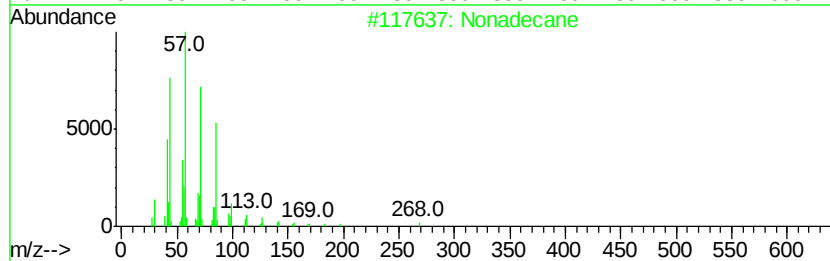
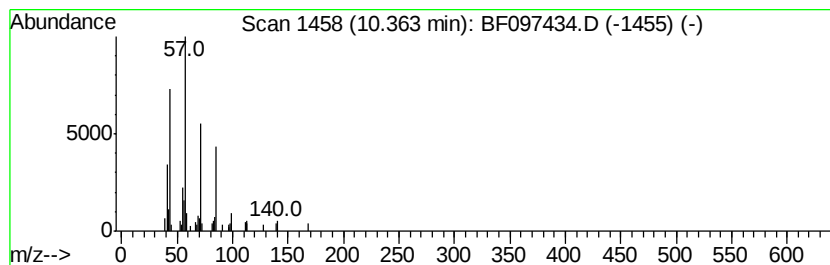
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.36	2.40 ng	70630	Phenanthrene-d10	10.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	80
2	Hexadecane		226	C16H34	000544-76-3	72
3	Tetratetracontane		619	C44H90	007098-22-8	72
4	Tetradecane, 1-iodo-		324	C14H29I	019218-94-1	64
5	Tetradecane		198	C14H30	000629-59-4	58



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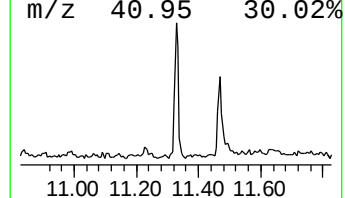
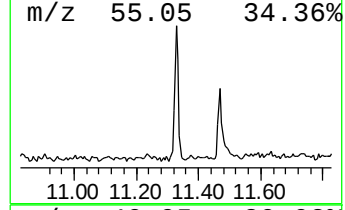
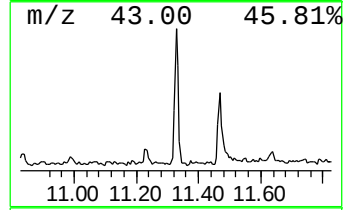
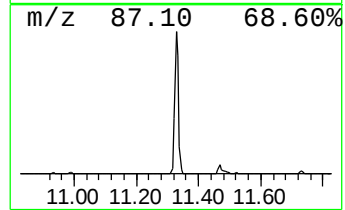
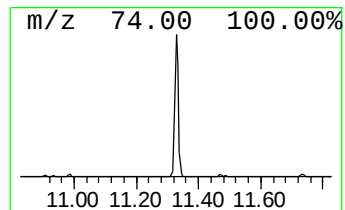
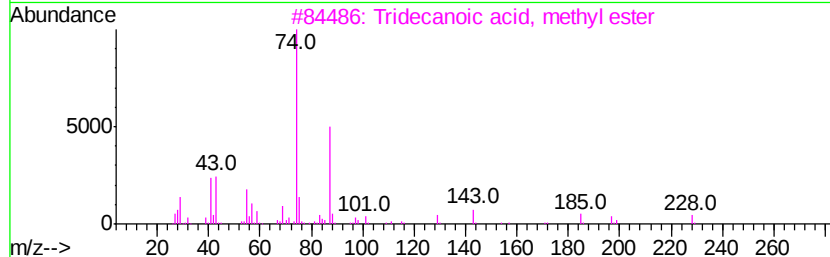
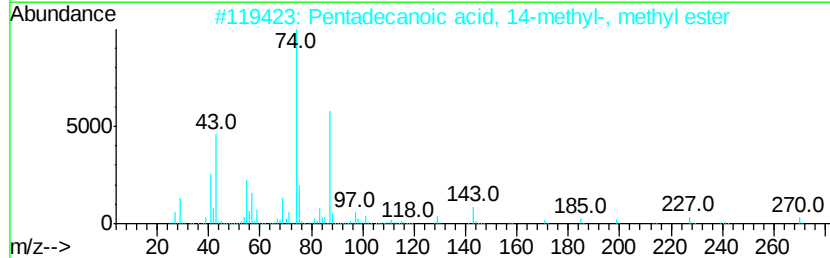
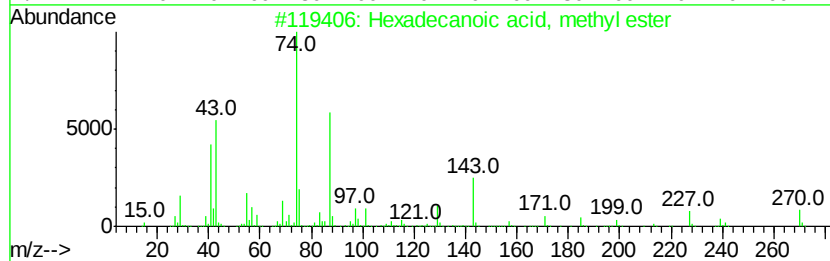
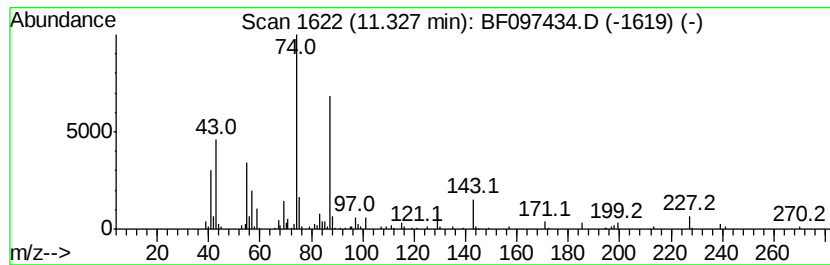
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.33	6.71 ng	197872	Phenanthrene-d10	10.91

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



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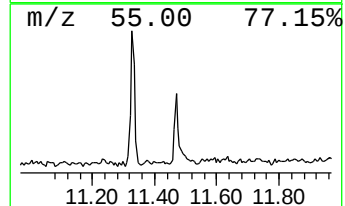
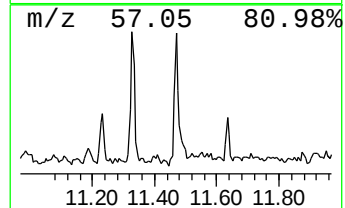
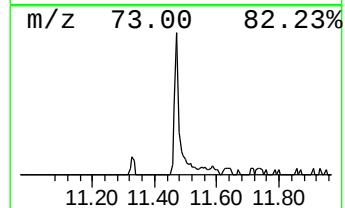
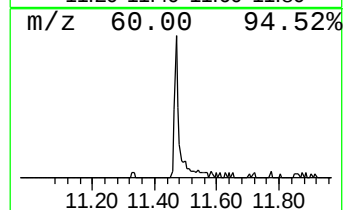
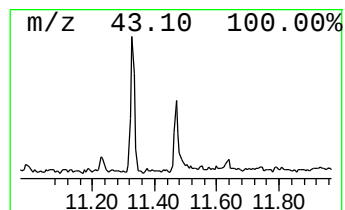
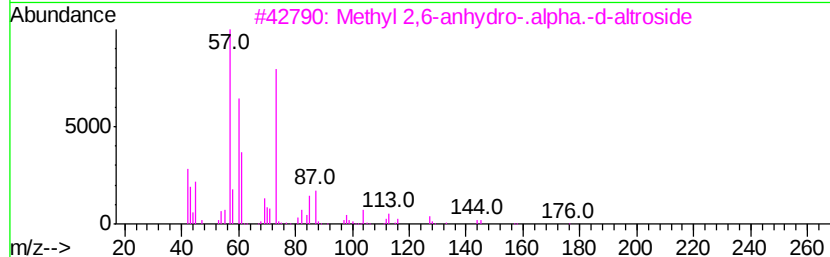
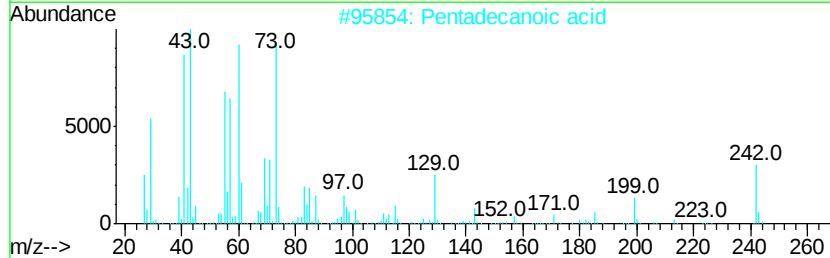
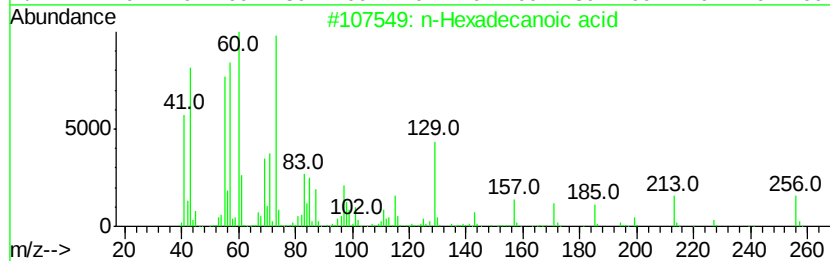
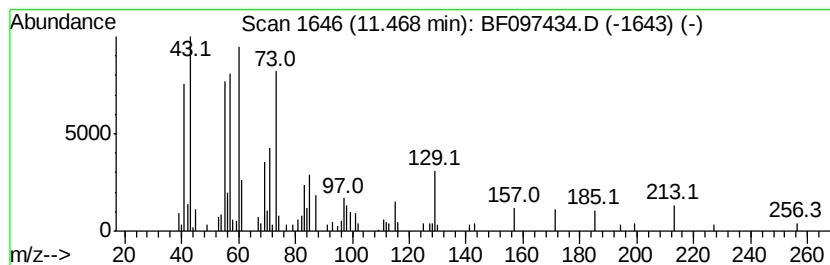
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	3.18 ng	93714	Phenanthrene-d10	10.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3		Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	22
4		Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	18
5		Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	18



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
Data File : BF097434.D
Acq On : 7 Aug 2017 17:34
Operator : SJ/JU
Sample : I4642-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-080417

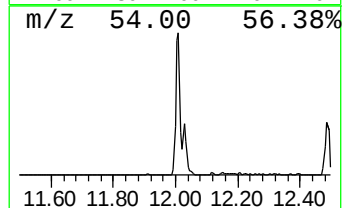
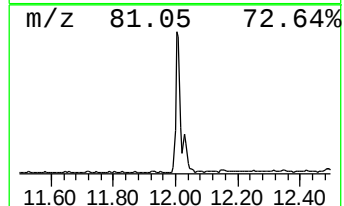
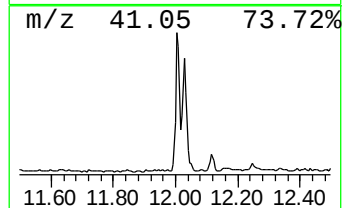
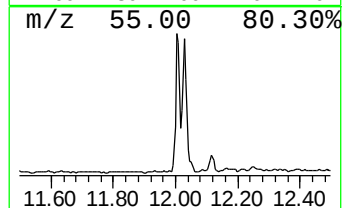
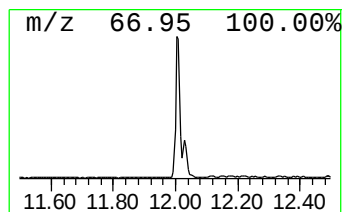
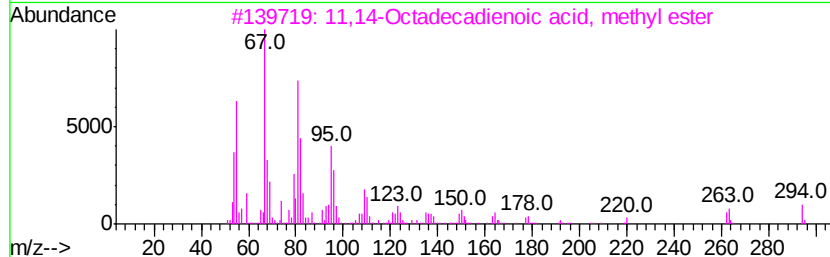
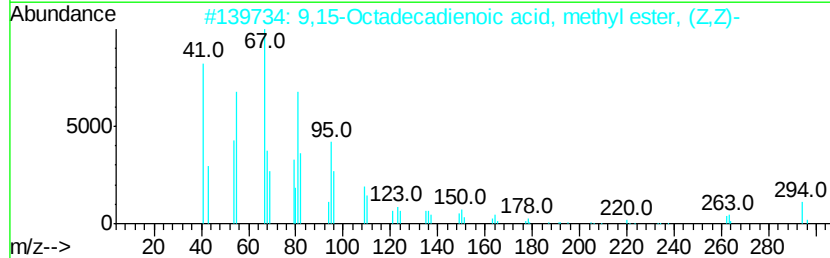
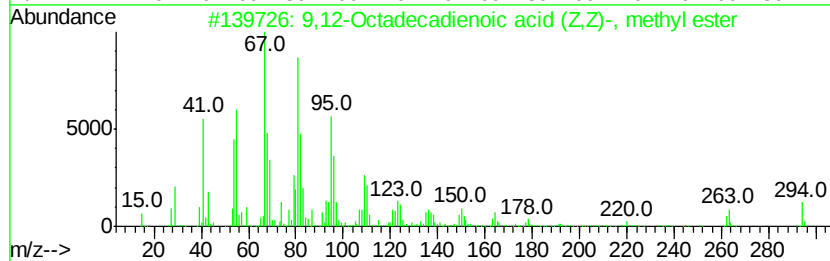
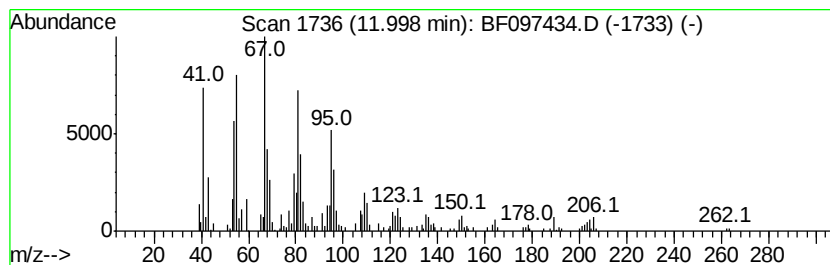
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9,12-Octadecadienoic acid (... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	26.14 ng	770146	Phenanthrene-d10	10.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2		9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	95
3		11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	94
4		11-Octadecynoic acid, methyl ester	294	C19H34O2	026543-37-3	92
5		2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	90



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Sample : I4642-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BU-03-080417

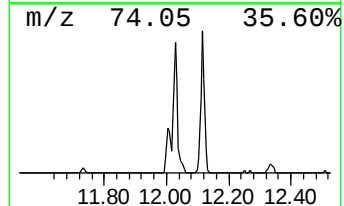
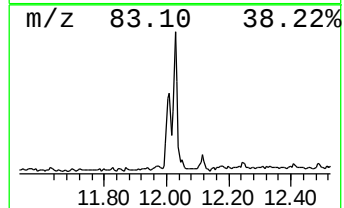
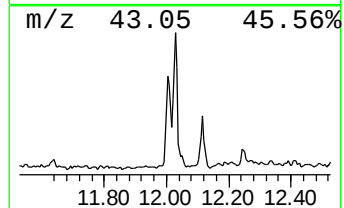
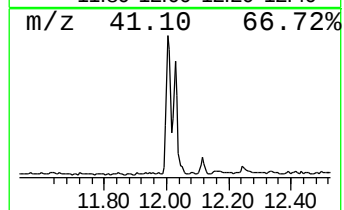
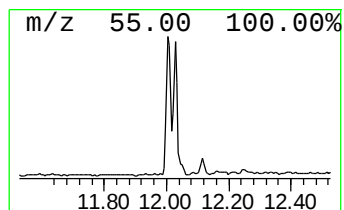
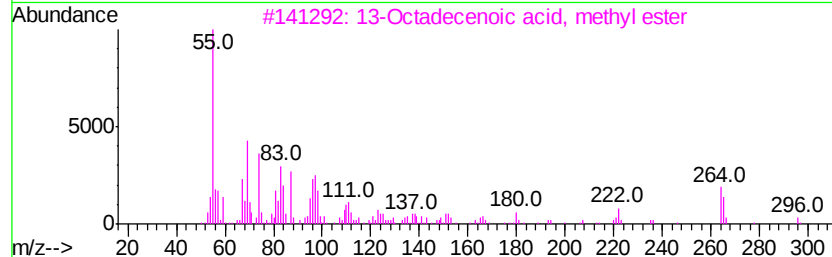
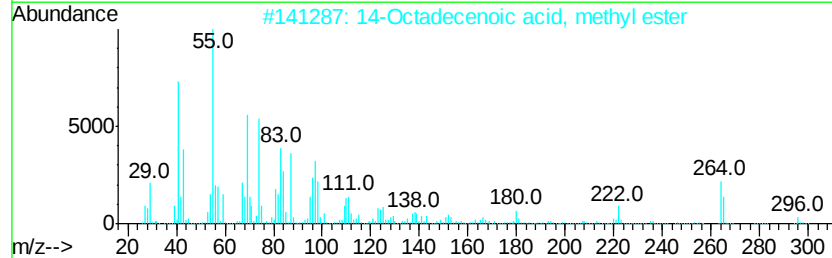
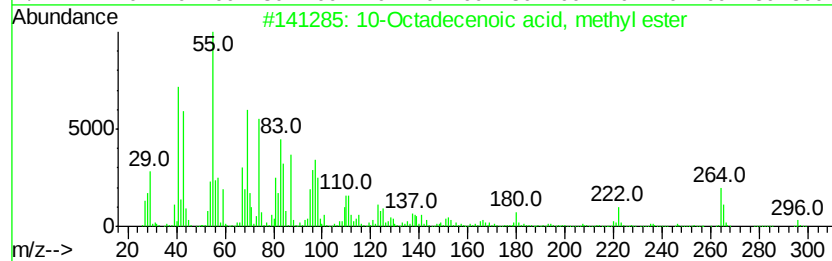
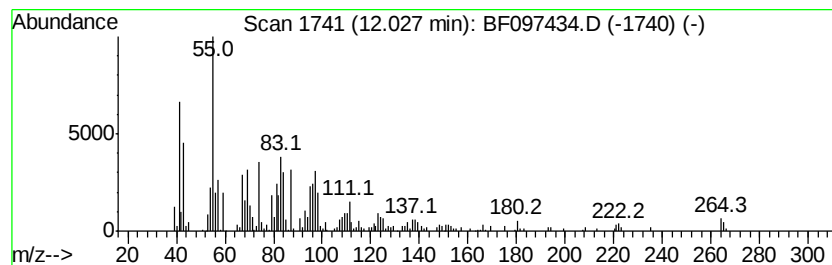
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 10-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.03	14.47 ng	426348	Phenanthrene-d10	10.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	87
2		14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	86
3		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	80
4		7-Hexadecenoic acid, methyl ester...	268	C17H32O2	056875-67-3	68
5		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	68



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Data File : BF097434.D
Acq On : 7 Aug 2017 17:34
Operator : SJ/JU
Sample : I4642-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-080417

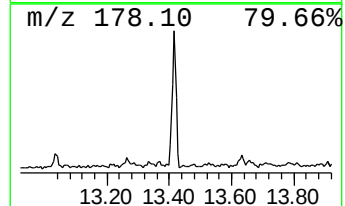
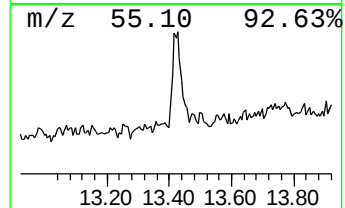
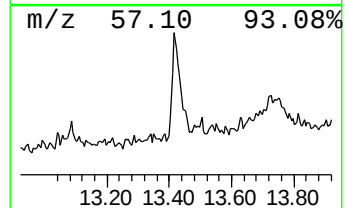
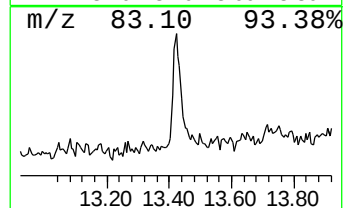
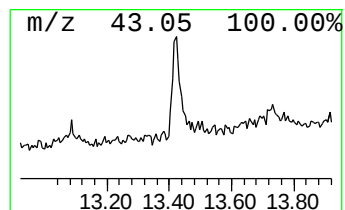
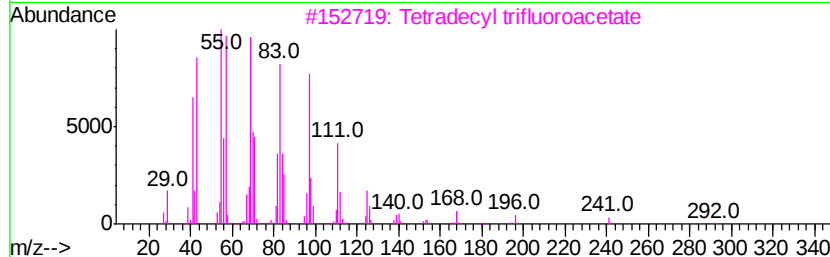
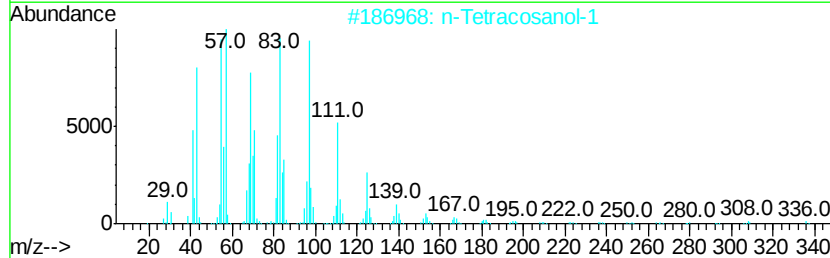
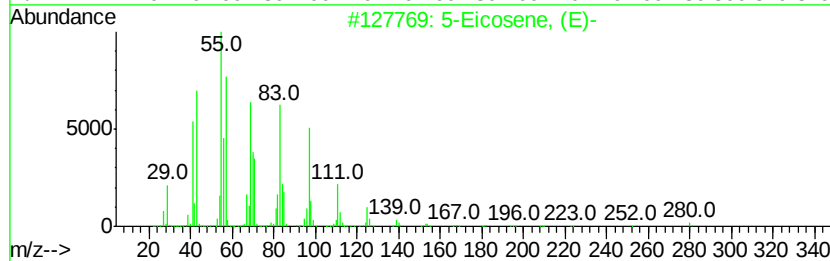
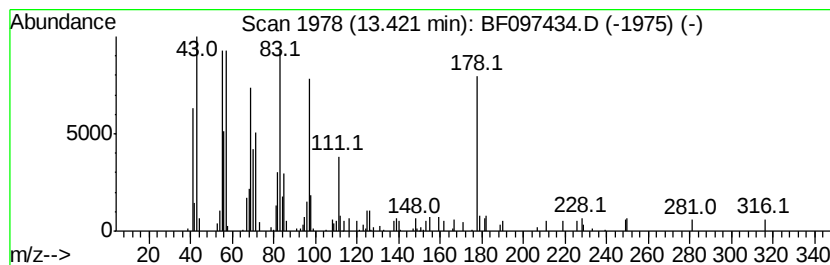
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.42 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.42	3.86 ng	140624	Chrysene-d12	13.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Eicosene, (E)-	280	C20H40	074685-30-6	46
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	46
3		Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	43
4		Cyclohexadecane	224	C16H32	000295-65-8	43
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	38



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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BU-03-080417

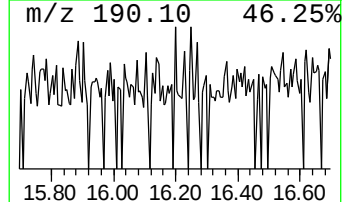
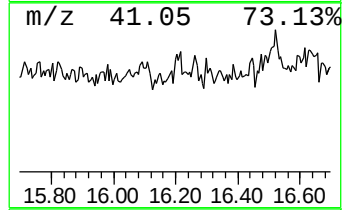
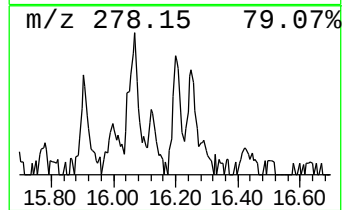
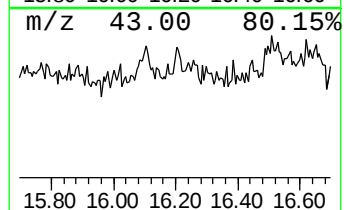
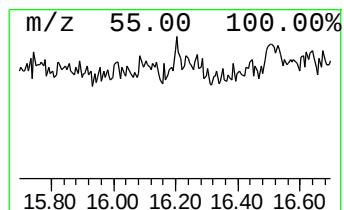
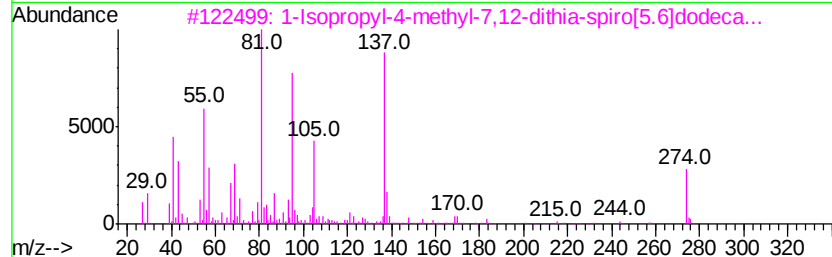
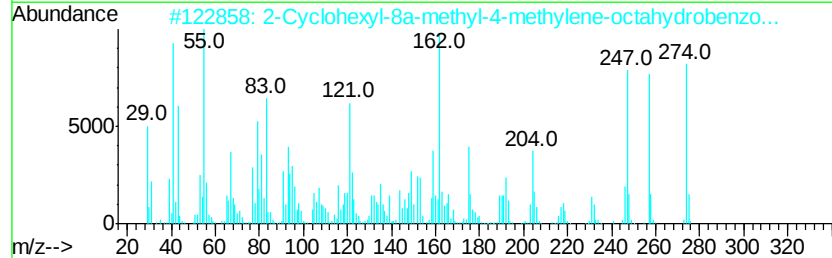
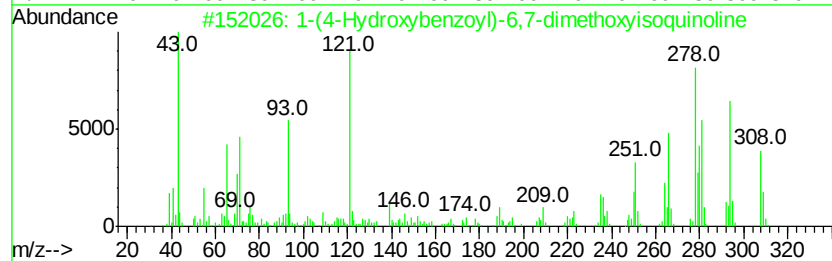
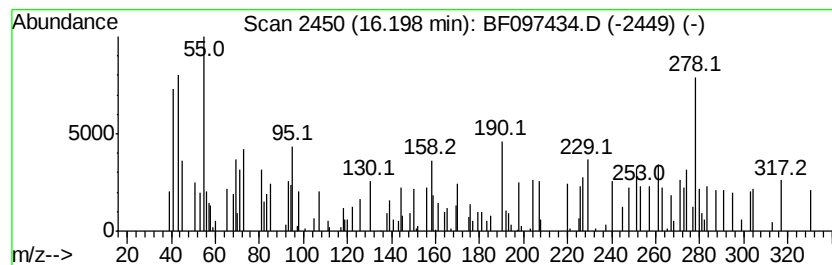
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.20 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	2.11 ng	40663	Perylene-d12	14.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(4-Hydroxybenzoyl)-6,7-dimetho...	309	C18H15N04	005544-57-0	11
2			2-Cyclohexyl-8a-methyl-4-methyle...	274	C17H26N2O	1000193-85-0	10
3			1-Isopropyl-4-methyl-7,12-dithia...	274	C14H26S2	1000190-40-2	10
4			1,11-Dibromoundecane	312	C11H22Br2	016696-65-4	10
5			Silane, dimethyl(2,2,2-trichloro...	320	C11H23Cl3O2Si	1000347-56-6	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080717\
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Sample : I4642-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-080417

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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unknown6.19	6.19	69.8	ng	1860730	1	6.41	532843	20.0
Nonadecane	10.36	2.4	ng	70630	4	10.91	589349	20.0
Hexadecanoic acid...	11.33	6.7	ng	197872	4	10.91	589349	20.0
n-Hexadecanoic acid	11.47	3.2	ng	93714	4	10.91	589349	20.0
9,12-Octadecadien...	12.00	26.1	ng	770146	4	10.91	589349	20.0
10-Octadecenoic a...	12.03	14.5	ng	426348	4	10.91	589349	20.0
unknown13.42	13.42	3.9	ng	140624	5	13.53	728297	20.0
unknown16.20	16.20	2.1	ng	40663	6	14.87	385962	20.0