

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080517\
 Data File : BF097399.D
 Acq On : 5 Aug 2017 16:09
 Operator : SJ/JU
 Sample : I4594-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-12000-R4

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	4.551	466	470	489	rBV	371314	648705	25.78%	2.951%
2	5.022	546	550	575	rBV	2119658	2516180	100.00%	11.447%
3	6.098	729	733	746	rBV	2176205	2369093	94.15%	10.778%
4	6.198	746	750	759	rVB	2324557	2262721	89.93%	10.294%
5	6.422	785	788	798	rBV	774849	705688	28.05%	3.210%
6	6.581	811	815	826	rBV	1533443	1513831	60.16%	6.887%
7	6.998	882	886	896	rBV	1456612	1421463	56.49%	6.467%
8	7.704	1003	1006	1017	rBV	1049533	1007998	40.06%	4.586%
9	8.786	1185	1190	1193	rBV	2417053	2107174	83.74%	9.586%
10	9.186	1254	1258	1267	rBV	355823	302301	12.01%	1.375%
11	9.451	1299	1303	1316	rVB	971137	926498	36.82%	4.215%
12	9.904	1377	1380	1383	rVB	36723	28804	1.14%	0.131%
13	10.239	1433	1437	1452	rBV	1299742	1361380	54.11%	6.193%
14	10.374	1457	1460	1468	rBV	43295	54096	2.15%	0.246%
15	10.816	1531	1535	1538	rBV2	27492	25950	1.03%	0.118%
16	10.922	1549	1553	1556	rBV	963704	832291	33.08%	3.786%
17	11.480	1644	1648	1655	rBV	216529	202736	8.06%	0.922%
18	12.127	1753	1758	1761	rBV	50676	47316	1.88%	0.215%
19	12.257	1777	1780	1790	rBV	106156	116261	4.62%	0.529%
20	12.351	1791	1796	1802	rVB2	69238	78098	3.10%	0.355%
21	12.504	1817	1822	1825	rBV	1479398	1463362	58.16%	6.657%
22	13.057	1911	1916	1920	rBV3	33153	45651	1.81%	0.208%
23	13.421	1974	1978	1987	rBV	114975	193972	7.71%	0.882%
24	13.539	1994	1998	2002	rBV	675724	670149	26.63%	3.049%
25	13.568	2002	2003	2008	rVB	42509	30902	1.23%	0.141%
26	14.139	2095	2100	2104	rBV3	24859	41851	1.66%	0.190%
27	14.186	2105	2108	2112	rBV	63699	76404	3.04%	0.348%
28	14.304	2125	2128	2134	rVB	38490	62409	2.48%	0.284%
29	14.539	2165	2168	2170	rBV	31406	34682	1.38%	0.158%
30	14.780	2206	2209	2215	rVB	31276	35599	1.41%	0.162%
31	14.833	2215	2218	2222	rBV	39954	37740	1.50%	0.172%
32	14.880	2222	2226	2230	rBV	501295	562713	22.36%	2.560%
33	15.262	2287	2291	2296	rVB2	30034	42192	1.68%	0.192%
34	15.657	2353	2358	2366	rVB4	27144	58154	2.31%	0.265%

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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	16.104	2428	2434	2445	rVB6	25413	68527	2.72%	0.312%
36	17.280	2632	2634	2644	rVB9	14083	28028	1.11%	0.128%

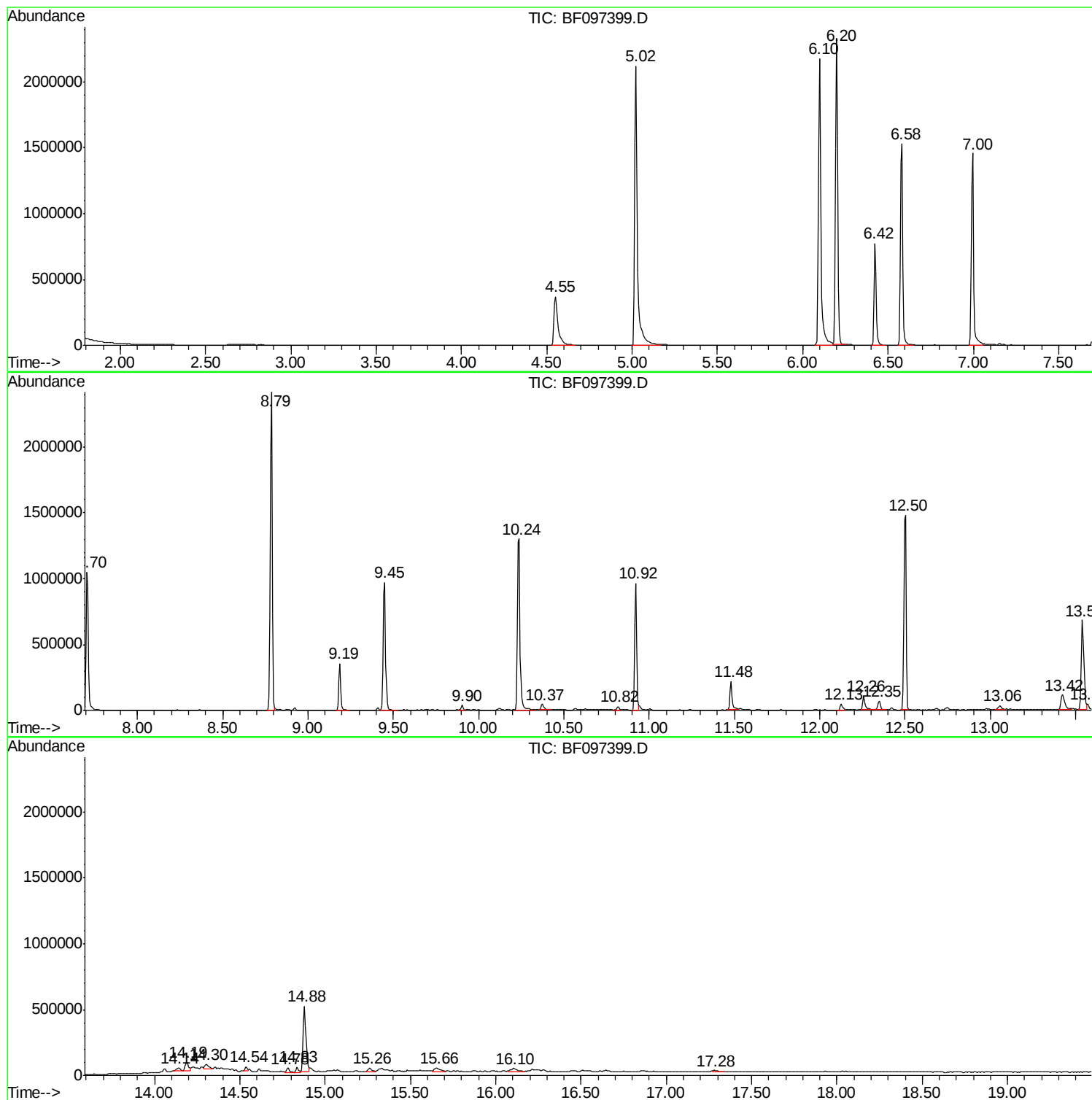
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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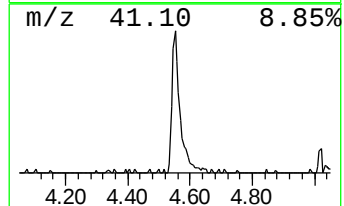
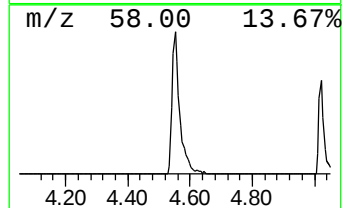
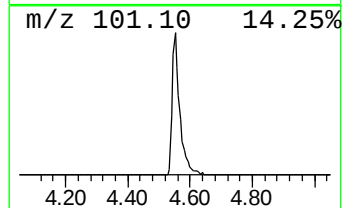
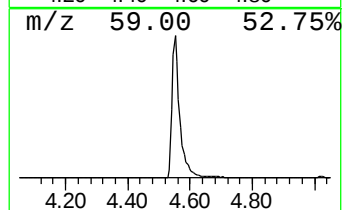
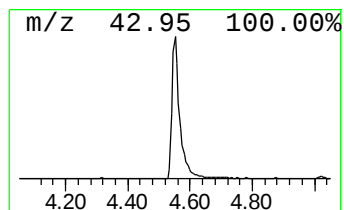
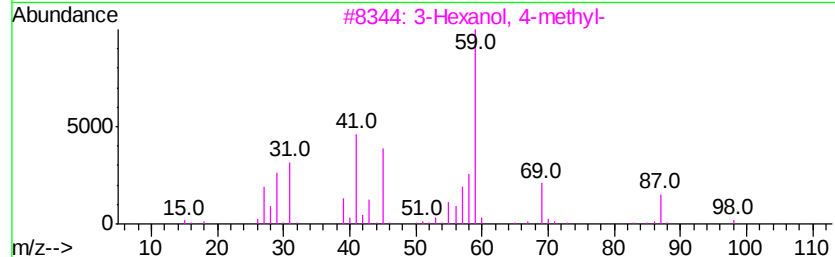
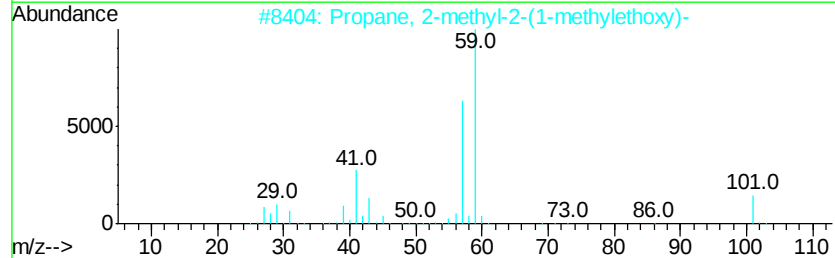
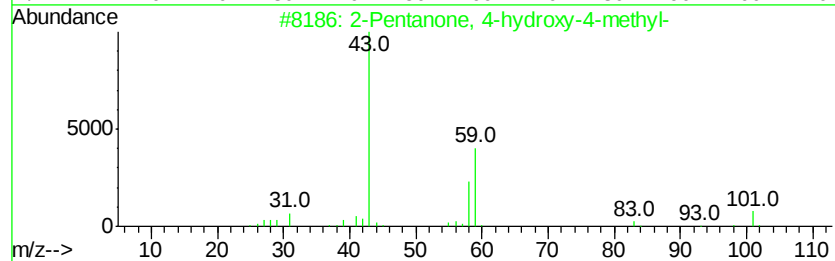
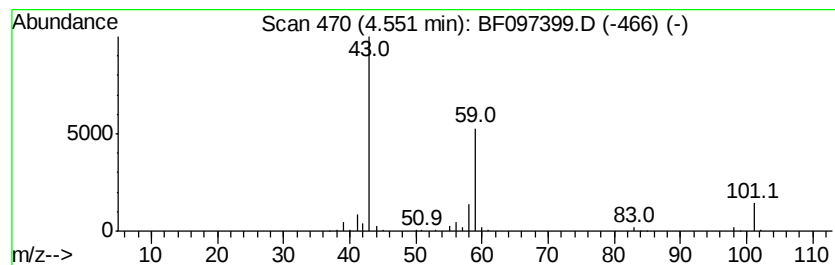
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	18.39 ng	648705	1,4-Dichlorobenzene-d4	6.42

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-methyleth...	116	C7H16O	017348-59-3	42
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	23



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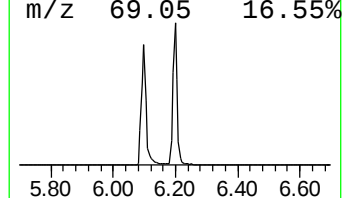
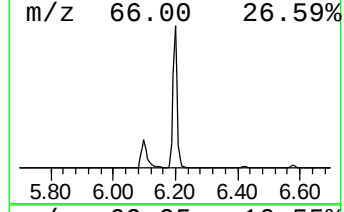
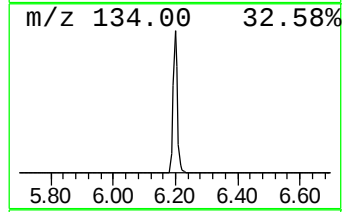
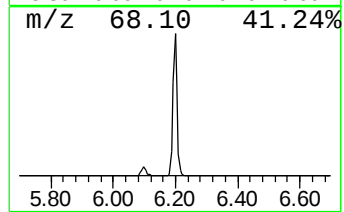
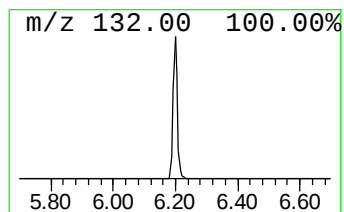
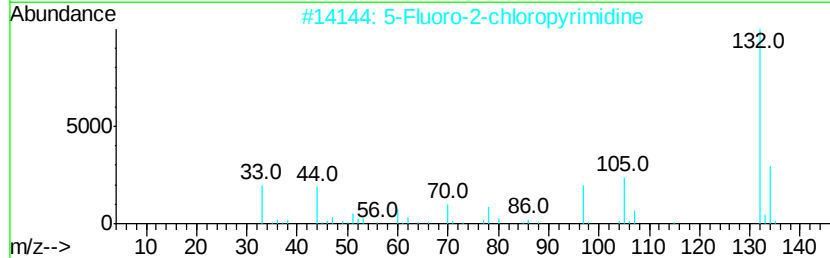
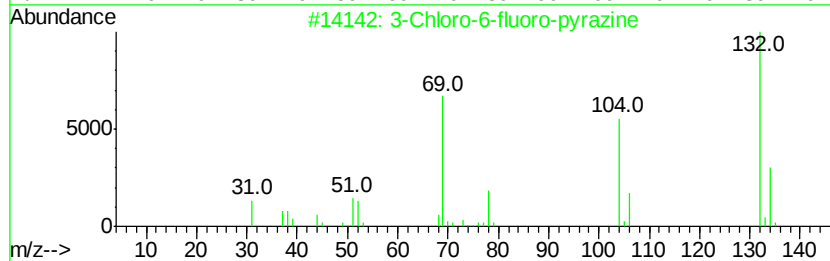
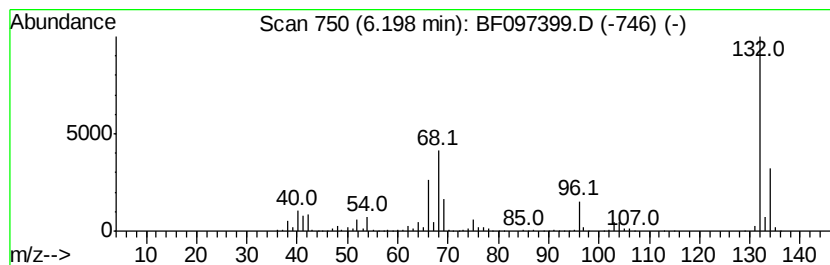
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.20	64.13 ng	2262720	1,4-Dichlorobenzene-d4	6.42

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



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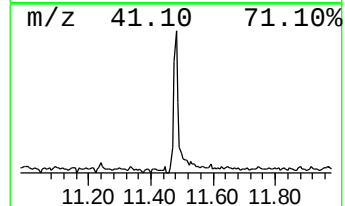
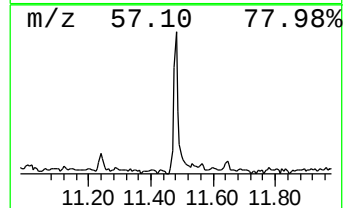
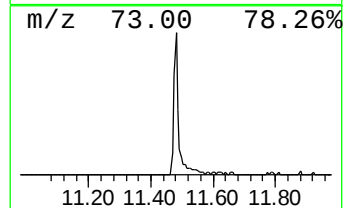
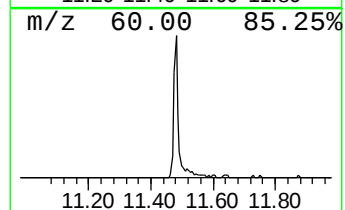
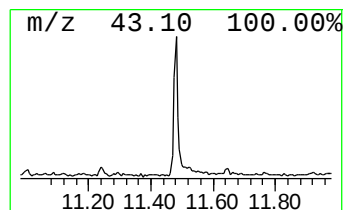
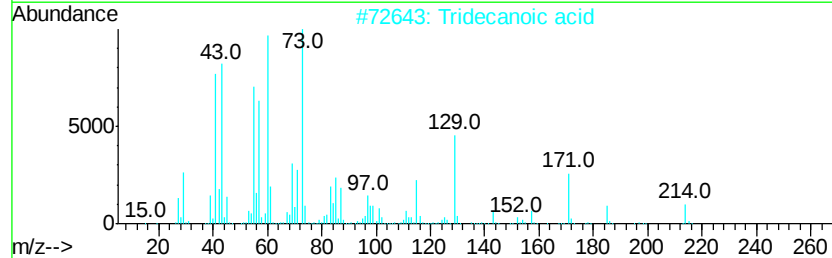
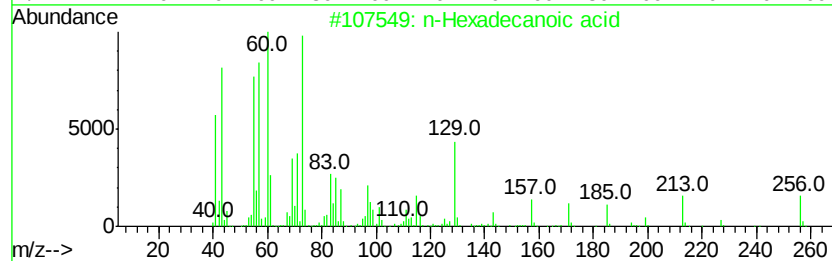
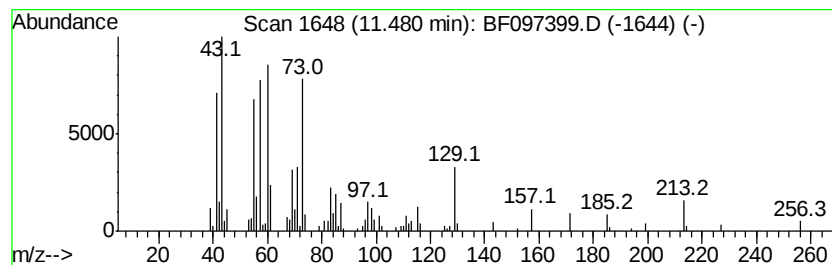
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.48	4.87 ng	202736	Phenanthrene-d10	10.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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ALS Vial : 10 Sample Multiplier: 1

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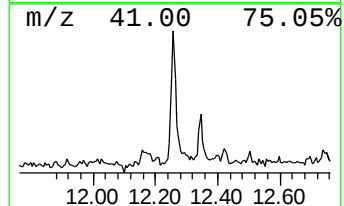
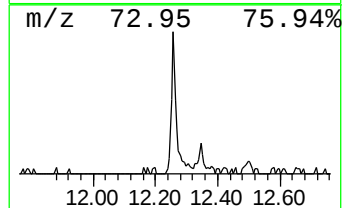
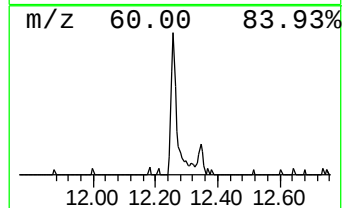
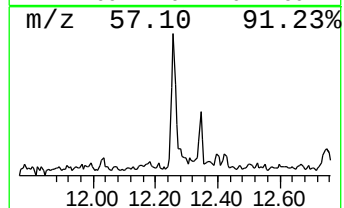
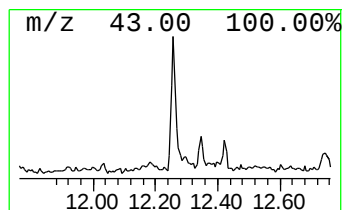
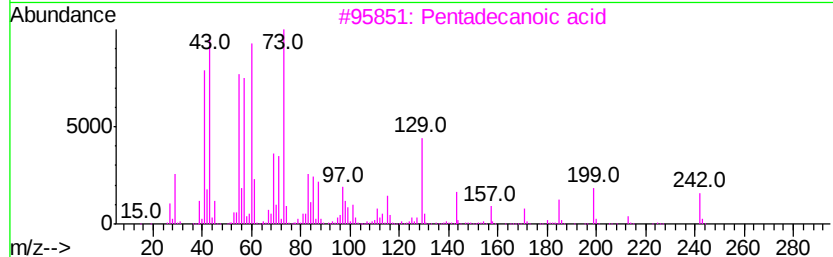
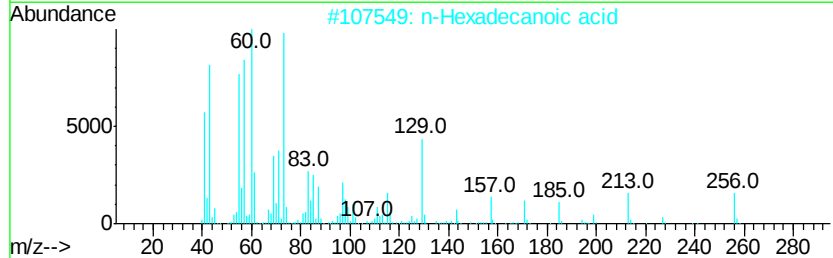
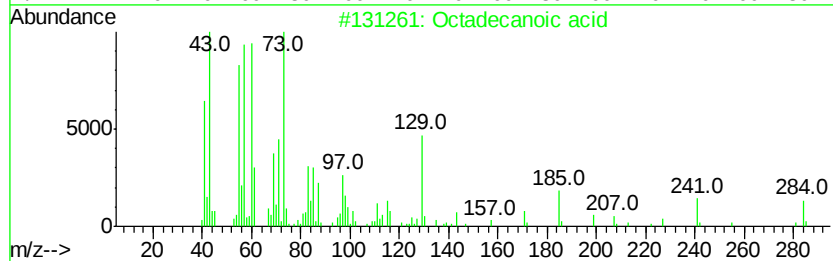
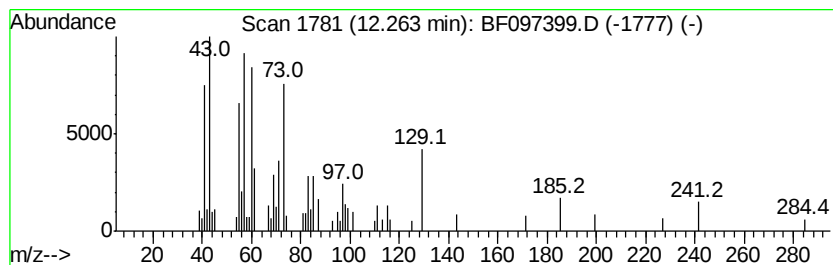
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	3.47 ng	116261	Chrysene-d12	13.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	97
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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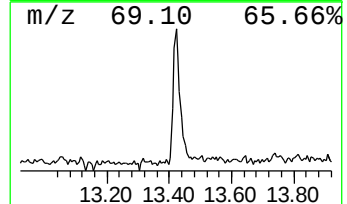
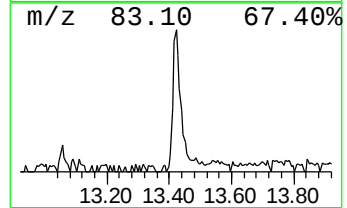
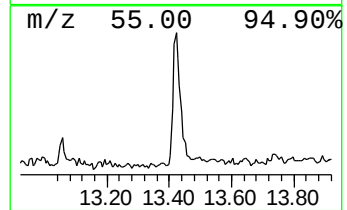
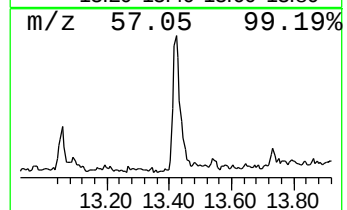
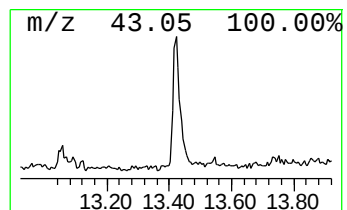
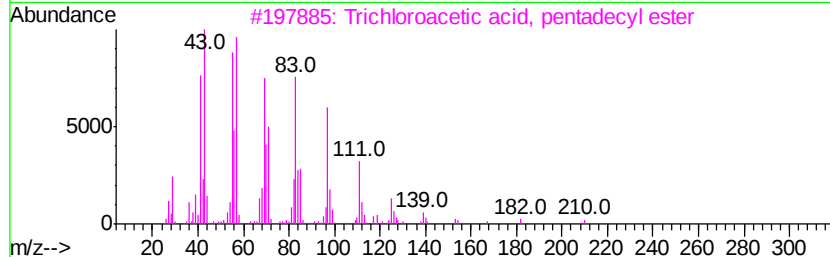
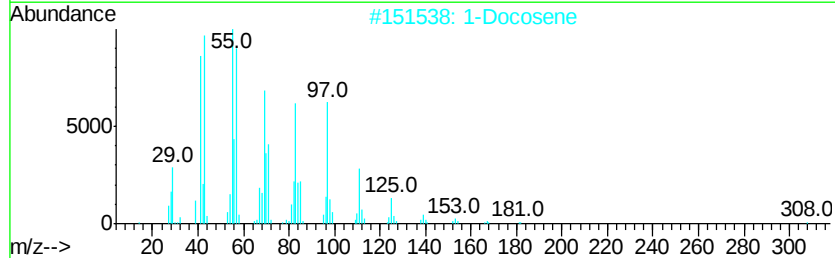
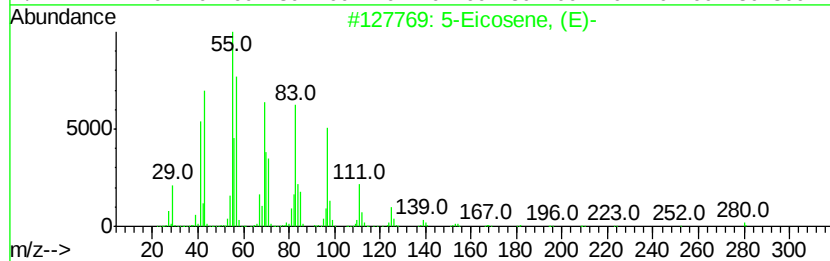
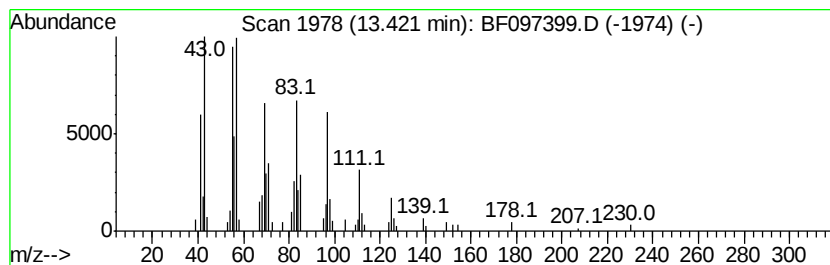
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.42	5.79 ng	193972	Chrysene-d12	13.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
2		1-Docosene	308	C22H44	001599-67-3	91
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90



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72-12000-R4

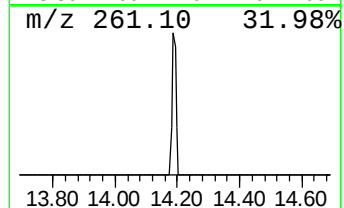
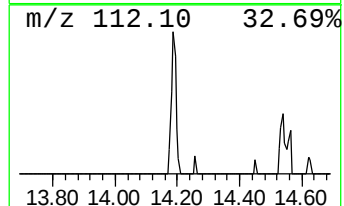
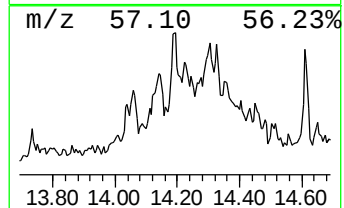
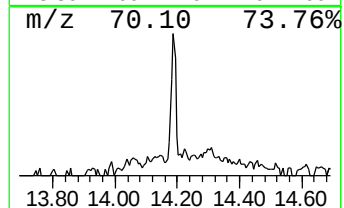
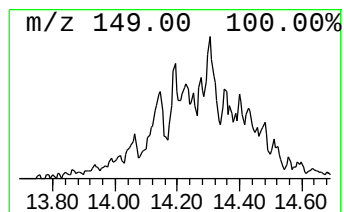
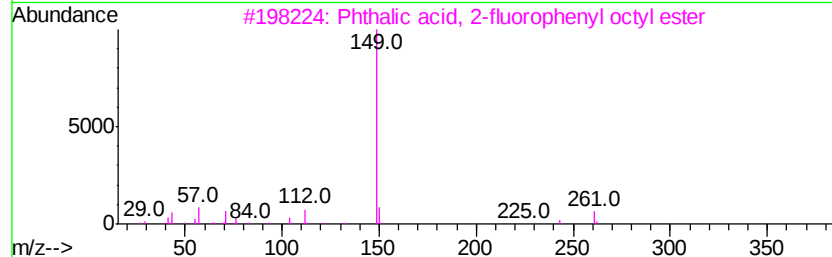
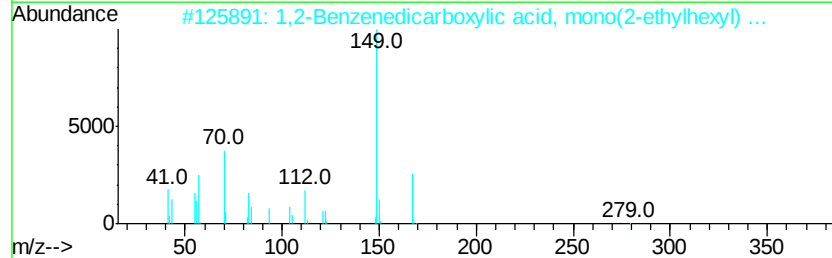
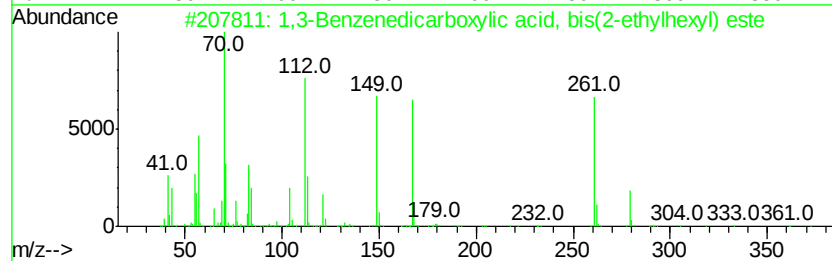
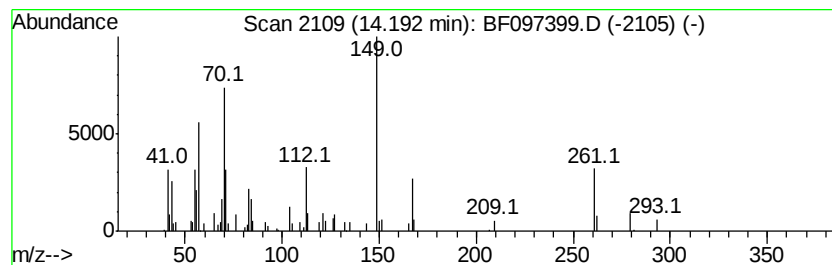
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.19 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	2.28 ng	76404	Chrysene-d12	13.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	47
2		1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	40
3		Phthalic acid, 2-fluorophenyl oc...	372	C22H25FO4	1000356-18-3	25
4		Dimethylmalonic acid, monochlori...	262	C13H23ClO3	1000361-64-8	22
5		Di-n-octyl phthalate	390	C24H38O4	000117-84-0	16



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080517\
Data File : BF097399.D
Acq On : 5 Aug 2017 16:09
Operator : SJ/JU
Sample : I4594-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000-R4

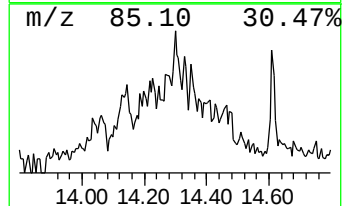
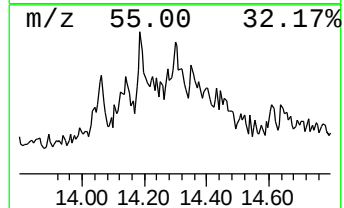
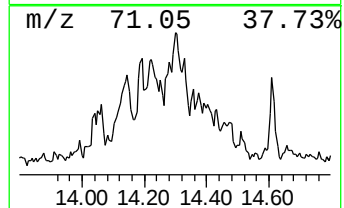
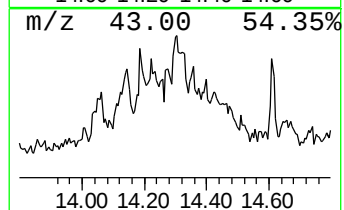
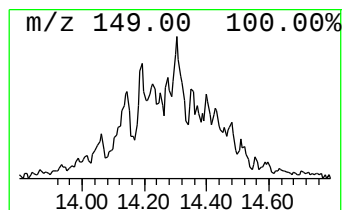
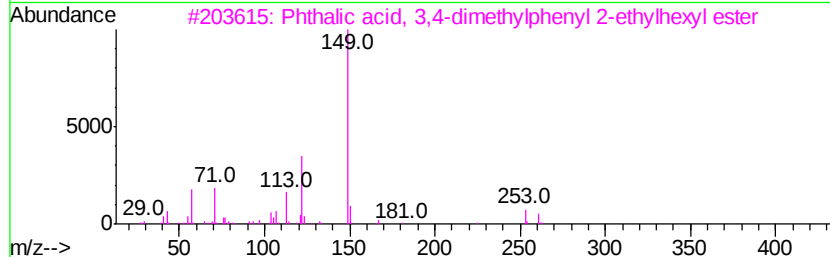
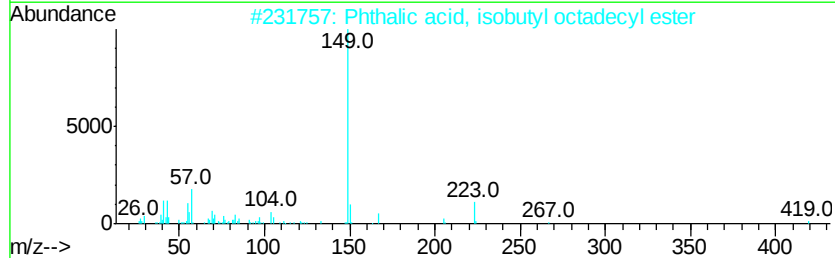
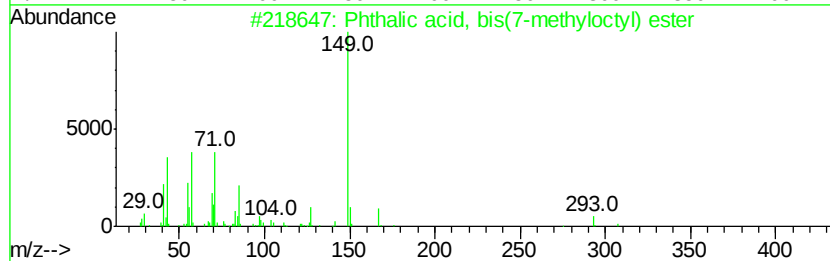
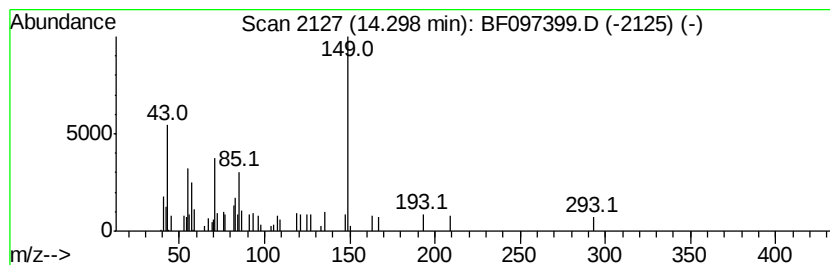
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Phthalic acid, bis(7-methyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.30	2.22 ng	62409	Perylene-d12	14.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, bis(7-methyloctyl...	418	C26H42O4	020548-62-3	53
2		Phthalic acid, isobutyl octadecyl...	474	C30H50O4	1000309-06-1	47
3		Phthalic acid, 3,4-dimethylphenyl...	382	C24H30O4	1000315-70-7	47
4		Phthalic acid, 3-methylbut-3-enyl...	360	C22H32O4	1000357-10-7	43
5		Phthalic acid, hex-3-yl isohexyl...	334	C20H30O4	1000356-95-6	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080517\
Data File : BF097399.D
Acq On : 5 Aug 2017 16:09
Operator : SJ/JU
Sample : I4594-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000-R4

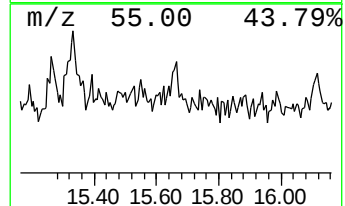
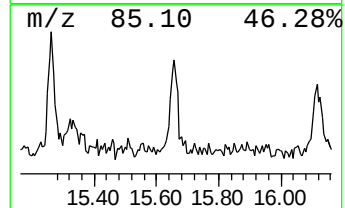
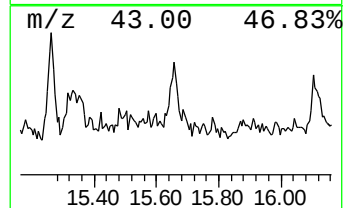
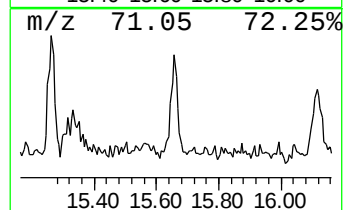
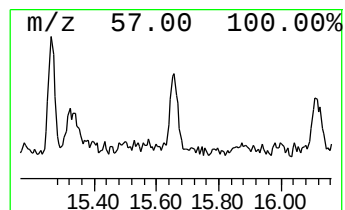
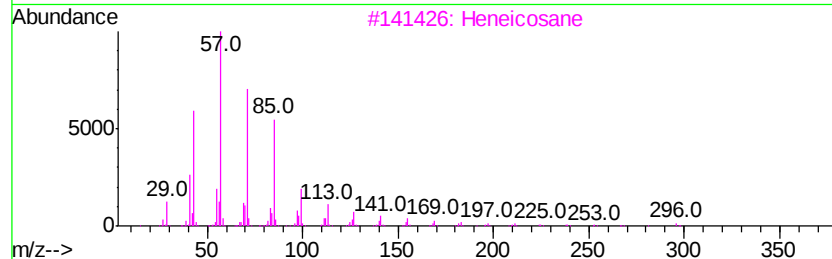
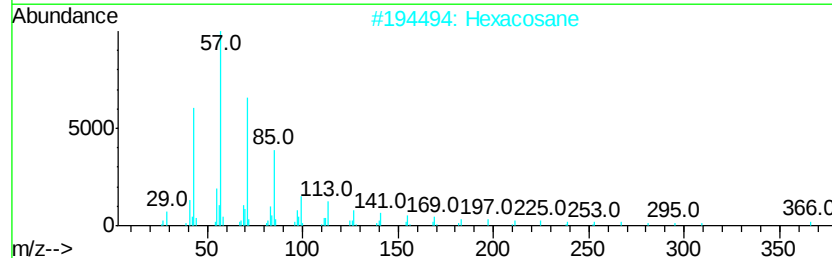
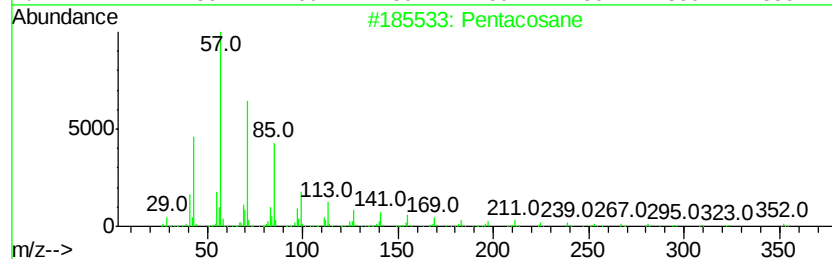
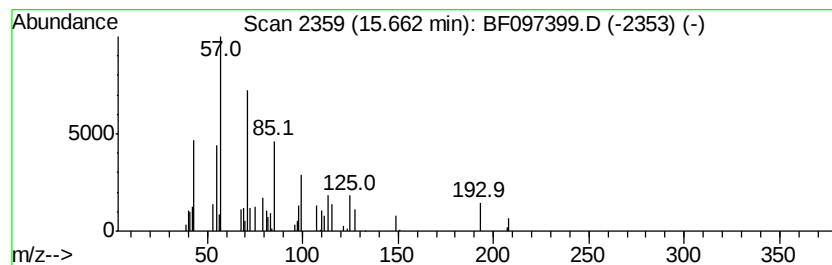
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	2.07 ng	58154	Perylene-d12	14.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	64
2		Hexacosane	366	C26H54	000630-01-3	64
3		Heneicosane	296	C21H44	000629-94-7	64
4		Eicosane, 10-methyl-	296	C21H44	054833-23-7	59
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	58



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080517\
Data File : BF097399.D
Acq On : 5 Aug 2017 16:09
Operator : SJ/JU
Sample : I4594-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000-R4

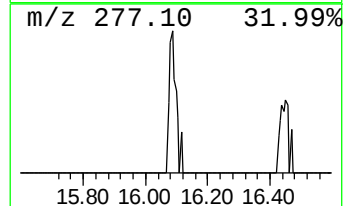
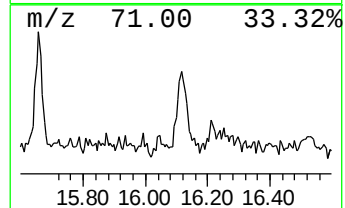
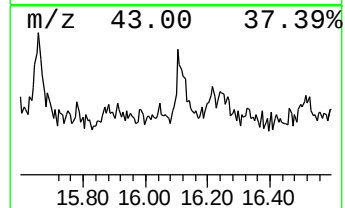
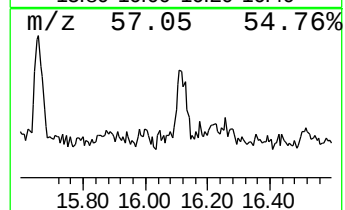
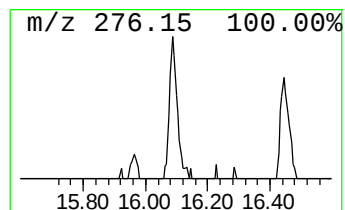
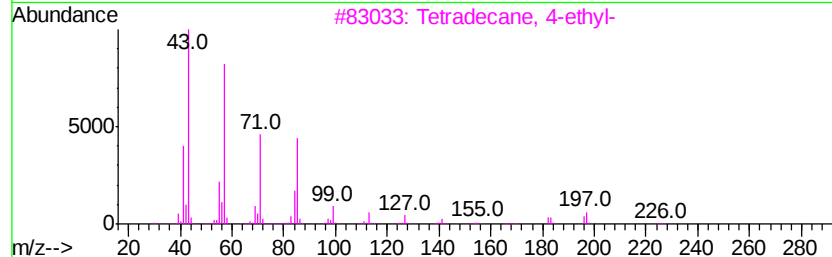
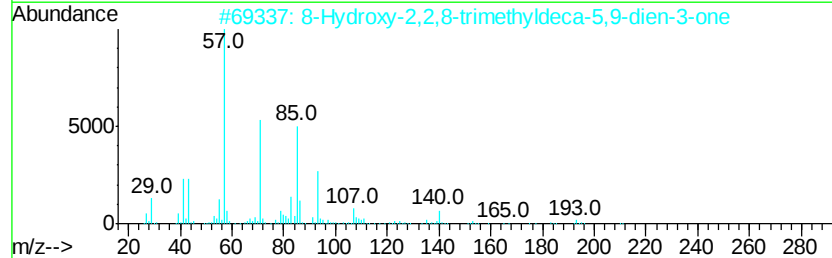
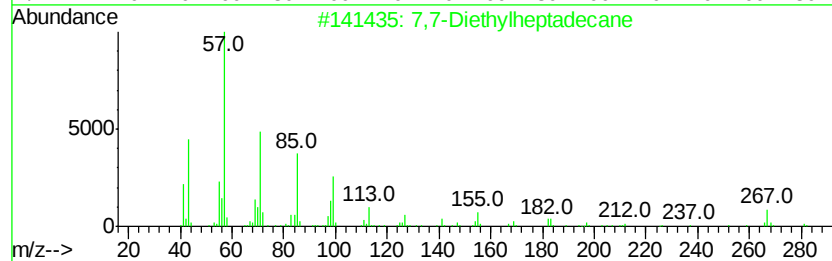
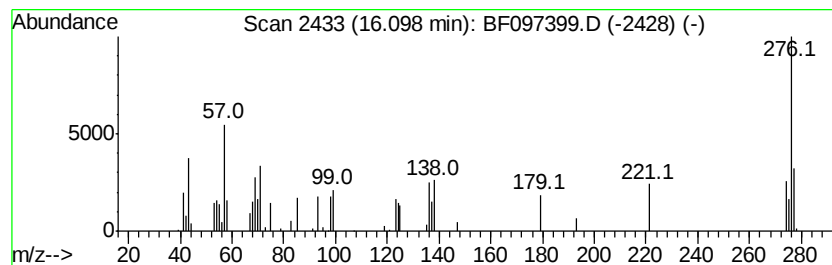
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.10 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.44 ng	68527	Perylene-d12	14.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7,7-Diethylheptadecane	296	C21H44	1000360-41-5	35
2		8-Hydroxy-2,2,8-trimethyldeca-5,...	210	C13H22O2	083040-92-0	27
3		Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	27
4		Undecane, 1-bromo-	234	C11H23Br	000693-67-4	27
5		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080517\
Data File : BF097399.D
Acq On : 5 Aug 2017 16:09
Operator : SJ/JU
Sample : I4594-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12000-R4

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
2-Pentanone, 4-hy...	4.55	18.4	ng	648705	1	6.42	705688	20.0
unknown6.20	6.20	64.1	ng	2262720	1	6.42	705688	20.0
n-Hexadecanoic acid	11.48	4.9	ng	202736	4	10.92	832291	20.0
Octadecanoic acid	12.26	3.5	ng	116261	5	13.54	670149	20.0
5-Eicosene, (E)-	13.42	5.8	ng	193972	5	13.54	670149	20.0
unknown14.19	14.19	2.3	ng	76404	5	13.54	670149	20.0
Phthalic acid, bi...	14.30	2.2	ng	62409	6	14.88	562713	20.0
Pentacosane	15.66	2.1	ng	58154	6	14.88	562713	20.0
unknown16.10	16.10	2.4	ng	68527	6	14.88	562713	20.0