

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
 Data File : BF096416.D
 Acq On : 2 Jul 2017 15:17
 Operator : SJ/MA
 Sample : I3950-15
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B6-4-6

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-BF070117.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	2.816	115	124	129	rVB4	17570	40581	1.07%	0.126%
2	3.745	274	282	287	rBV3	24203	37955	1.00%	0.118%
3	4.939	480	485	493	rBV	485391	684847	18.12%	2.135%
4	5.316	545	549	550	rBV	46080	37912	1.00%	0.118%
5	5.357	550	556	559	rVB	3490354	3779494	100.00%	11.781%
6	5.581	591	594	599	rVB2	42011	48303	1.28%	0.151%
7	6.275	705	712	717	rBV3	33302	51383	1.36%	0.160%
8	6.339	717	723	724	rBV2	40668	48500	1.28%	0.151%
9	6.375	724	729	732	rVB	3151869	3726039	98.59%	11.614%
10	6.504	746	751	755	rBV	3334376	3621209	95.81%	11.287%
11	6.563	759	761	763	rBV2	45133	39368	1.04%	0.123%
12	6.733	786	790	793	rBV	1144619	904490	23.93%	2.819%
13	6.798	798	801	805	rBV2	35970	40711	1.08%	0.127%
14	6.892	810	817	820	rBV	2834877	2589696	68.52%	8.072%
15	7.298	879	886	889	rBV	2227948	2294946	60.72%	7.153%
16	7.345	891	894	897	rVB2	50522	43572	1.15%	0.136%
17	7.392	897	902	906	rBV2	55206	69924	1.85%	0.218%
18	8.016	1004	1008	1010	rBV	1450025	1188580	31.45%	3.705%
19	8.033	1010	1011	1014	rVB	80724	51779	1.37%	0.161%
20	8.451	1077	1082	1086	rBV	53340	49086	1.30%	0.153%
21	8.622	1108	1111	1113	rBV	72753	58522	1.55%	0.182%
22	8.727	1123	1129	1132	rBV	116572	94871	2.51%	0.296%
23	8.827	1142	1146	1149	rVB	94361	83572	2.21%	0.260%
24	9.092	1186	1191	1194	rBV	3347335	3008529	79.60%	9.378%
25	9.186	1204	1207	1210	rVB2	100123	87730	2.32%	0.273%
26	9.351	1229	1235	1241	rBV2	35498	54836	1.45%	0.171%
27	9.427	1245	1248	1250	rBV	66522	60474	1.60%	0.188%
28	9.451	1250	1252	1254	rBV	53596	41677	1.10%	0.130%
29	9.486	1254	1258	1260	rBV	581436	513733	13.59%	1.601%
30	9.710	1294	1296	1300	rVB	101853	88283	2.34%	0.275%
31	9.769	1300	1306	1309	rBV	1143584	1087041	28.76%	3.388%
32	9.969	1337	1340	1343	rVB	61822	56653	1.50%	0.177%
33	10.174	1371	1375	1379	rBV3	30217	49176	1.30%	0.153%
34	10.210	1379	1381	1384	rVB	135519	101128	2.68%	0.315%

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35	10.433	1415	1419	1421	rBV	43731	49865	1.32%	0.155%
36	10.469	1421	1425	1430	rVB5	28849	41124	1.09%	0.128%
37	10.551	1435	1439	1443	rVB	1737219	1618454	42.82%	5.045%
38	10.680	1459	1461	1468	rBV3	139105	211274	5.59%	0.659%
39	11.127	1535	1537	1540	rBV	86398	73339	1.94%	0.229%
40	11.245	1553	1557	1560	rBV	986723	826530	21.87%	2.576%
41	11.480	1594	1597	1602	rBV3	70047	65465	1.73%	0.204%
42	11.557	1607	1610	1612	rBV	60435	49604	1.31%	0.155%
43	11.786	1644	1649	1652	rBV2	133079	155198	4.11%	0.484%
44	11.851	1657	1660	1663	rBV	41559	40779	1.08%	0.127%
45	11.963	1675	1679	1687	rVB2	44250	55409	1.47%	0.173%
46	12.298	1733	1736	1740	rBV	351364	299469	7.92%	0.933%
47	12.351	1743	1745	1748	rVB	85091	79530	2.10%	0.248%
48	12.451	1759	1762	1766	rBV2	55876	58170	1.54%	0.181%
49	12.568	1779	1782	1786	rBV2	60405	70137	1.86%	0.219%
50	12.827	1822	1826	1830	rBV	1725072	1710117	45.25%	5.330%
51	13.045	1860	1863	1865	rBV	56076	53398	1.41%	0.166%
52	13.286	1900	1904	1906	rBV	78428	102084	2.70%	0.318%
53	13.315	1906	1909	1914	rVB	280336	269469	7.13%	0.840%
54	13.380	1918	1920	1923	rBV3	32075	42385	1.12%	0.132%
55	13.415	1923	1926	1929	rVV4	38788	40676	1.08%	0.127%
56	13.733	1977	1980	1987	rVB2	160017	192531	5.09%	0.600%
57	13.874	2000	2004	2007	rBV	862177	788055	20.85%	2.456%
58	15.286	2240	2244	2248	rVB	379907	454681	12.03%	1.417%

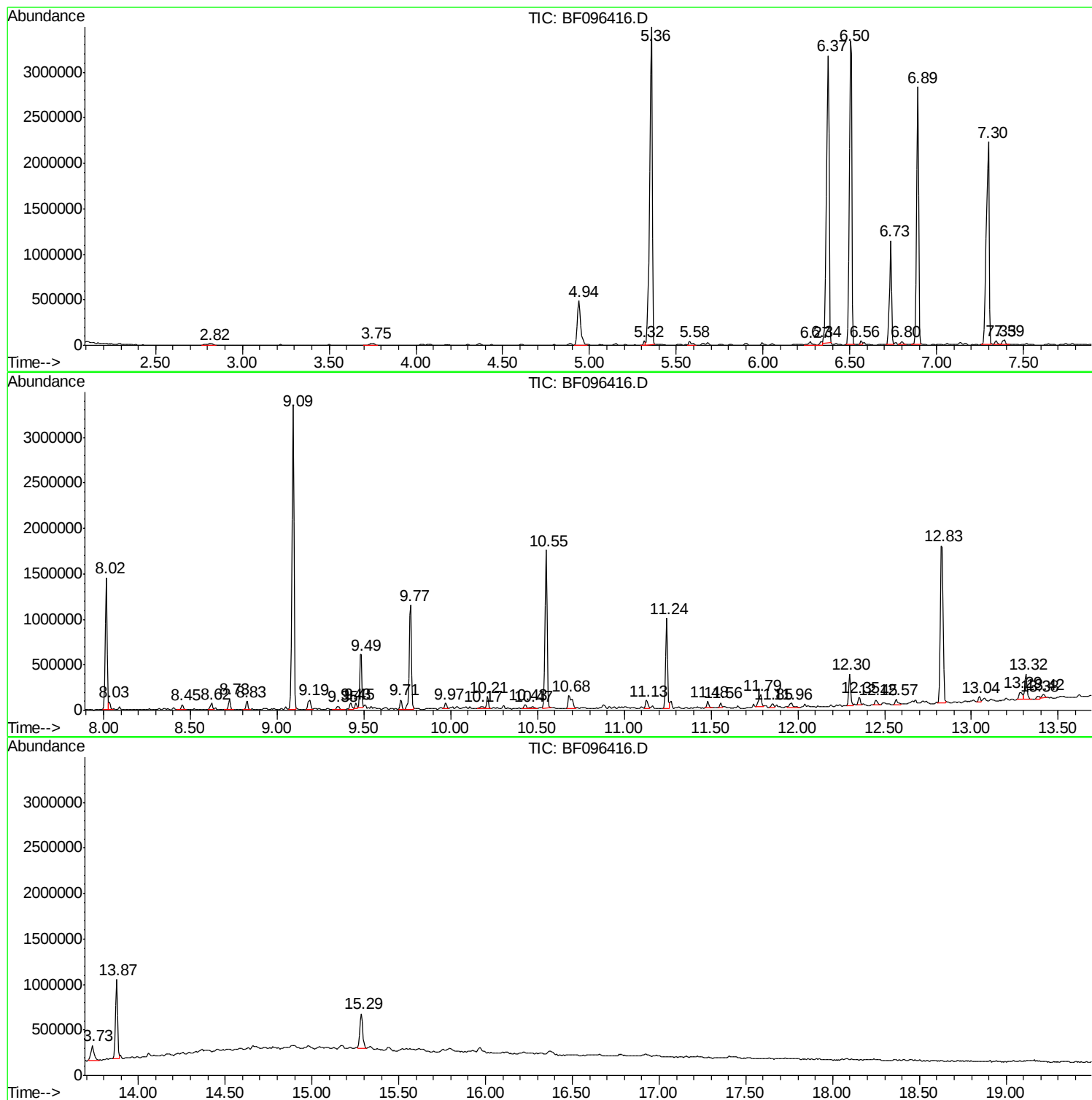
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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ClientSampleId :
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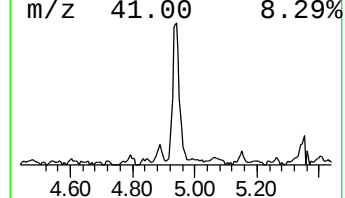
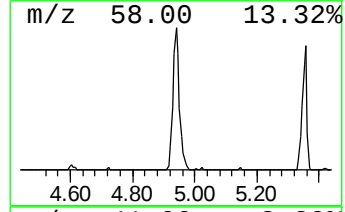
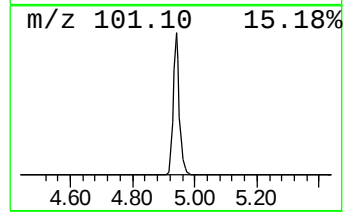
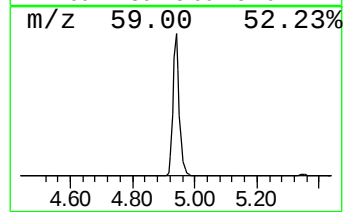
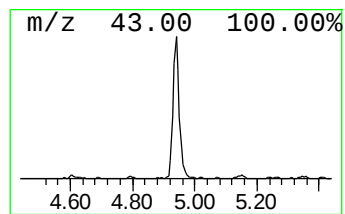
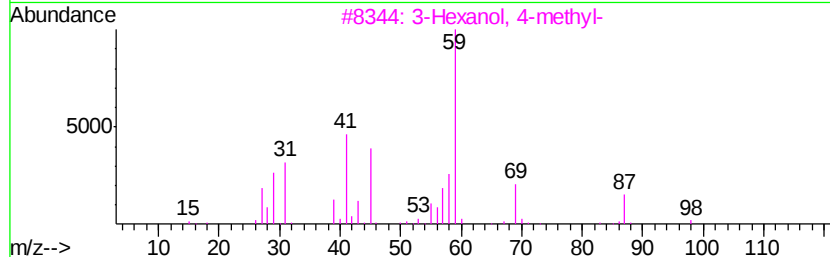
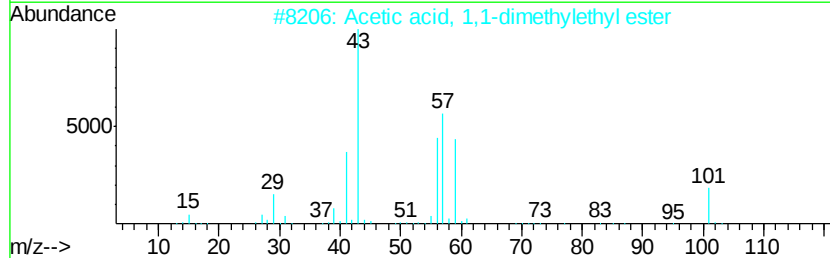
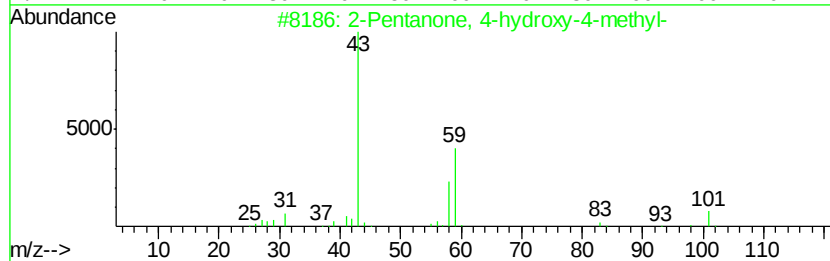
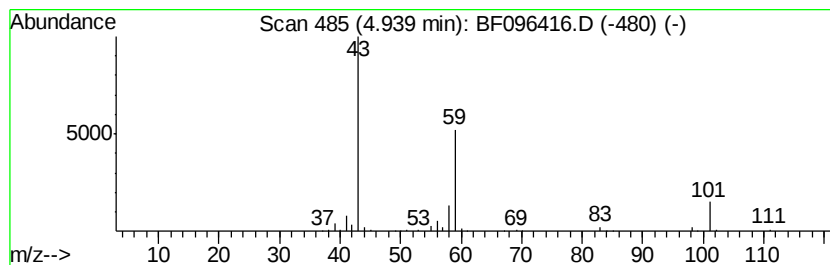
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	15.14 ng	684847	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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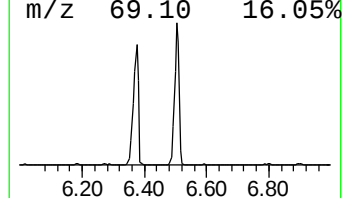
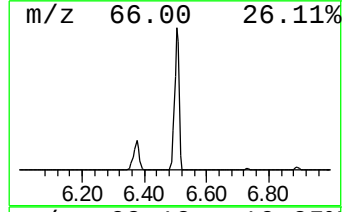
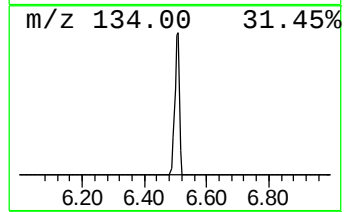
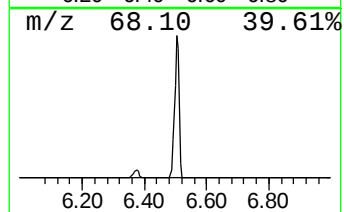
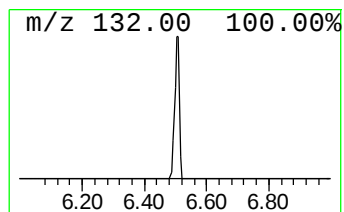
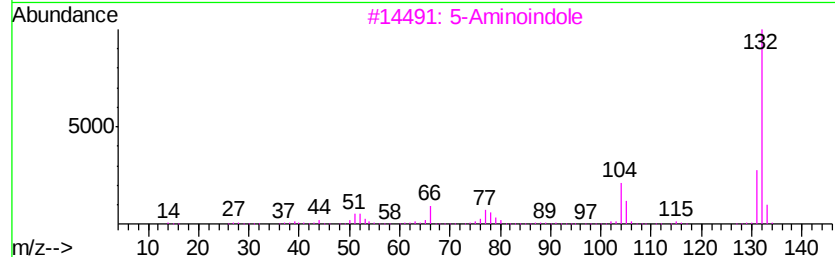
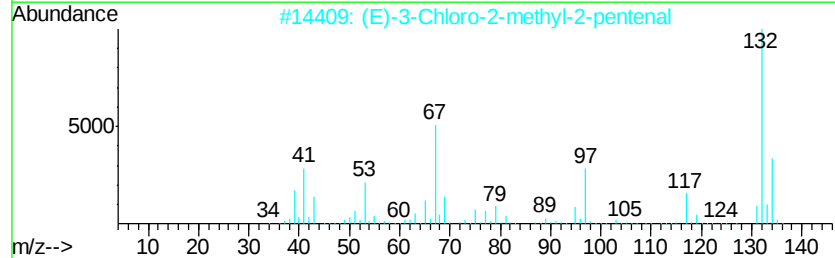
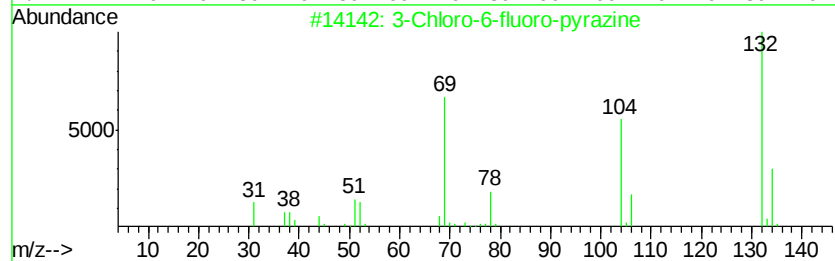
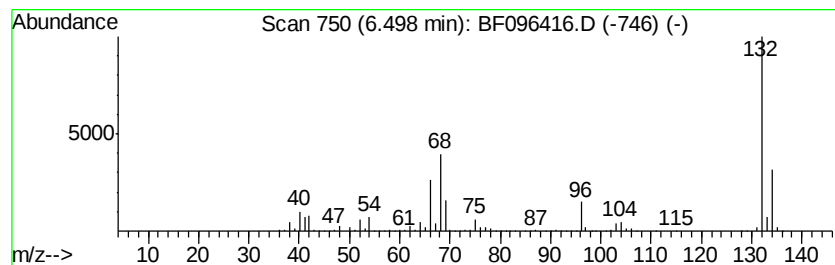
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	80.07 ng	3621210	1,4-Dichlorobenzene-d4	6.73

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	17
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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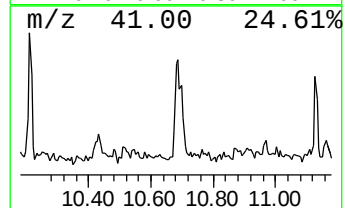
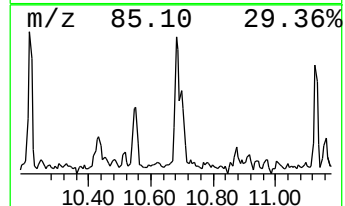
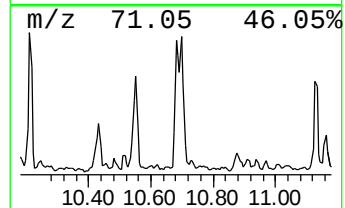
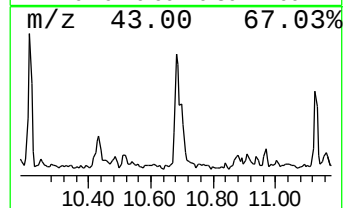
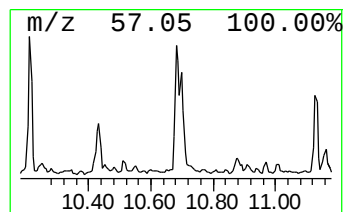
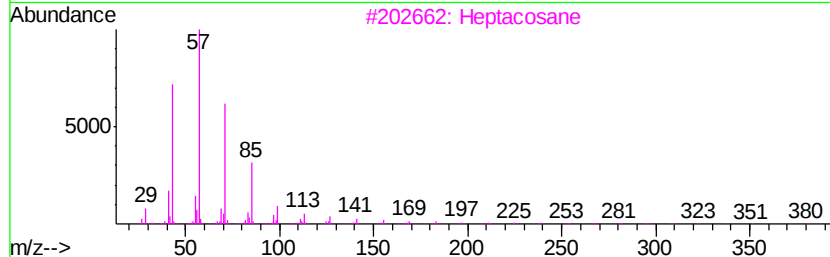
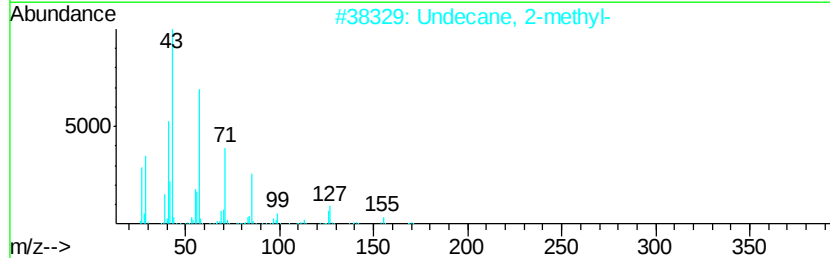
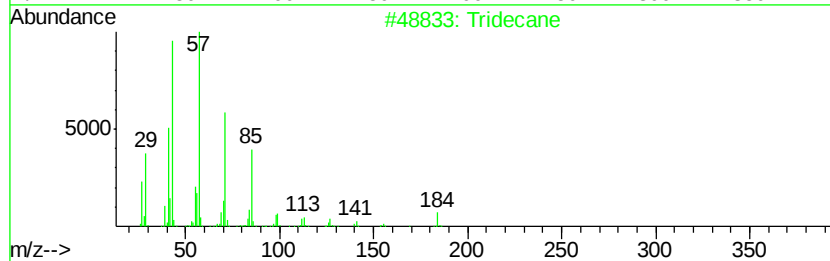
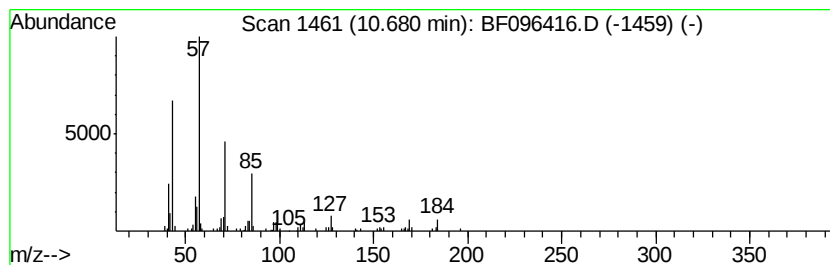
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.68	5.11 ng	211274	Phenanthrene-d10		11.24
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	94
2	Undecane, 2-methyl-	170	C12H26	007045-71-8	80
3	Heptacosane	380	C27H56	000593-49-7	80
4	Eicosane	282	C20H42	000112-95-8	80
5	5-Ethyldecane	170	C12H26	017302-36-2	80



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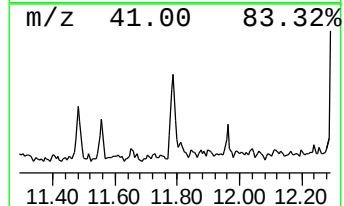
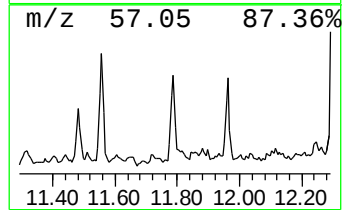
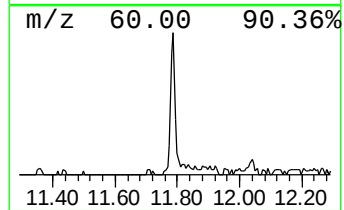
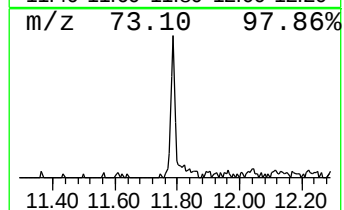
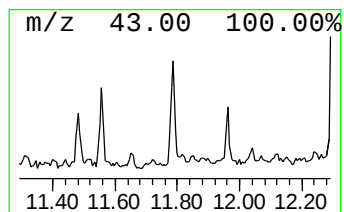
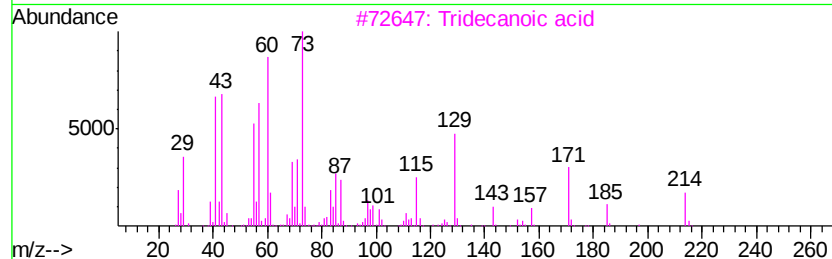
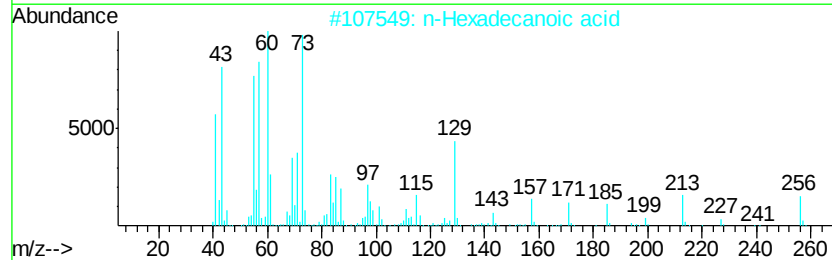
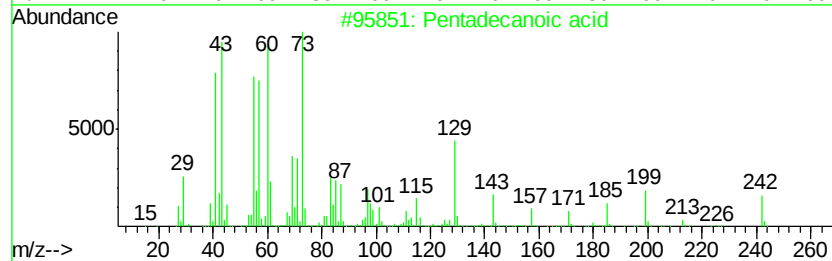
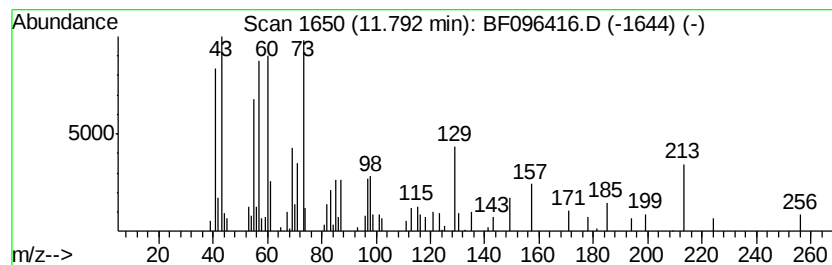
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	3.76 ng	155198	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	89
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		Dodecanoic acid	200	C12H24O2	000143-07-7	72



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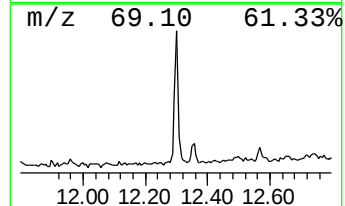
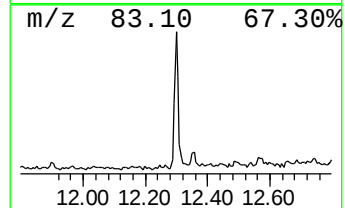
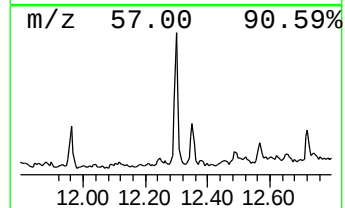
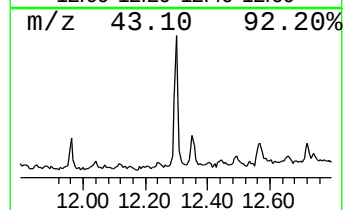
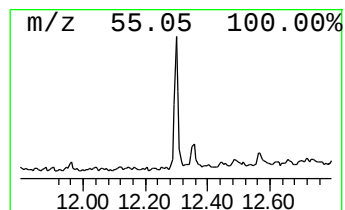
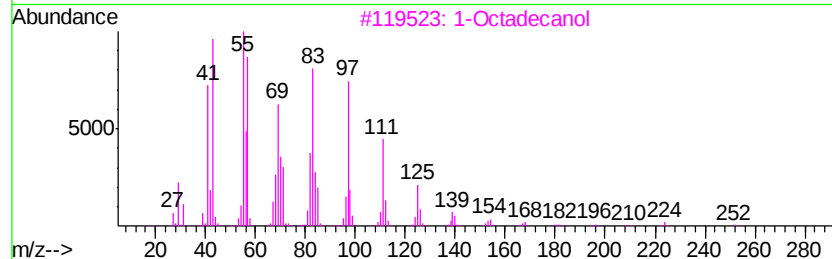
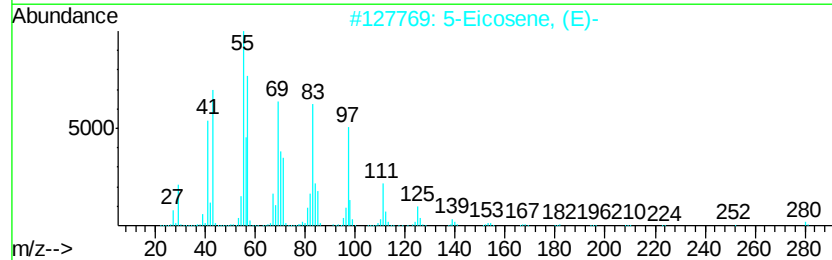
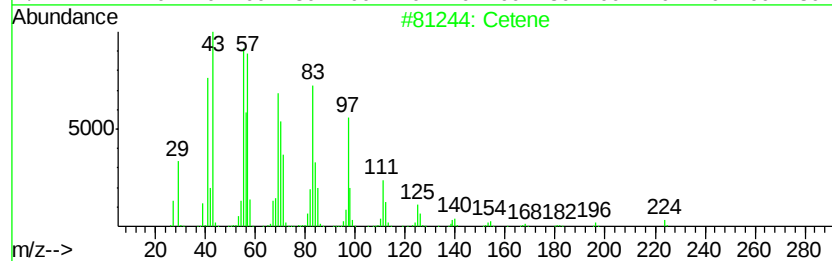
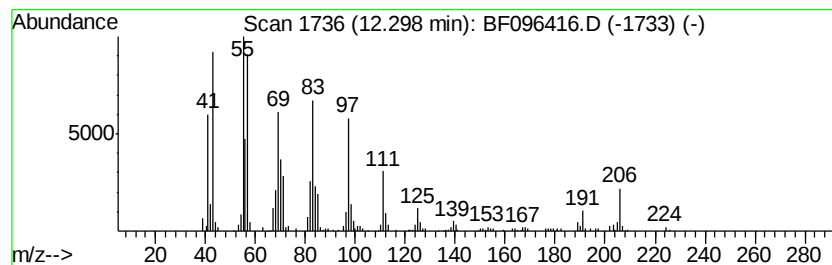
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BNA_F
ClientSampleId :
B6-4-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cetene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	7.25 ng	299469	Phenanthrene-d10	11.24
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Cetene	224 C16H32	000629-73-2	92
2	5-Eicosene, (E)-	280 C20H40	074685-30-6	87
3	1-Octadecanol	270 C18H38O	000112-92-5	87
4	Pentafluoropropionic acid, tetra...	360 C17H29F5O2	006222-06-6	83
5	3-Chloropropionic acid, heptadec...	346 C20H39ClO2	1000283-05-1	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096416.D
Acq On : 2 Jul 2017 15:17
Operator : SJ/MA
Sample : I3950-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B6-4-6

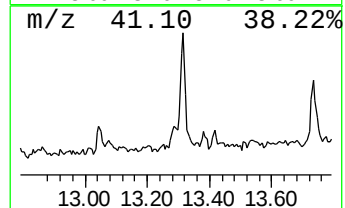
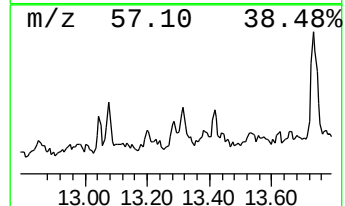
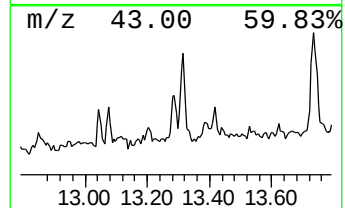
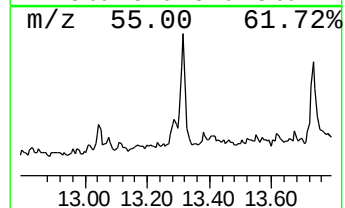
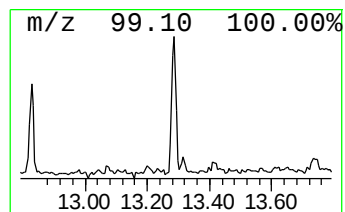
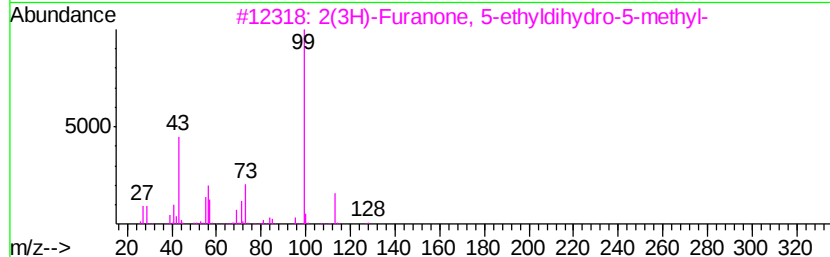
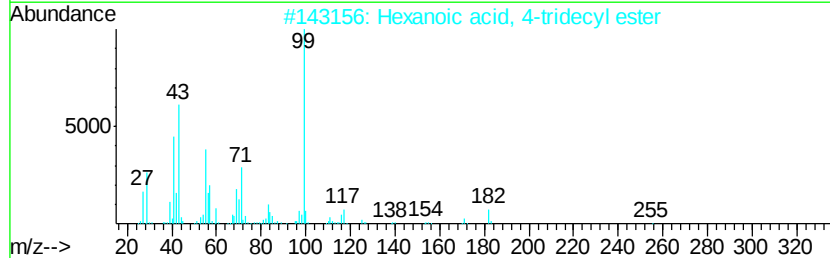
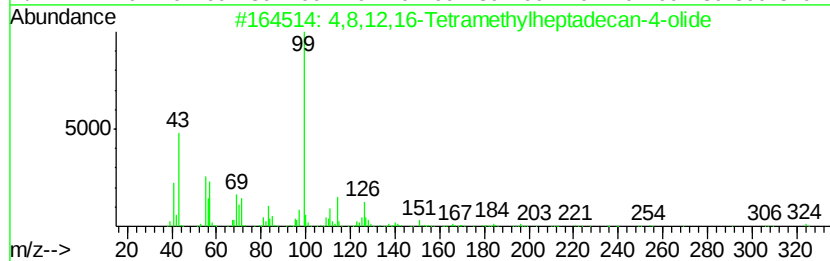
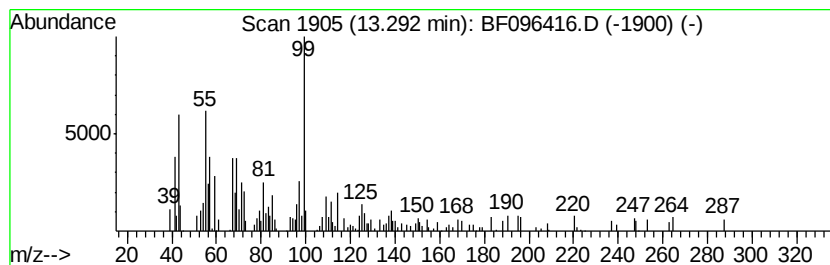
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4,8,12,16-Tetramethylheptad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.29	2.59 ng	102084	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	72	
2	Hexanoic acid, 4-tridecyl ester	298	C19H38O2	1000279-29-3	53	
3	2(3H)-Furanone, 5-ethylidihydro-5...	128	C7H12O2	002865-82-9	50	
4	Hexanamide, N-allyl-	155	C9H17NO	1000340-13-9	50	
5	2(3H)-Furanone, 5-butyldihydro-4...	156	C9H16O2	055013-32-6	47	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096416.D
Acq On : 2 Jul 2017 15:17
Operator : SJ/MA
Sample : I3950-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B6-4-6

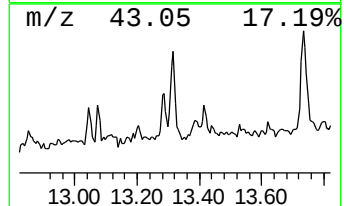
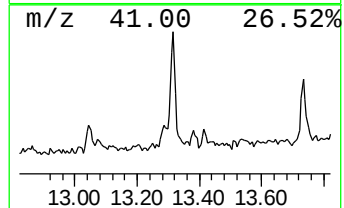
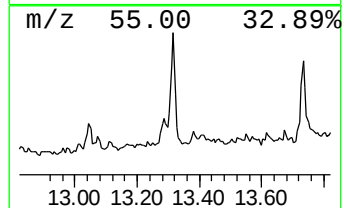
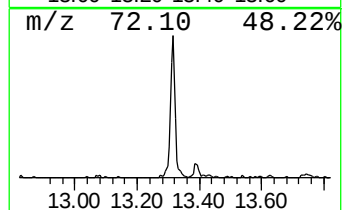
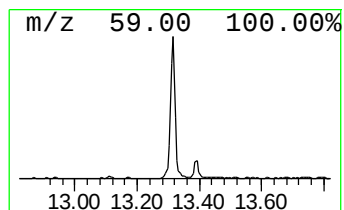
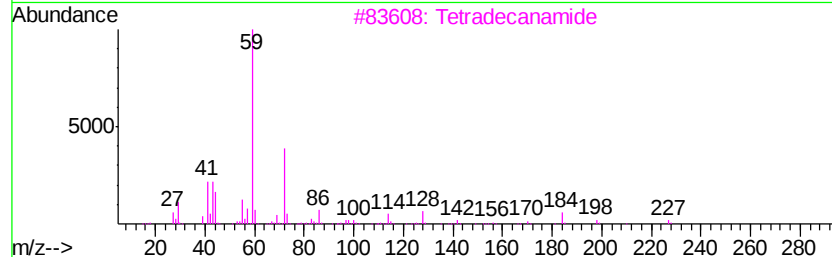
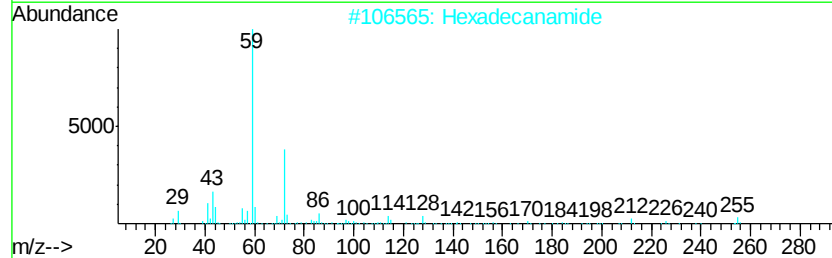
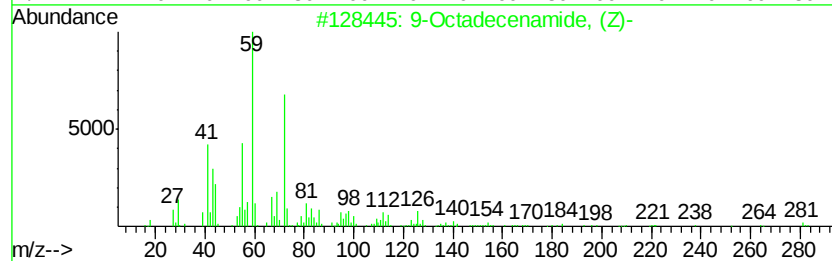
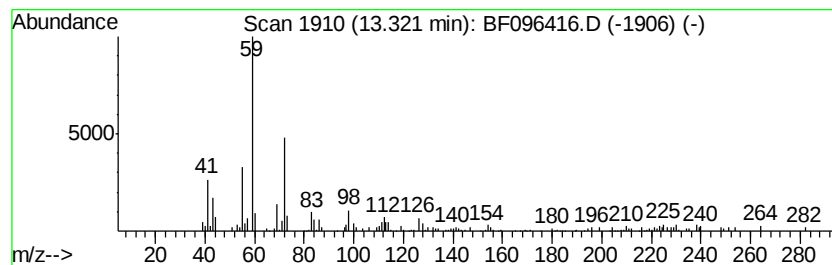
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	6.84 ng	269469	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2		Hexadecanamide	255	C16H33NO	000629-54-9	78
3		Tetradecanamide	227	C14H29NO	000638-58-4	72
4		Nonadecanamide	297	C19H39NO	058185-32-3	64
5		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096416.D
Acq On : 2 Jul 2017 15:17
Operator : SJ/MA
Sample : I3950-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

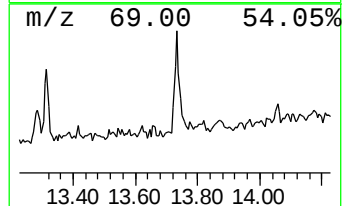
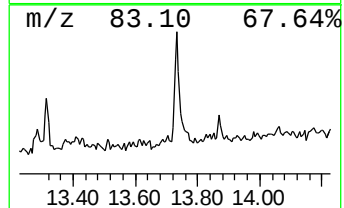
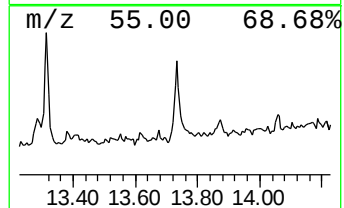
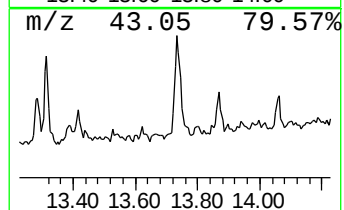
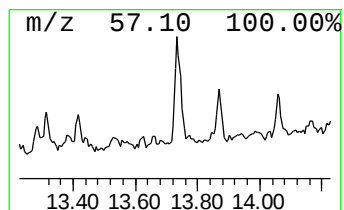
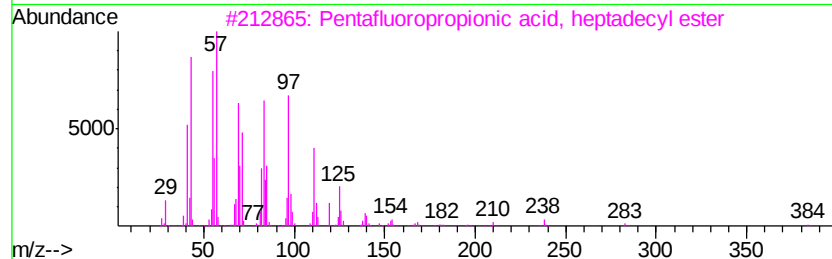
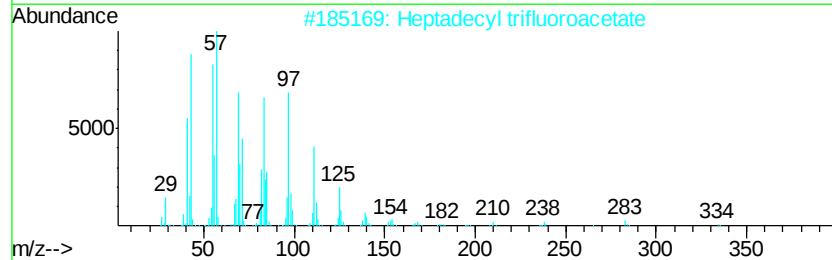
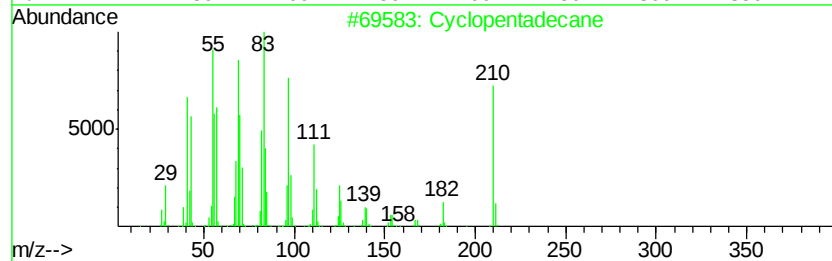
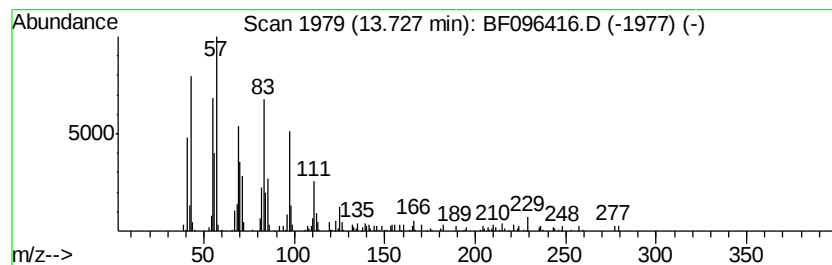
Instrument :
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ClientSampleID :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclopentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.89 ng	192531	Chrysene-d12	13.87
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Cyclopentadecane	210 C15H30	000295-48-7	94
2	Heptadecyl trifluoroacetate	352 C19H35F3O2	1000351-87-0	93
3	Pentafluoropropionic acid, hepta...	402 C20H35F5O2	959218-78-1	93
4	Pentafluoropropionic acid, hexad...	388 C19H33F5O2	006222-07-7	91
5	10-Heneicosene (c,t)	294 C21H42	095008-11-0	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070217\
Data File : BF096416.D
Acq On : 2 Jul 2017 15:17
Operator : SJ/MA
Sample : I3950-15
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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...	4.94	15.1	ng	684847	1	6.73	904490	20.0
unknown6.50	6.50	80.1	ng	3621210	1	6.73	904490	20.0
Tridecane	10.68	5.1	ng	211274	4	11.24	826530	20.0
Pentadecanoic acid	11.79	3.8	ng	155198	4	11.24	826530	20.0
Cetene	12.30	7.3	ng	299469	4	11.24	826530	20.0
4,8,12,16-Tetrame...	13.29	2.6	ng	102084	5	13.87	788055	20.0
9-Octadecenamide,...	13.32	6.8	ng	269469	5	13.87	788055	20.0
Cyclopentadecane	13.73	4.9	ng	192531	5	13.87	788055	20.0