

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
 Data File : BF096545.D
 Acq On : 6 Jul 2017 20:43
 Operator : SJ/MA
 Sample : I3972-04
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B4A-18-18.5

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	4.904	475	479	491	rVB	277401	389638	14.99%	1.709%
2	5.334	546	552	555	rBV	2388166	2526668	97.20%	11.082%
3	6.357	720	726	738	rVB	2407145	2599467	100.00%	11.401%
4	6.487	743	748	751	rBV	2624784	2460806	94.67%	10.793%
5	6.716	783	787	790	rBV	761882	672787	25.88%	2.951%
6	6.869	809	813	817	rBV	1941074	1842292	70.87%	8.080%
7	7.275	877	882	885	rBV	1678095	1498889	57.66%	6.574%
8	7.375	894	899	904	rBV2	23376	26076	1.00%	0.114%
9	7.992	1000	1004	1007	rBV	1002203	959883	36.93%	4.210%
10	8.710	1122	1126	1129	rBV	48686	41431	1.59%	0.182%
11	8.804	1139	1142	1146	rVB	35339	33993	1.31%	0.149%
12	9.075	1183	1188	1191	rBV	2683489	2307525	88.77%	10.121%
13	9.469	1251	1255	1258	rBV	251757	229411	8.83%	1.006%
14	9.698	1290	1294	1298	rVB	33175	28819	1.11%	0.126%
15	9.751	1298	1303	1306	rBV	933509	834201	32.09%	3.659%
16	9.781	1306	1308	1311	rVB	88998	65797	2.53%	0.289%
17	9.951	1335	1337	1341	rVB	43466	33501	1.29%	0.147%
18	10.192	1375	1378	1381	rVB	59810	48207	1.85%	0.211%
19	10.292	1393	1395	1399	rBV	61751	46945	1.81%	0.206%
20	10.416	1412	1416	1419	rBV	22269	29863	1.15%	0.131%
21	10.533	1432	1436	1441	rBV	1229987	1134374	43.64%	4.975%
22	10.663	1455	1458	1467	rBV	69297	91498	3.52%	0.401%
23	11.116	1531	1535	1538	rBV3	46018	48985	1.88%	0.215%
24	11.228	1550	1554	1557	rBV	767925	682989	26.27%	2.996%
25	11.251	1557	1558	1562	rVB	183898	110094	4.24%	0.483%
26	11.304	1562	1567	1570	rVB	44181	45402	1.75%	0.199%
27	11.839	1655	1658	1661	rBV	34858	36907	1.42%	0.162%
28	12.439	1756	1760	1763	rBV	199057	170955	6.58%	0.750%
29	12.486	1765	1768	1774	rVB	69618	63579	2.45%	0.279%
30	12.663	1793	1798	1802	rBV	170512	184251	7.09%	0.808%
31	12.816	1820	1824	1827	rVB	1690175	1504845	57.89%	6.600%
32	13.063	1863	1866	1869	rVB	37852	31984	1.23%	0.140%
33	13.098	1869	1872	1875	rBV	21848	27223	1.05%	0.119%
34	13.722	1973	1978	1985	rBV2	107400	143905	5.54%	0.631%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096545.D
Acq On : 6 Jul 2017 20:43
Operator : SJ/MA
Sample : I3972-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B4A-18-18.5

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

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

35	13.863	1995	2002	2005	rBV	858353	881189	33.90%	3.865%
36	13.886	2005	2006	2009	rVB	80093	47808	1.84%	0.210%
37	13.969	2017	2020	2024	rBV4	28789	38733	1.49%	0.170%
38	14.351	2082	2085	2088	rBV3	20841	26904	1.03%	0.118%
39	14.716	2144	2147	2151	rBV4	20080	30429	1.17%	0.133%
40	14.868	2170	2173	2176	rBV	62081	88173	3.39%	0.387%
41	14.968	2187	2190	2198	rBV4	38698	71145	2.74%	0.312%
42	15.157	2219	2222	2227	rVB	36318	43703	1.68%	0.192%
43	15.216	2228	2232	2237	rVB	48889	61360	2.36%	0.269%
44	15.274	2237	2242	2246	rBV	439855	520339	20.02%	2.282%
45	15.321	2248	2250	2257	rVB5	27514	37060	1.43%	0.163%

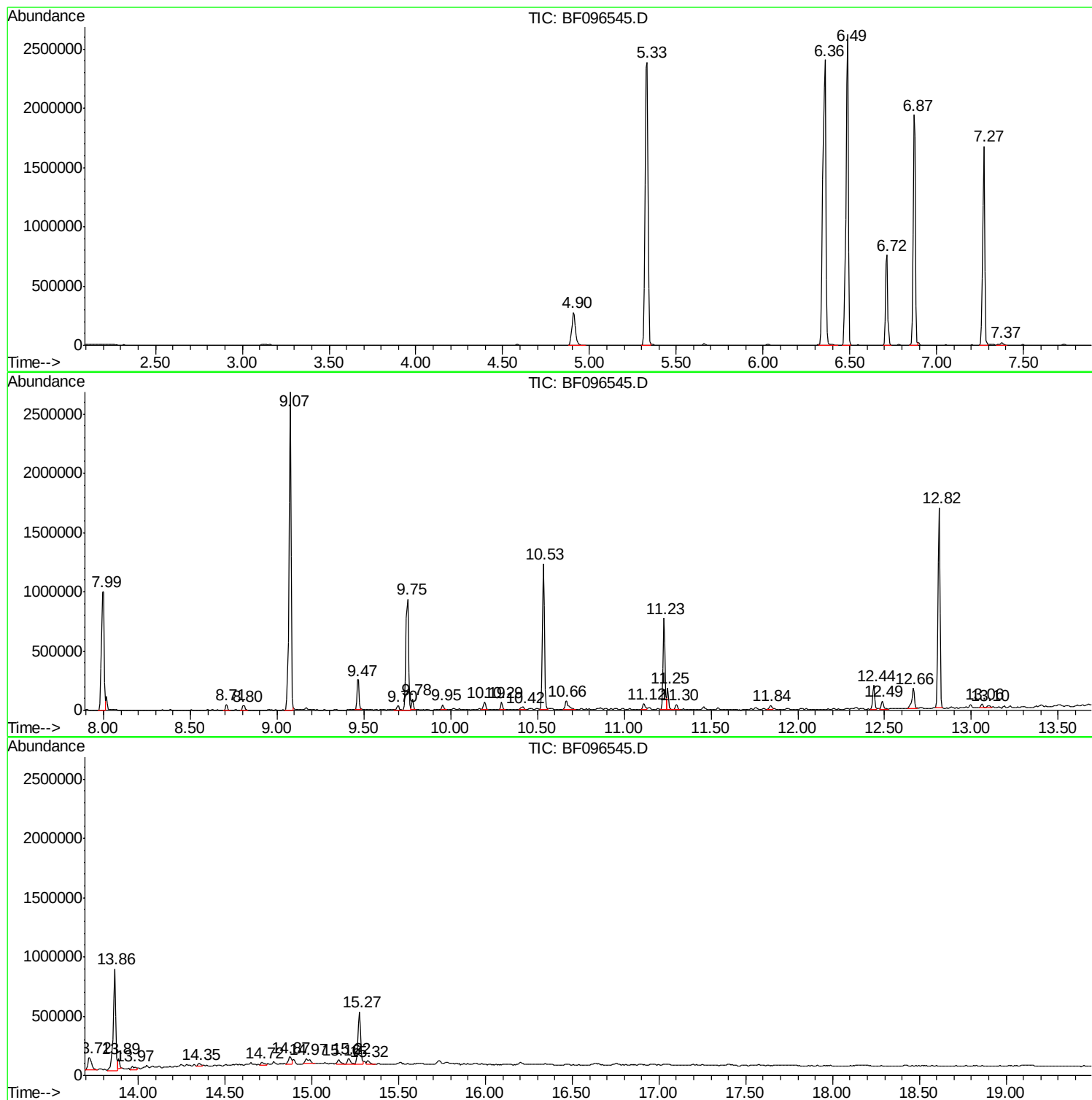
Sum of corrected areas: 22800033

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096545.D
Acq On : 6 Jul 2017 20:43
Operator : SJ/MA
Sample : I3972-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
B4A-18-18.5

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096545.D
Acq On : 6 Jul 2017 20:43
Operator : SJ/MA
Sample : I3972-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B4A-18-18.5

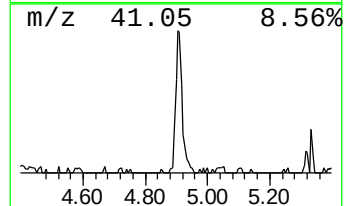
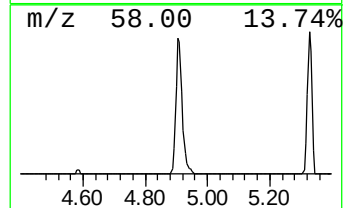
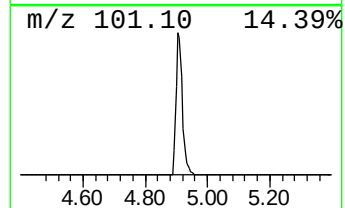
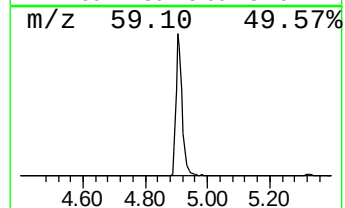
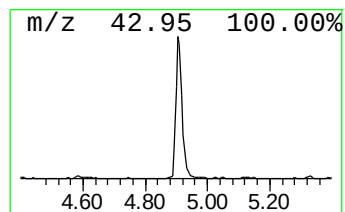
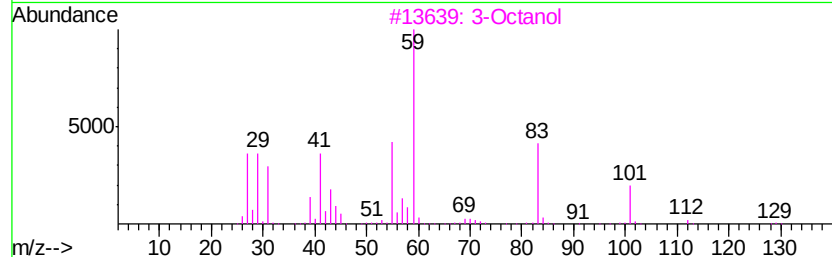
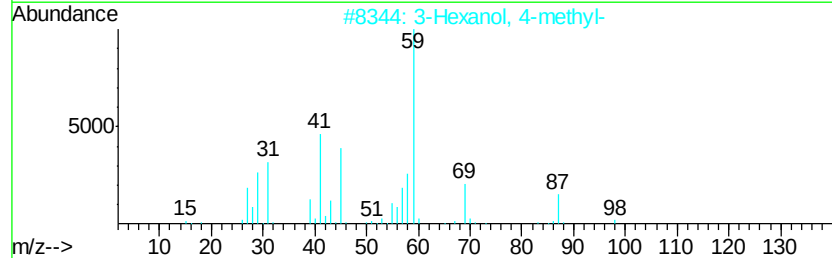
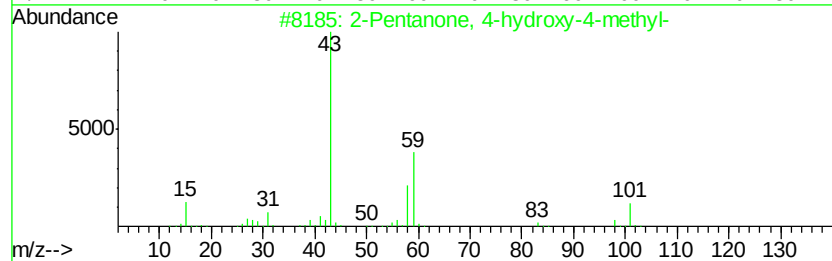
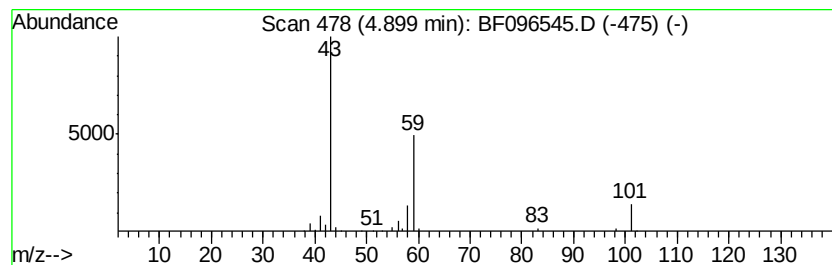
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.90	11.58 ng	389638	1,4-Dichlorobenzene-d4	6.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
3	3-Octanol	130	C8H18O	000589-98-0	33	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096545.D
Acq On : 6 Jul 2017 20:43
Operator : SJ/MA
Sample : I3972-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B4A-18-18.5

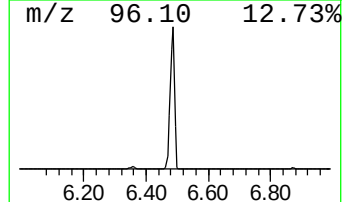
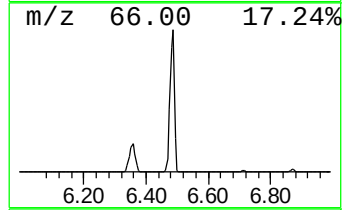
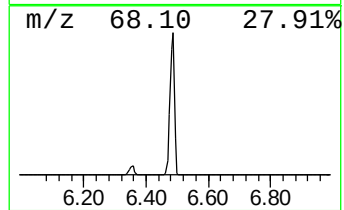
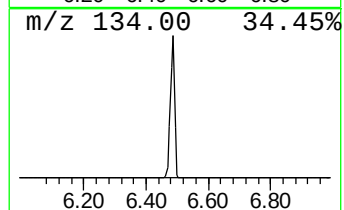
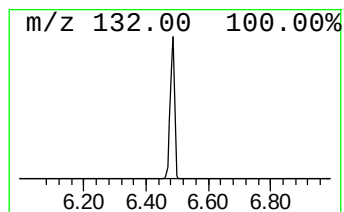
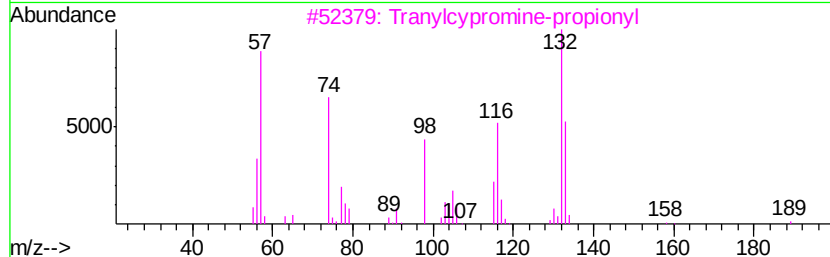
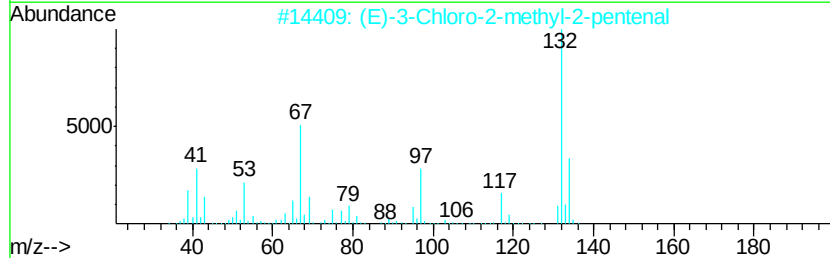
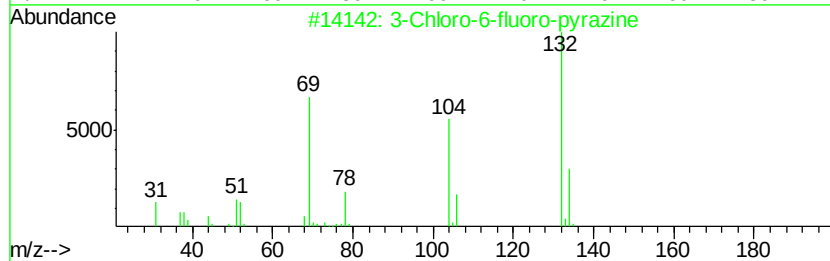
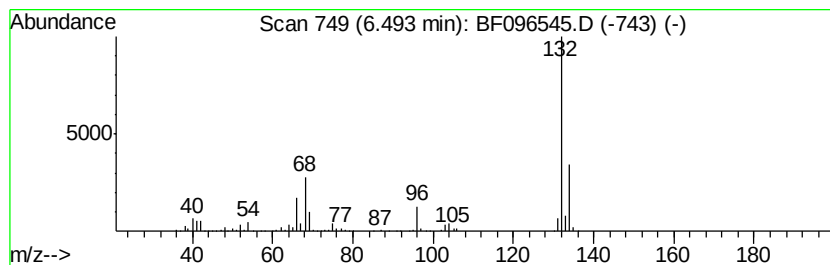
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	73.15 ng	2460810	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096545.D
Acq On : 6 Jul 2017 20:43
Operator : SJ/MA
Sample : I3972-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B4A-18-18.5

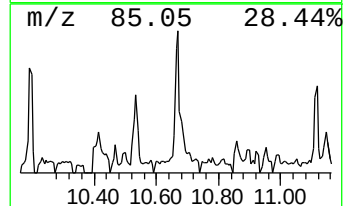
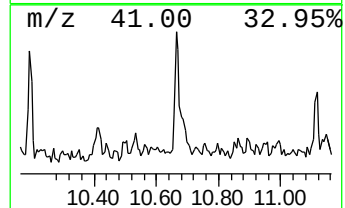
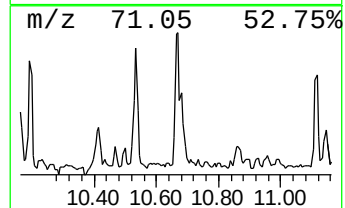
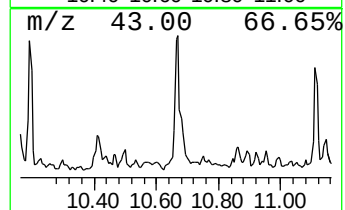
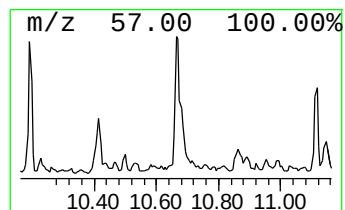
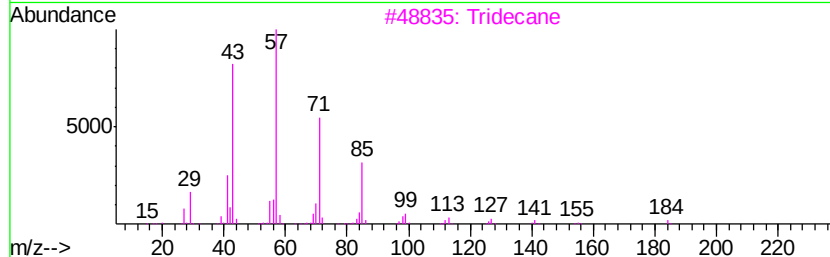
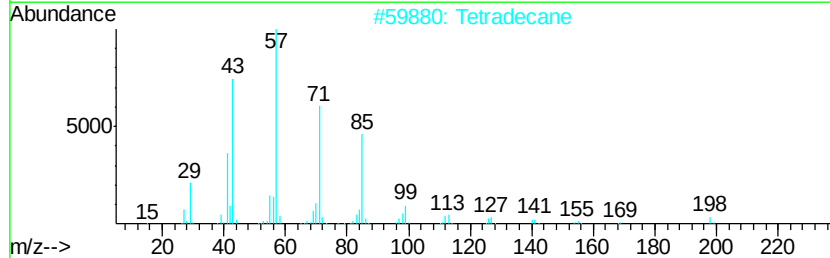
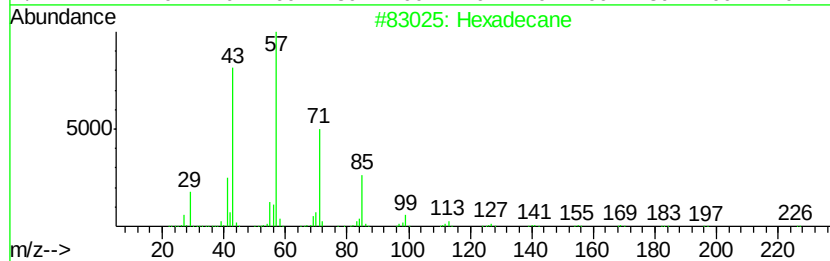
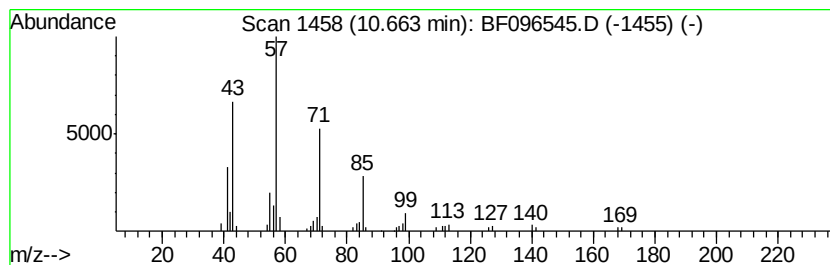
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.68 ng	91498	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Tetradecane		198	C14H30	000629-59-4	86
3	Tridecane		184	C13H28	000629-50-5	80
4	Tridecane, 2-methyl-		198	C14H30	001560-96-9	72
5	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096545.D
Acq On : 6 Jul 2017 20:43
Operator : SJ/MA
Sample : I3972-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B4A-18-18.5

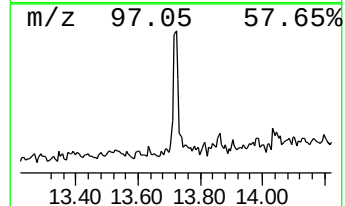
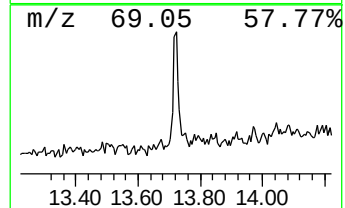
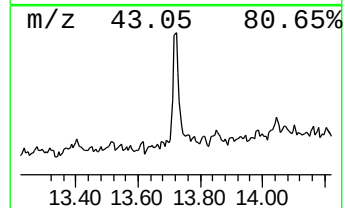
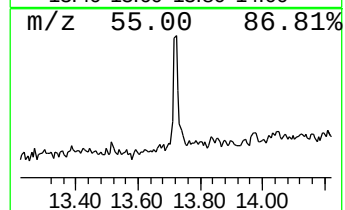
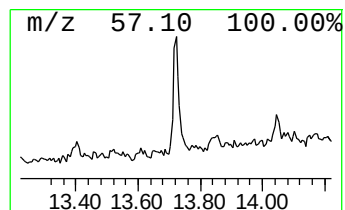
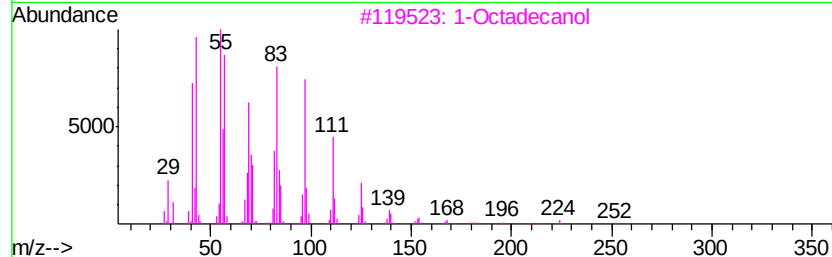
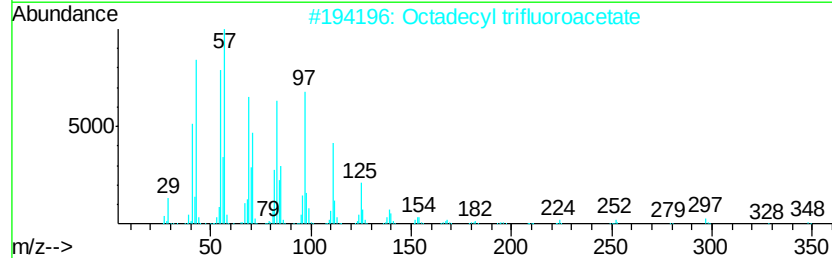
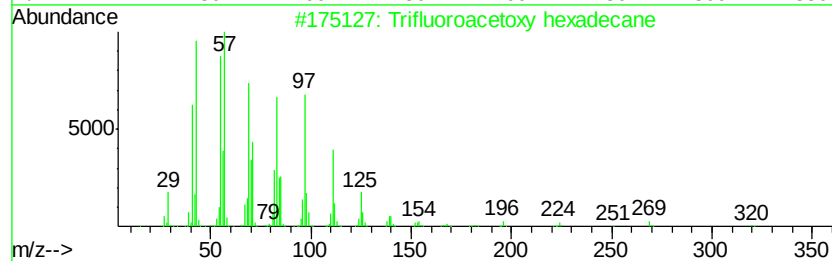
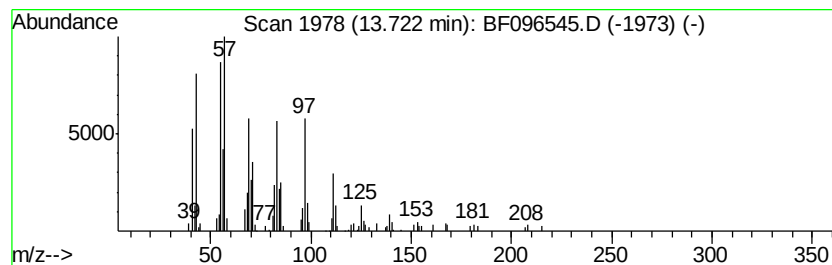
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	3.27 ng	143905	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3		1-Octadecanol	270	C18H38O	000112-92-5	91
4		1-Hexadecanol	242	C16H34O	036653-82-4	91
5		11-Tricosene	322	C23H46	052078-56-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096545.D
Acq On : 6 Jul 2017 20:43
Operator : SJ/MA
Sample : I3972-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B4A-18-18.5

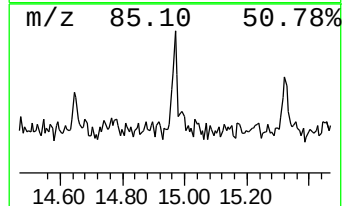
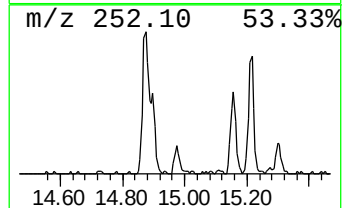
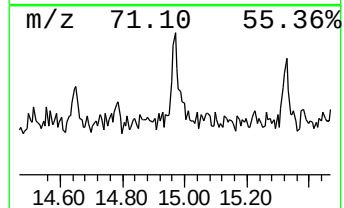
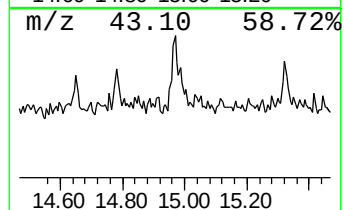
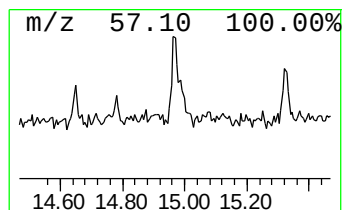
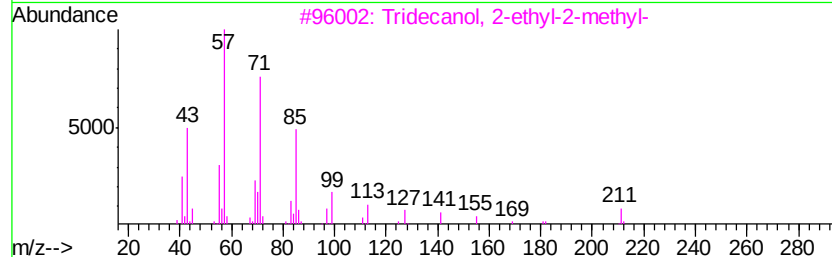
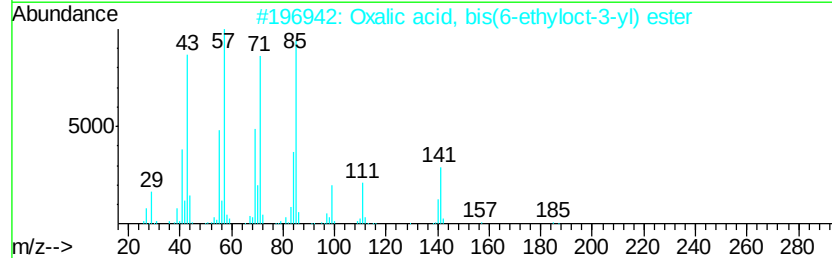
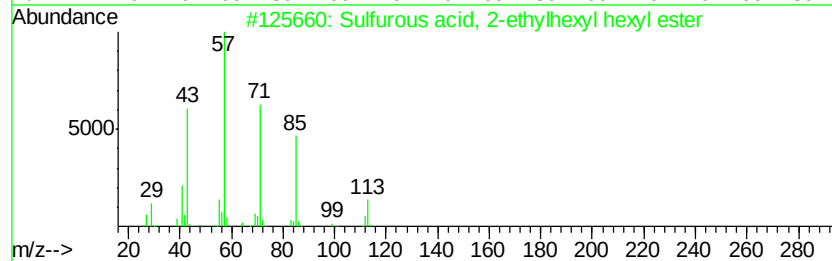
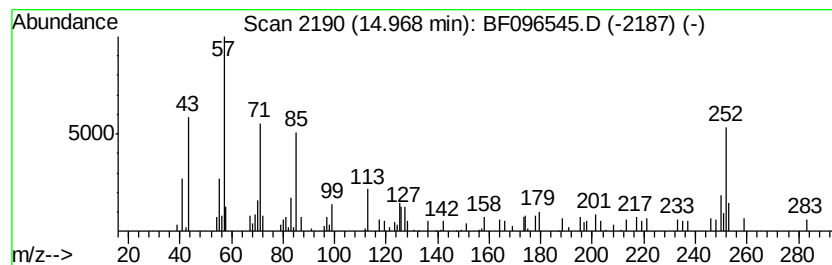
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.97 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	2.73 ng	71145	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	38
2		Oxalic acid, bis(6-ethyloct-3-yl...	370	C22H42O4	1000309-34-6	35
3		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	35
4		Undecane	156	C11H24	001120-21-4	35
5		Benzo[e]pyrene	252	C20H12	000192-97-2	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096545.D
Acq On : 6 Jul 2017 20:43
Operator : SJ/MA
Sample : I3972-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B4A-18-18.5

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...	4.90	11.6	ng	389638	1	6.72	672787	20.0
unknown6.49	6.49	73.2	ng	2460810	1	6.72	672787	20.0
Hexadecane	10.66	2.7	ng	91498	4	11.23	682989	20.0
Trifluoroacetoxy ...	13.72	3.3	ng	143905	5	13.86	881189	20.0
unknown14.97	14.97	2.7	ng	71145	6	15.27	520339	20.0