

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082317\
 Data File : BF097998.D
 Acq On : 23 Aug 2017 15:16
 Operator : SJ/JU
 Sample : I4908-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-04-082117-B

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-BF081517.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	3.099	168	172	189	rBV	86558	169823	4.32%	0.406%
2	4.934	481	484	496	rVB	318554	493776	12.55%	1.181%
3	5.351	549	555	558	rBV	3254099	3689779	93.76%	8.823%
4	6.381	724	730	733	rBV	3382545	3935548	100.00%	9.411%
5	6.510	747	752	755	rBV	3379702	3646031	92.64%	8.718%
6	6.739	787	791	794	rBV	1107354	900733	22.89%	2.154%
7	6.898	813	818	821	rBV	2952297	2766579	70.30%	6.616%
8	7.304	881	887	890	rBV	2312899	2414778	61.36%	5.774%
9	7.392	897	902	905	rVB4	36127	46256	1.18%	0.111%
10	8.022	1004	1009	1012	rBV	1429209	1196578	30.40%	2.861%
11	9.098	1186	1192	1195	rBV	3515812	3737808	94.98%	8.938%
12	9.492	1255	1259	1263	rVB	556006	445325	11.32%	1.065%
13	9.633	1279	1283	1288	rBV	169629	157530	4.00%	0.377%
14	9.775	1300	1307	1310	rBV	1316801	1204953	30.62%	2.881%
15	9.975	1338	1341	1344	rBV2	51414	46844	1.19%	0.112%
16	10.210	1378	1381	1385	rBV2	52553	46681	1.19%	0.112%
17	10.316	1396	1399	1405	rBV2	44057	55083	1.40%	0.132%
18	10.427	1412	1418	1423	rBV3	48783	99291	2.52%	0.237%
19	10.557	1436	1440	1444	rBV	1607196	1637737	41.61%	3.916%
20	10.680	1458	1461	1469	rBV3	102660	159741	4.06%	0.382%
21	11.127	1535	1537	1539	rBV2	49601	40705	1.03%	0.097%
22	11.157	1540	1542	1546	rVB2	71459	68438	1.74%	0.164%
23	11.251	1555	1558	1561	rBV	1083136	1035877	26.32%	2.477%
24	11.274	1561	1562	1567	rVV	340070	251839	6.40%	0.602%
25	11.327	1568	1571	1574	rVB	131254	114602	2.91%	0.274%
26	11.751	1641	1643	1646	rVB	54539	45072	1.15%	0.108%
27	11.780	1646	1648	1653	rBV2	90188	104421	2.65%	0.250%
28	11.827	1654	1656	1658	rVB2	57916	44598	1.13%	0.107%
29	11.863	1658	1662	1665	rBV	129461	157911	4.01%	0.378%
30	12.051	1691	1694	1696	rBV	44108	42539	1.08%	0.102%
31	12.304	1734	1737	1739	rBV	76472	77189	1.96%	0.185%
32	12.386	1748	1751	1752	rBV2	52130	49683	1.26%	0.119%
33	12.463	1760	1764	1767	rVB	731744	626047	15.91%	1.497%
34	12.692	1797	1803	1806	rBV	595393	691597	17.57%	1.654%

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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	12.810	1820	1823	1824	rBV	47567	45515	1.16%	0.109%
36	12.839	1824	1828	1832	rVV	2406382	2462256	62.56%	5.888%
37	12.992	1852	1854	1856	rBV2	49966	56059	1.42%	0.134%
38	13.015	1856	1858	1862	rVB	129376	121948	3.10%	0.292%
39	13.086	1867	1870	1872	rVB2	88324	89415	2.27%	0.214%
40	13.121	1873	1876	1879	rBV2	98739	99791	2.54%	0.239%
41	13.210	1889	1891	1894	rVB	64135	58108	1.48%	0.139%
42	13.245	1894	1897	1900	rBV	59155	64926	1.65%	0.155%
43	13.739	1978	1981	1988	rVB3	192957	265999	6.76%	0.636%
44	13.886	2001	2006	2008	rBV2	1063892	1321747	33.58%	3.161%
45	13.910	2008	2010	2013	rVB	375157	295459	7.51%	0.707%
46	14.304	2075	2077	2080	rVB	75796	61167	1.55%	0.146%
47	14.374	2085	2089	2101	rVV3	266668	473192	12.02%	1.132%
48	14.898	2175	2178	2186	rBV	412347	770535	19.58%	1.843%
49	15.009	2194	2197	2201	rVB2	214449	271459	6.90%	0.649%
50	15.186	2224	2227	2233	rVB	263880	324335	8.24%	0.776%
51	15.245	2233	2237	2243	rBV	388369	447027	11.36%	1.069%
52	15.304	2243	2247	2251	rBV	535741	698432	17.75%	1.670%
53	15.804	2329	2332	2340	rVB4	120239	219044	5.57%	0.524%
54	16.674	2476	2480	2491	rVB2	163159	339266	8.62%	0.811%
55	17.092	2547	2551	2560	rVB	127760	246588	6.27%	0.590%
56	17.233	2570	2575	2584	rBV6	124174	277383	7.05%	0.663%
57	19.192	2897	2908	2925	rVB4	771597	2608457	66.28%	6.237%

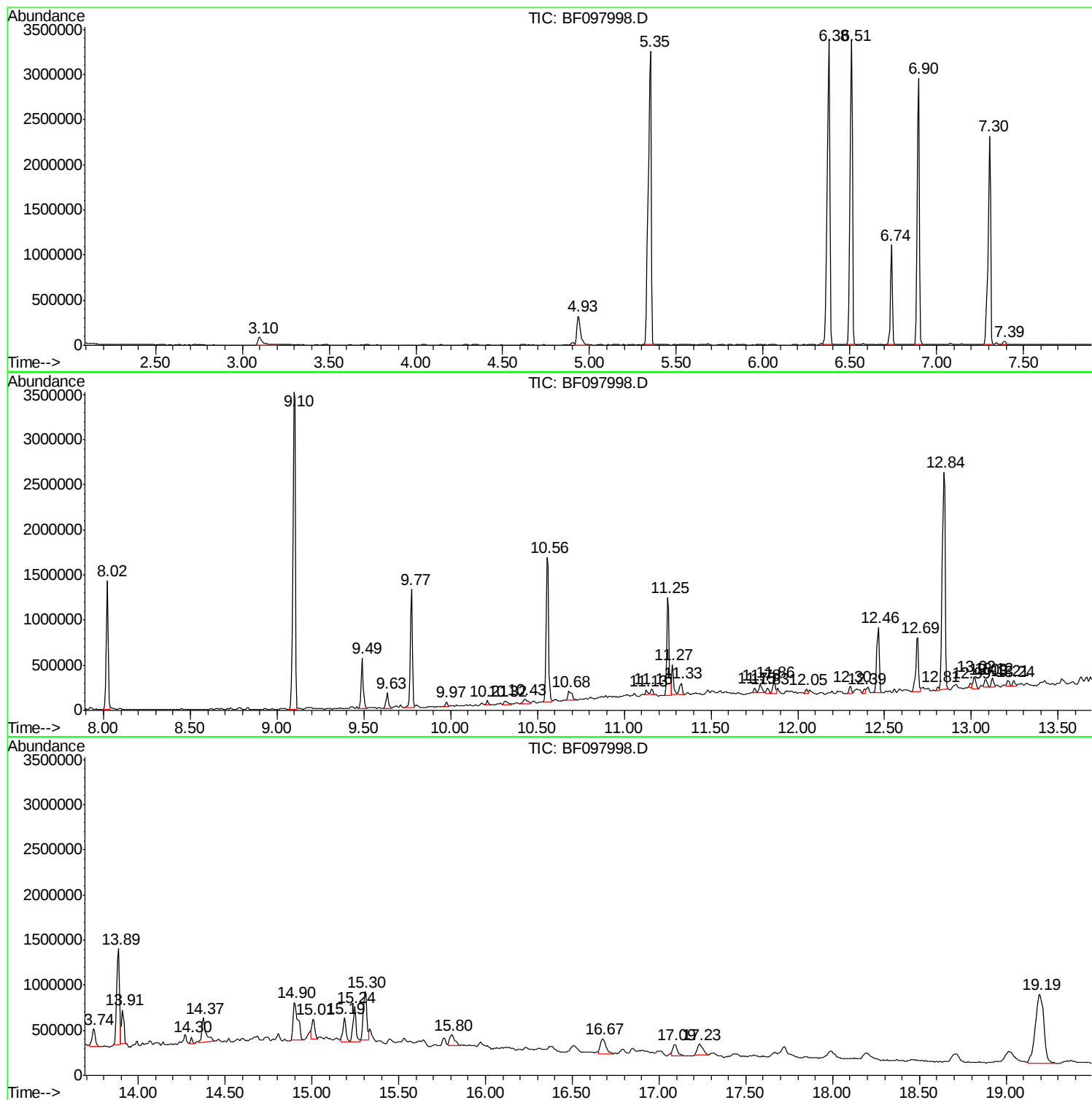
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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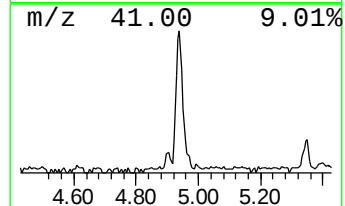
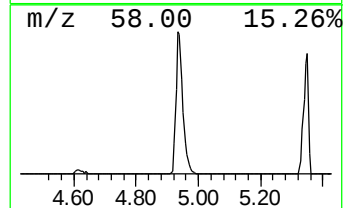
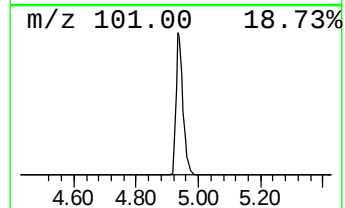
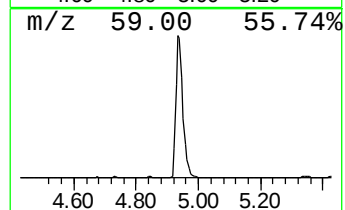
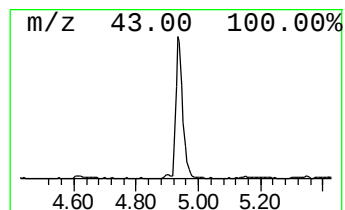
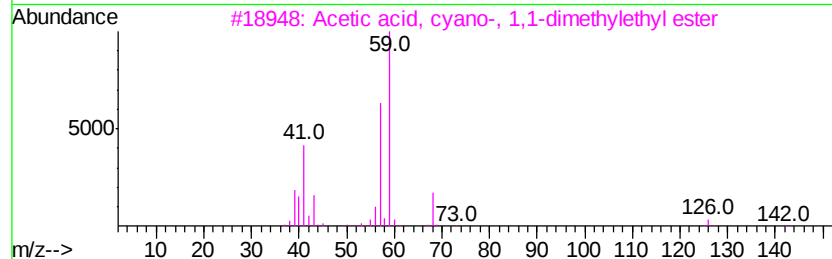
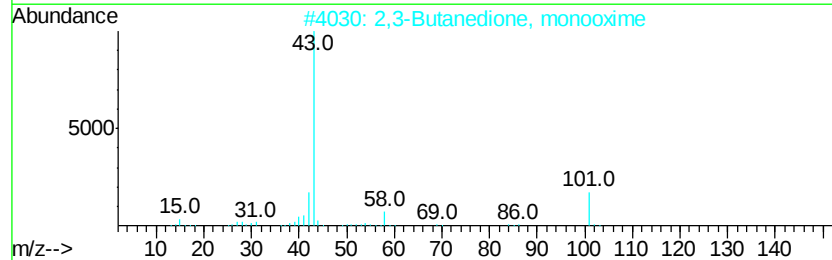
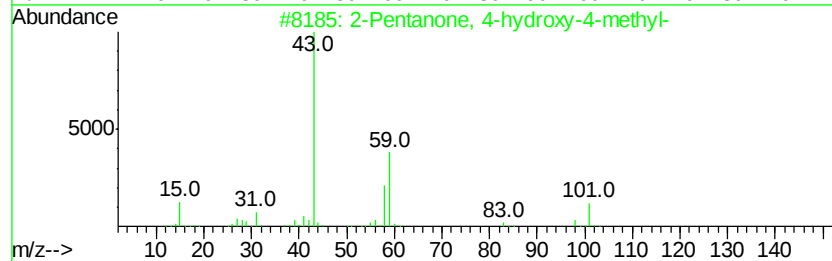
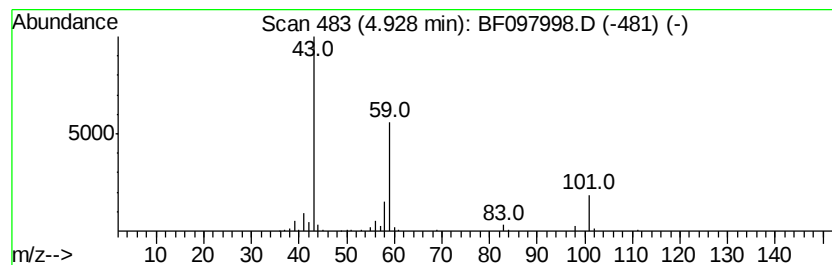
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	10.96 ng	493776	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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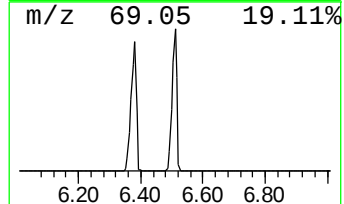
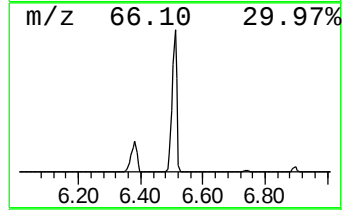
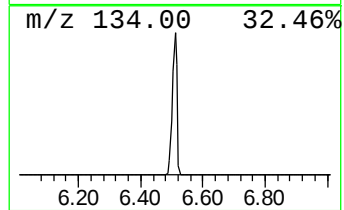
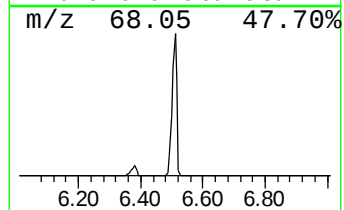
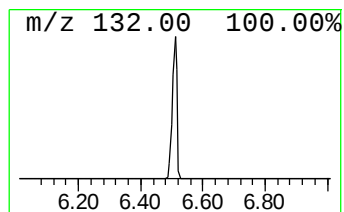
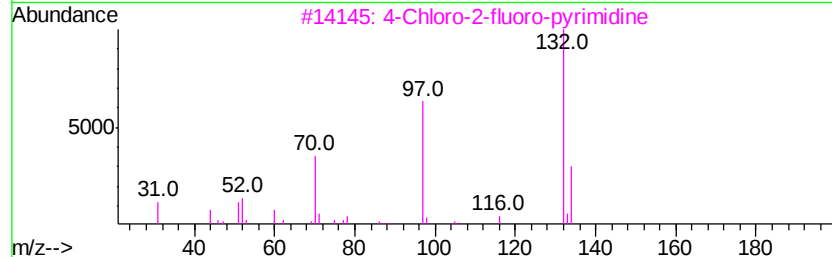
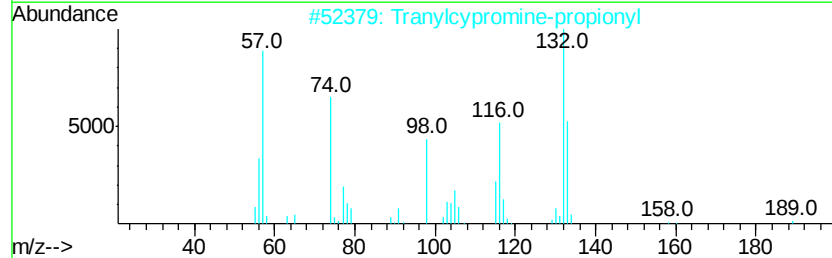
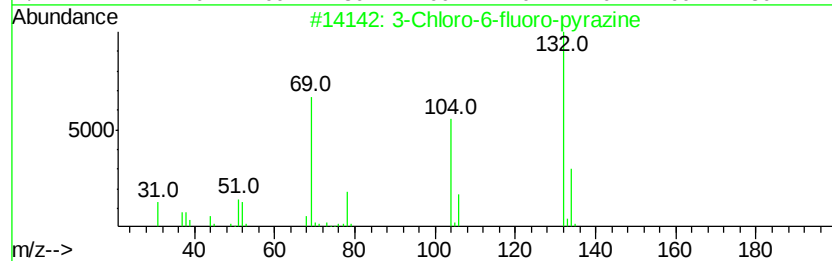
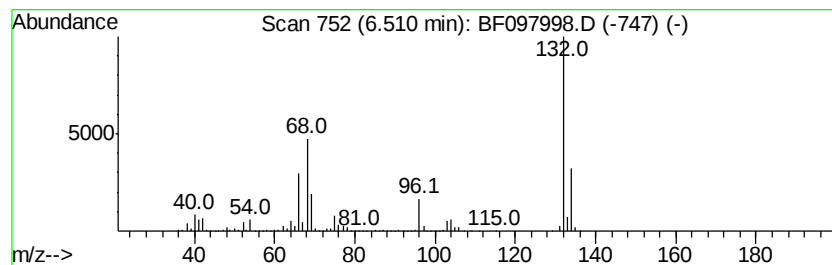
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	80.96 ng	3646030	1,4-Dichlorobenzene-d4	6.74

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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Xenon	132	Xe	007440-63-3	9



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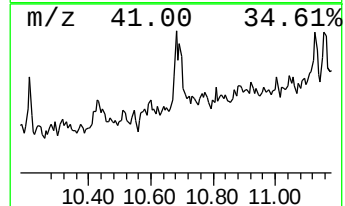
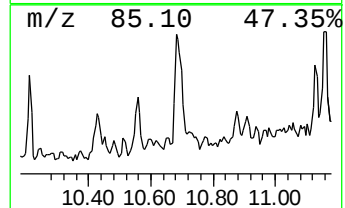
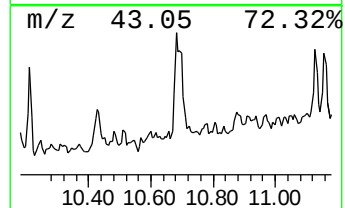
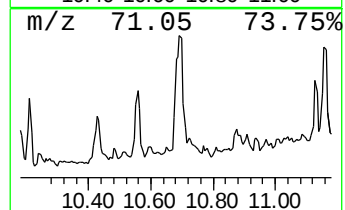
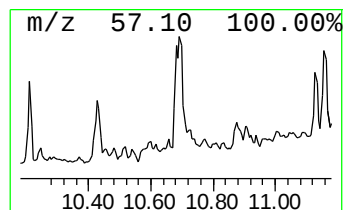
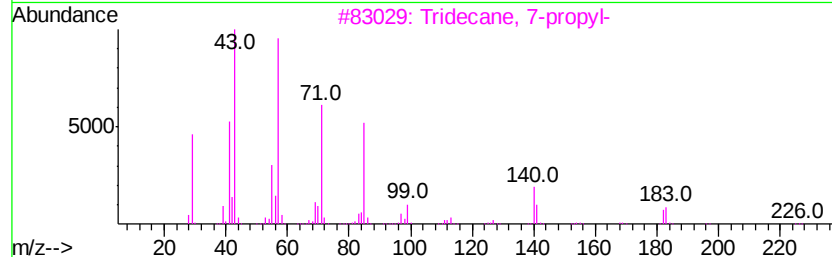
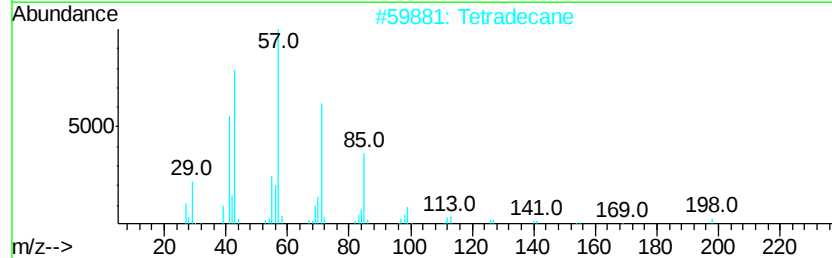
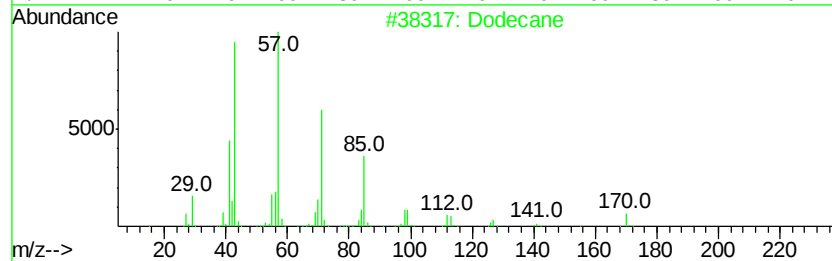
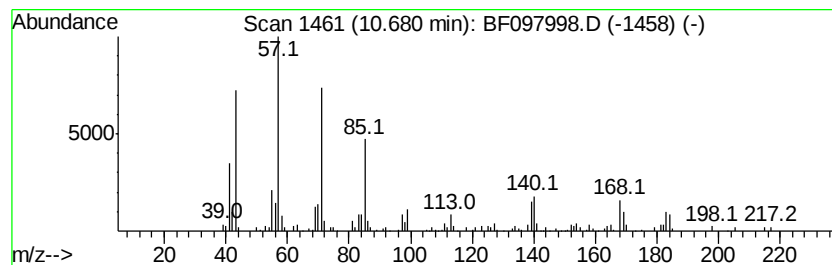
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Dodecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.68	3.08 ng	159741	Phenanthrene-d10	11.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	70
2	Tetradecane	198	C14H30	000629-59-4	64
3	Tridecane, 7-propyl-	226	C16H34	055045-09-5	64
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
5	Tridecane	184	C13H28	000629-50-5	62



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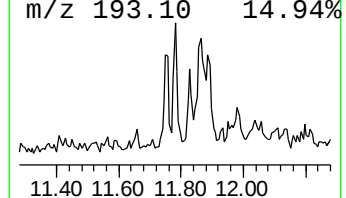
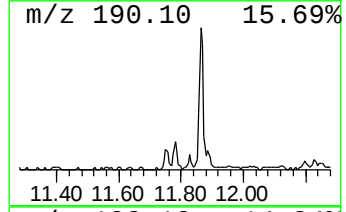
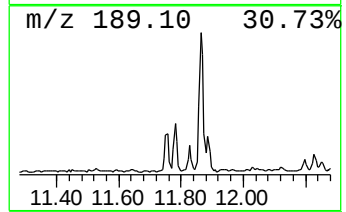
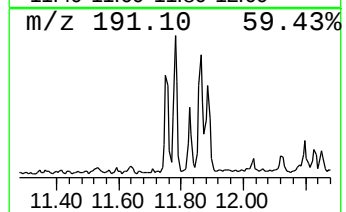
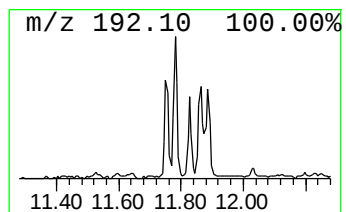
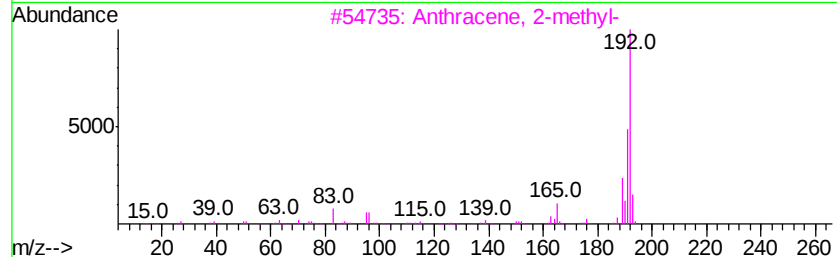
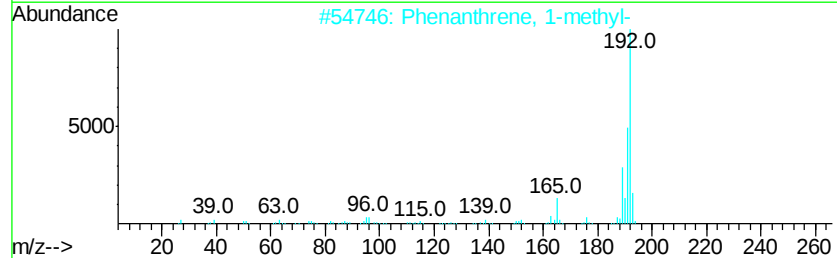
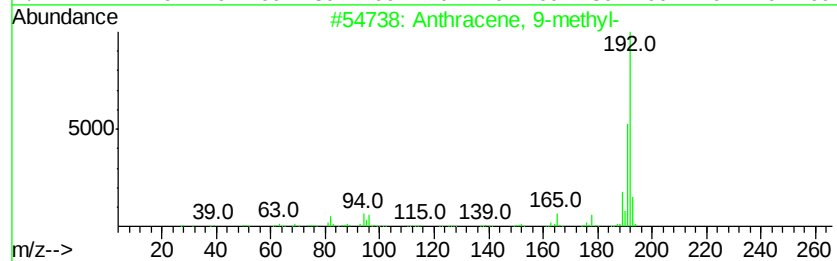
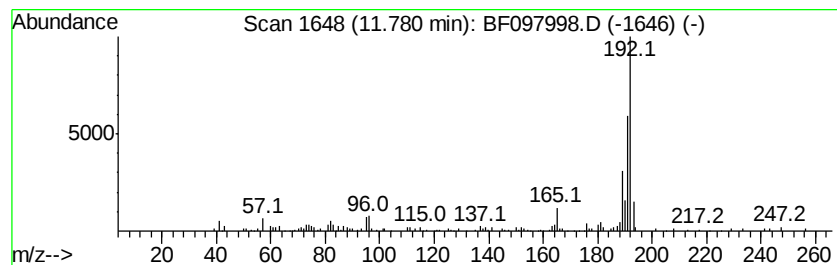
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Anthracene, 9-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	2.02 ng	104421	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	94
2		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
3		Anthracene, 2-methyl-	192	C15H12	000613-12-7	90
4		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	87
5		Anthracene, 1-methyl-	192	C15H12	000610-48-0	87



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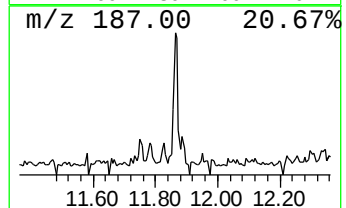
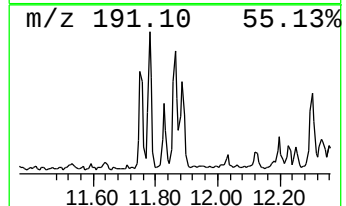
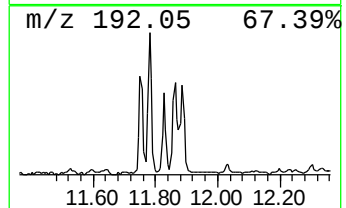
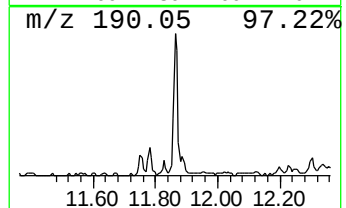
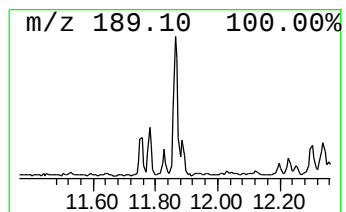
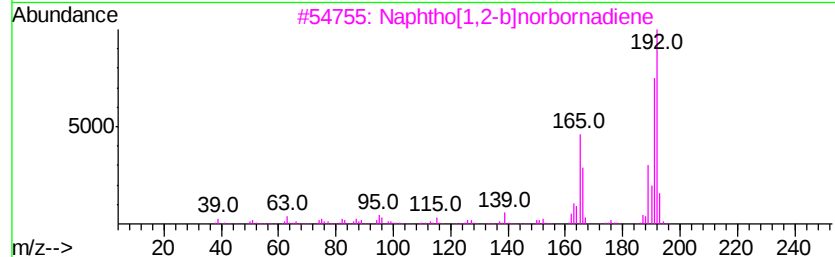
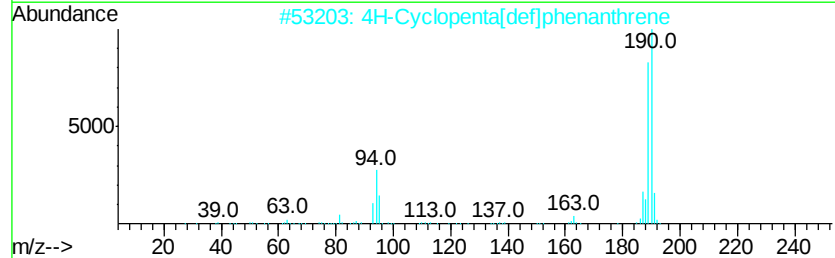
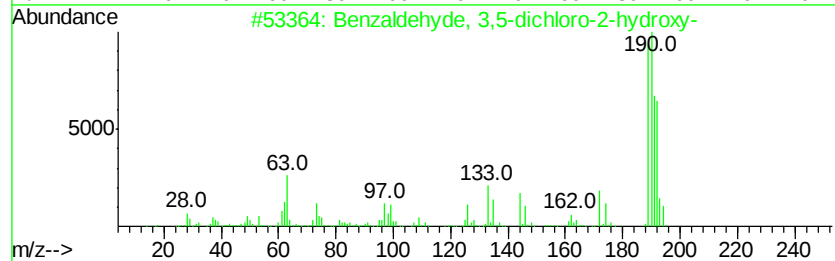
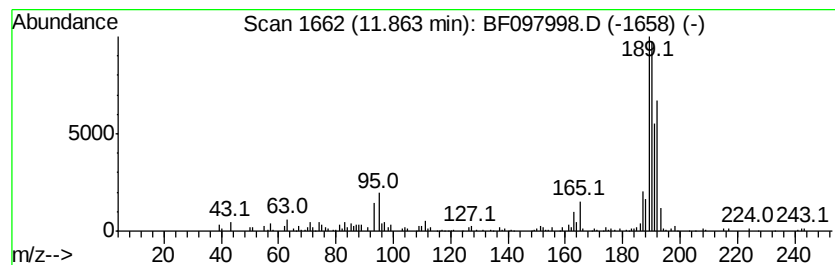
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ClientSampleId :
TR-04-082117-B

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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 Benzaldehyde, 3,5-dichloro-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.86	3.05 ng	157911	Phenanthrene-d10	11.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	62
3	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	42
4	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	38
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF082317\
Data File : BF097998.D
Acq On : 23 Aug 2017 15:16
Operator : SJ/JU
Sample : I4908-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-082117-B

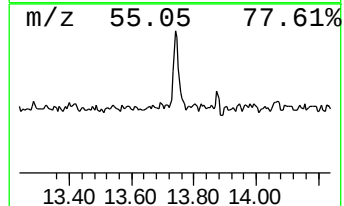
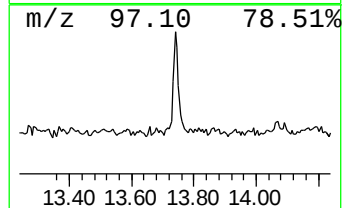
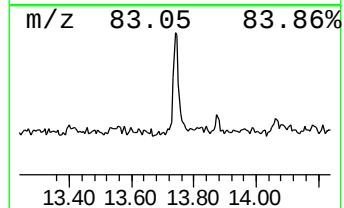
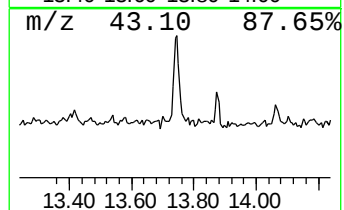
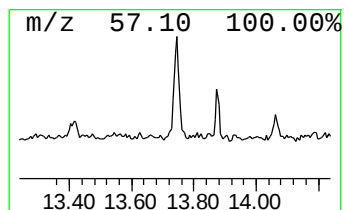
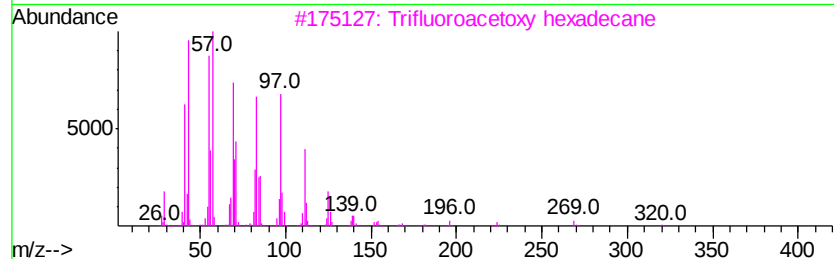
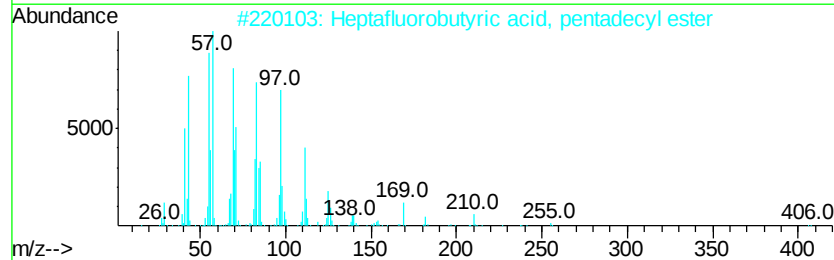
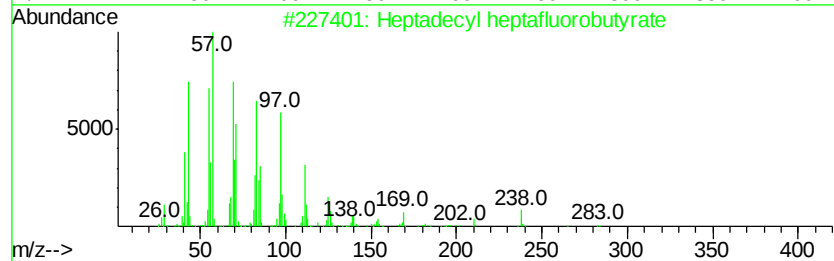
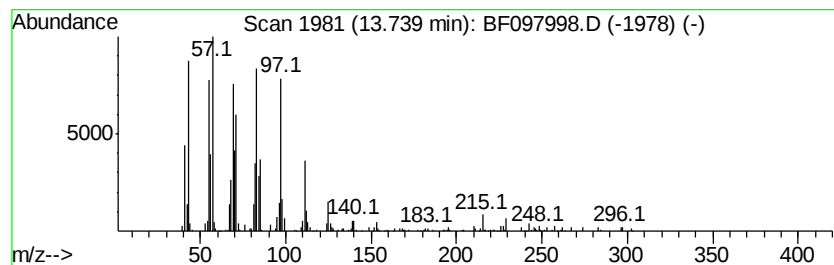
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecyl heptafluorobutyrate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	4.02 ng	265999	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4		1-Heneicosanol	312	C21H44O	015594-90-8	91
5		Behenic alcohol	326	C22H46O	000661-19-8	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF082317\
Data File : BF097998.D
Acq On : 23 Aug 2017 15:16
Operator : SJ/JU
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Misc :
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Instrument :
BNA_F
ClientSampleId :
TR-04-082117-B

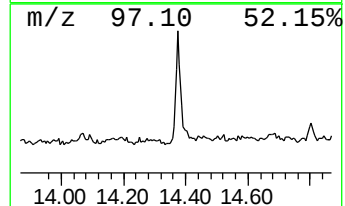
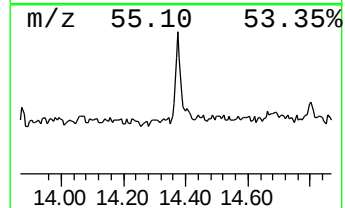
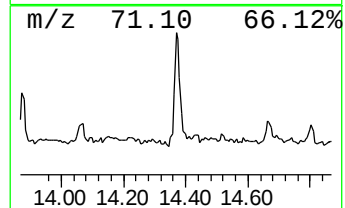
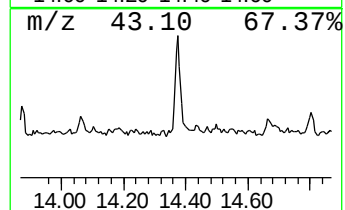
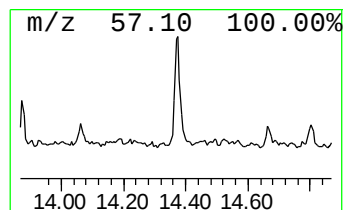
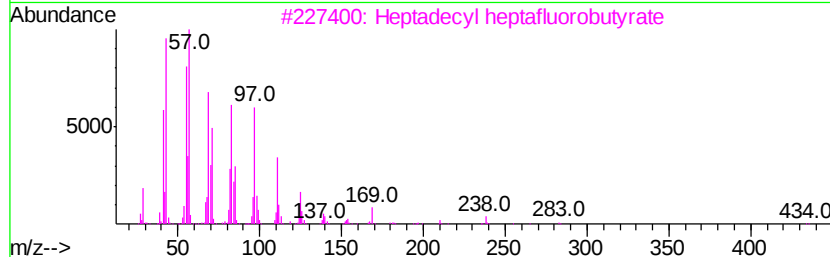
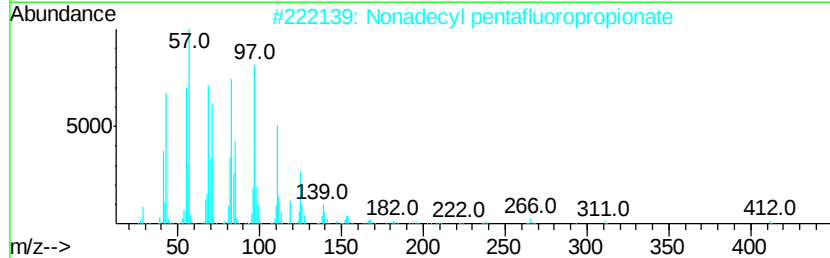
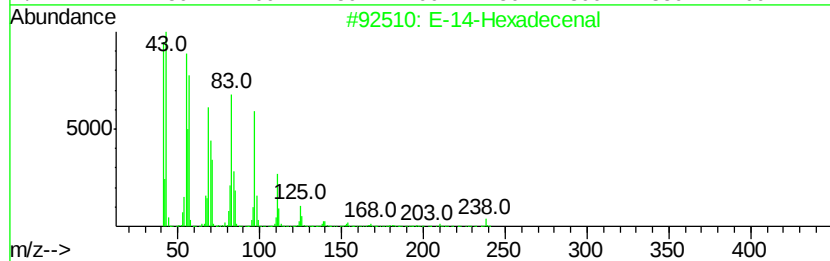
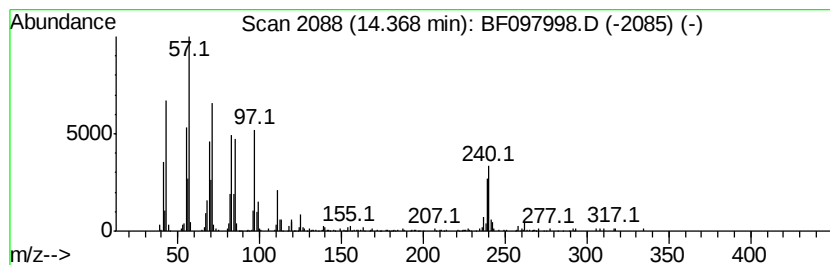
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 E-14-Hexadecenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	7.16 ng	473192	Chrysene-d12	13.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-14-Hexadecenal			238	C16H30O	330207-53-9	91
2	Nonadecyl pentafluoropropionate			430	C22H39F5O2	1000351-88-8	91
3	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	87
4	Ethanol, 2-(tetradecyloxy)-			258	C16H34O2	002136-70-1	87
5	9-Eicosene, (E)-			280	C20H40	074685-29-3	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF082317\
Data File : BF097998.D
Acq On : 23 Aug 2017 15:16
Operator : SJ/JU
Sample : I4908-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

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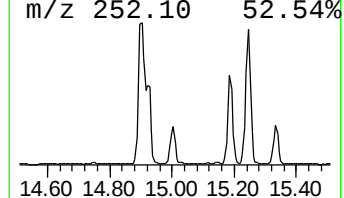
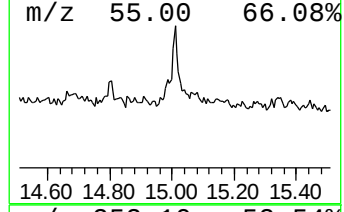
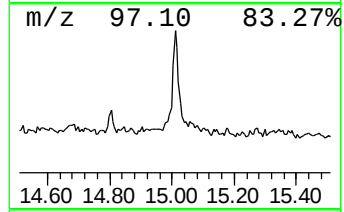
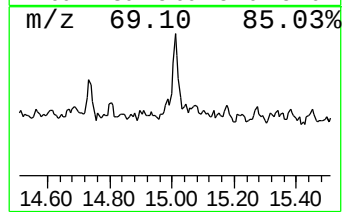
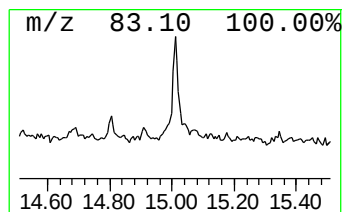
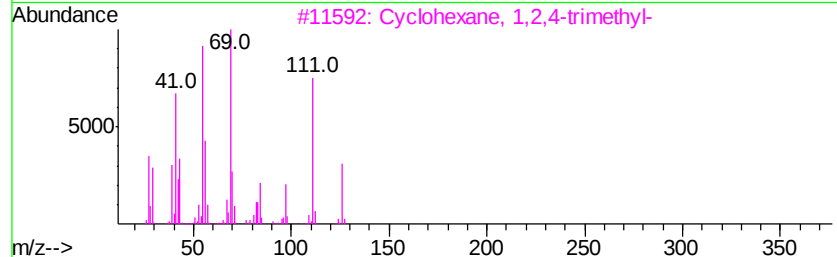
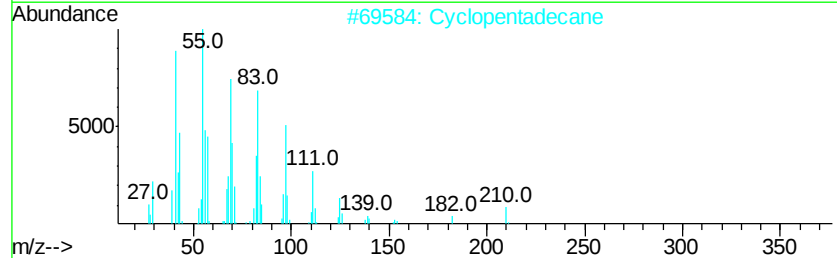
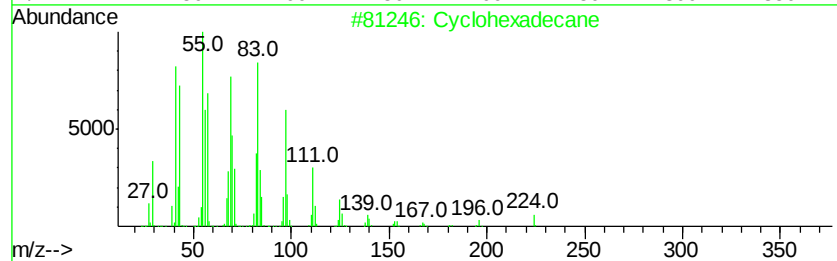
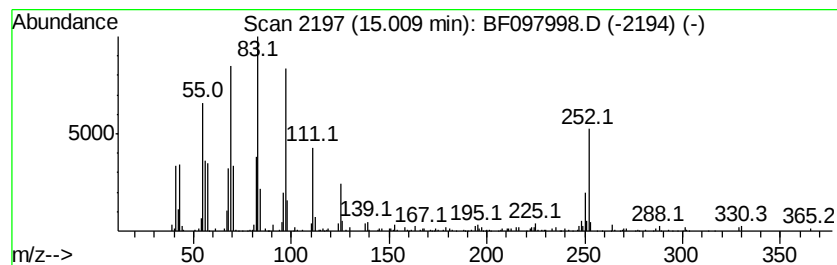
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclohexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	7.77 ng	271459	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexadecane	224	C16H32	000295-65-8	59
2		Cyclopentadecane	210	C15H30	000295-48-7	43
3		Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	38
4		Cyclopentane, 1,1,3,4-tetramethyl-	126	C9H18	020309-77-7	35
5		2-Thiopheneacetic acid, cyclohexyl-	224	C12H16O2S	1000278-95-9	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082317\
Data File : BF097998.D
Acq On : 23 Aug 2017 15:16
Operator : SJ/JU
Sample : I4908-04
Misc :
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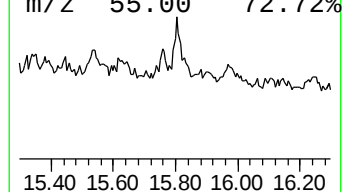
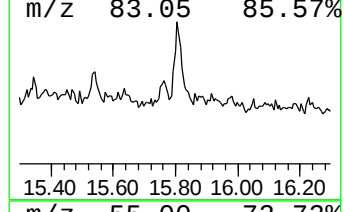
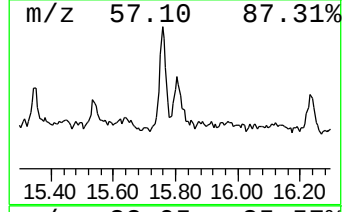
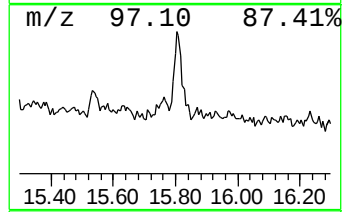
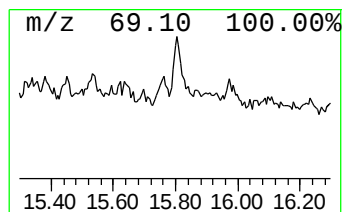
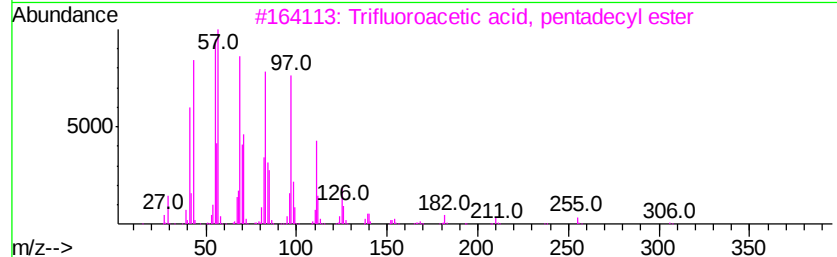
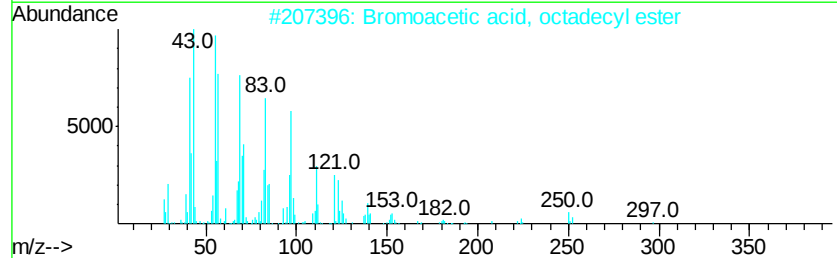
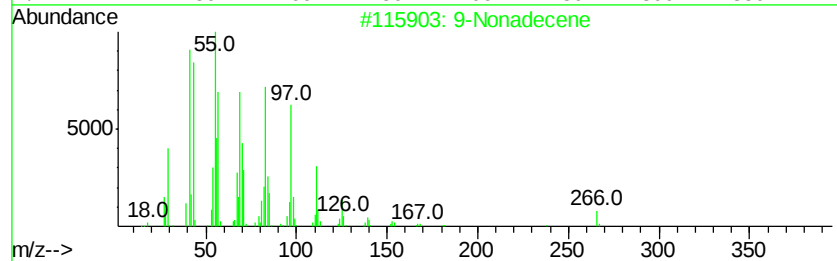
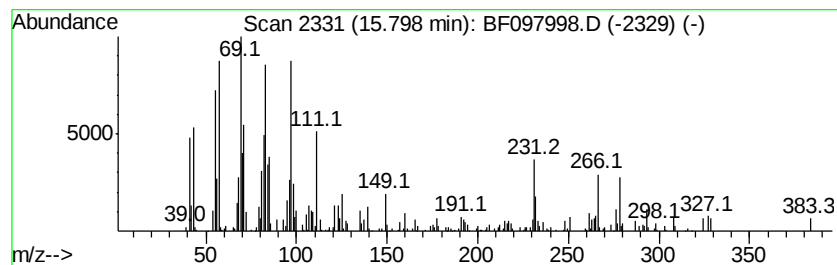
Instrument :
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 9-Nonadecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	6.27 ng	219044	Perylene-d12	15.30
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	9-Nonadecene	266 C19H38	031035-07-1	70
2	Bromoacetic acid, octadecyl ester	390 C20H39BrO2	018992-03-5	68
3	Trifluoroacetic acid, pentadecyl...	324 C17H31F3O2	959010-23-2	64
4	Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5	64
5	Pentafluoropropionic acid, penta...	374 C18H31F5O2	959092-08-1	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082317\
Data File : BF097998.D
Acq On : 23 Aug 2017 15:16
Operator : SJ/JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
TR-04-082117-B

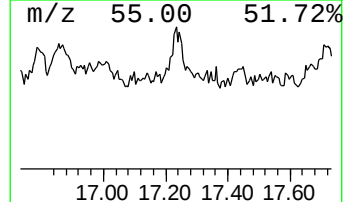
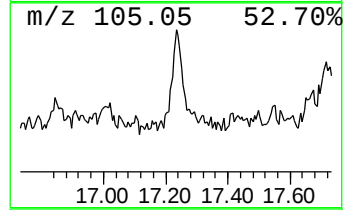
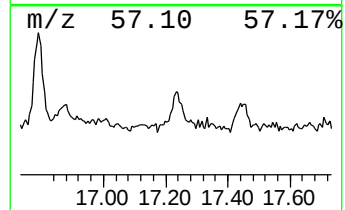
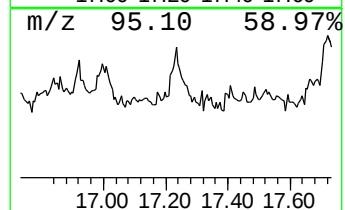
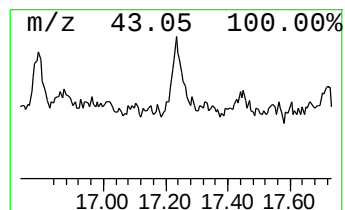
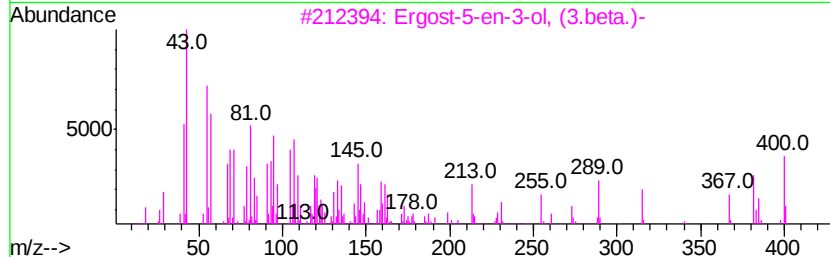
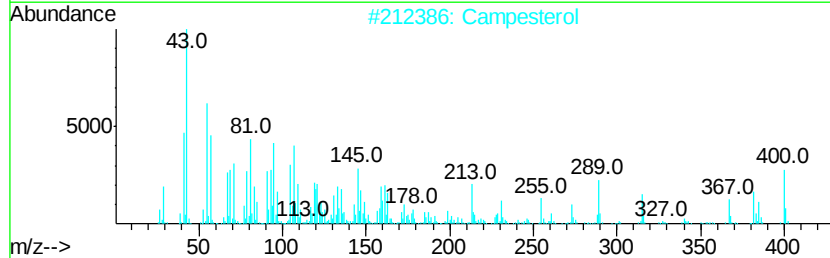
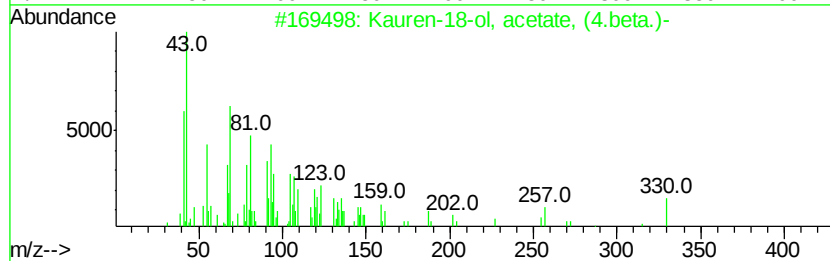
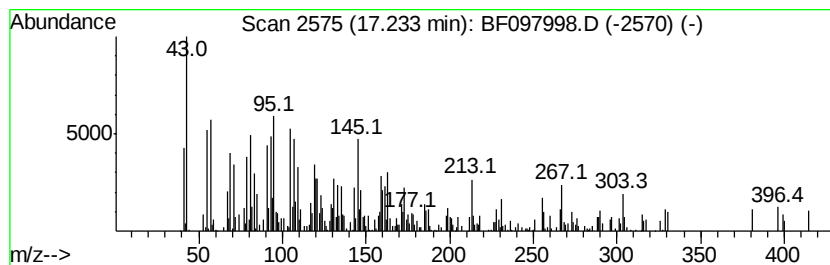
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.23 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.23	7.94 ng	277383	Perylene-d12	15.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Kauren-18-ol, acetate, (4.beta.)-	330	C22H34O2	072150-74-4	49
2			Campesterol	400	C28H48O	000474-62-4	43
3			Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	38
4			Isocholesterol methyl ether	400	C28H48O	029944-53-4	32
5			8-Methyl-9,11-tridecadienol prop...	266	C17H30O2	1000130-96-9	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082317\
Data File : BF097998.D
Acq On : 23 Aug 2017 15:16
Operator : SJ/JU
Sample : I4908-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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...	4.93	11.0	ng	493776	1	6.74	900733	20.0
unknown6.51	6.51	81.0	ng	3646030	1	6.74	900733	20.0
Dodecane	10.68	3.1	ng	159741	4	11.25	1035880	20.0
Anthracene, 9-met...	11.78	2.0	ng	104421	4	11.25	1035880	20.0
Benzaldehyde, 3,5...	11.86	3.0	ng	157911	4	11.25	1035880	20.0
Heptadecyl hepta...	13.74	4.0	ng	265999	5	13.89	1321750	20.0
E-14-Hexadecenal	14.37	7.2	ng	473192	5	13.89	1321750	20.0
Cyclohexadecane	15.01	7.8	ng	271459	6	15.30	698432	20.0
9-Nonadecene	15.80	6.3	ng	219044	6	15.30	698432	20.0
unknown17.23	17.23	7.9	ng	277383	6	15.30	698432	20.0
5-Bromo-4-oxo-4,5...	19.19	74.7	ng	2608460	6	15.30	698432	20.0