

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
 Data File : BF096488.D
 Acq On : 5 Jul 2017 17:10
 Operator : SJ/MA
 Sample : I3871-07
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 POSTEX-53-20170622

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	474	479	490	rBV	341772	501547	18.43%	2.156%
2	5.328	546	551	554	rBV	2728210	2696965	99.09%	11.592%
3	6.351	720	725	728	rBV	2473800	2721687	100.00%	11.698%
4	6.481	742	747	751	rBV	2603584	2662367	97.82%	11.443%
5	6.710	782	786	790	rBV	831923	681459	25.04%	2.929%
6	6.869	809	813	816	rVB	2238739	1954799	71.82%	8.402%
7	7.275	876	882	885	rBV	1758839	1640337	60.27%	7.050%
8	7.375	894	899	908	rVB	31619	39868	1.46%	0.171%
9	7.992	1000	1004	1008	rBV	1053344	841423	30.92%	3.617%
10	9.075	1183	1188	1191	rBV	2732309	2447629	89.93%	10.520%
11	9.463	1251	1254	1258	rBV	551475	448011	16.46%	1.926%
12	9.745	1298	1302	1306	rBV2	915855	789196	29.00%	3.392%
13	10.192	1375	1378	1381	rVB	46298	35981	1.32%	0.155%
14	10.533	1431	1436	1439	rBV	1327465	1234812	45.37%	5.307%
15	10.663	1455	1458	1467	rBV	46616	52406	1.93%	0.225%
16	11.110	1527	1534	1538	rBV4	28598	35713	1.31%	0.153%
17	11.227	1550	1554	1556	rBV	719322	612824	22.52%	2.634%
18	11.251	1556	1558	1562	rVB	66061	49590	1.82%	0.213%
19	11.463	1589	1594	1598	rBV3	82150	81594	3.00%	0.351%
20	12.280	1730	1733	1737	rBV	276970	256358	9.42%	1.102%
21	12.339	1741	1743	1745	rVB2	67247	49462	1.82%	0.213%
22	12.433	1755	1759	1763	rBV	129074	109991	4.04%	0.473%
23	12.663	1792	1798	1801	rBV	109956	116353	4.28%	0.500%
24	12.816	1819	1824	1827	rVB	1594293	1493530	54.88%	6.419%
25	13.033	1857	1861	1863	rBV	39765	38976	1.43%	0.168%
26	13.268	1898	1901	1904	rBV	66551	58971	2.17%	0.253%
27	13.716	1972	1977	1982	rBV2	127082	149131	5.48%	0.641%
28	13.857	1996	2001	2004	rBV	705270	689390	25.33%	2.963%
29	13.880	2004	2005	2012	rVB	60215	49680	1.83%	0.214%
30	14.615	2128	2130	2133	rBV	40953	32737	1.20%	0.141%
31	14.715	2143	2147	2151	rBV	83925	82209	3.02%	0.353%
32	14.862	2169	2172	2175	rBV2	48717	68349	2.51%	0.294%
33	15.151	2217	2221	2225	rBV	34928	44365	1.63%	0.191%
34	15.204	2227	2230	2234	rBV	41452	47364	1.74%	0.204%

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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	15.268	2236	2241	2245	rBV	387460	451099	16.57%	1.939%
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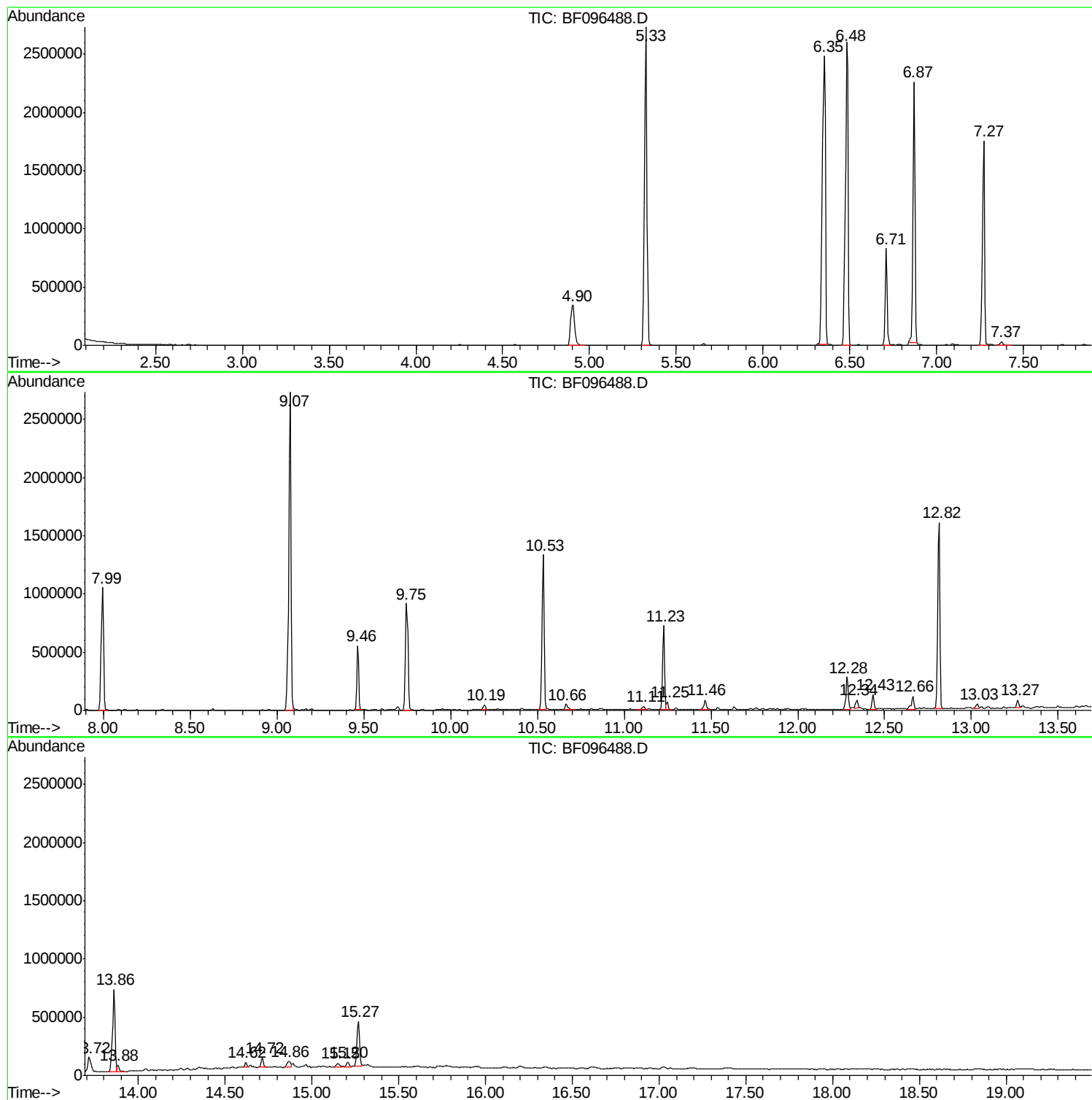
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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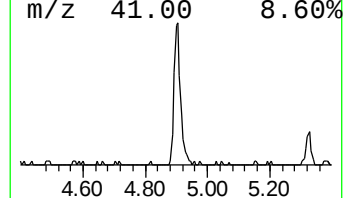
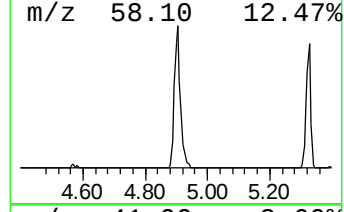
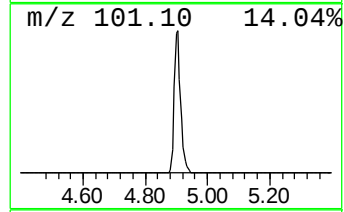
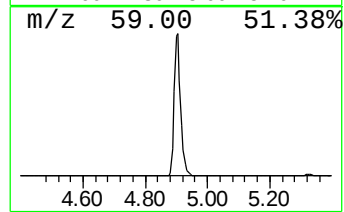
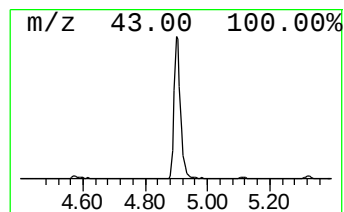
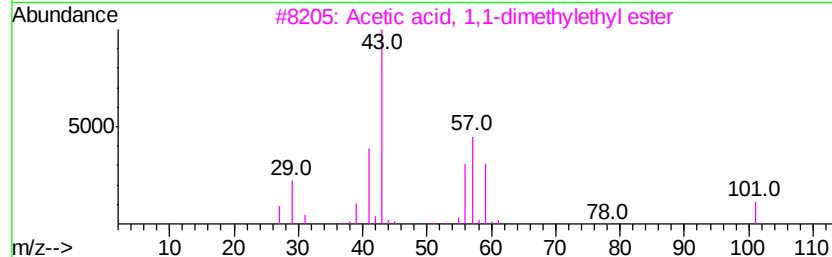
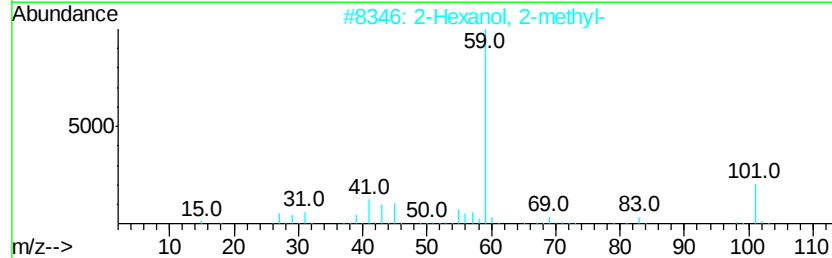
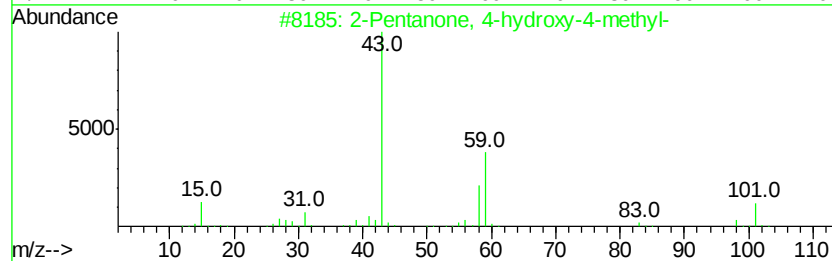
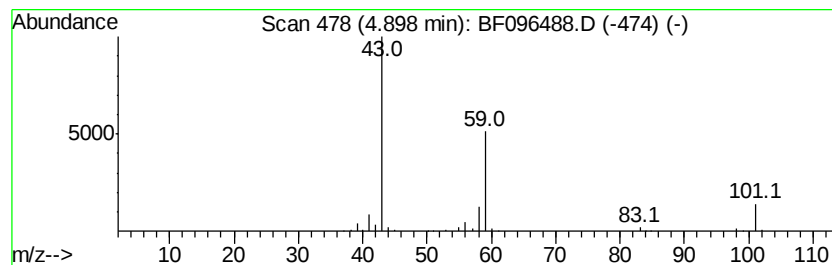
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	14.72 ng	501547	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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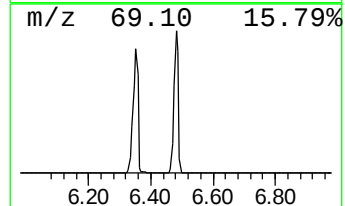
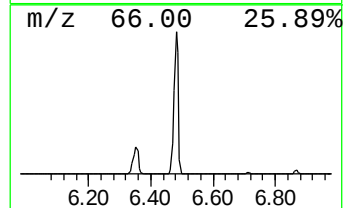
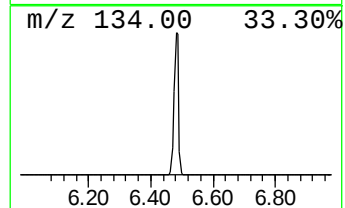
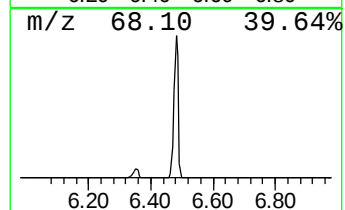
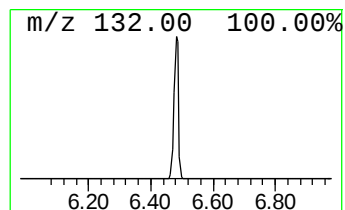
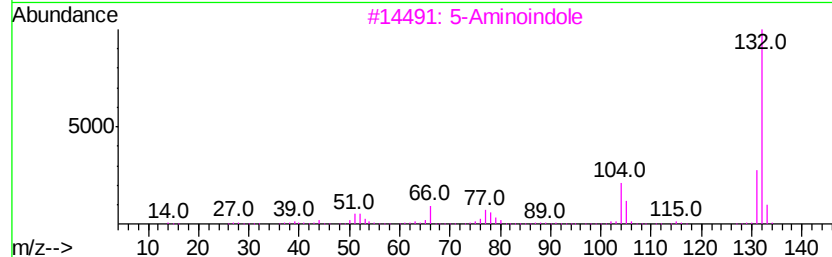
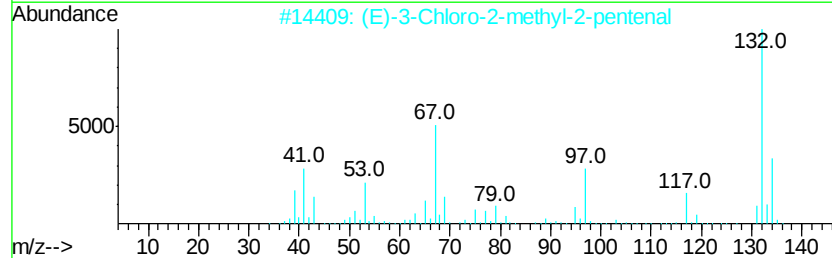
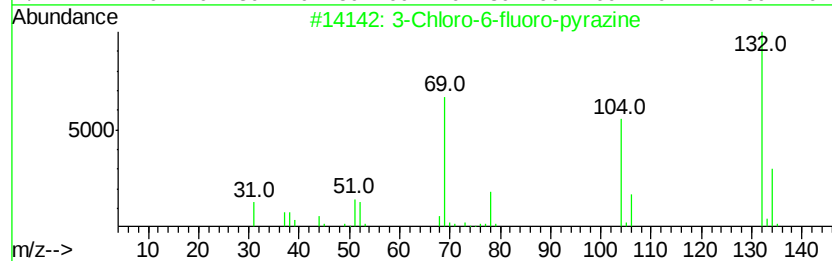
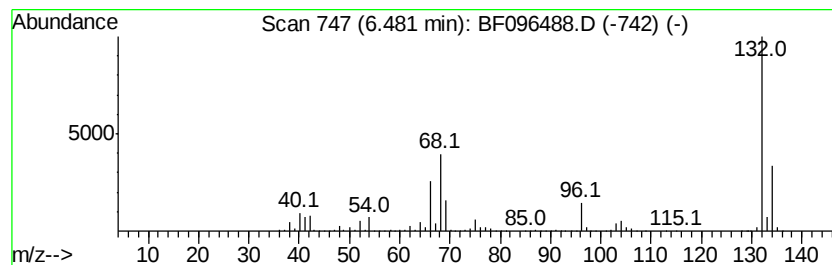
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	78.14 ng	2662370	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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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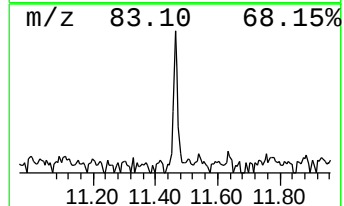
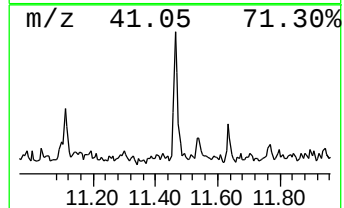
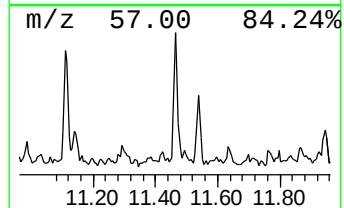
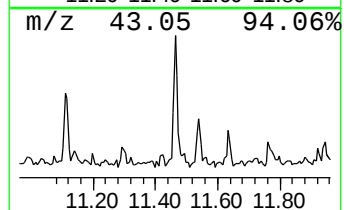
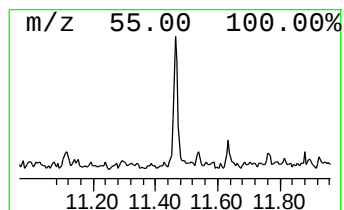
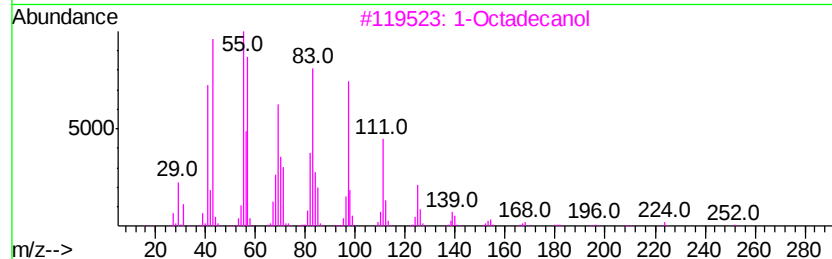
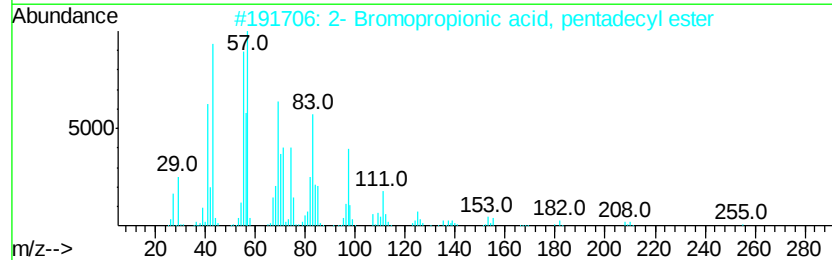
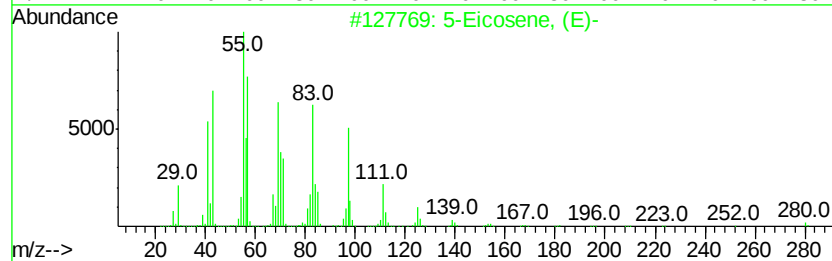
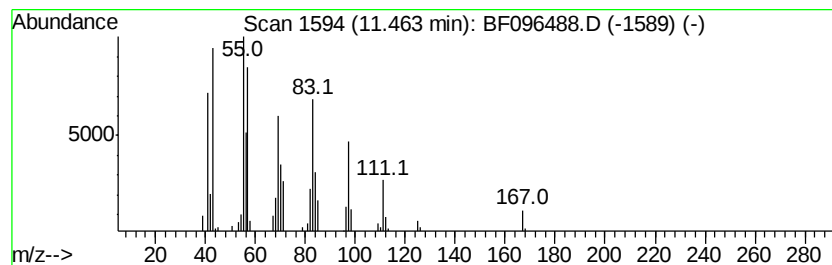
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.46	2.66 ng	81594	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	91
2	2- Bromopropionic acid, pentadec...		362	C18H35BrO2	1000292-44-2	87
3	1-Octadecanol		270	C18H38O	000112-92-5	87
4	Trichloroacetic acid, tetradecyl...		358	C16H29Cl3O2	074339-52-9	80
5	1-Heneicosanol		312	C21H44O	015594-90-8	74



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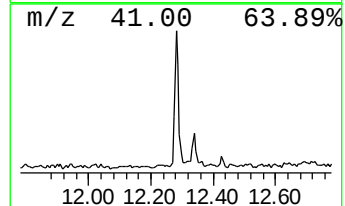
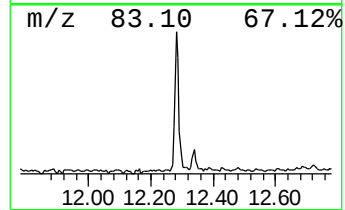
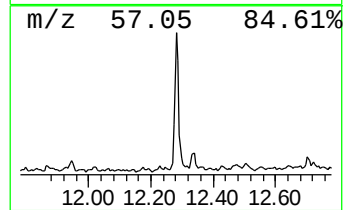
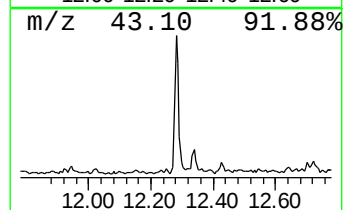
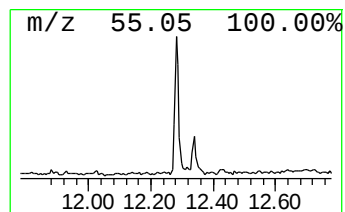
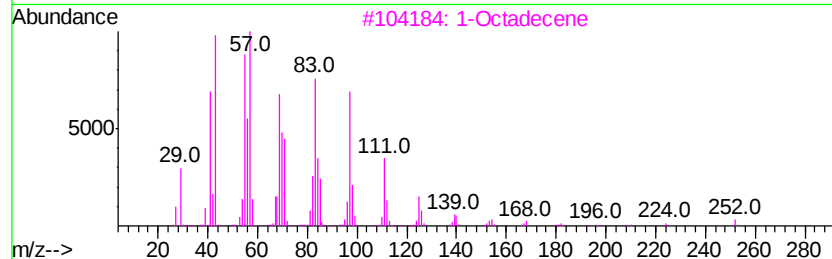
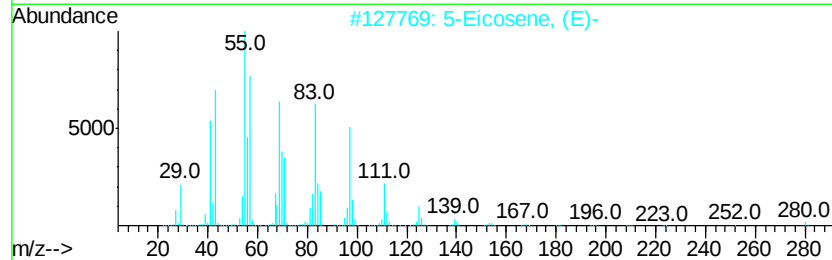
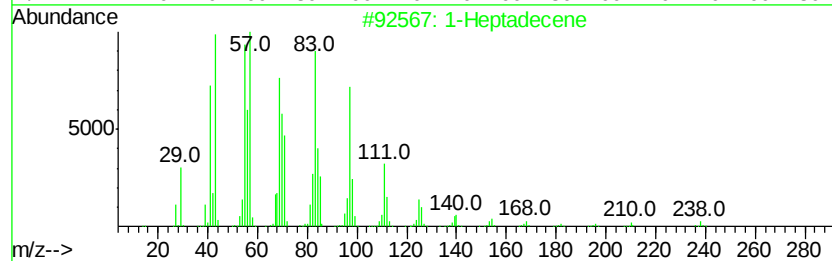
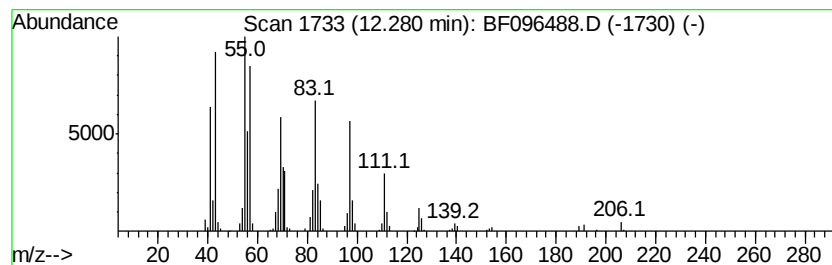
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Heptadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	8.37 ng	256358	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecene		238	C17H34	006765-39-5	90
2	5-Eicosene, (E)-		280	C20H40	074685-30-6	90
3	1-Octadecene		252	C18H36	000112-88-9	87
4	11-Tricosene		322	C23H46	052078-56-5	87
5	n-Heptadecanol-1		256	C17H36O	001454-85-9	87



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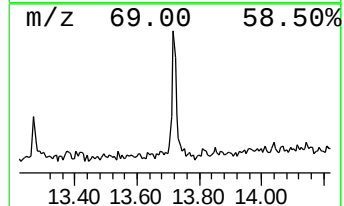
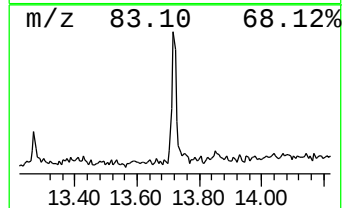
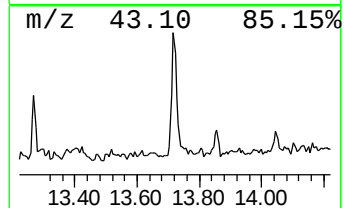
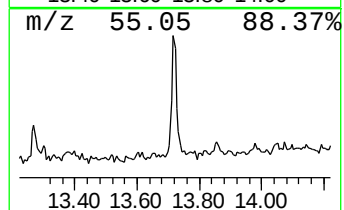
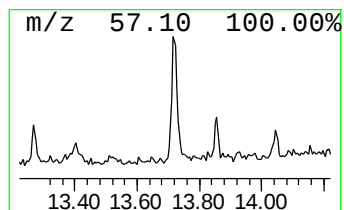
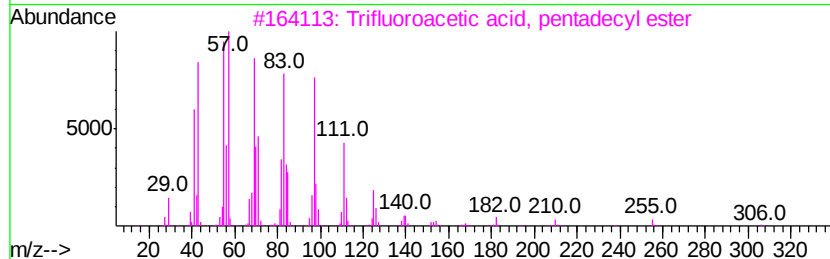
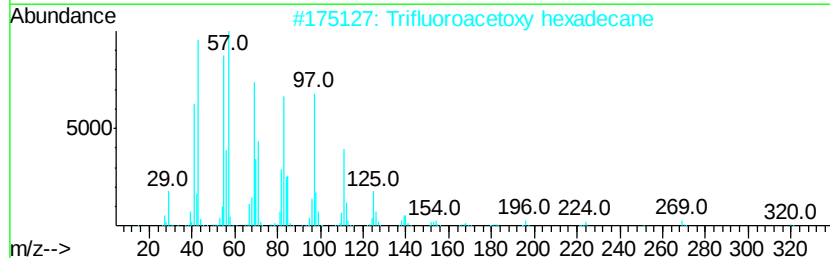
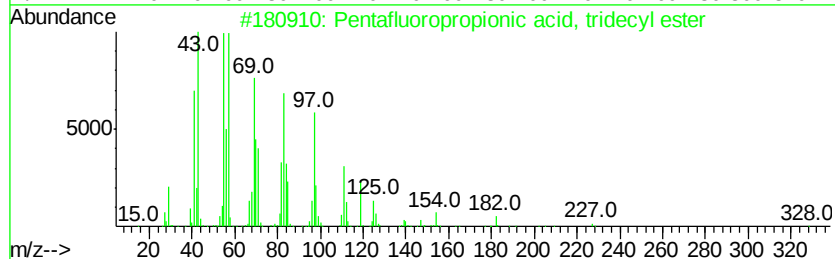
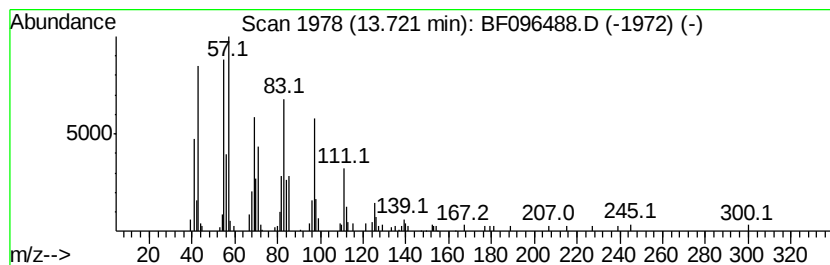
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.33 ng	149131	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, tridecyl...	346	C16H27F5O2	959261-22-4	95
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4		Heptadecyl heptafluorobutyrte	452	C21H35F7O2	959085-66-6	93
5		1-Heneicosyl formate	340	C22H44O2	077899-03-7	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096488.D
Acq On : 5 Jul 2017 17:10
Operator : SJ/MA
Sample : I3871-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
POSTEX-53-20170622

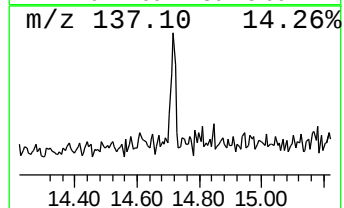
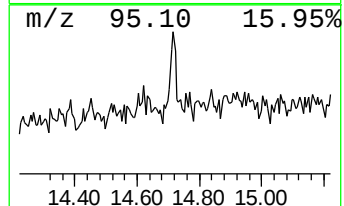
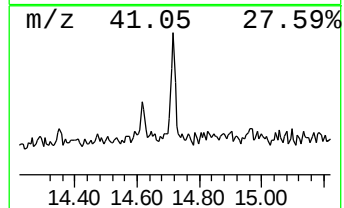
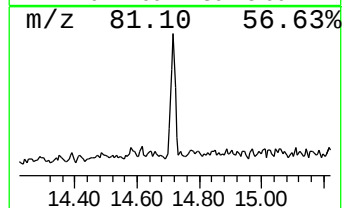
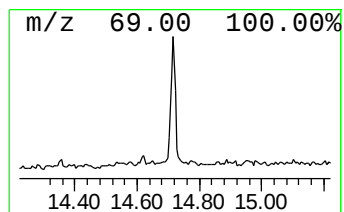
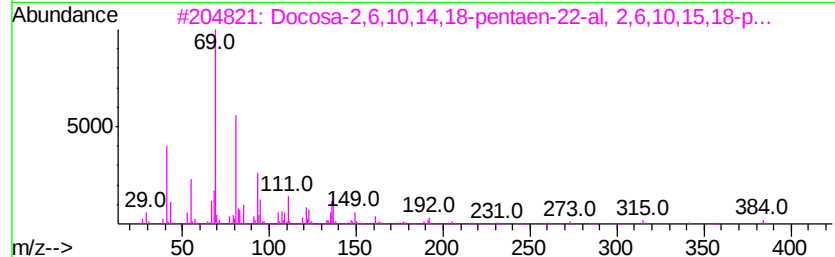
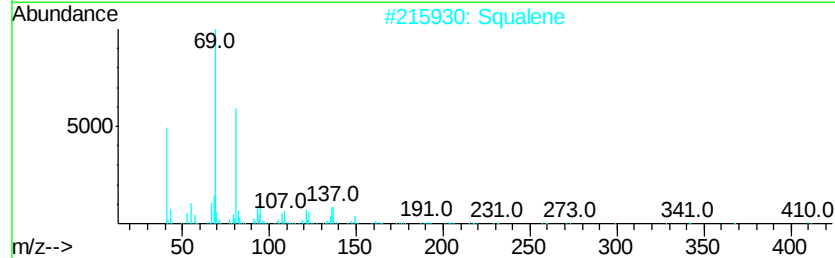
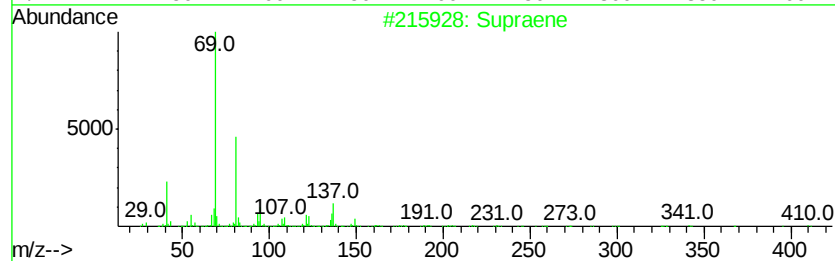
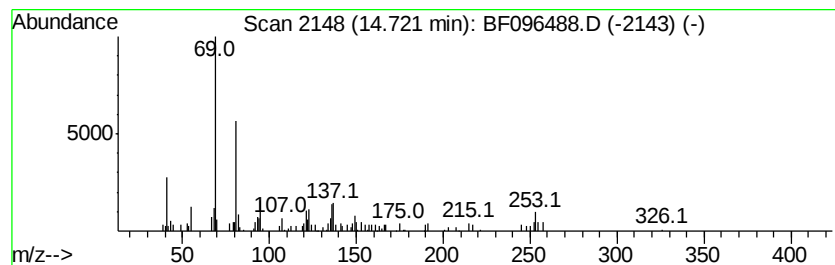
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	3.64 ng	82209	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	87
2		Squalene	410	C30H50	000111-02-4	83
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80
4		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
5		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
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Sample : I3871-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
POSTEX-53-20170622

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	14.7	ng	501547	1	6.71	681459	20.0
unknown6.48	6.48	78.1	ng	2662370	1	6.71	681459	20.0
5-Eicosene, (E)-	11.46	2.7	ng	81594	4	11.23	612824	20.0
1-Heptadecene	12.28	8.4	ng	256358	4	11.23	612824	20.0
Pentafluoropropio...	13.72	4.3	ng	149131	5	13.86	689390	20.0
Supraene	14.72	3.6	ng	82209	6	15.27	451099	20.0