

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
 Data File : BF096541.D
 Acq On : 6 Jul 2017 18:54
 Operator : SJ/MA
 Sample : I3999-03
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS3-1-4-COMP

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	489	rVB	317315	428069	17.32%	1.954%
2	5.328	546	551	554	rBV	2478547	2454255	99.29%	11.201%
3	6.351	720	725	737	rVB	2233826	2471896	100.00%	11.282%
4	6.487	743	748	751	rBV	2451238	2335606	94.49%	10.660%
5	6.716	783	787	790	rBV	780167	686396	27.77%	3.133%
6	6.869	809	813	817	rBV	1909533	1766677	71.47%	8.063%
7	7.275	877	882	885	rBV	1628852	1471192	59.52%	6.715%
8	7.375	893	899	905	rVB2	30391	35932	1.45%	0.164%
9	7.992	1001	1004	1008	rBV	1021184	949714	38.42%	4.335%
10	9.075	1183	1188	1191	rBV	2451136	2035625	82.35%	9.291%
11	9.169	1199	1204	1208	rVB2	39514	35226	1.43%	0.161%
12	9.469	1251	1255	1258	rBV	497265	415533	16.81%	1.896%
13	9.698	1291	1294	1297	rVB	70483	57648	2.33%	0.263%
14	9.751	1297	1303	1306	rBV	953188	835022	33.78%	3.811%
15	10.163	1363	1373	1376	rBV4	17457	27584	1.12%	0.126%
16	10.192	1376	1378	1382	rVB	80617	69791	2.82%	0.319%
17	10.416	1412	1416	1419	rBV	29940	37337	1.51%	0.170%
18	10.533	1432	1436	1440	rBV	1099201	980873	39.68%	4.477%
19	10.669	1456	1459	1468	rBV	87614	117581	4.76%	0.537%
20	11.116	1532	1535	1538	rBV2	65221	59129	2.39%	0.270%
21	11.145	1538	1540	1543	rVB	33505	27679	1.12%	0.126%
22	11.227	1551	1554	1557	rBV	649955	613340	24.81%	2.799%
23	11.251	1557	1558	1563	rVB	119867	81050	3.28%	0.370%
24	11.304	1563	1567	1570	rBV2	39185	38256	1.55%	0.175%
25	11.539	1604	1607	1609	rBV	49328	40471	1.64%	0.185%
26	11.763	1642	1645	1649	rVB	28011	28671	1.16%	0.131%
27	11.839	1655	1658	1661	rBV2	32378	35073	1.42%	0.160%
28	11.945	1673	1676	1679	rBV	42058	32608	1.32%	0.149%
29	12.286	1730	1734	1736	rBV3	23961	25827	1.04%	0.118%
30	12.339	1740	1743	1745	rVB	57732	53489	2.16%	0.244%
31	12.439	1757	1760	1763	rBV	163990	138520	5.60%	0.632%
32	12.668	1793	1799	1802	rBV	133806	162897	6.59%	0.743%
33	12.710	1803	1806	1809	rVB2	59560	51744	2.09%	0.236%
34	12.816	1820	1824	1828	rBV	1539289	1448257	58.59%	6.610%

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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

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Peak separation: 5

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35	12.998	1853	1855	1859	rVB2	29608	26037	1.05%	0.119%
36	13.063	1863	1866	1869	rVB	73284	67232	2.72%	0.307%
37	13.404	1921	1924	1929	rVB	67117	58455	2.36%	0.267%
38	13.721	1975	1978	1987	rVB4	126380	185058	7.49%	0.845%
39	13.863	1998	2002	2005	rBV	749186	721643	29.19%	3.294%
40	14.051	2031	2034	2037	rVB	82376	69705	2.82%	0.318%
41	14.351	2083	2085	2088	rBV	83382	72131	2.92%	0.329%
42	14.651	2134	2136	2141	rVB	89142	92456	3.74%	0.422%
43	14.968	2188	2190	2196	rVB2	96654	122168	4.94%	0.558%
44	15.280	2239	2243	2246	rVB	396210	446689	18.07%	2.039%

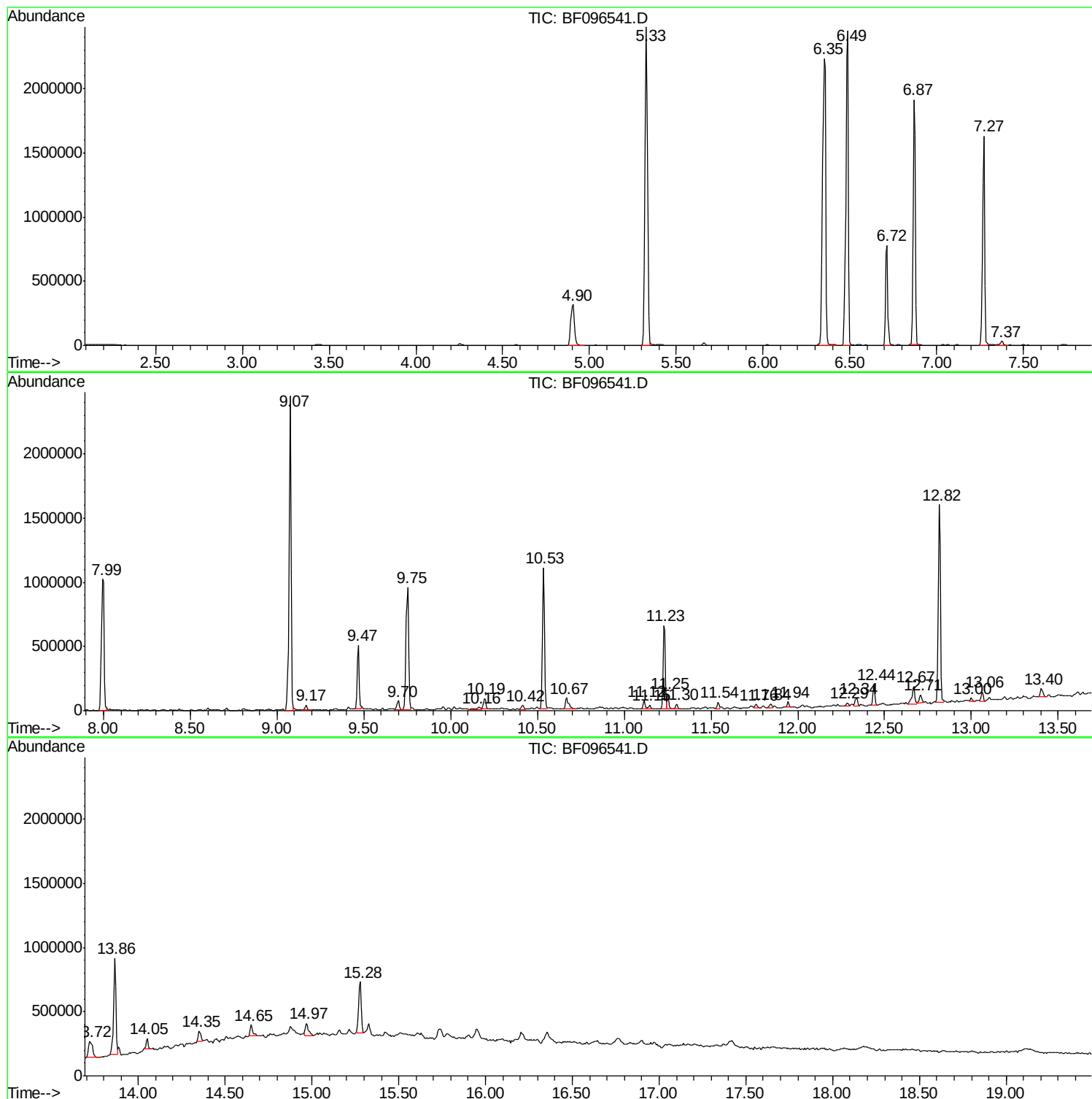
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Instrument :
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ClientSampled :
SS3-1-4-COMP

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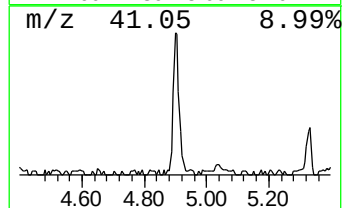
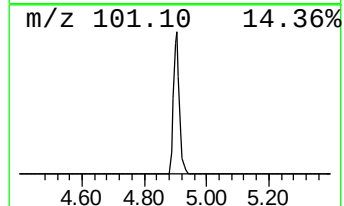
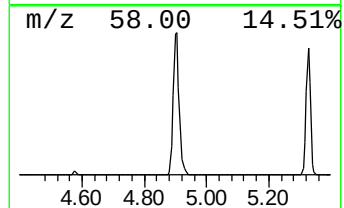
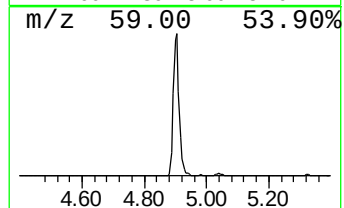
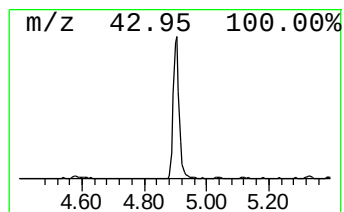
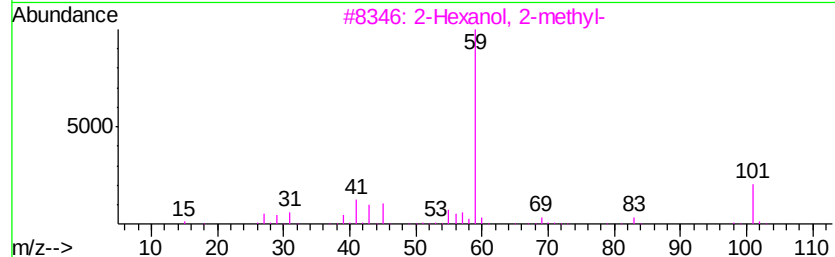
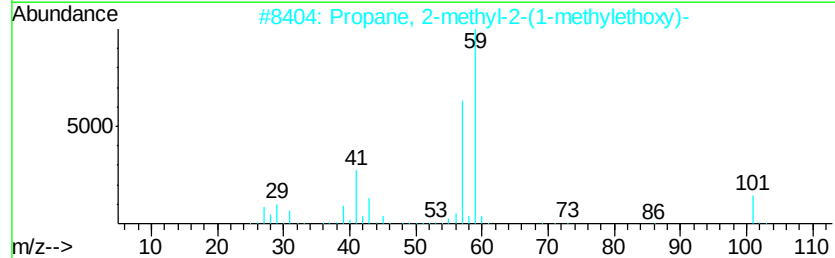
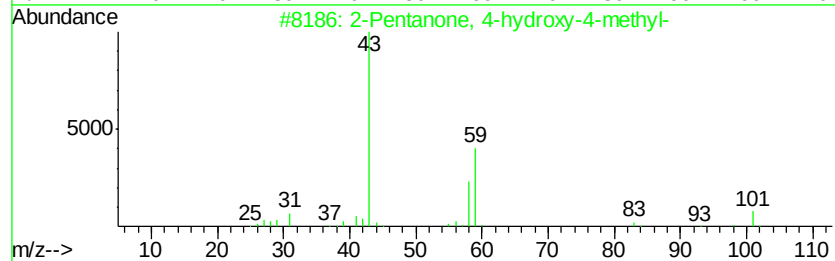
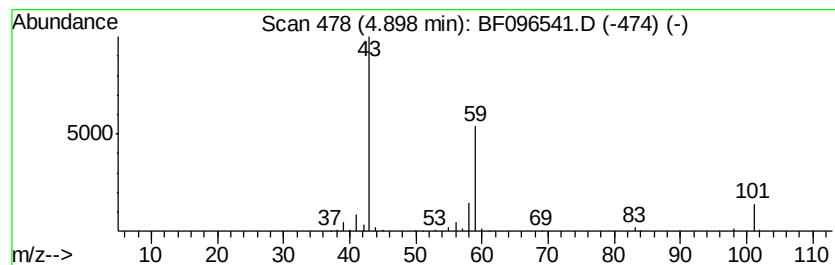
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.90	12.47 ng	428069	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			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	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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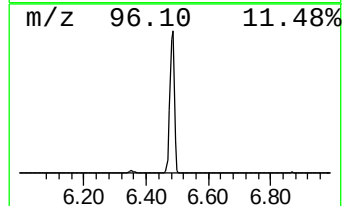
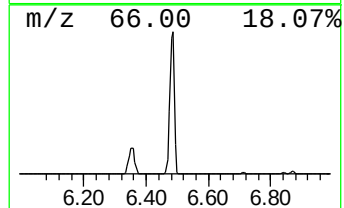
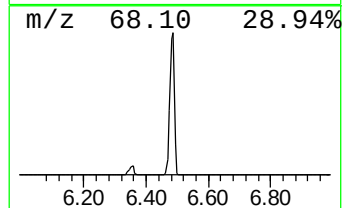
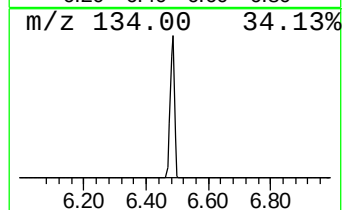
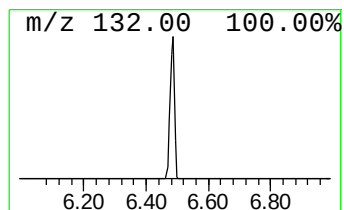
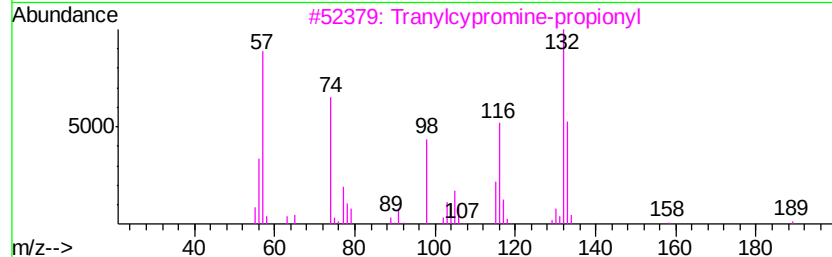
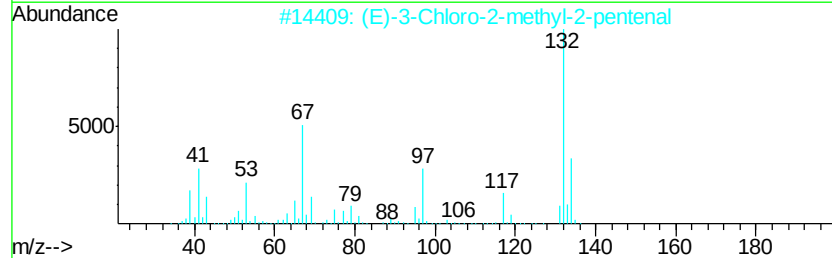
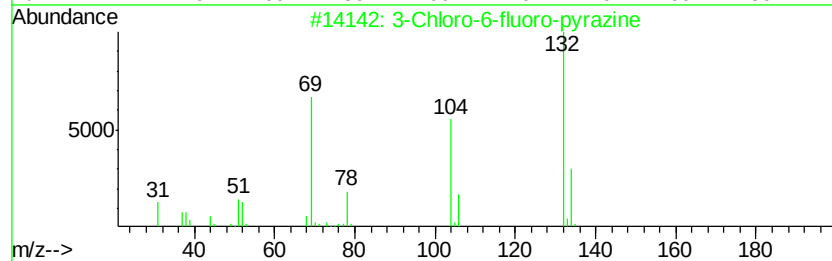
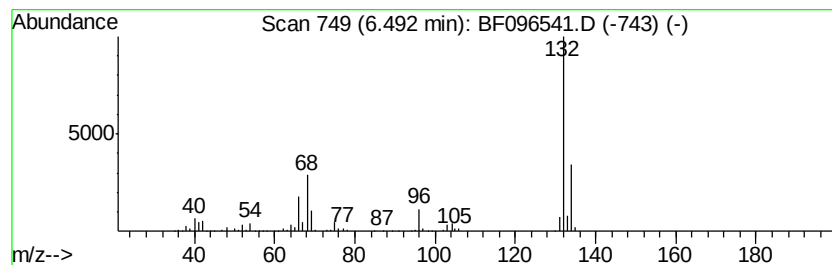
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	68.05 ng	2335610	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		Amphetaminil	250	C17H18N2	017590-01-1	12
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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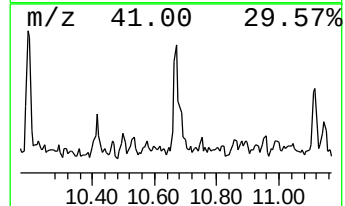
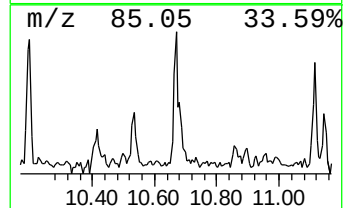
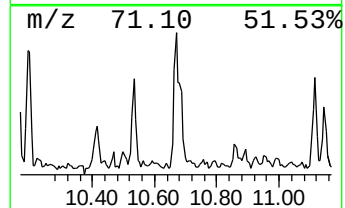
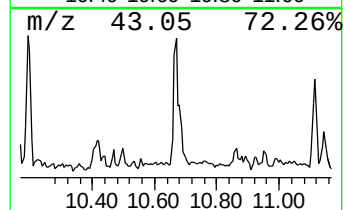
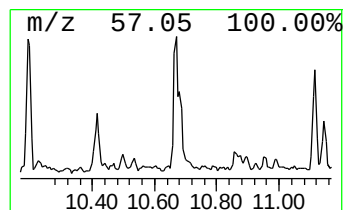
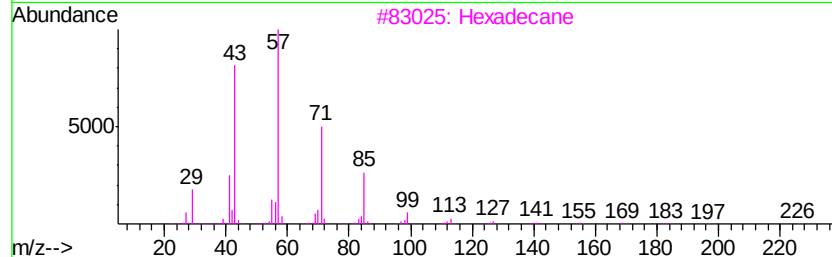
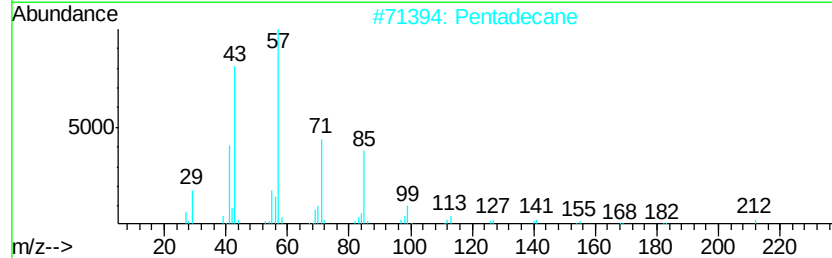
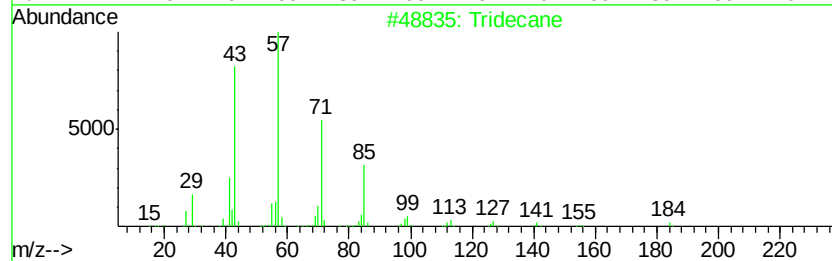
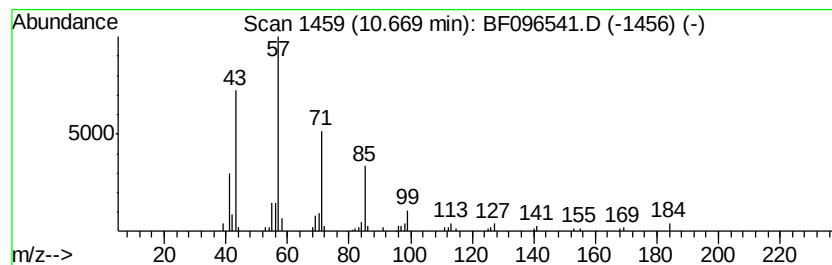
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	3.83 ng	117581	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane		184	C13H28	000629-50-5	95
2	Pentadecane		212	C15H32	000629-62-9	91
3	Hexadecane		226	C16H34	000544-76-3	90
4	Heptadecane		240	C17H36	000629-78-7	83
5	Tetradecane		198	C14H30	000629-59-4	80



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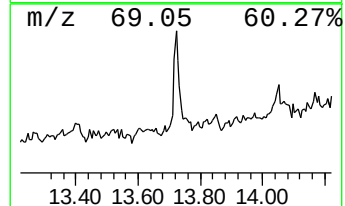
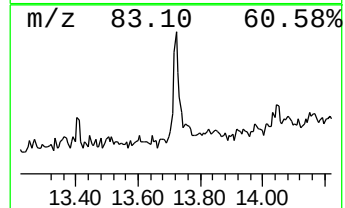
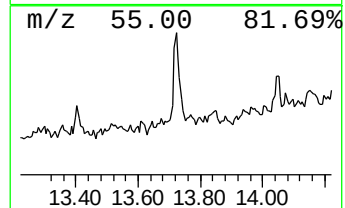
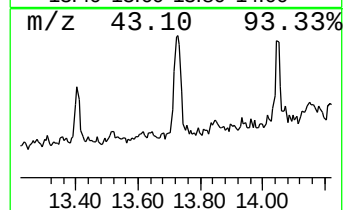
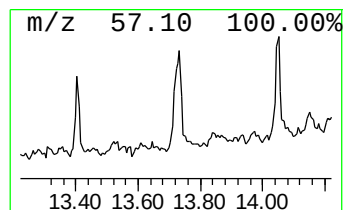
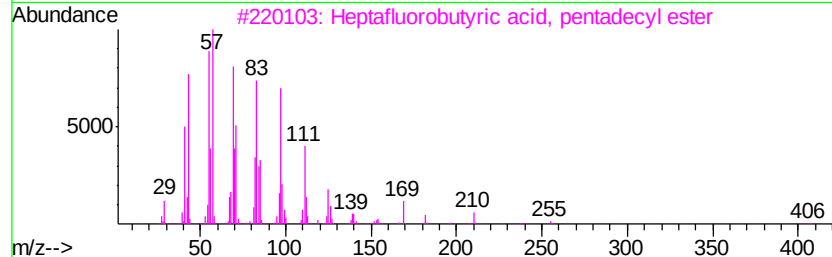
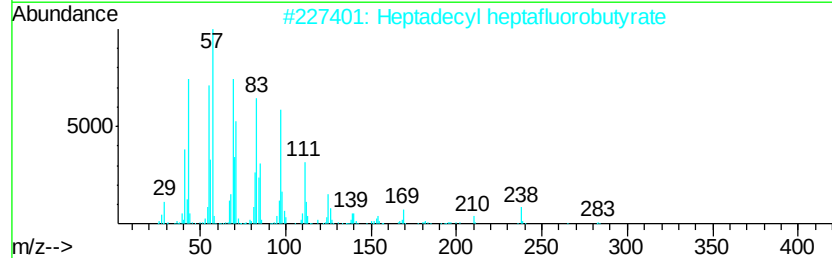
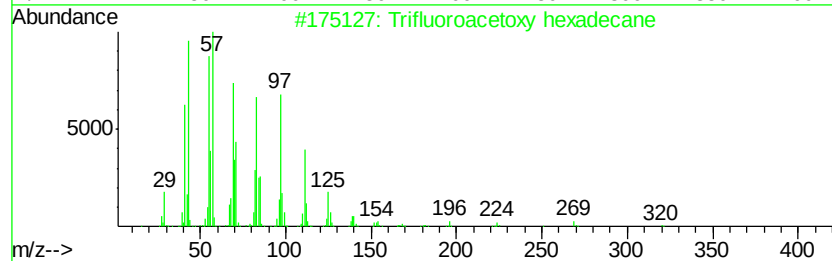
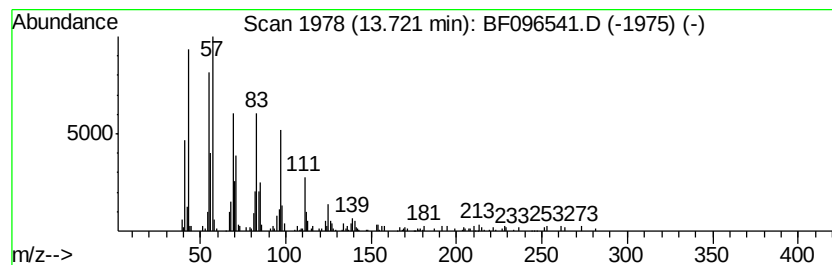
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.72	5.13 ng	185058	Chrysene-d12	13.86		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



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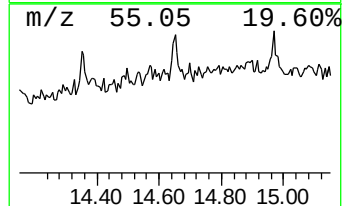
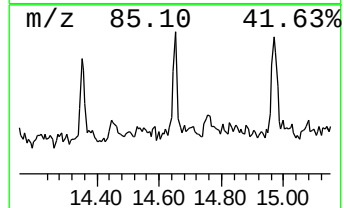
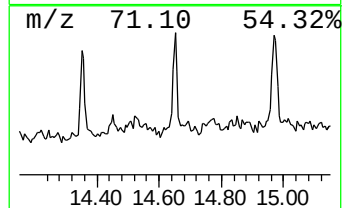
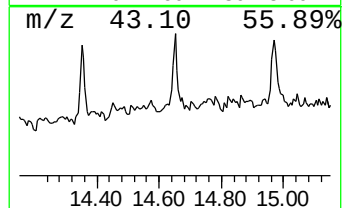
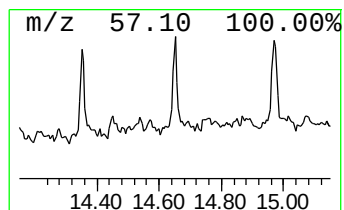
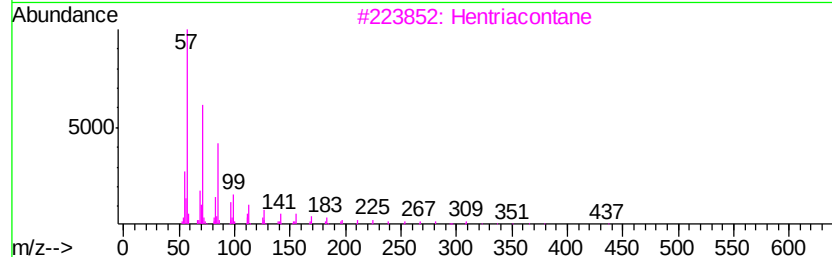
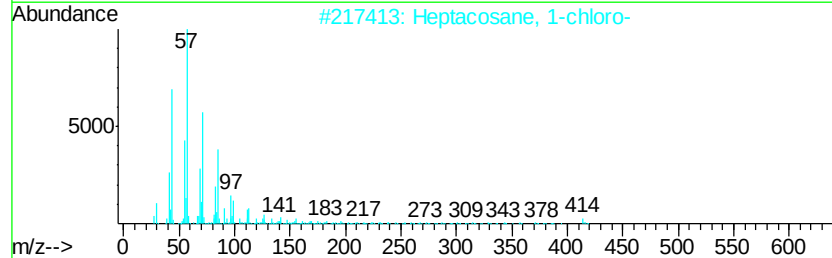
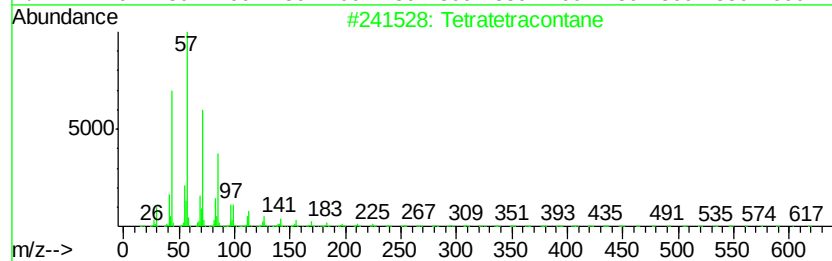
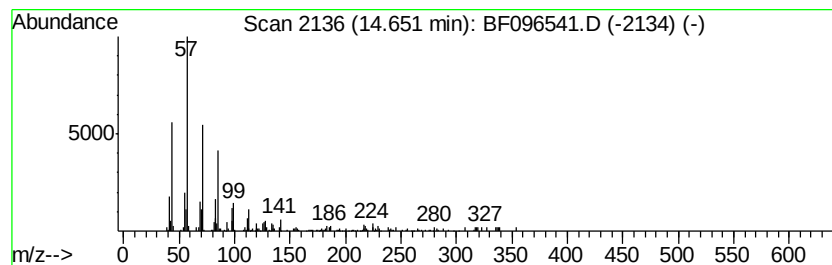
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	4.14 ng	92456	Perylene-d12	15.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	90
2			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	87
3			Hentriacontane	437	C31H64	000630-04-6	87
4			Octacosane	394	C28H58	000630-02-4	87
5			Docosane, 11-decyl-	451	C32H66	055401-55-3	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096541.D
Acq On : 6 Jul 2017 18:54
Operator : SJ/MA
Sample : I3999-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

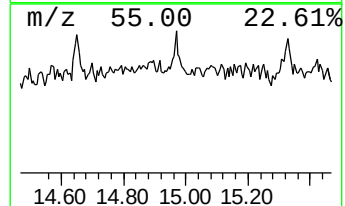
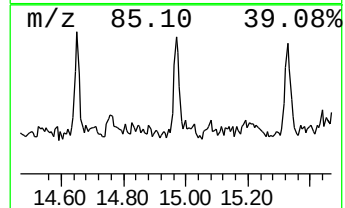
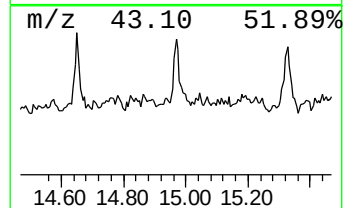
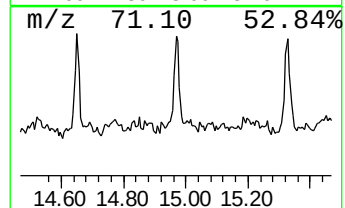
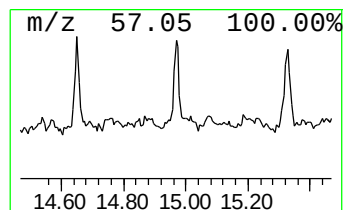
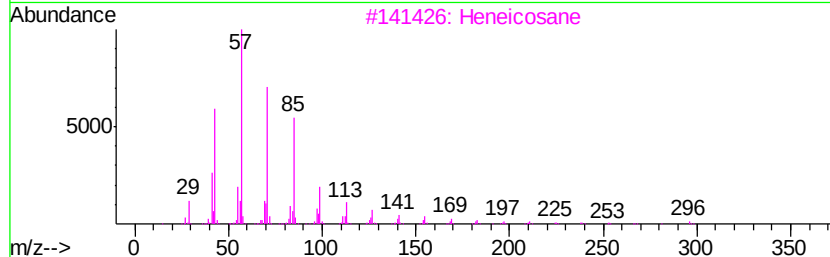
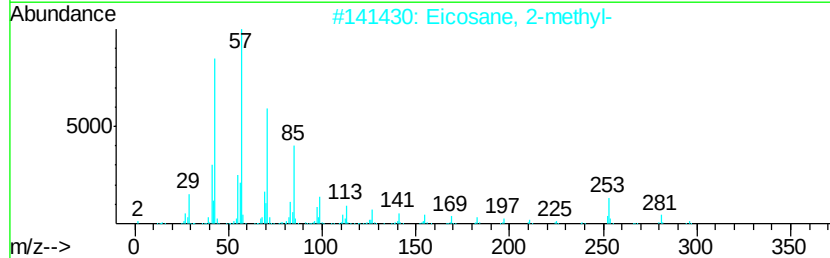
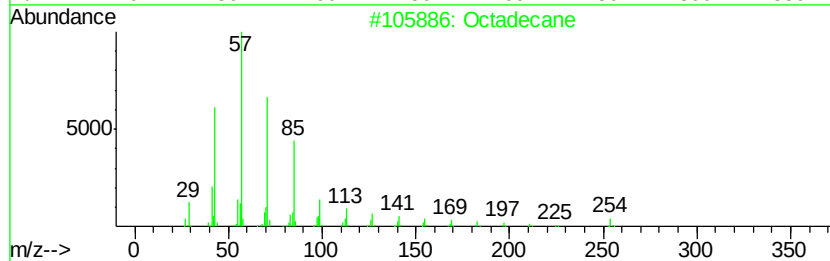
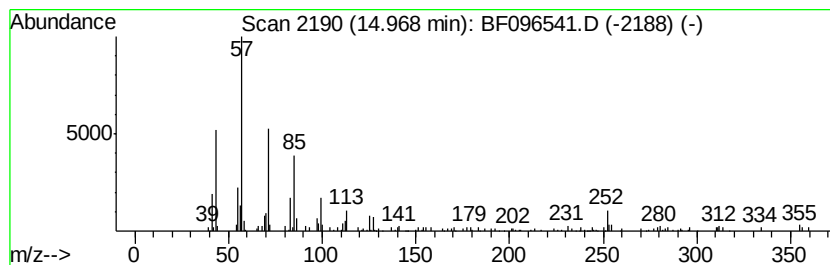
Instrument :
BNA_F
ClientSampleId :
SS3-1-4-COMP

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 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	5.47 ng	122168	Perylene-d12	15.28
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecane	254 C18H38	000593-45-3	91
2	Eicosane, 2-methyl-	296 C21H44	001560-84-5	91
3	Heneicosane	296 C21H44	000629-94-7	91
4	Hexadecane	226 C16H34	000544-76-3	87
5	Docosane	310 C22H46	000629-97-0	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070617\
Data File : BF096541.D
Acq On : 6 Jul 2017 18:54
Operator : SJ/MA
Sample : I3999-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS3-1-4-COMP

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	12.5	ng	428069	1	6.72	686396	20.0
unknown6.49	6.49	68.0	ng	2335610	1	6.72	686396	20.0
Tridecane	10.67	3.8	ng	117581	4	11.23	613340	20.0
Trifluoroacetoxy ...	13.72	5.1	ng	185058	5	13.86	721643	20.0
Tetratetracontane	14.65	4.1	ng	92456	6	15.28	446689	20.0
Octadecane	14.97	5.5	ng	122168	6	15.28	446689	20.0