

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
 Data File : BF096508.D
 Acq On : 6 Jul 2017 3:19
 Operator : SJ/MA
 Sample : I3976-08
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B10-4-6

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	4.904	475	479	488	rBV	331975	464013	17.45%	2.036%
2	5.328	546	551	555	rBV	2477628	2590913	97.45%	11.371%
3	5.998	661	665	668	rBV	175464	151015	5.68%	0.663%
4	6.351	720	725	731	rVB	2369183	2633434	99.05%	11.558%
5	6.487	743	748	751	rBV	2766979	2658787	100.00%	11.669%
6	6.710	783	786	790	rBV	752598	689086	25.92%	3.024%
7	6.869	809	813	817	rVB	2000698	1854099	69.73%	8.137%
8	7.275	876	882	885	rBV	1568514	1426050	53.64%	6.259%
9	7.375	894	899	903	rBV2	30218	35149	1.32%	0.154%
10	7.992	1000	1004	1008	rBV	937936	834065	31.37%	3.661%
11	9.075	1183	1188	1191	rBV	2550520	2247369	84.53%	9.863%
12	9.169	1198	1204	1208	rVB	130418	115350	4.34%	0.506%
13	9.422	1242	1247	1249	rBV3	25422	35705	1.34%	0.157%
14	9.463	1251	1254	1257	rVV	512333	452826	17.03%	1.987%
15	9.698	1290	1294	1297	rVB	134346	115407	4.34%	0.506%
16	9.751	1298	1303	1306	rBV	738177	707856	26.62%	3.107%
17	10.192	1375	1378	1382	rVB	69463	62080	2.33%	0.272%
18	10.533	1432	1436	1440	rBV	1223004	1030344	38.75%	4.522%
19	10.669	1456	1459	1467	rBV	58455	92576	3.48%	0.406%
20	11.116	1532	1535	1538	rBV3	43310	42750	1.61%	0.188%
21	11.145	1538	1540	1546	rVB2	31829	32386	1.22%	0.142%
22	11.227	1550	1554	1557	rVV	710892	616826	23.20%	2.707%
23	11.251	1557	1558	1562	rVB	109523	67569	2.54%	0.297%
24	11.298	1563	1566	1570	rBV3	39116	44292	1.67%	0.194%
25	11.469	1590	1595	1598	rBV5	34186	47983	1.80%	0.211%
26	11.639	1621	1624	1628	rVB3	27473	30498	1.15%	0.134%
27	11.839	1655	1658	1661	rBV3	46659	57040	2.15%	0.250%
28	11.945	1674	1676	1681	rVB2	30526	32600	1.23%	0.143%
29	12.098	1700	1702	1704	rBV2	35969	35604	1.34%	0.156%
30	12.227	1722	1724	1727	rVB	42466	33639	1.27%	0.148%
31	12.333	1740	1742	1745	rBV2	47020	44170	1.66%	0.194%
32	12.439	1757	1760	1763	rBV	110755	110581	4.16%	0.485%
33	12.480	1763	1767	1772	rVV2	50560	89622	3.37%	0.393%
34	12.545	1776	1778	1781	rBV3	25237	29172	1.10%	0.128%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.704	1803	1805	1808	rBV	50406	52118	1.96%	0.229%
36	12.816	1820	1824	1827	rBV	1662574	1495110	56.23%	6.562%
37	13.063	1863	1866	1868	rBV3	60074	54633	2.05%	0.240%
38	13.186	1885	1887	1891	rBV2	63491	65050	2.45%	0.285%
39	13.298	1904	1906	1913	rVB2	132363	146221	5.50%	0.642%
40	13.721	1975	1978	1982	rBV	156371	163670	6.16%	0.718%
41	13.862	1995	2002	2005	rBV	756036	841895	31.66%	3.695%
42	14.145	2048	2050	2054	rBV2	70496	79740	3.00%	0.350%
43	15.274	2238	2242	2248	rVB	307004	375960	14.14%	1.650%

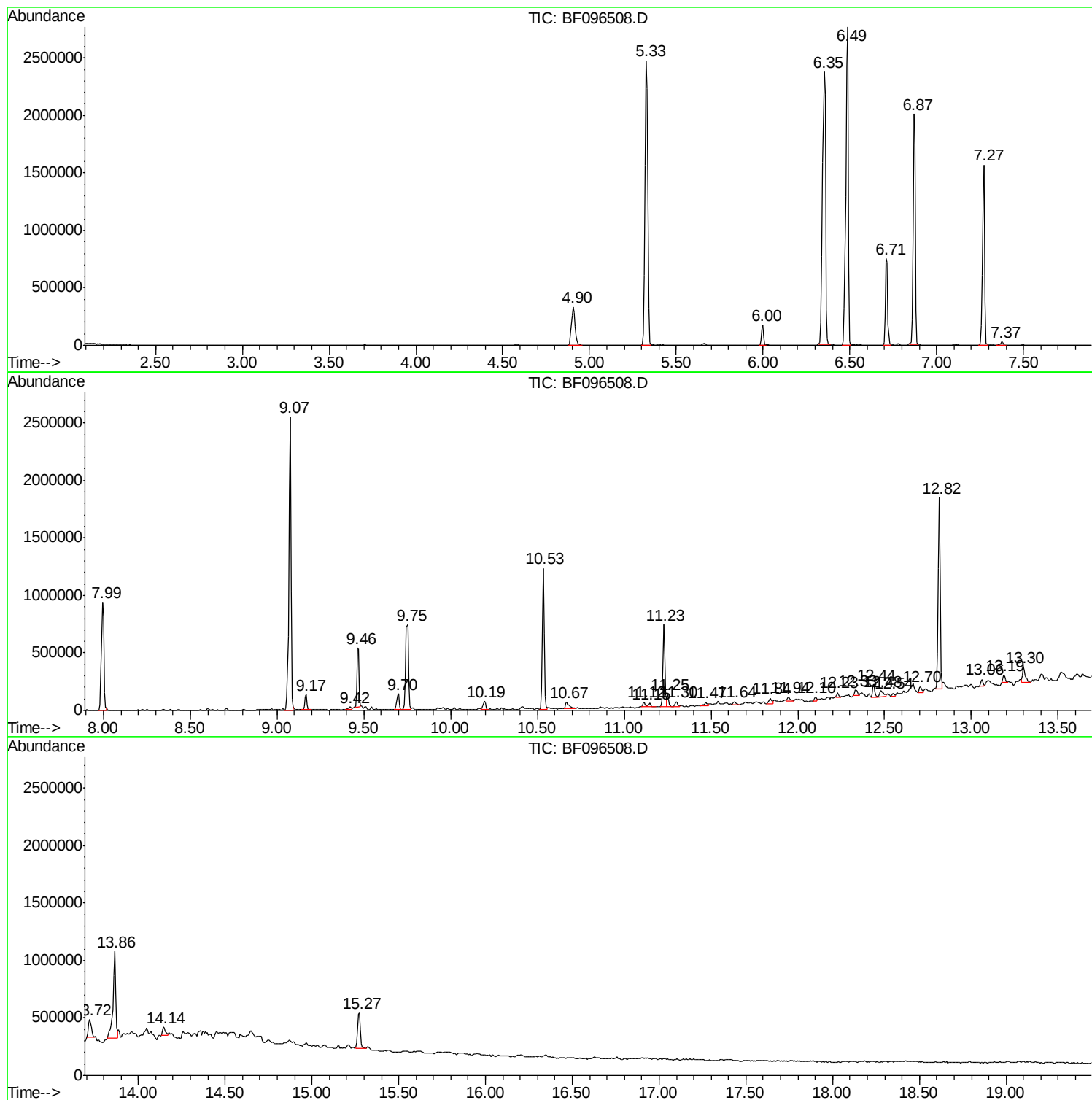
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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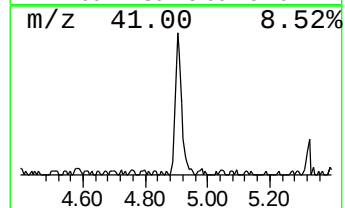
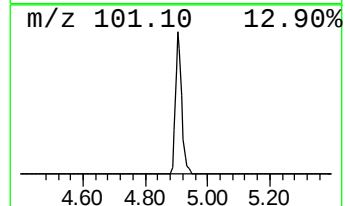
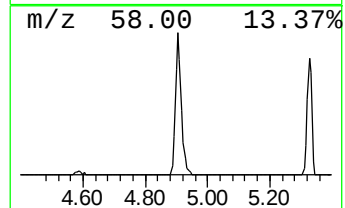
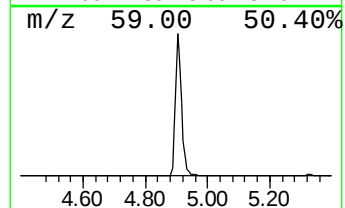
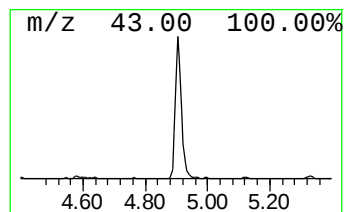
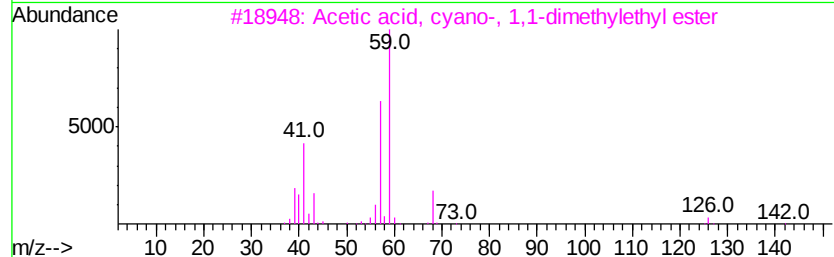
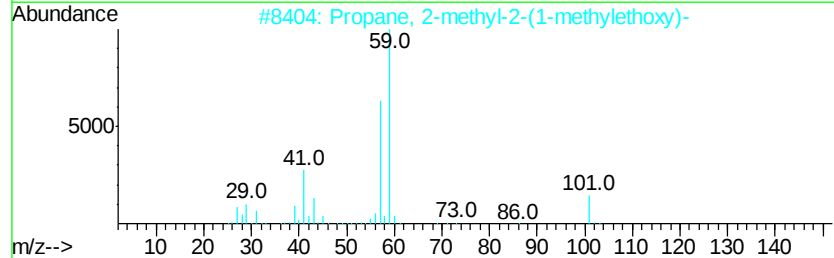
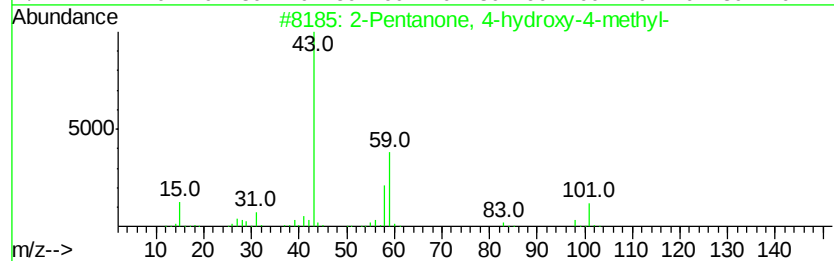
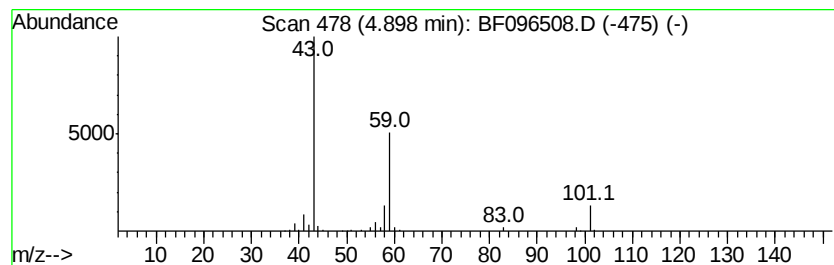
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	13.47 ng	464013	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	53	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36	
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9	



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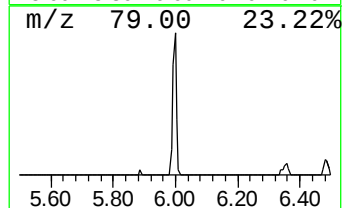
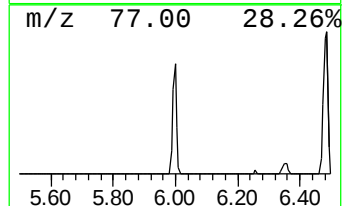
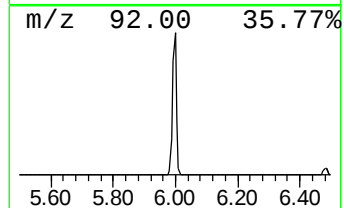
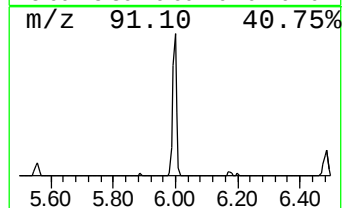
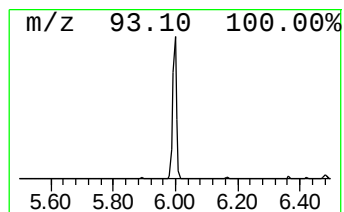
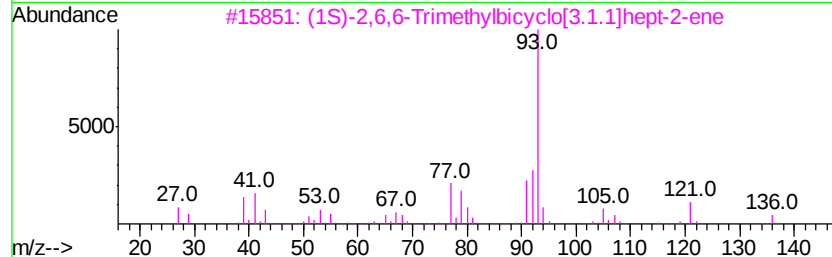
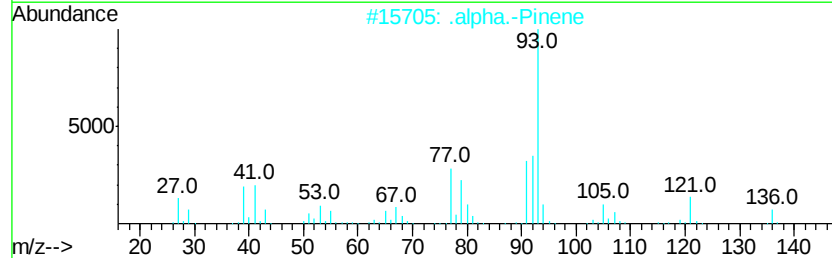
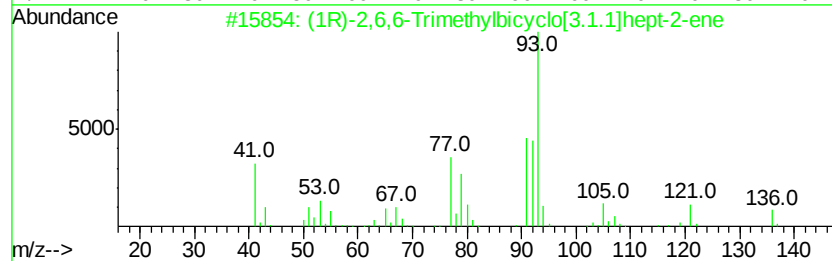
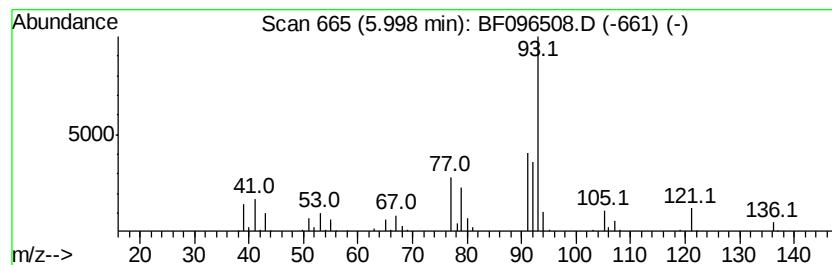
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Peak Number 2 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.00	4.38 ng	151015	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	96
2		.alpha.-Pinene	136	C10H16	000080-56-8	96
3		(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-26-4	94
4		Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	94
5		Tricyclo[2.2.1.0(2,6)]heptane, 1,4-dichloro-	136	C10H16	000508-32-7	91



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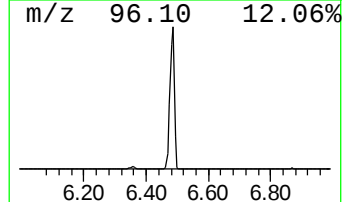
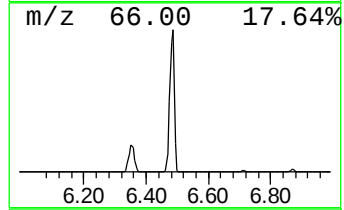
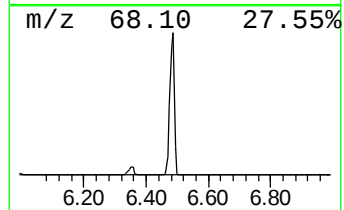
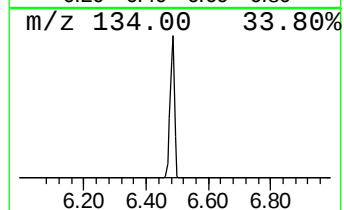
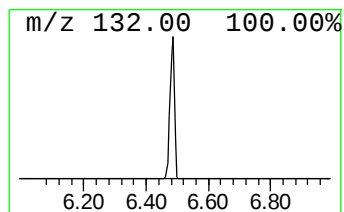
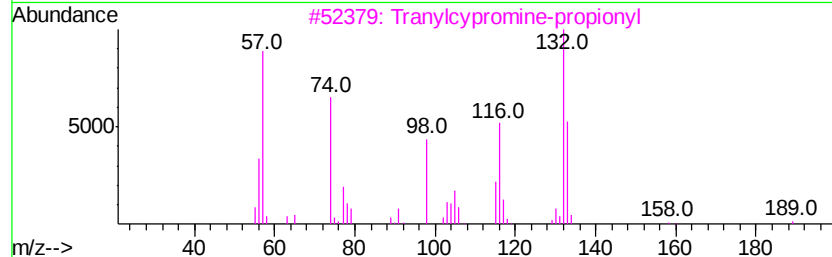
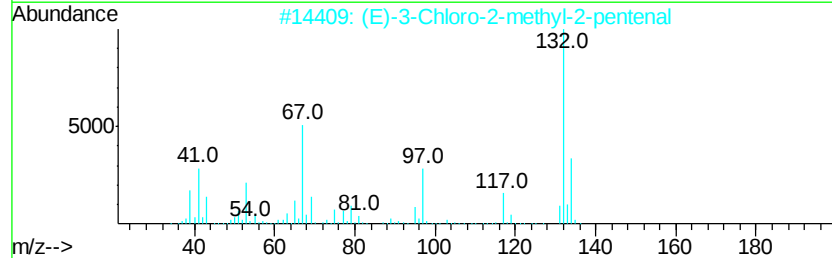
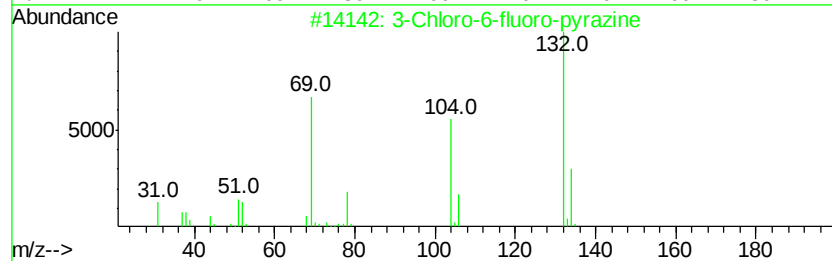
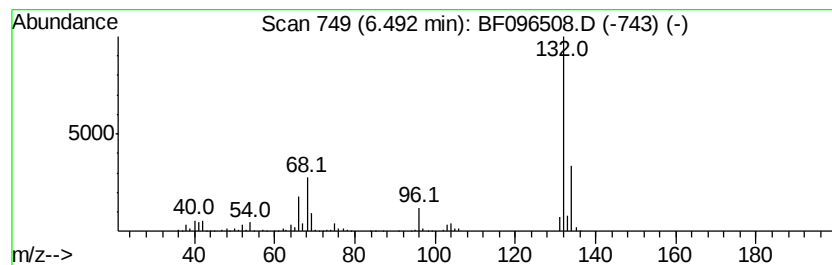
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	77.17 ng	2658790	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		Tranvlcypropine-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



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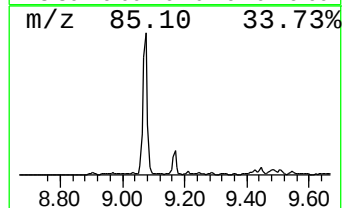
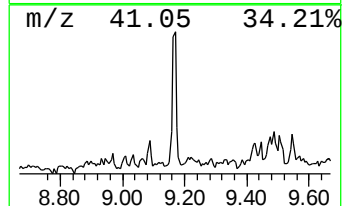
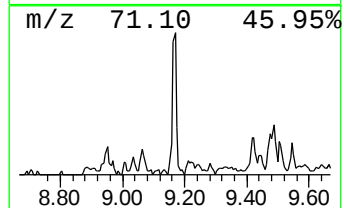
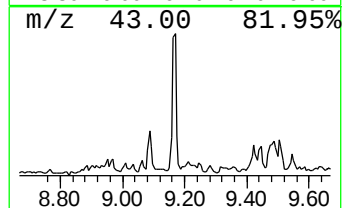
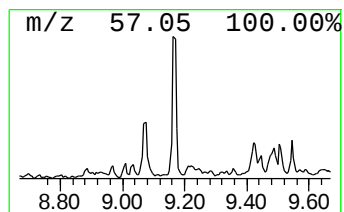
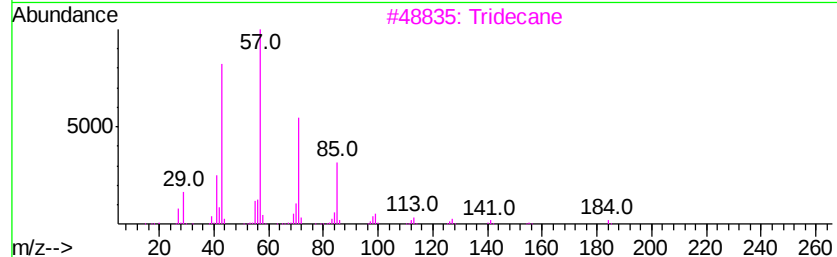
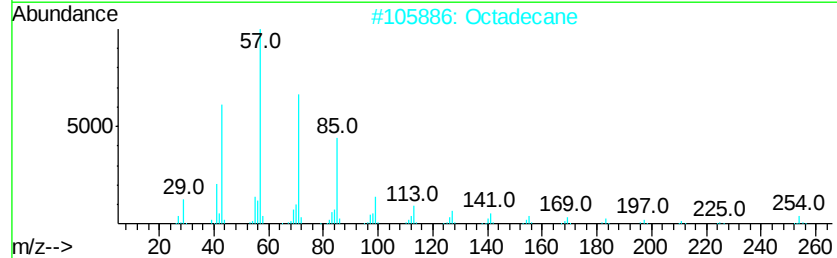
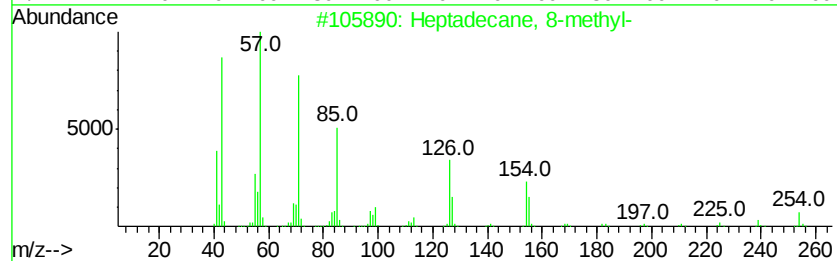
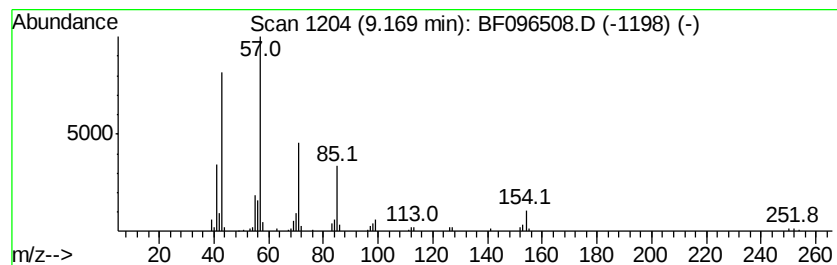
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heptadecane, 8-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.17	3.26 ng	115350	Acenaphthene-d10	9.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	87
2		Octadecane	254	C18H38	000593-45-3	74
3		Tridecane	184	C13H28	000629-50-5	72
4		Dodecane	170	C12H26	000112-40-3	64
5		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	64



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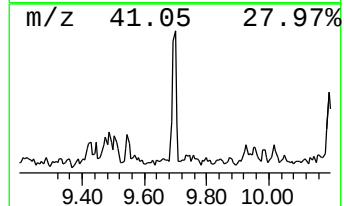
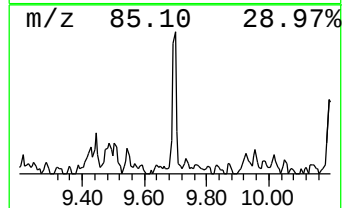
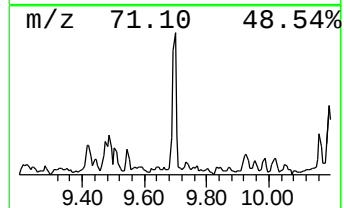
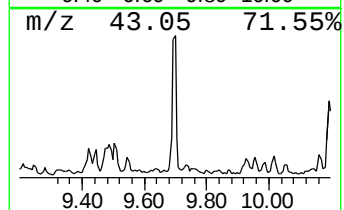
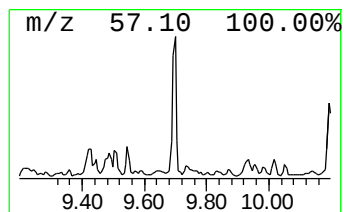
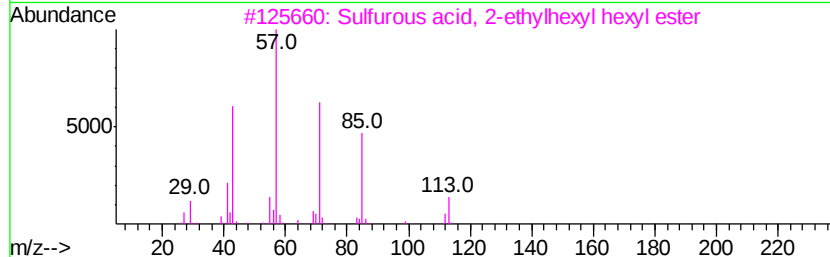
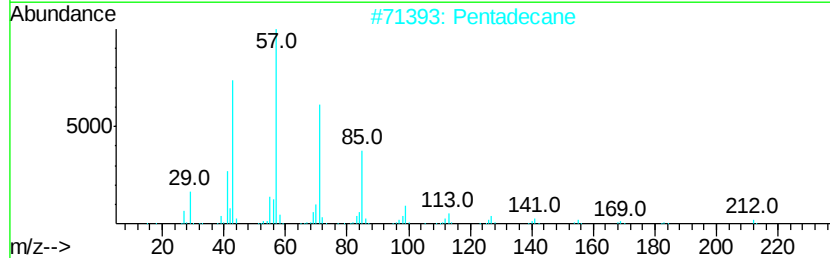
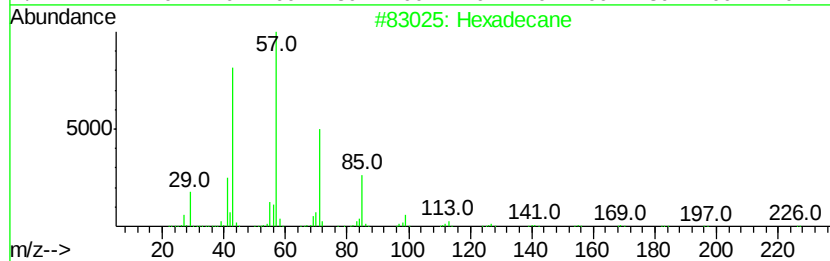
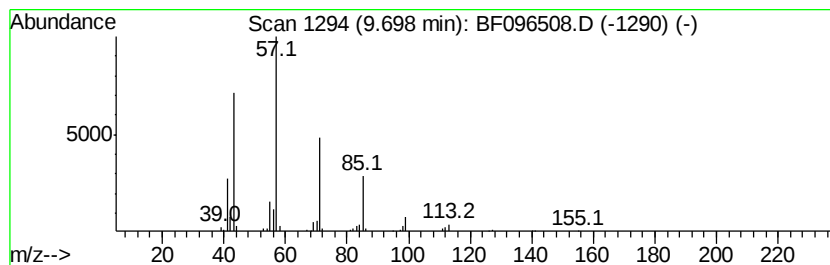
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.70	3.26 ng	115407	Acenaphthene-d10	9.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Pentadecane		212	C15H32	000629-62-9	90
3	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	80
4	Tridecane		184	C13H28	000629-50-5	78
5	Tetradecane		198	C14H30	000629-59-4	78



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
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Acq On : 6 Jul 2017 3:19
Operator : SJ/MA
Sample : I3976-08
Misc :
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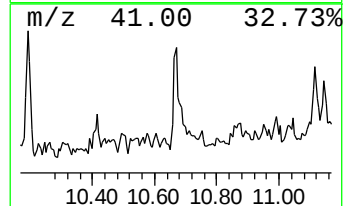
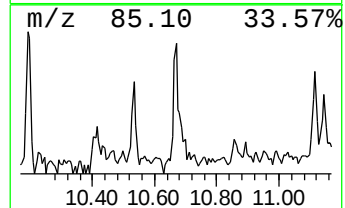
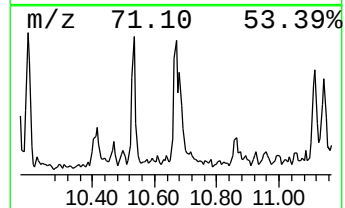
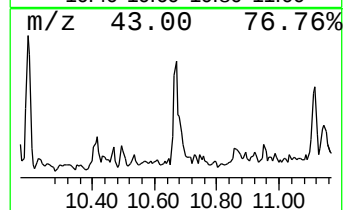
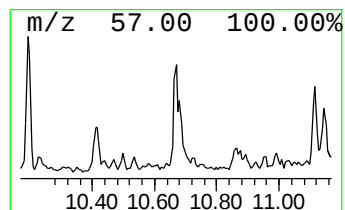
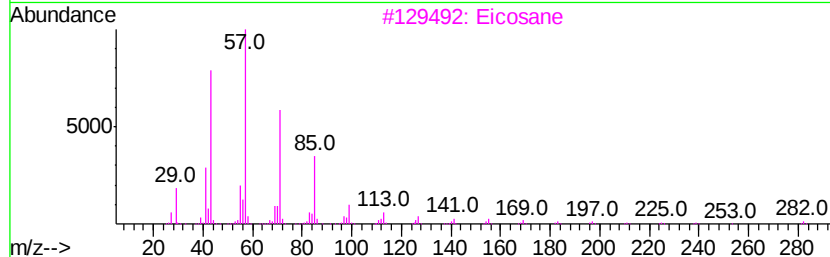
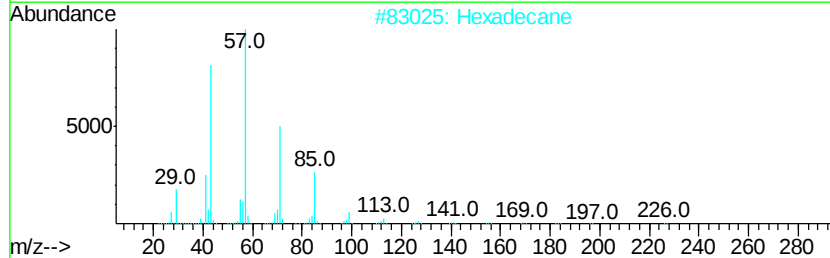
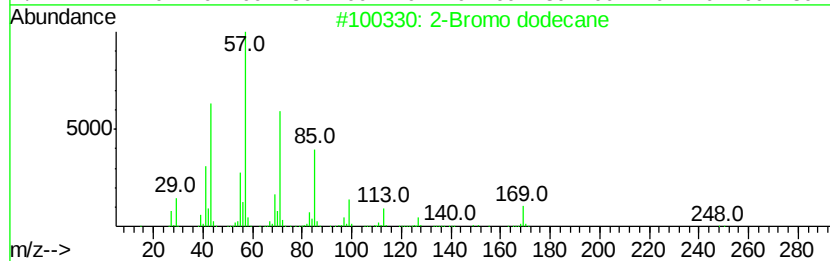
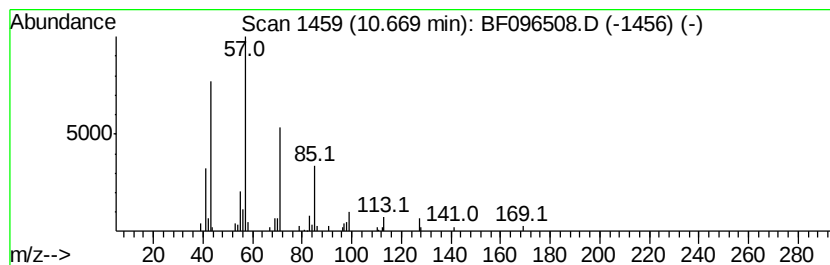
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Bromo dodecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.67	3.00 ng	92576	Phenanthrene-d10		11.23	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane		248	C12H25Br	013187-99-0	90
2	Hexadecane		226	C16H34	000544-76-3	86
3	Eicosane		282	C20H42	000112-95-8	86
4	Heneicosane		296	C21H44	000629-94-7	86
5	Heptacosane		380	C27H56	000593-49-7	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
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Operator : SJ/MA
Sample : I3976-08
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B10-4-6

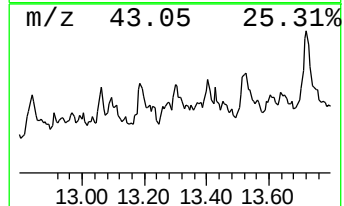
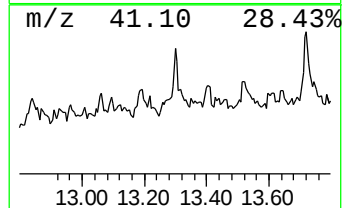
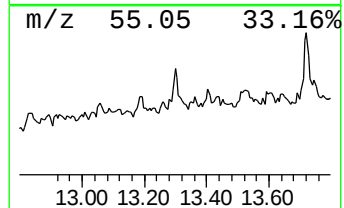
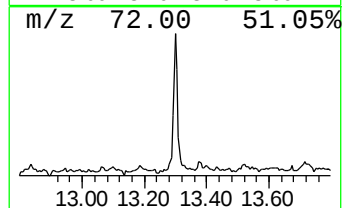
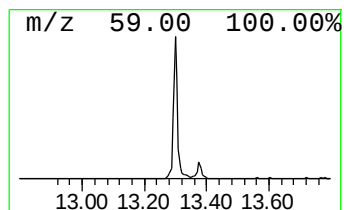
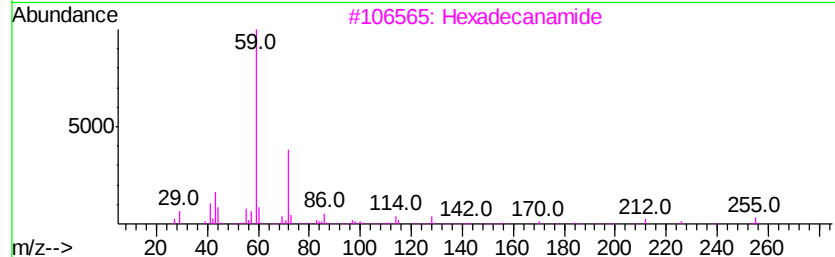
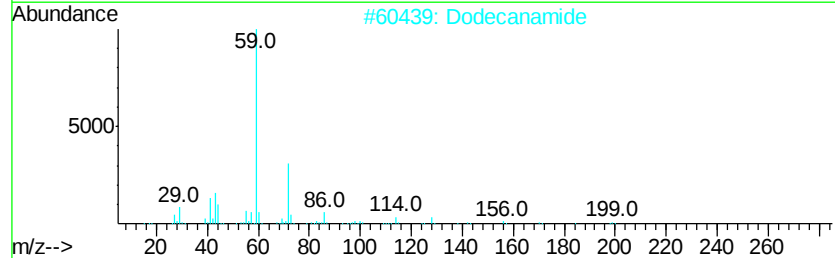
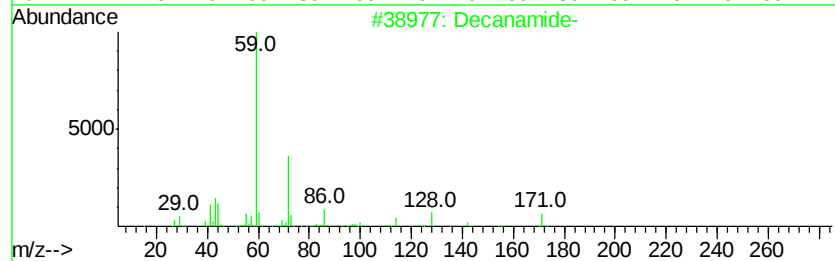
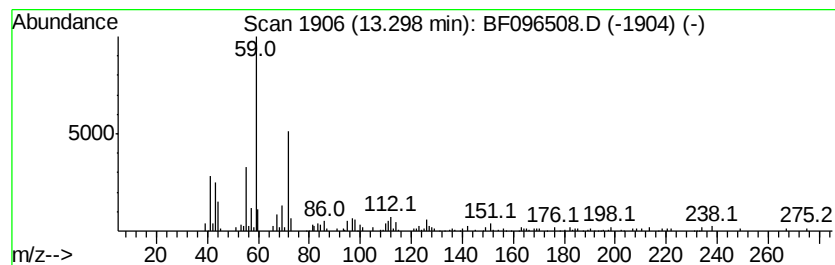
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Decanamide- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	3.47 ng	146221	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decanamide-	171	C10H21NO	002319-29-1	78
2		Dodecanamide	199	C12H25NO	001120-16-7	59
3		Hexadecanamide	255	C16H33NO	000629-54-9	59
4		Tetradecanamide	227	C14H29NO	000638-58-4	59
5		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	56



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096508.D
Acq On : 6 Jul 2017 3:19
Operator : SJ/MA
Sample : I3976-08
Misc :
ALS Vial : 36 Sample Multiplier: 1

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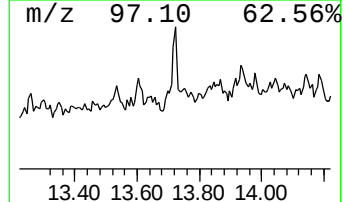
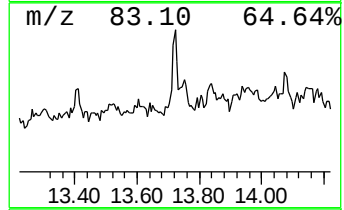
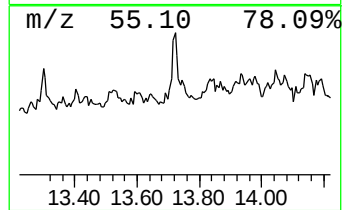
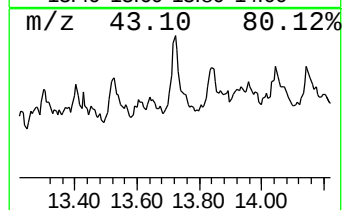
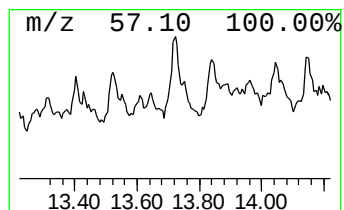
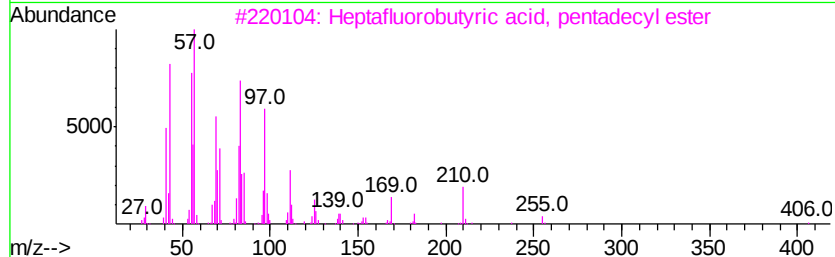
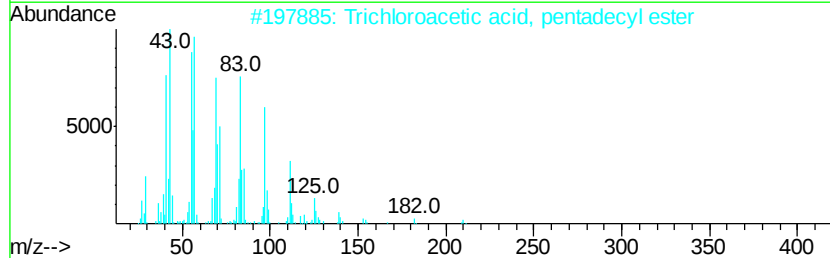
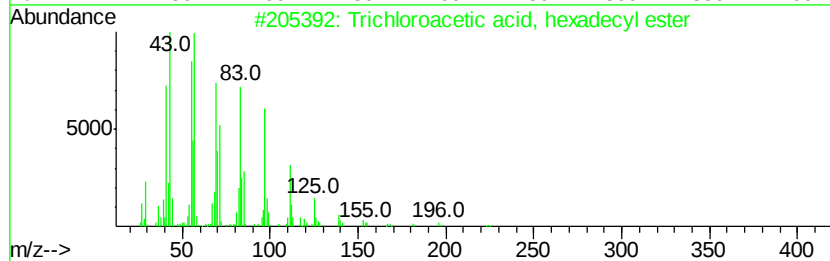
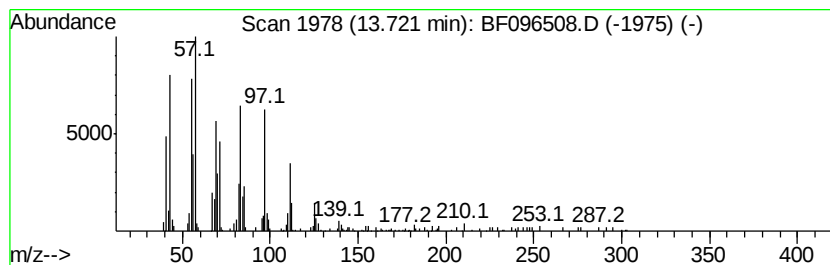
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	3.89 ng	163670	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	87
4		Z-5-Nonadecene	266	C19H38	1000131-11-8	83
5		1-Hexacosanol	382	C26H54O	000506-52-5	74



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Misc :
ALS Vial : 36 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...	4.90	13.5	ng	464013	1	6.72	689086	20.0
(1R)-2,6,6-Trimet...	6.00	4.4	ng	151015	1	6.72	689086	20.0
unknown6.49	6.49	77.2	ng	2658790	1	6.72	689086	20.0
Heptadecane, 8-me...	9.17	3.3	ng	115350	3	9.75	707856	20.0
Hexadecane	9.70	3.3	ng	115407	3	9.75	707856	20.0
2-Bromo dodecane	10.67	3.0	ng	92576	4	11.23	616826	20.0
Decanamide-	13.30	3.5	ng	146221	5	13.86	841895	20.0
Trichloroacetic a...	13.72	3.9	ng	163670	5	13.86	841895	20.0