

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091917\
 Data File : BF098651.D
 Acq On : 19 Sep 2017 19:52
 Operator : SJ/JU
 Sample : I5276-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-ENV-117-4(5-10)

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-BF091117.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	4.110	340	344	352	rBV	90383	120131	2.24%	0.281%
2	4.598	424	427	437	rVB	73225	89635	1.67%	0.210%
3	4.810	459	463	480	rBV	356593	663134	12.37%	1.551%
4	5.239	531	536	539	rBV	3579112	3682643	68.71%	8.613%
5	6.286	708	714	717	rBV	3126073	3994514	74.53%	9.342%
6	6.404	729	734	737	rBV	3885714	3997086	74.58%	9.348%
7	6.622	768	771	780	rBV	871610	841256	15.70%	1.967%
8	6.781	793	798	802	rBV	2761448	2638173	49.22%	6.170%
9	7.204	864	870	873	rBV	2307566	2556329	47.70%	5.979%
10	7.910	985	990	1004	rVB	1352674	1191434	22.23%	2.786%
11	8.992	1167	1174	1177	rBV	5104367	5359701	100.00%	12.535%
12	9.386	1236	1241	1244	rBV	553415	487352	9.09%	1.140%
13	9.663	1282	1288	1291	rBV	1760366	1747622	32.61%	4.087%
14	10.457	1416	1423	1426	rBV	3183442	3417610	63.76%	7.993%
15	11.145	1535	1540	1543	rBV	1915072	1776520	33.15%	4.155%
16	11.686	1627	1632	1634	rBV2	102049	94345	1.76%	0.221%
17	12.357	1742	1746	1754	rVB	103630	128350	2.39%	0.300%
18	12.580	1782	1784	1789	rVB	85850	77763	1.45%	0.182%
19	12.733	1802	1810	1813	rBV	4361212	5251758	97.99%	12.283%
20	13.210	1886	1891	1896	rBV	116814	117551	2.19%	0.275%
21	13.286	1901	1904	1909	rVV	61376	55589	1.04%	0.130%
22	13.621	1957	1961	1969	rBV2	161504	223954	4.18%	0.524%
23	13.780	1984	1988	1991	rVV	2196558	2029056	37.86%	4.745%
24	13.804	1991	1992	1998	rVB2	56734	54713	1.02%	0.128%
25	13.962	2013	2019	2027	rBV9	30021	84453	1.58%	0.198%
26	14.404	2091	2094	2099	rVB	66664	70766	1.32%	0.166%
27	14.527	2111	2115	2117	rBV	322548	331721	6.19%	0.776%
28	14.786	2157	2159	2166	rVB	51793	76603	1.43%	0.179%
29	15.180	2220	2226	2235	rVB	1214682	1496384	27.92%	3.500%
30	16.515	2448	2453	2460	rBV6	43165	101727	1.90%	0.238%

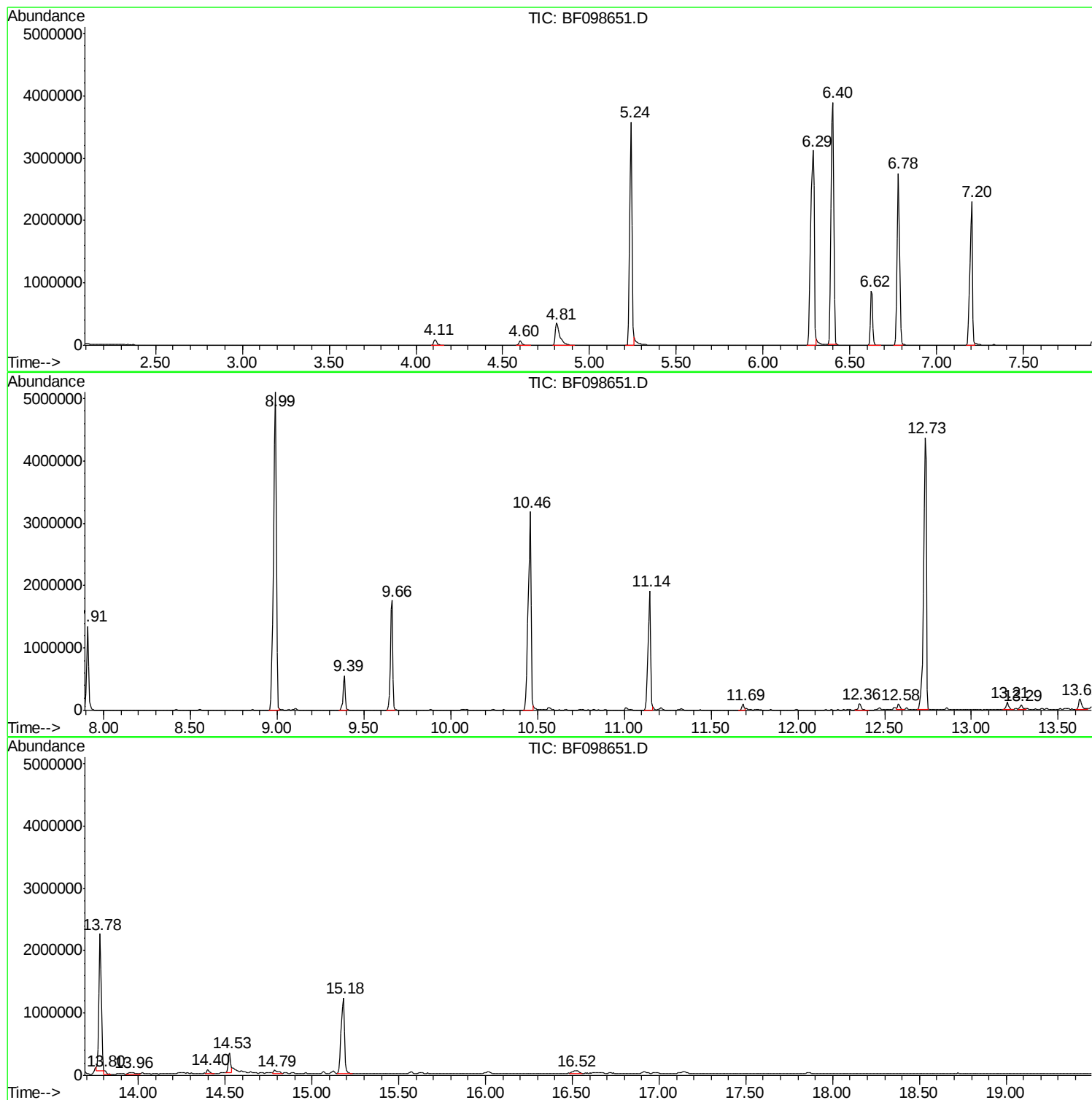
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SASP2P-ENV-117-4(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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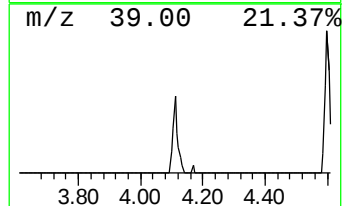
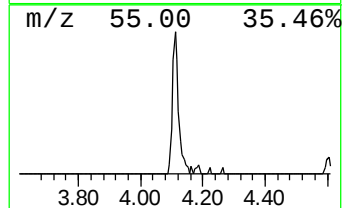
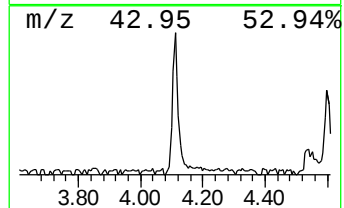
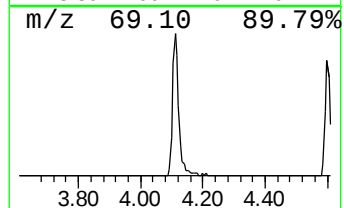
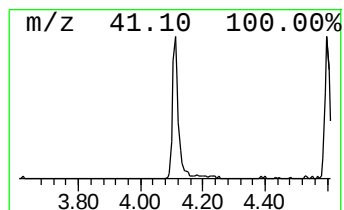
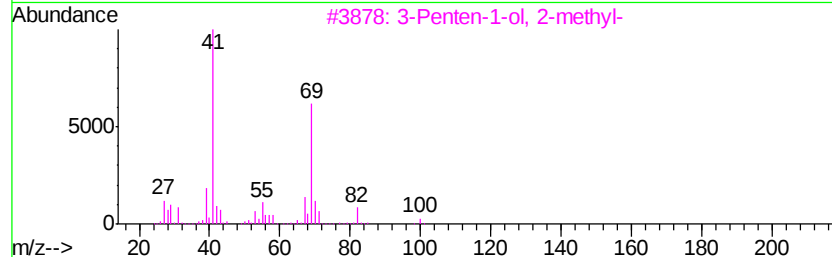
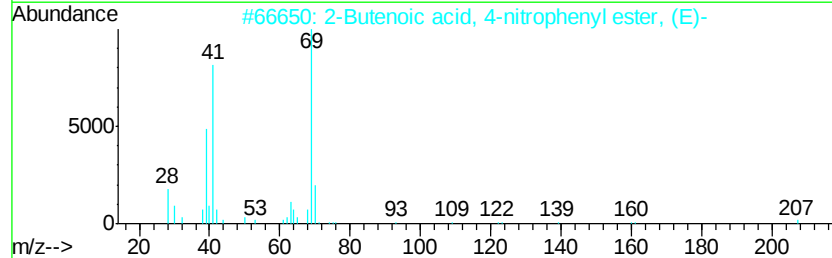
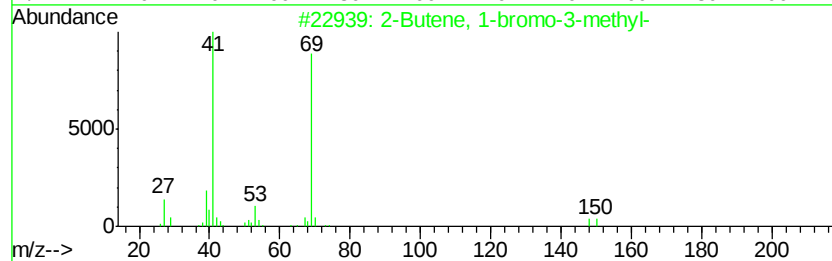
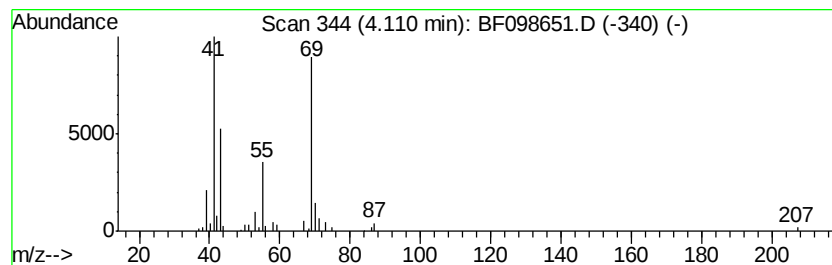
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Butene, 1-bromo-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.11	2.86 ng	120131	1,4-Dichlorobenzene-d4	6.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butene, 1-bromo-3-methyl-	148	C5H9Br	000870-63-3	64
2			2-Butenoic acid, 4-nitrophenyl e...	207	C10H9NO4	014617-88-0	53
3			3-Penten-1-ol, 2-methyl-	100	C6H12O	062238-37-3	40
4			1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	39
5			1-Butene, 3,3-dimethyl-	84	C6H12	000558-37-2	39



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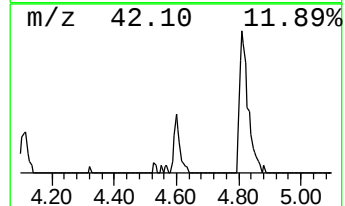
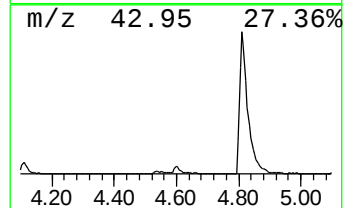
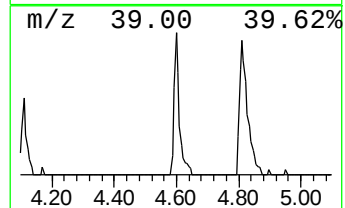
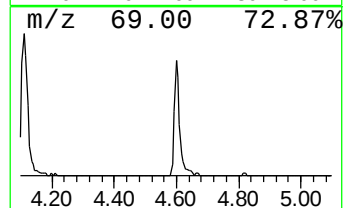
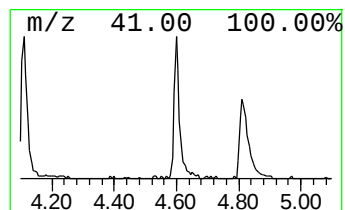
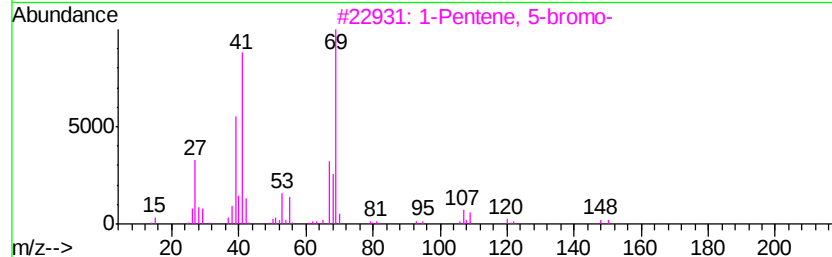
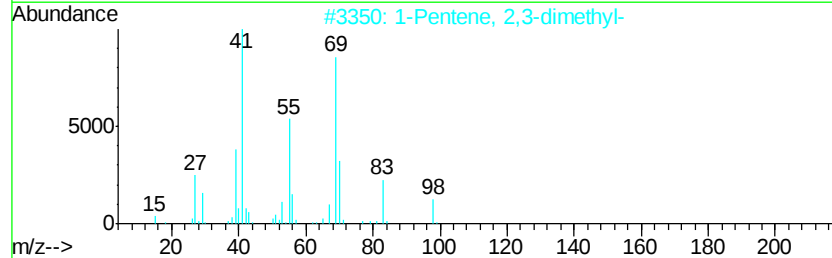
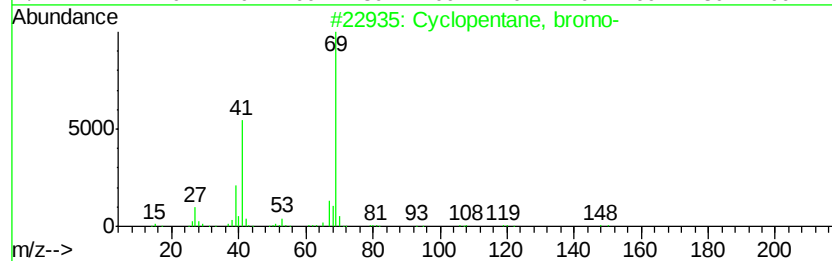
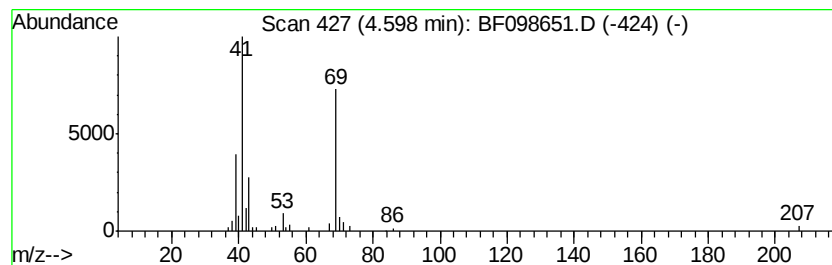
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Peak Number 2 unknown4.60 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.60	2.13 ng	89635	1,4-Dichlorobenzene-d4	6.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, bromo-	148	C5H9Br	000137-43-9	40
2			1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	39
3			1-Pentene, 5-bromo-	148	C5H9Br	001119-51-3	38
4			(Z)-1,3-Butadien-1-ol	70	C4H6O	070415-58-6	33
5			Vinyl crotonate	112	C6H8O2	014861-06-4	33



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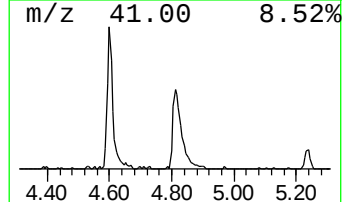
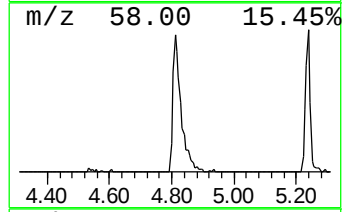
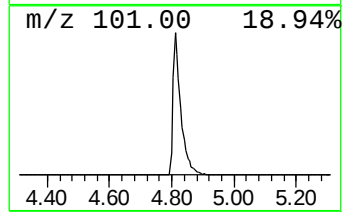
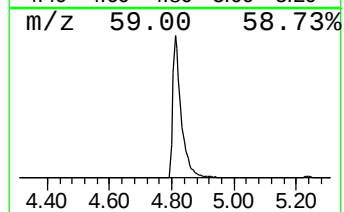
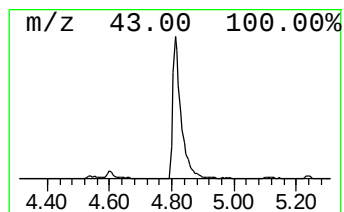
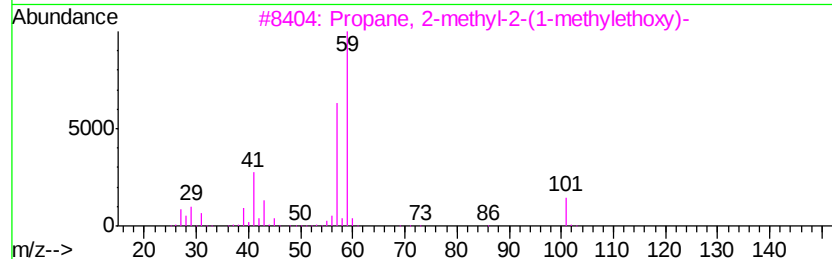
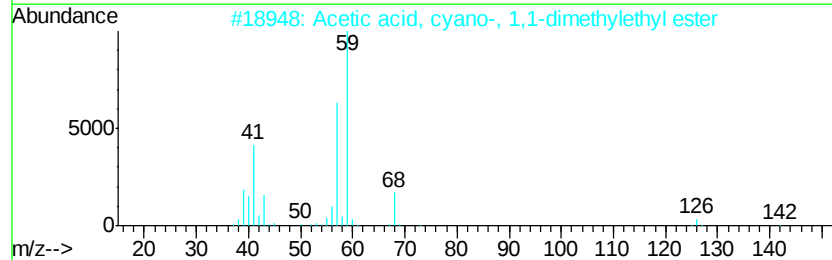
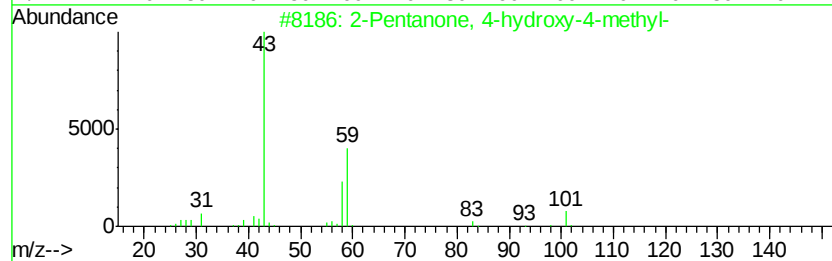
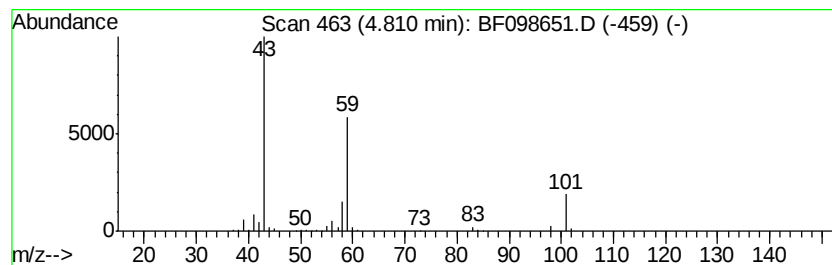
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	15.77 ng	663134	1,4-Dichlorobenzene-d4	6.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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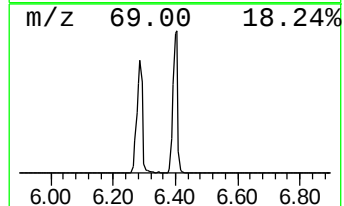
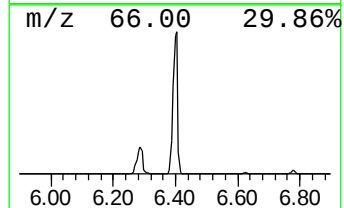
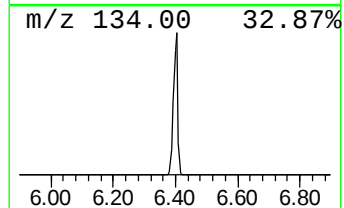
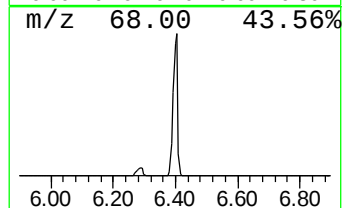
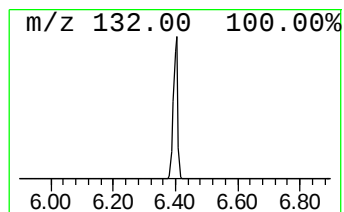
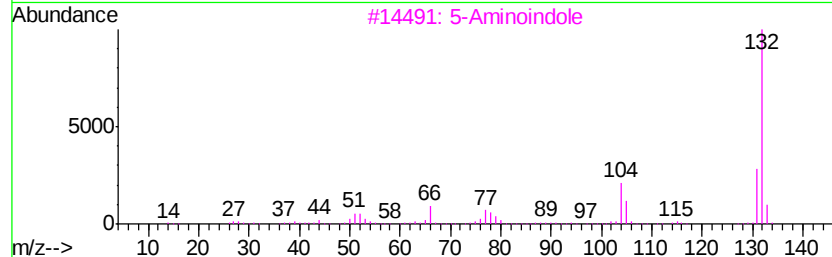
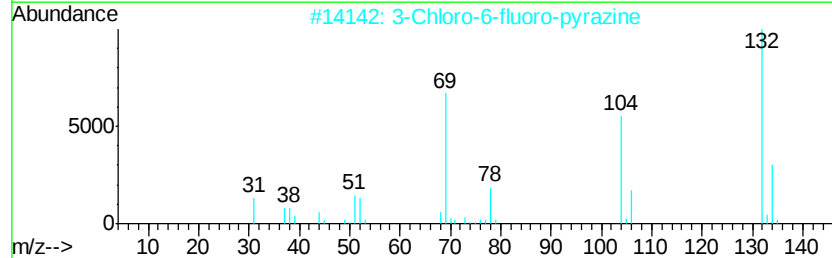
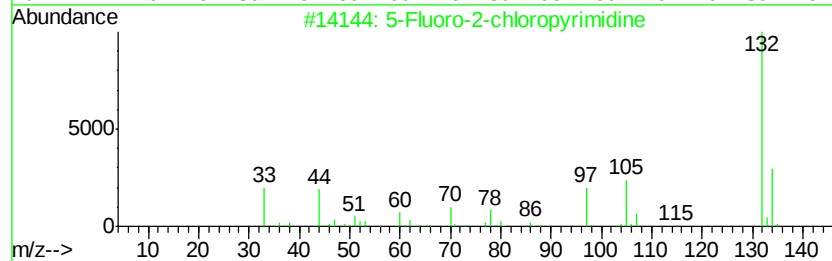
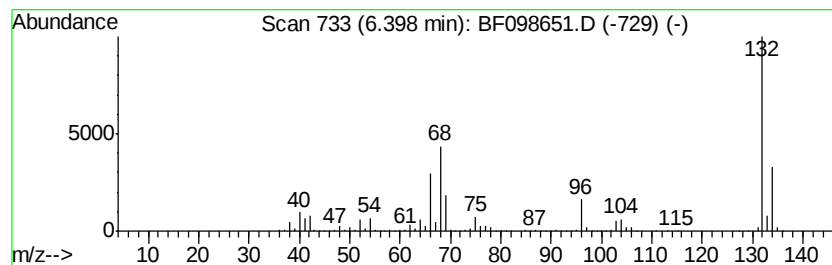
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Peak Number 4 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	95.03 ng	3997090	1,4-Dichlorobenzene-d4	6.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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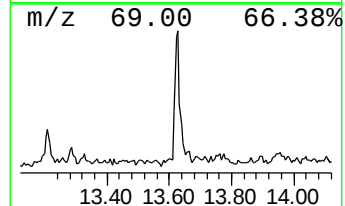
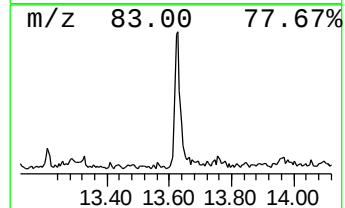
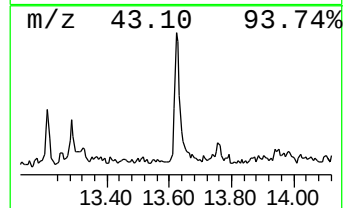
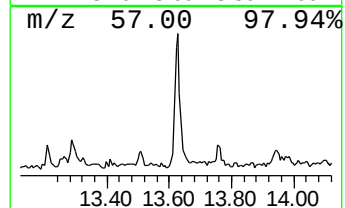
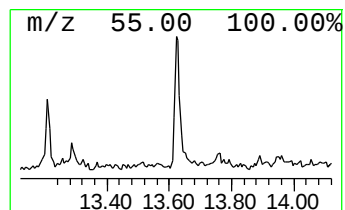
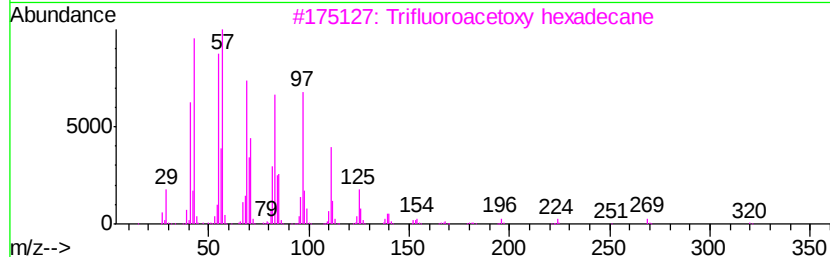
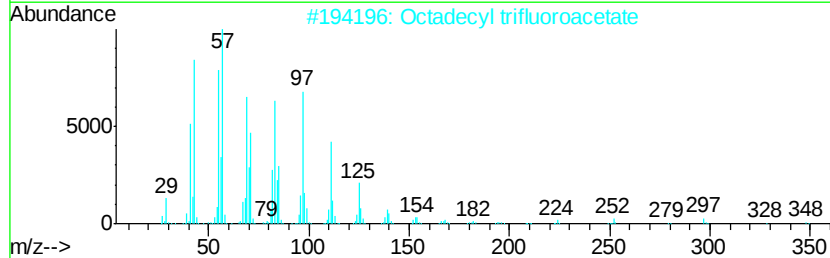
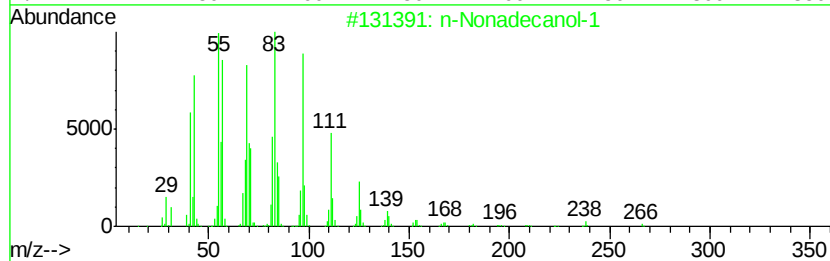
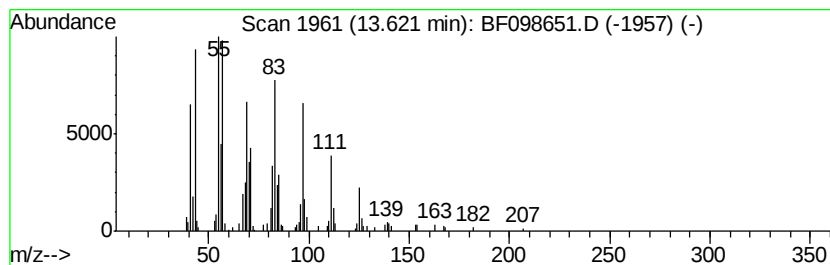
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Peak Number 6 n-Nonadecanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.62	2.21 ng	223954	Chrysene-d12	13.78	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	1-Docosene	308	C22H44	001599-67-3	91



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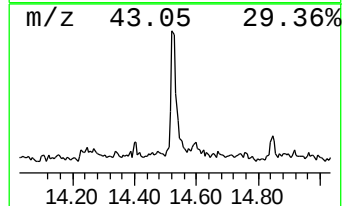
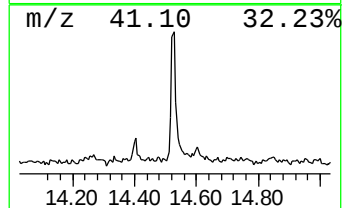
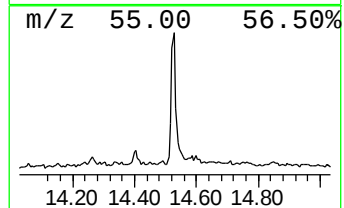
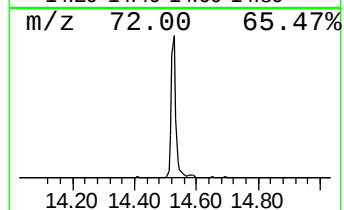
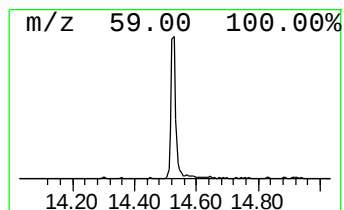
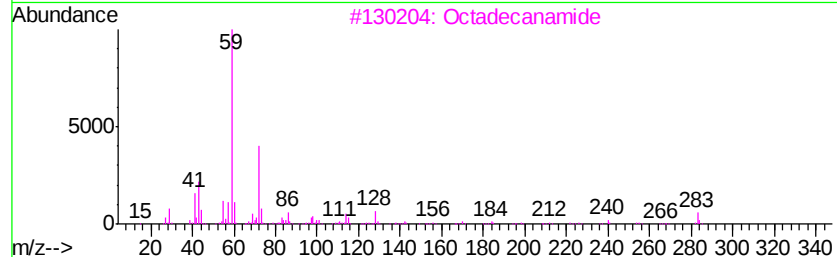
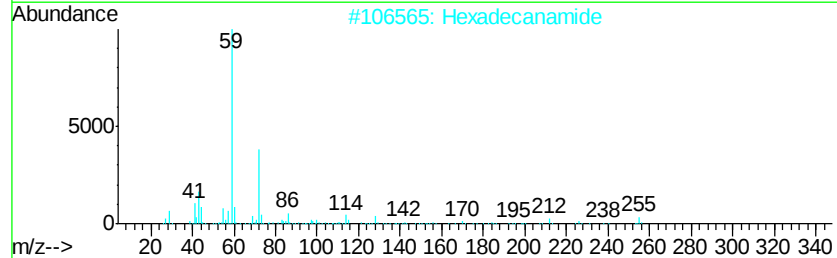
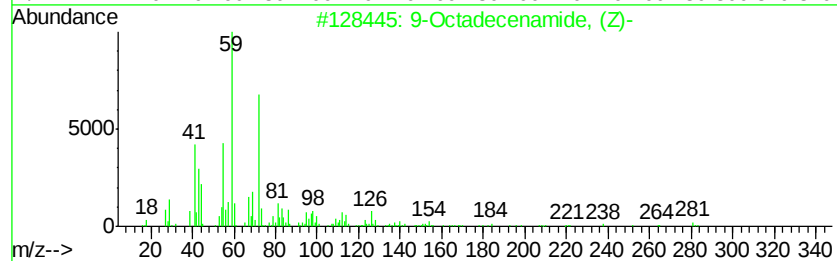
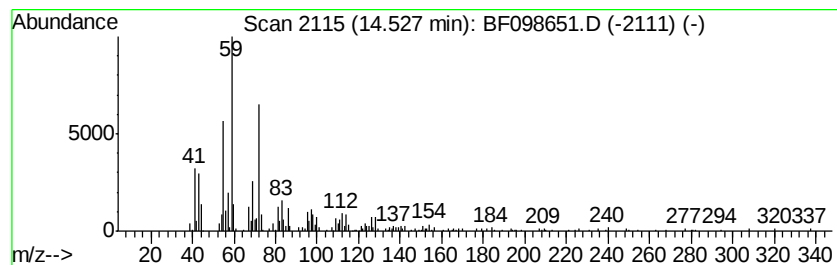
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	4.43 ng	331721	Perylene-d12	15.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2		Hexadecanamide	255	C16H33NO	000629-54-9	64
3		Octadecanamide	283	C18H37NO	000124-26-5	58
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	53
5		Cyclooctanemethanol, .alpha.,.al...	170	C11H22O	016624-06-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091917\
Data File : BF098651.D
Acq On : 19 Sep 2017 19:52
Operator : SJ/JU
Sample : I5276-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-117-4(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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-Butene, 1-bromo...	4.11	2.9	ng	120131	1	6.63	841256	20.0
unknown4.60	4.60	2.1	ng	89635	1	6.63	841256	20.0
2-Pentanone, 4-hy...	4.81	15.8	ng	663134	1	6.63	841256	20.0
unknown6.40	6.40	95.0	ng	3997090	1	6.63	841256	20.0
n-Nonadecanol-1	13.62	2.2	ng	223954	5	13.78	2029060	20.0
9-Octadecenamide, ...	14.53	4.4	ng	331721	6	15.18	1496380	20.0