

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
 Data File : BF096291.D
 Acq On : 29 Jun 2017 14:58
 Operator : SJ/MA
 Sample : I3949-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-C2-(0-8)

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-BF062717.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	4.975	486	491	499	rBV	618295	794658	19.95%	2.473%
2	5.387	556	561	565	rVB	3655784	3940994	98.92%	12.266%
3	6.404	728	734	737	rBV	3845404	3983890	100.00%	12.399%
4	6.540	752	757	761	rBV	3754876	3705832	93.02%	11.534%
5	6.769	792	796	800	rBV	1186790	1069332	26.84%	3.328%
6	6.928	819	823	827	rVB	2912017	2565335	64.39%	7.984%
7	7.328	886	891	894	rBV	2506520	2363657	59.33%	7.356%
8	7.422	903	907	911	rVB	68245	70246	1.76%	0.219%
9	7.757	958	964	966	rBV	76785	93671	2.35%	0.292%
10	8.051	1010	1014	1020	rBV	1602894	1387710	34.83%	4.319%
11	8.486	1084	1088	1092	rBV	44945	46011	1.15%	0.143%
12	8.657	1113	1117	1120	rBV	56657	49034	1.23%	0.153%
13	9.128	1192	1197	1201	rBV	3022532	2719450	68.26%	8.464%
14	9.222	1210	1213	1217	rBV2	91430	78612	1.97%	0.245%
15	9.522	1260	1264	1266	rBV	720381	606902	15.23%	1.889%
16	9.751	1300	1303	1307	rVB	128940	105097	2.64%	0.327%
17	9.804	1307	1312	1316	rBV	1386903	1181768	29.66%	3.678%
18	10.010	1344	1347	1350	rVB	64238	50497	1.27%	0.157%
19	10.251	1385	1388	1391	rVB	128154	106639	2.68%	0.332%
20	10.469	1421	1425	1427	rBV2	37918	44672	1.12%	0.139%
21	10.586	1441	1445	1449	rBV	1571946	1403339	35.23%	4.368%
22	10.686	1458	1462	1465	rBV	153259	121421	3.05%	0.378%
23	10.722	1465	1468	1474	rVV	133699	142692	3.58%	0.444%
24	11.169	1541	1544	1547	rBV2	83009	61809	1.55%	0.192%
25	11.286	1560	1564	1567	rBV	1070586	953615	23.94%	2.968%
26	11.592	1613	1616	1619	rBV	46069	45502	1.14%	0.142%
27	11.816	1651	1654	1659	rBV2	224169	229429	5.76%	0.714%
28	11.892	1664	1667	1670	rBV2	40042	41451	1.04%	0.129%
29	11.998	1682	1685	1694	rVB3	40233	60052	1.51%	0.187%
30	12.080	1694	1699	1704	rBV3	35989	51771	1.30%	0.161%
31	12.333	1739	1742	1745	rVB	48848	48462	1.22%	0.151%
32	12.492	1766	1769	1773	rBV2	62152	67591	1.70%	0.210%
33	12.604	1784	1788	1795	rBV7	47783	65173	1.64%	0.203%
34	12.721	1802	1808	1810	rBV	48044	52583	1.32%	0.164%

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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

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Peak separation: 5

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35	12.868	1829	1833	1836	rBV	2029850	1747785	43.87%	5.440%
36	13.427	1923	1928	1930	rBV5	27547	46285	1.16%	0.144%
37	13.768	1983	1986	1995	rVB	285169	298400	7.49%	0.929%
38	13.915	2007	2011	2014	rBV	1083152	979886	24.60%	3.050%
39	14.404	2091	2094	2096	rBV4	45934	44341	1.11%	0.138%
40	15.339	2249	2253	2260	rBV2	562176	704871	17.69%	2.194%

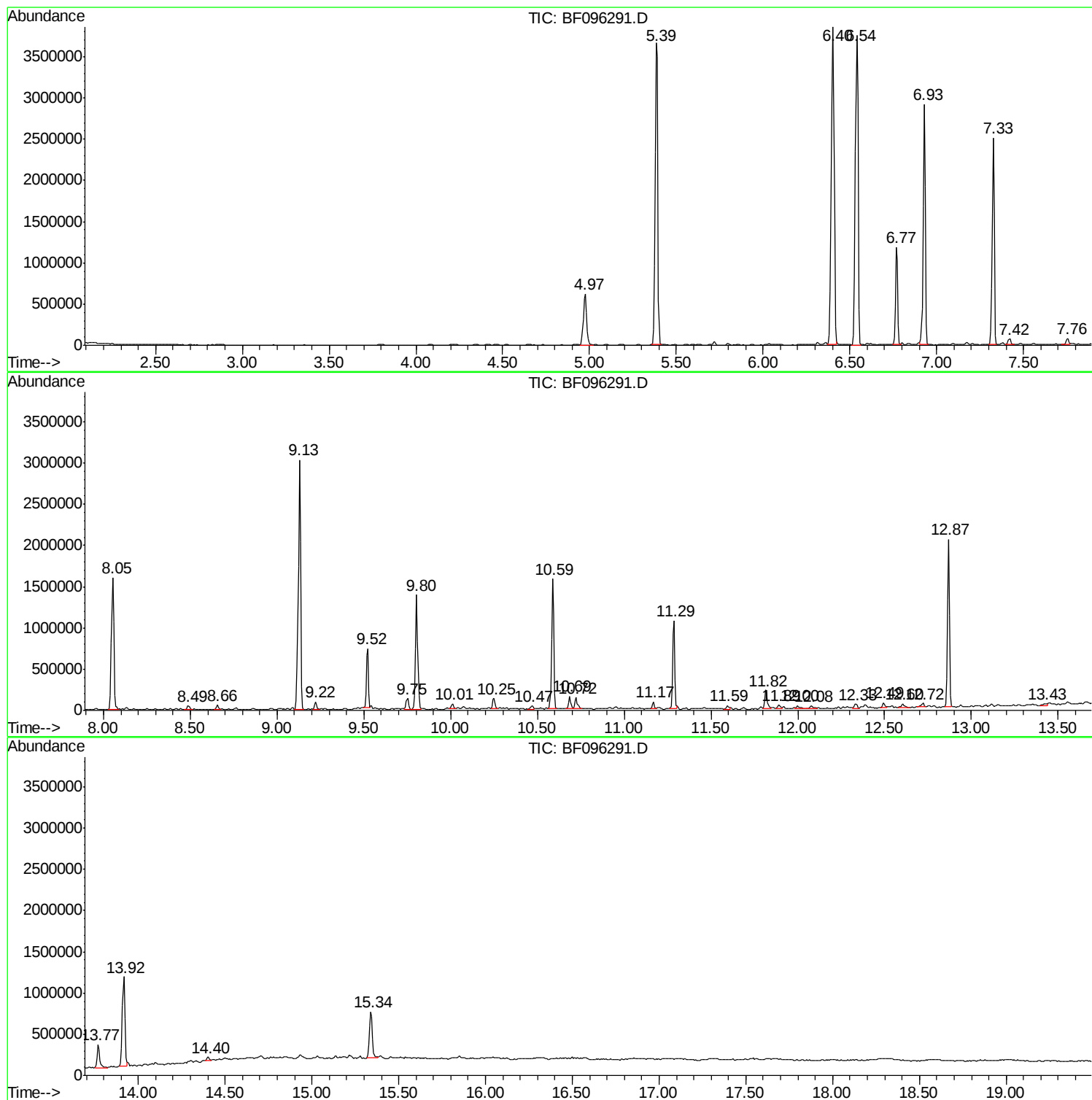
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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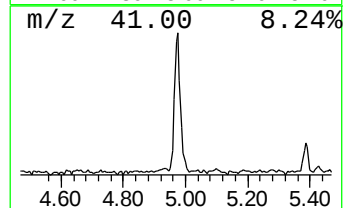
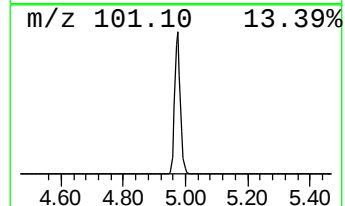
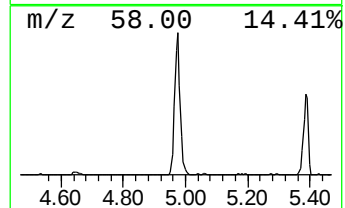
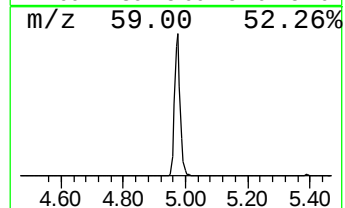
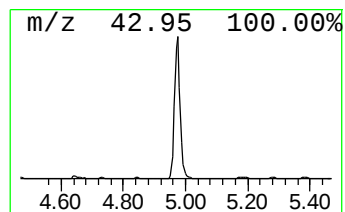
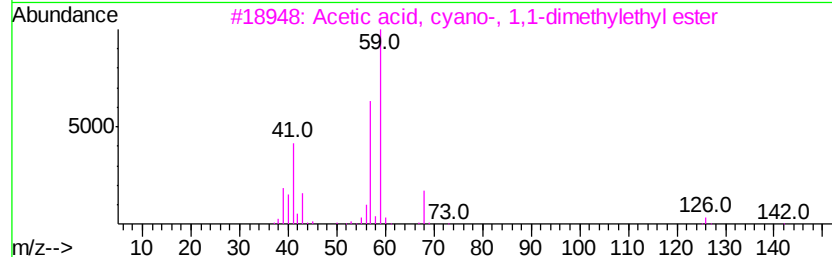
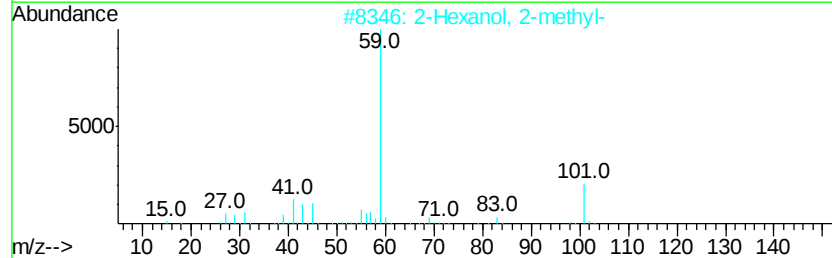
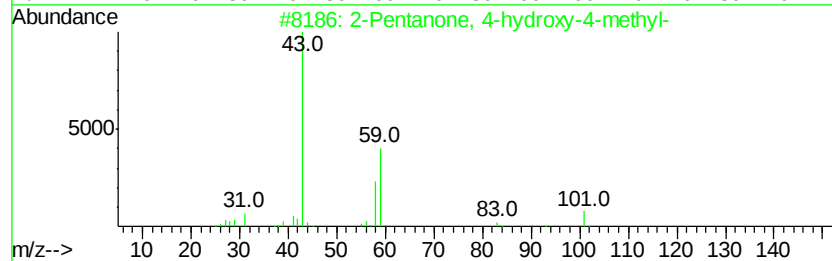
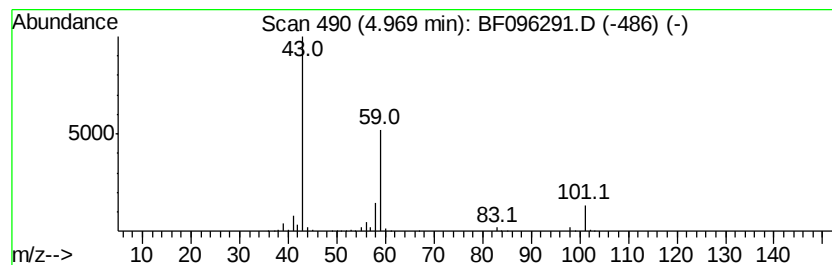
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.97	14.86 ng	794658	1,4-Dichlorobenzene-d4	6.77

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	28
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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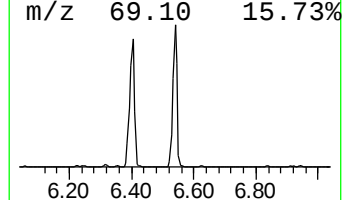
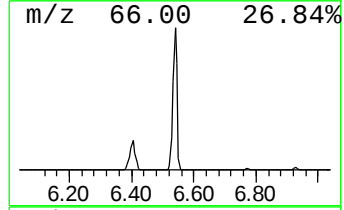
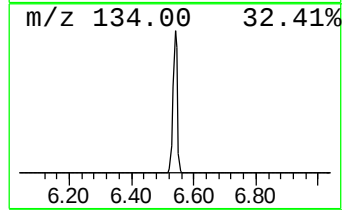
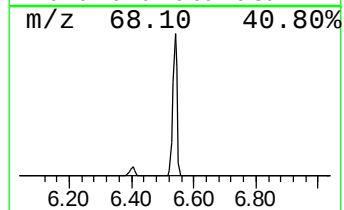
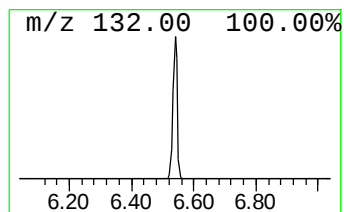
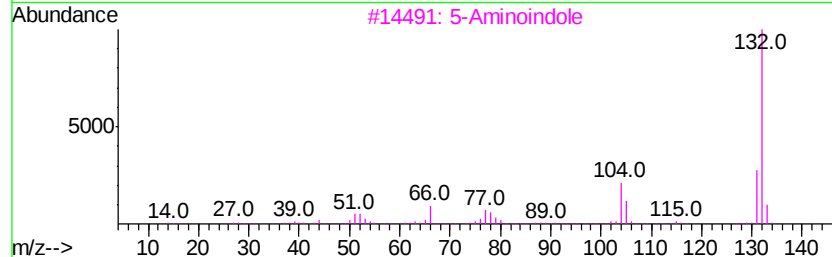
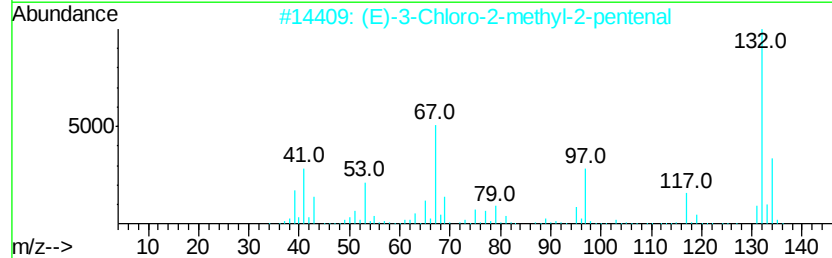
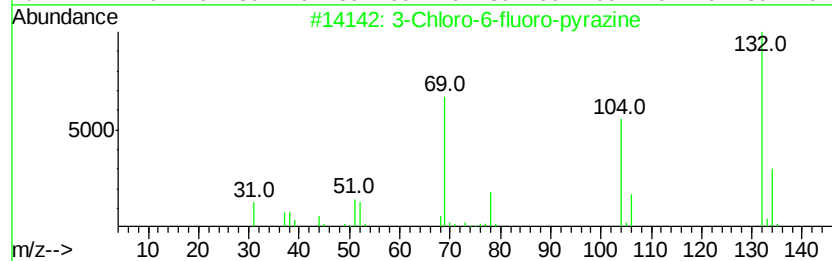
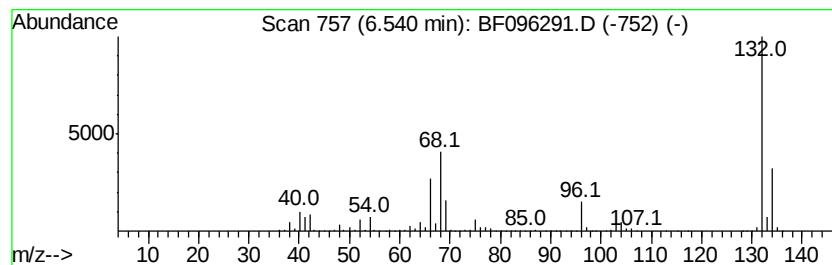
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Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	69.31 ng	3705830	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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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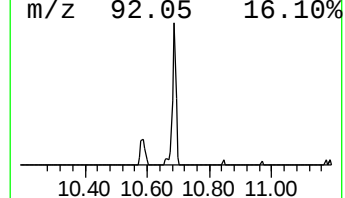
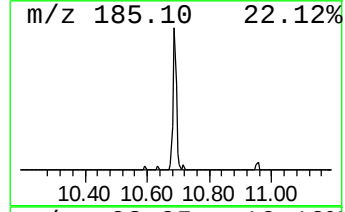
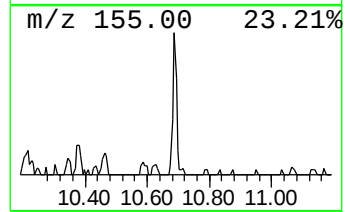
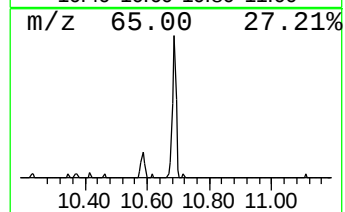
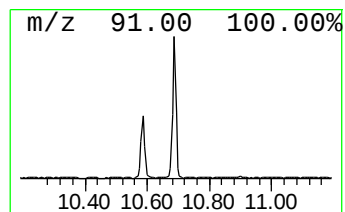
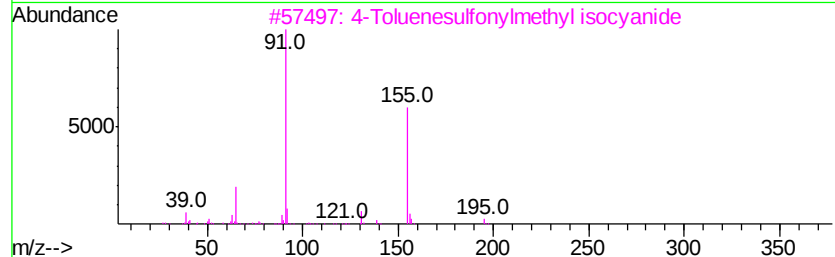
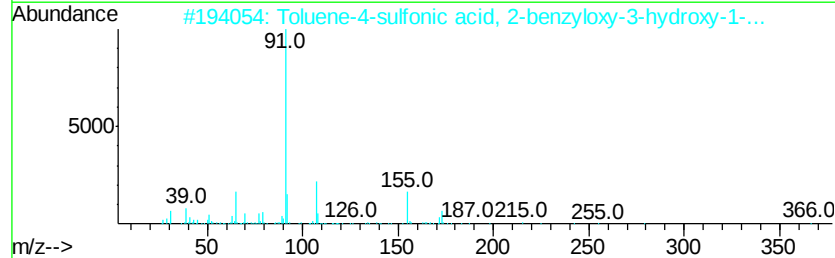
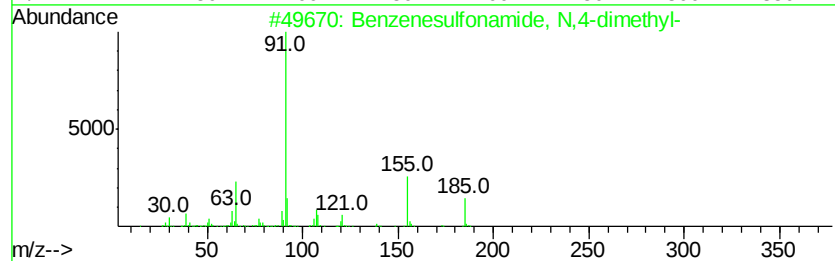
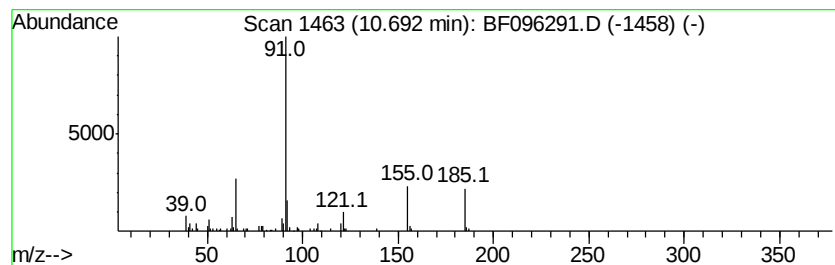
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzenesulfonamide, N,4-dim... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.69	2.55 ng	121421	Phenanthrene-d10	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	91
2		Toluene-4-sulfonic acid, 2-benzy...	366	C18H22O6S	118653-93-3	59
3		4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	59
4		(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	59
5		Toluene-4-sulfonic acid, 4-benzy...	354	C20H18O4S	1000295-51-0	47



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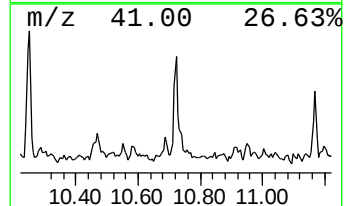
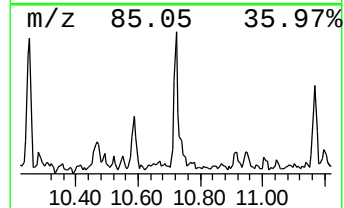
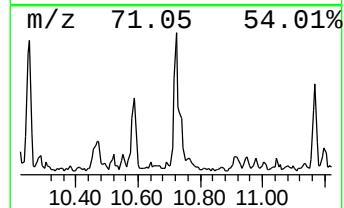
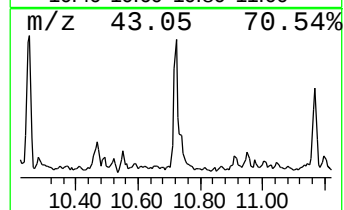
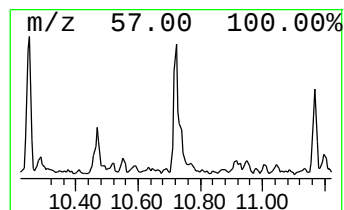
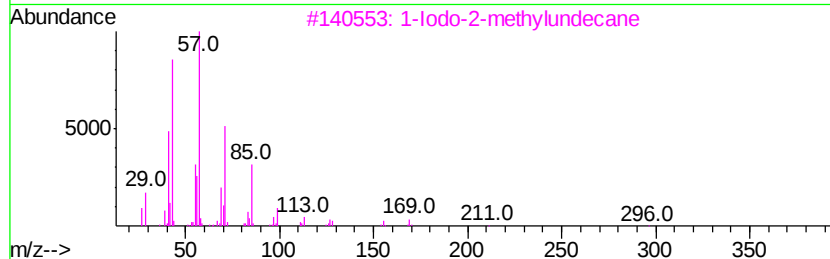
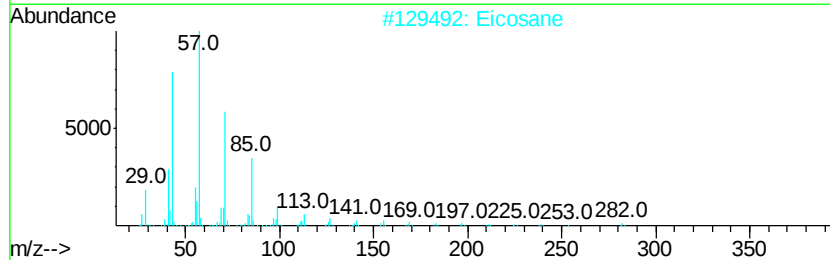
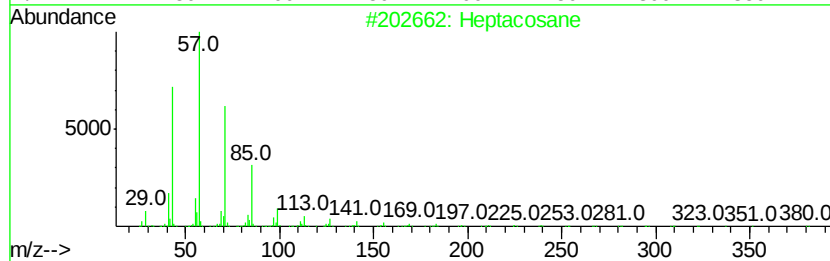
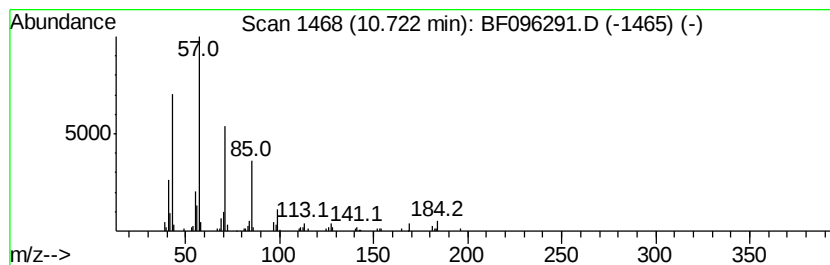
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Peak Number 5 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.72	2.99 ng	142692	Phenanthrene-d10	11.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	87
2	Eicosane	282	C20H42	000112-95-8	87
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	80



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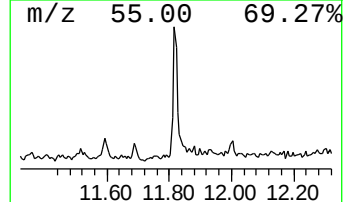
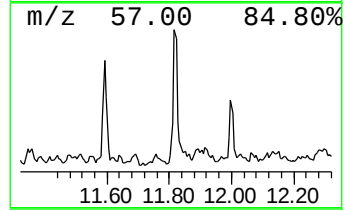
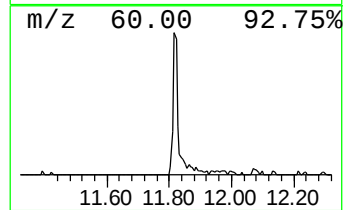
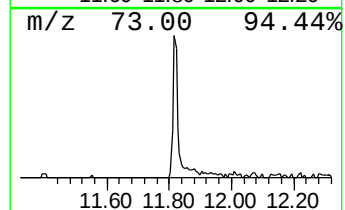
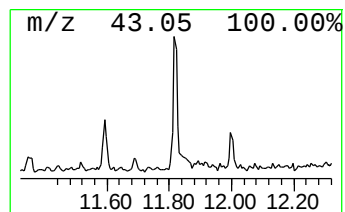
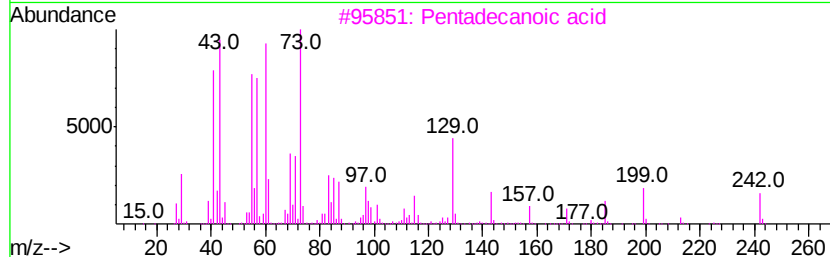
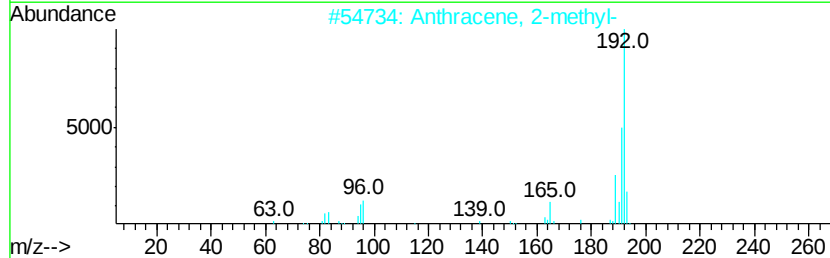
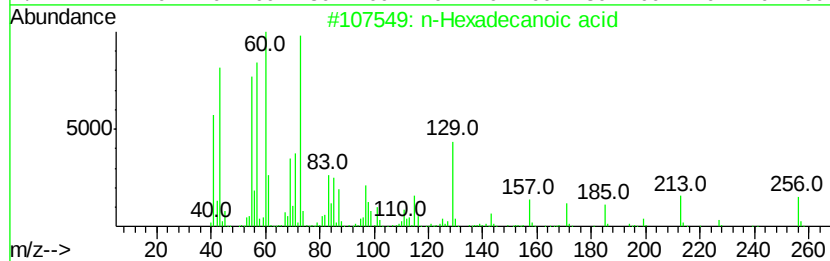
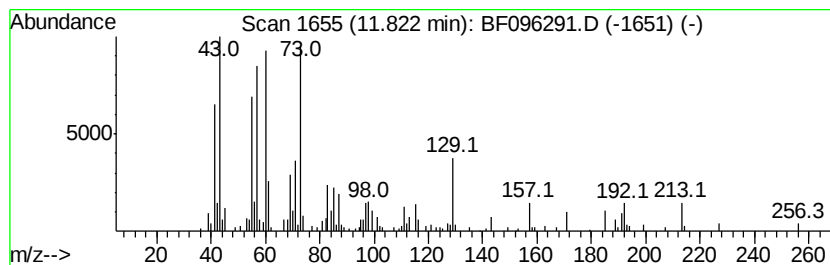
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	4.81 ng	229429	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	60
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096291.D
Acq On : 29 Jun 2017 14:58
Operator : SJ/MA
Sample : I3949-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C2-(0-8)

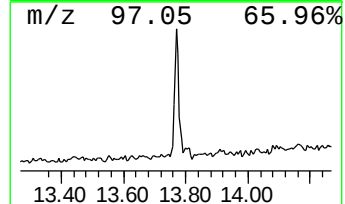
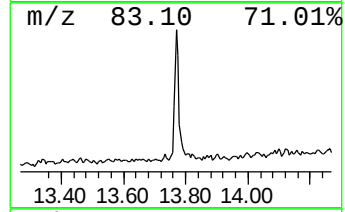
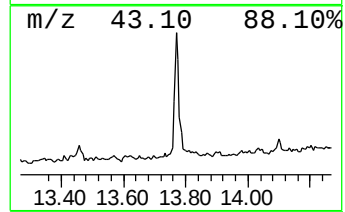
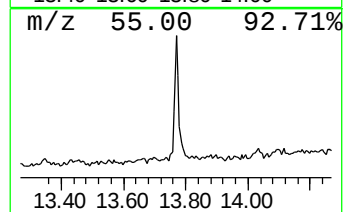
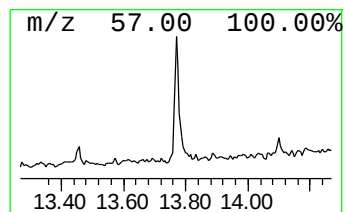
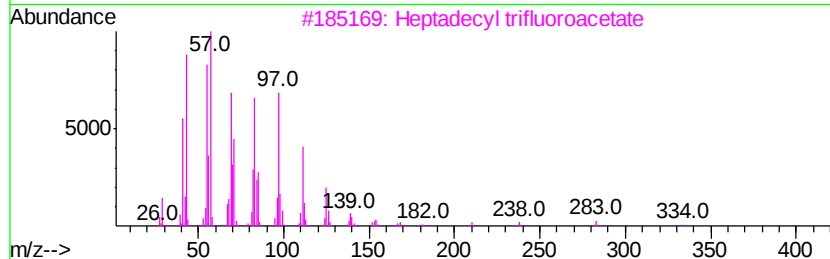
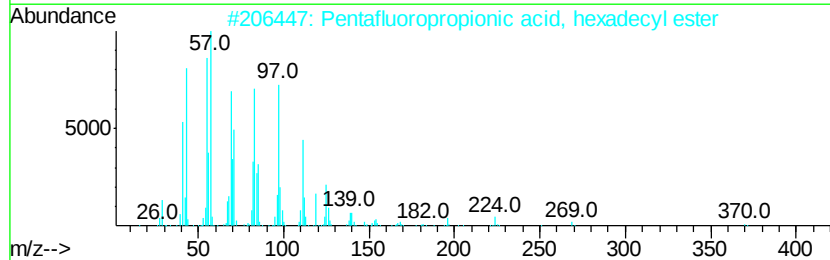
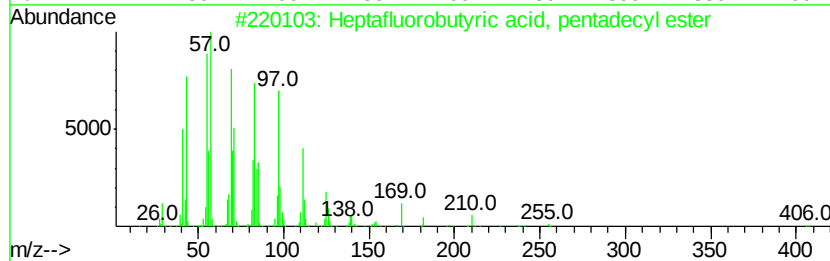
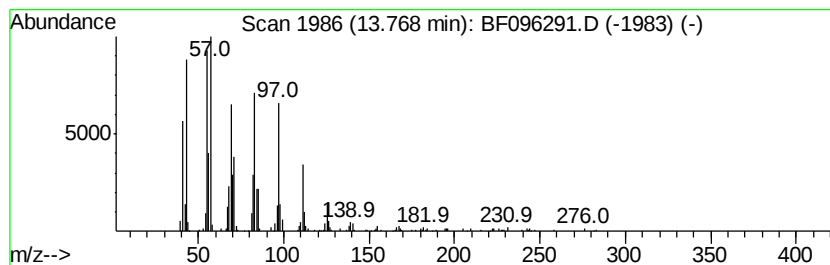
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	6.09 ng	298400	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4		1-Docosene	308	C22H44	001599-67-3	94
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062917\
Data File : BF096291.D
Acq On : 29 Jun 2017 14:58
Operator : SJ/MA
Sample : I3949-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-C2-(0-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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...	4.97	14.9	ng	794658	1	6.77	1069330	20.0
unknown6.54	6.54	69.3	ng	3705830	1	6.77	1069330	20.0
Benzenesulfonamid...	10.69	2.5	ng	121421	4	11.29	953615	20.0
Heptacosane	10.72	3.0	ng	142692	4	11.29	953615	20.0
n-Hexadecanoic acid	11.82	4.8	ng	229429	4	11.29	953615	20.0
Heptafluorobutyri...	13.77	6.1	ng	298400	5	13.92	979886	20.0