

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF110417\
 Data File : BF100178.D
 Acq On : 4 Nov 2017 15:09
 Operator : SJ/JU
 Sample : I6313-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PET-BF010-01

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-BF102317.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	4.987	489	493	518	rBV	143538	264234	12.16%	1.492%
2	5.393	559	562	589	rBV	1276103	1661466	76.49%	9.380%
3	6.416	733	736	753	rBV	1531187	1700435	78.28%	9.600%
4	6.540	753	757	770	rVB	1894260	1795349	82.65%	10.136%
5	6.763	792	795	806	rBV	550914	507629	23.37%	2.866%
6	6.916	818	821	844	rBV	1460555	1351474	62.21%	7.630%
7	7.334	889	892	912	rBV	990594	1063884	48.98%	6.006%
8	8.045	1010	1013	1032	rBV	802752	730766	33.64%	4.126%
9	9.116	1191	1195	1208	rBV	2411573	2172271	100.00%	12.264%
10	9.516	1260	1263	1270	rBV	112736	100934	4.65%	0.570%
11	9.798	1307	1311	1320	rVB	974110	849873	39.12%	4.798%
12	10.592	1443	1446	1460	rBV	1184810	1215001	55.93%	6.859%
13	10.722	1465	1468	1482	rBV	100772	126138	5.81%	0.712%
14	11.286	1561	1564	1574	rBV	840094	836213	38.49%	4.721%
15	11.804	1648	1652	1660	rBV	60178	64626	2.98%	0.365%
16	12.586	1780	1785	1792	rBV6	18574	28604	1.32%	0.161%
17	12.869	1829	1833	1836	rBV	2041655	1927064	88.71%	10.880%
18	13.745	1978	1982	1987	rBV	81570	94854	4.37%	0.536%
19	13.939	2012	2015	2022	rBV	544165	532499	24.51%	3.006%
20	14.463	2101	2104	2105	rBV3	24050	27887	1.28%	0.157%
21	14.657	2133	2137	2145	rVB	162943	180411	8.31%	1.019%
22	15.398	2259	2263	2278	rVB	327219	481119	22.15%	2.716%

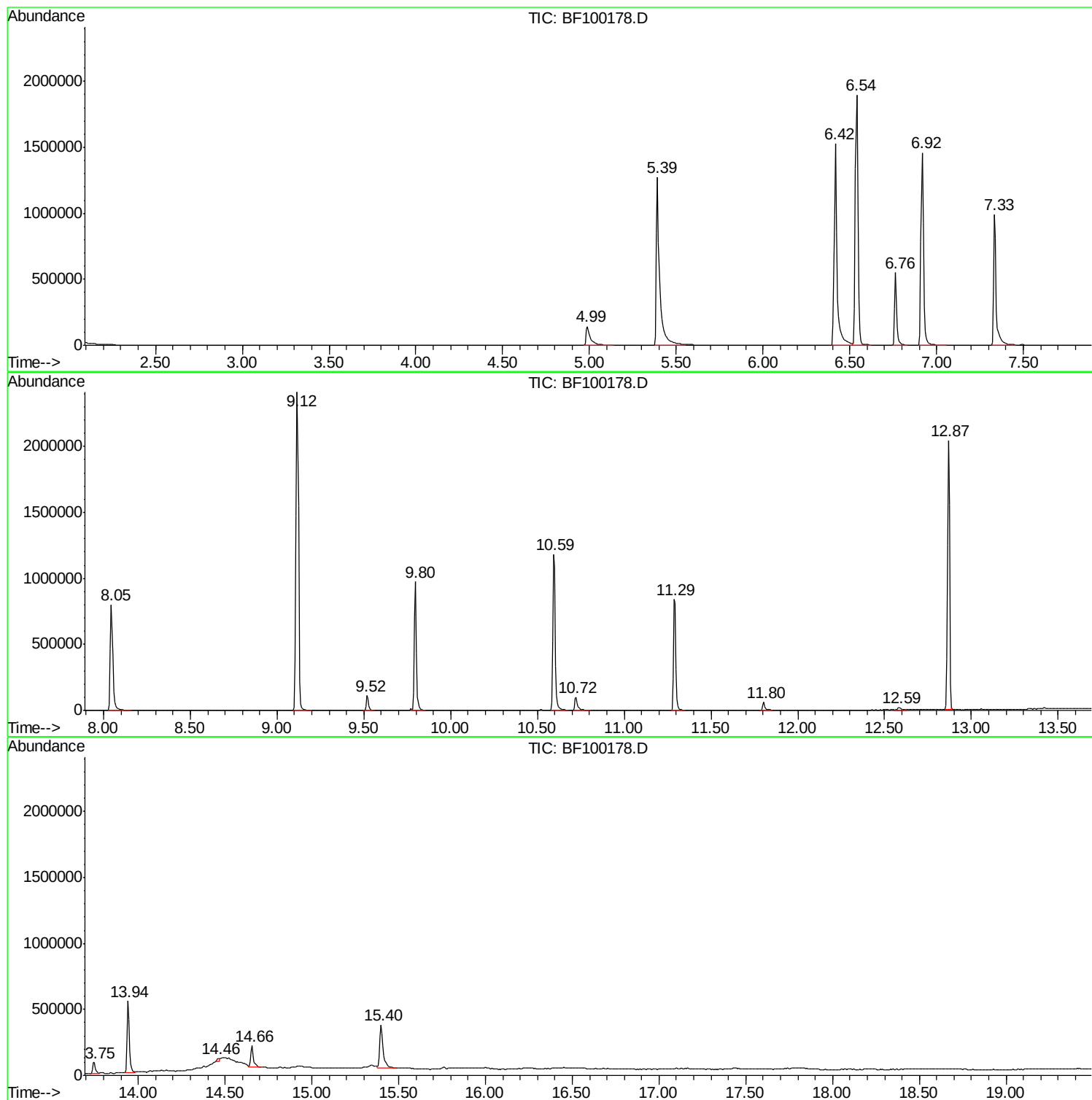
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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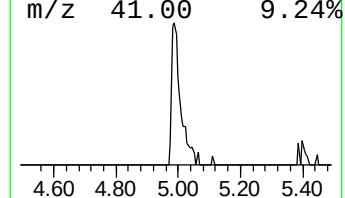
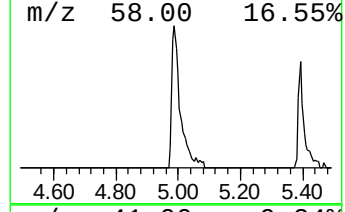
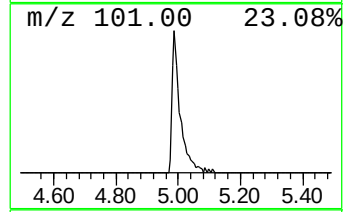
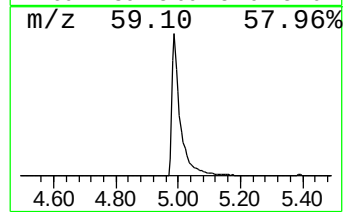
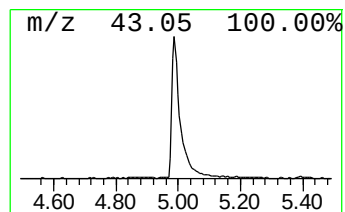
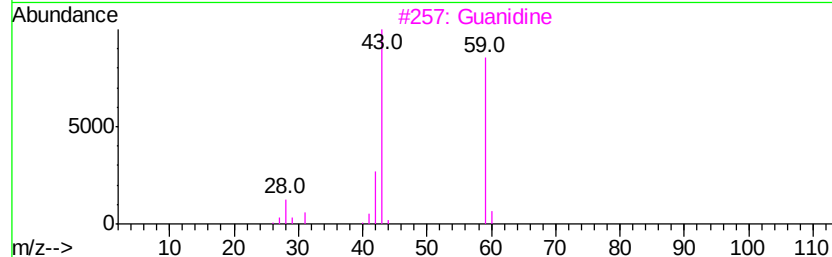
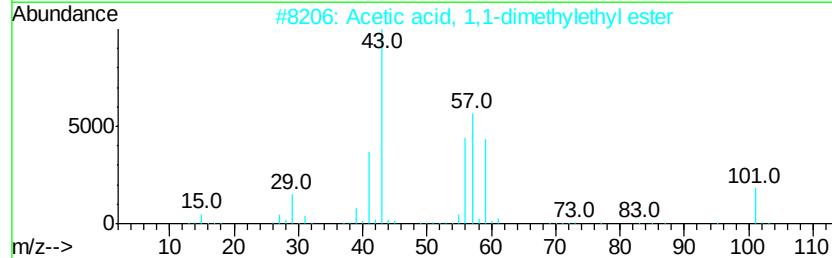
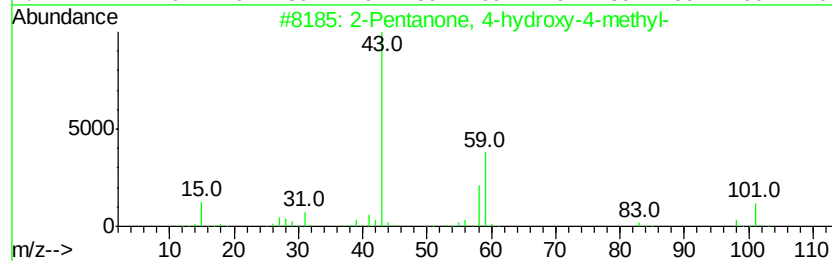
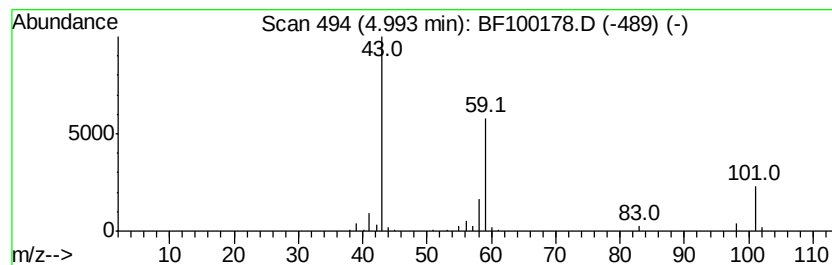
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.99	10.41 ng	264234	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		Guanidine	59	CH5N3	000113-00-8	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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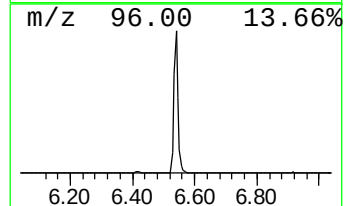
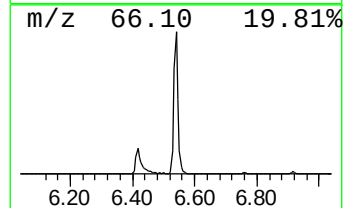
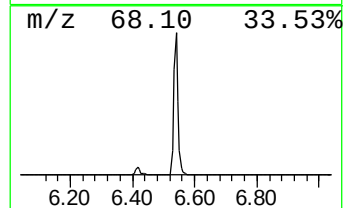
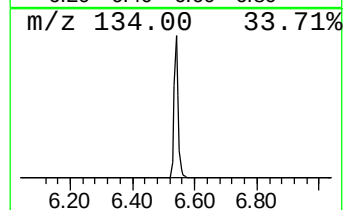
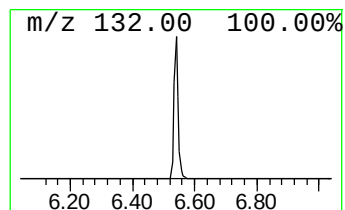
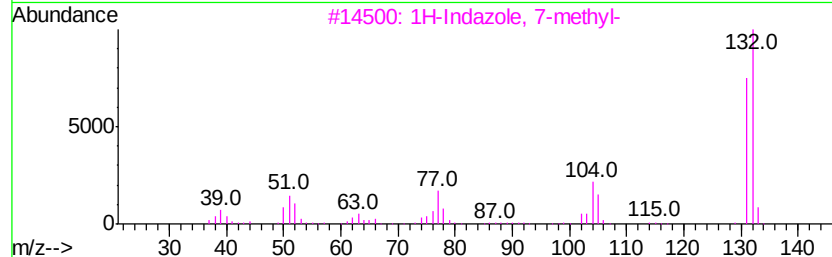
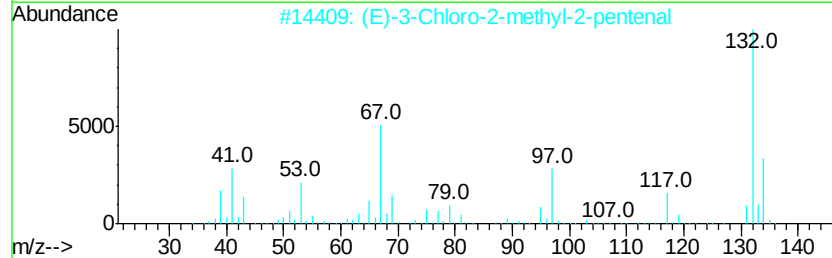
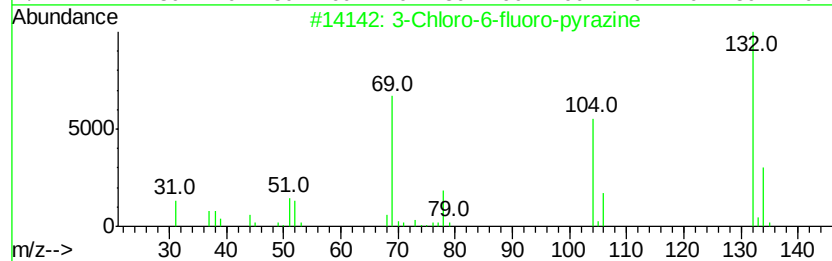
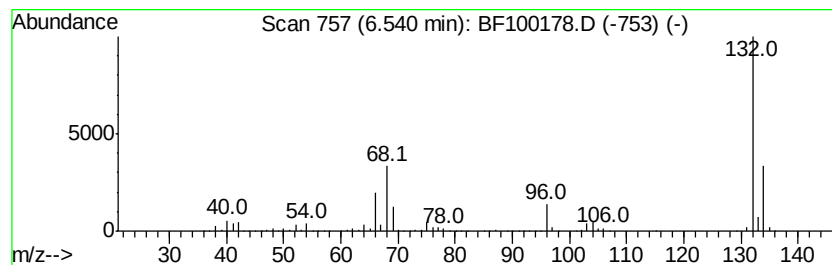
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	70.73 ng	1795350	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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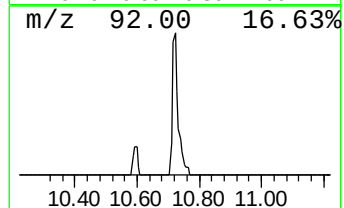
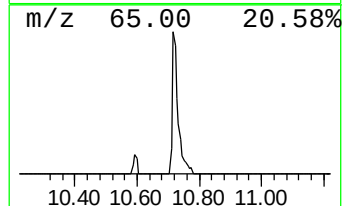
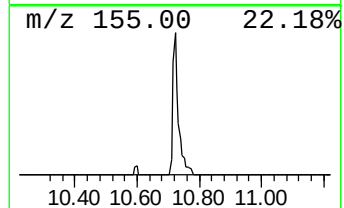
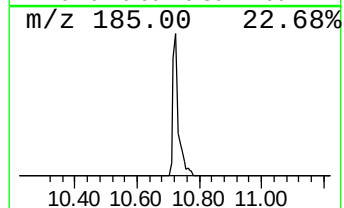
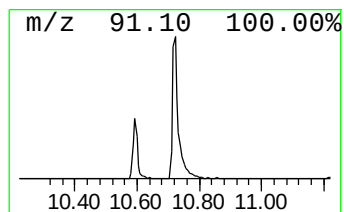
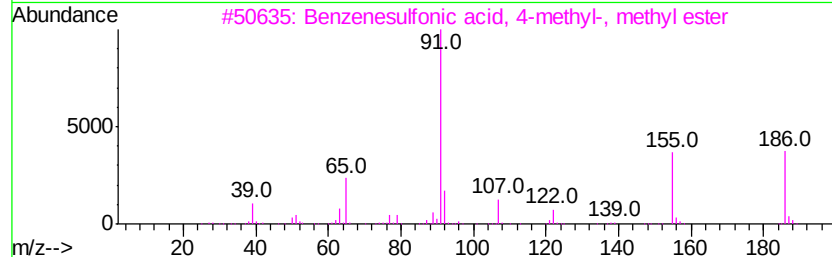
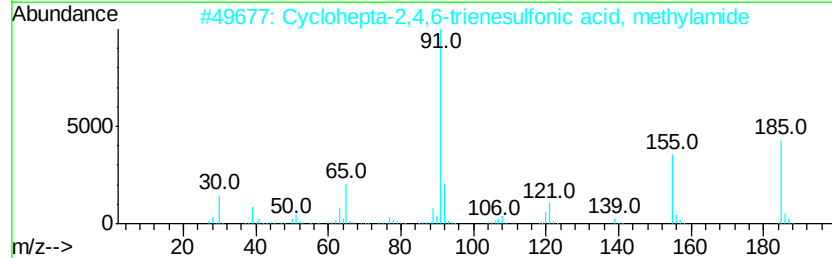
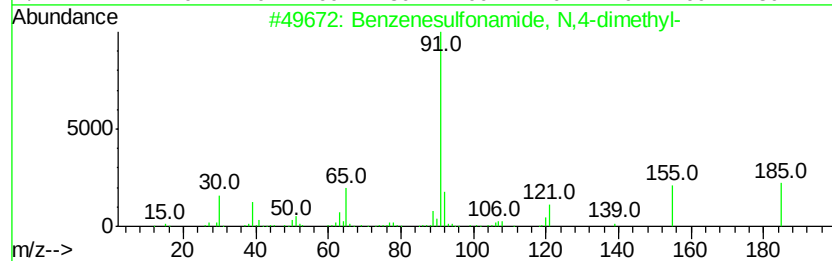
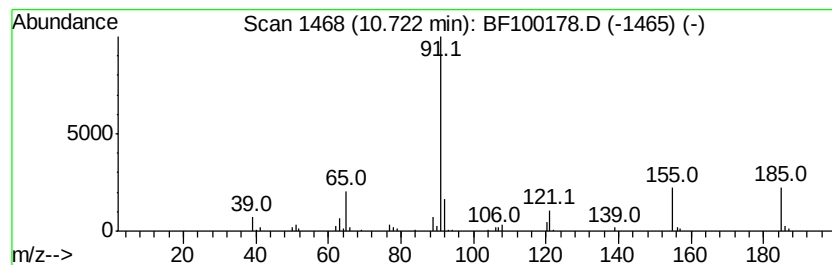
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Peak Number 4 Benzenesulfonamide, N,4-dim... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.72	3.02 ng	126138	Phenanthrene-d10	11.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	94
2	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	62
3	Benzenesulfonic acid, 4-methyl-,...	186	C8H10O3S	000080-48-8	53
4	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	50
5	p-Toluenesulfonylacetonitrile	195	C9H9NO2S	005697-44-9	47



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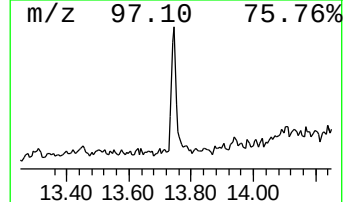
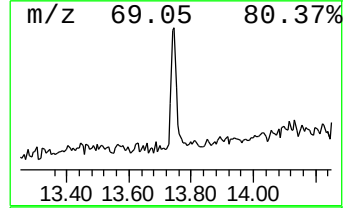
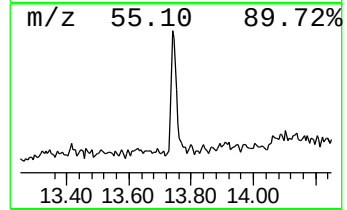
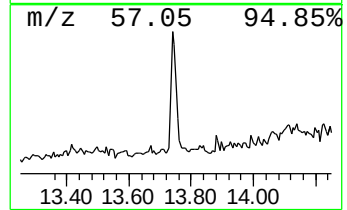
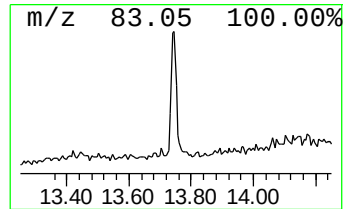
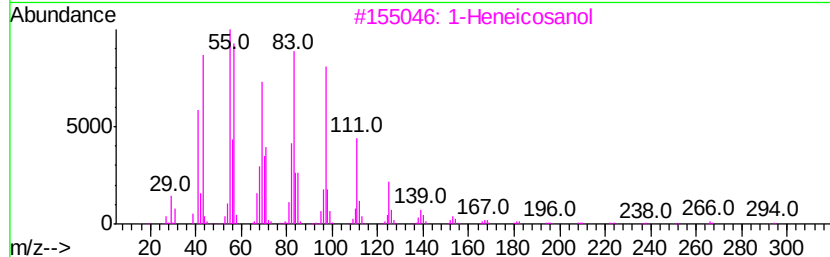
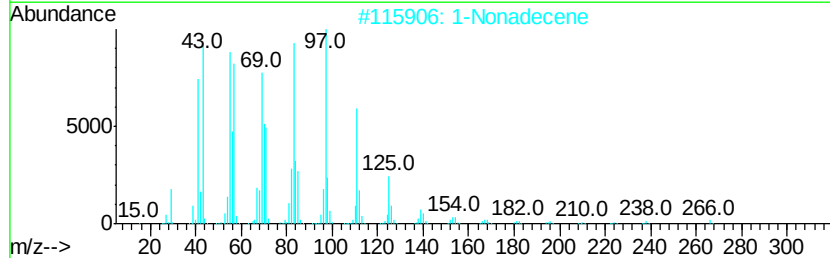
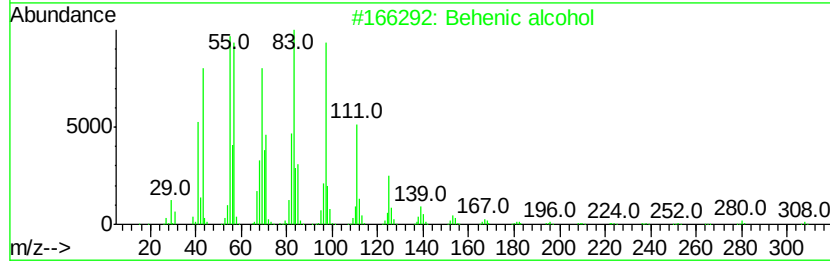
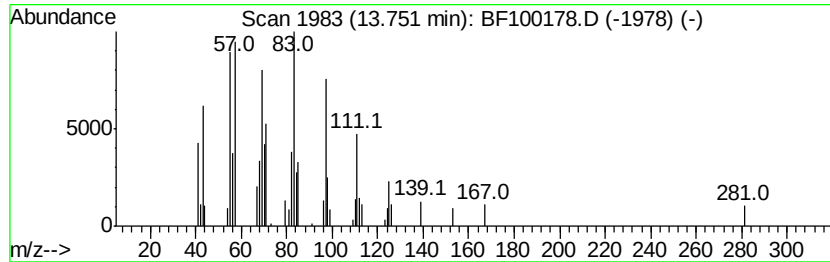
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Peak Number 5 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.75	3.56 ng	94854	Chrysene-d12	13.94	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	1-Nonadecene	266	C19H38	018435-45-5	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91



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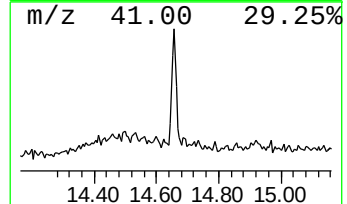
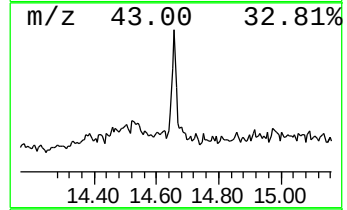
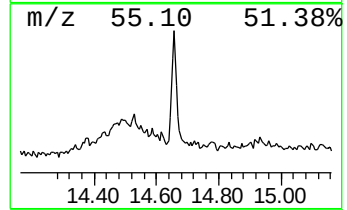
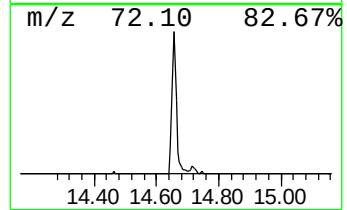
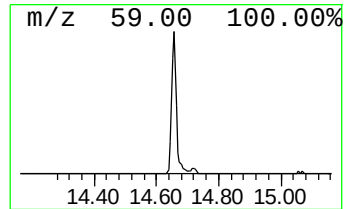
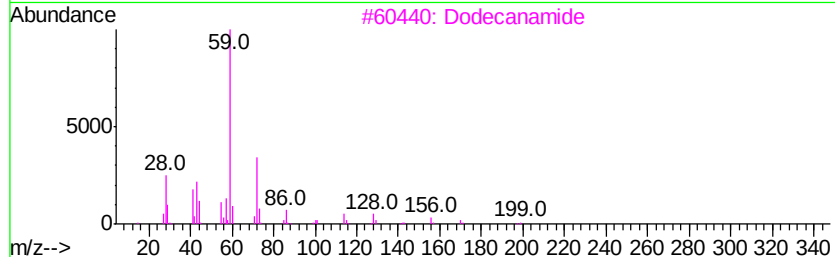
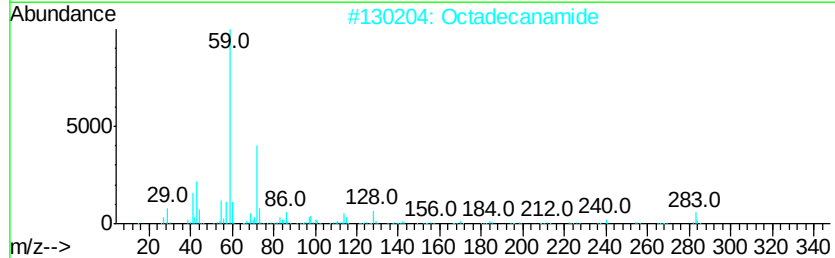
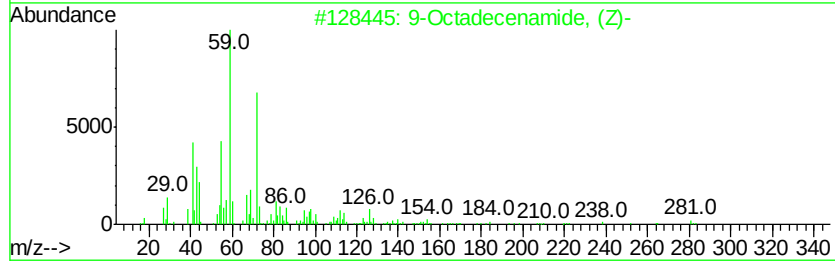
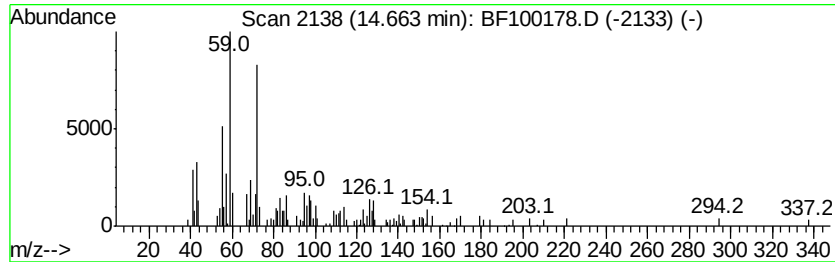
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Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	6.78 ng	180411	Chrysene-d12	13.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2			Octadecanamide	283	C18H37NO	000124-26-5	43
3			Dodecanamide	199	C12H25NO	001120-16-7	43
4			3-Tridecanone	198	C13H26O	001534-26-5	35
5			3-Tetradecanol	214	C14H30O	001653-32-3	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.99	10.4	ng	264234	1	6.76	507629	20.0
unknown6.54	6.54	70.7	ng	1795350	1	6.76	507629	20.0
Benzenesulfonamid...	10.72	3.0	ng	126138	4	11.29	836213	20.0
Behenic alcohol	13.75	3.6	ng	94854	5	13.94	532499	20.0
9-Octadecenamide,...	14.66	6.8	ng	180411	5	13.94	532499	20.0