

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112017\
 Data File : BF100758.D
 Acq On : 21 Nov 2017 3:55
 Operator : SJ/JU
 Sample : I6535-04
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-4252-RT-3025-RT-2342

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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	2.157	9	12	30	rVB3	58641	136468	5.98%	0.900%
2	4.481	404	407	413	rBB	26502	29931	1.31%	0.197%
3	5.092	507	511	522	rVB	204706	236411	10.36%	1.560%
4	5.487	574	578	582	rBV	1151823	1054828	46.22%	6.959%
5	6.492	745	749	757	rBV	837513	738871	32.38%	4.875%
6	6.639	770	774	778	rBV	1743176	1710213	74.94%	11.283%
7	6.875	810	814	817	rBV	551501	479259	21.00%	3.162%
8	7.028	836	840	844	rBV	1714054	1614537	70.75%	10.652%
9	7.439	904	910	913	rBV	1210333	1270441	55.67%	8.382%
10	8.151	1027	1031	1035	rBV	683585	602388	26.40%	3.974%
11	9.227	1209	1214	1217	rBV	2409404	2281969	100.00%	15.055%
12	9.616	1277	1280	1284	rVB	93277	74179	3.25%	0.489%
13	9.910	1326	1330	1334	rBV	661182	559339	24.51%	3.690%
14	10.621	1447	1451	1454	rBV	69257	60027	2.63%	0.396%
15	10.698	1460	1464	1467	rBV	1113492	948543	41.57%	6.258%
16	11.392	1579	1582	1586	rBV	515140	451271	19.78%	2.977%
17	11.910	1667	1670	1676	rBV	67079	66103	2.90%	0.436%
18	12.698	1800	1804	1810	rBV	39721	41369	1.81%	0.273%
19	12.980	1847	1852	1855	rBV	1840201	1679309	73.59%	11.079%
20	13.445	1921	1931	1937	rBV6	9178	24441	1.07%	0.161%
21	13.862	1998	2002	2010	rBV	153295	166666	7.30%	1.100%
22	14.033	2027	2031	2035	rVB	604833	515191	22.58%	3.399%
23	15.504	2276	2281	2287	rBV	319351	415499	18.21%	2.741%

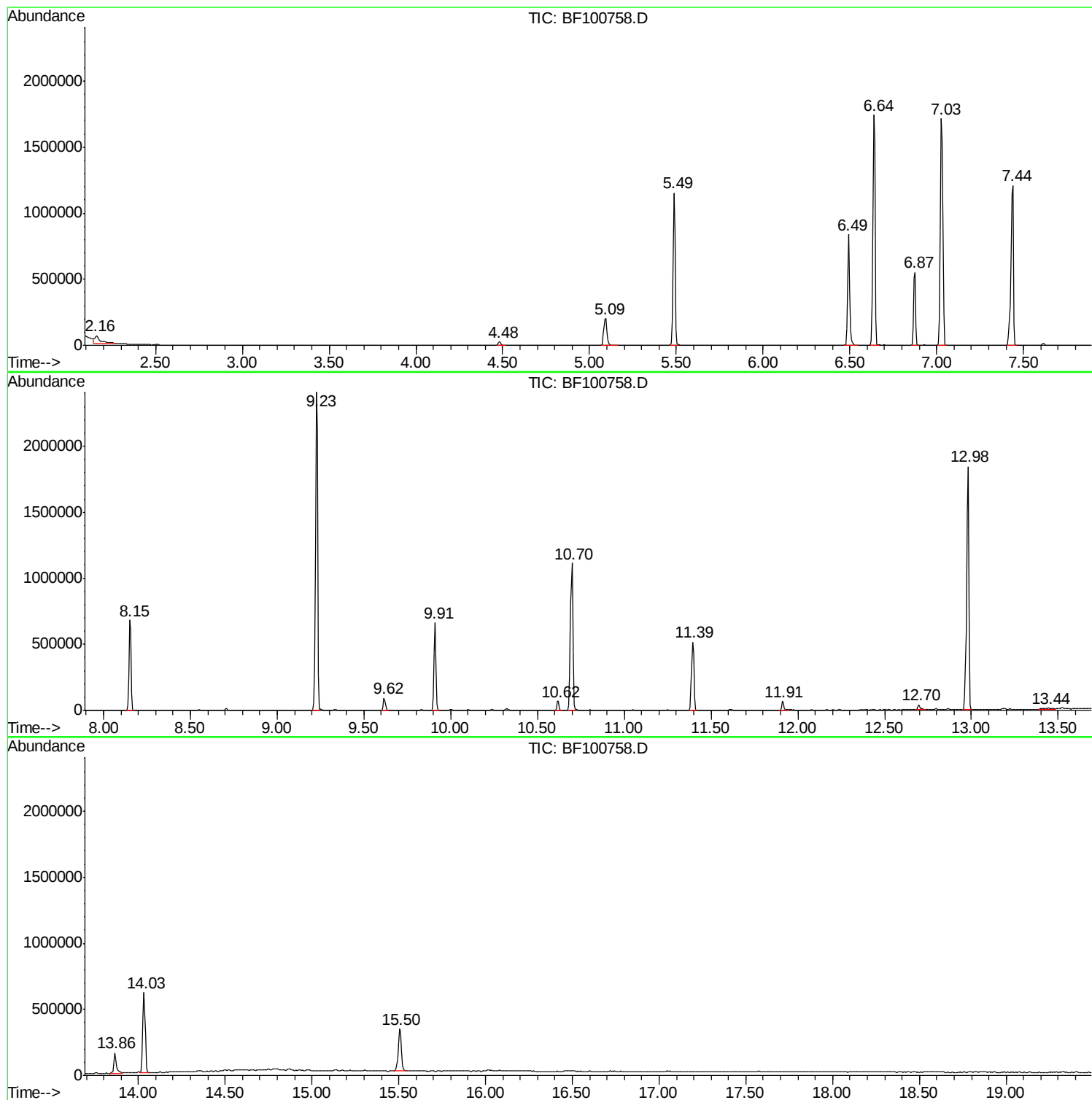
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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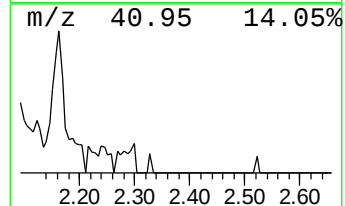
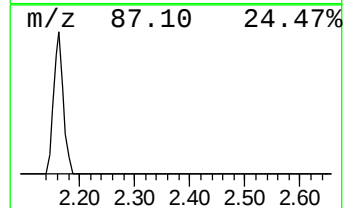
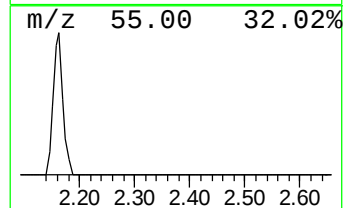
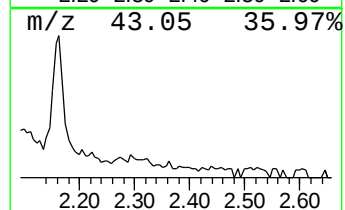
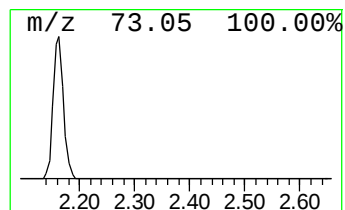
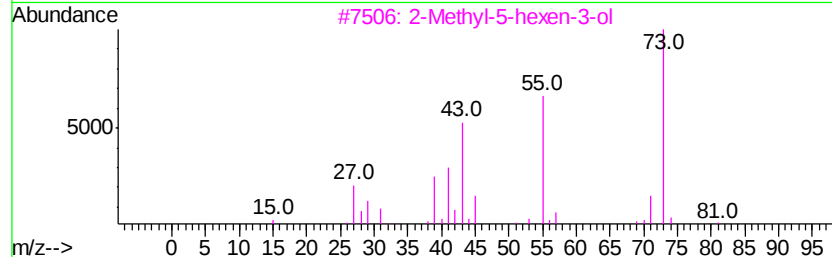
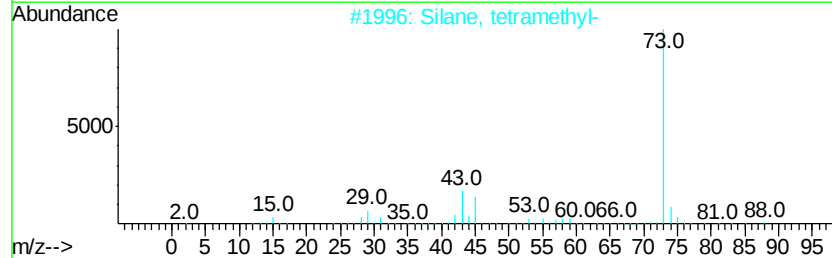
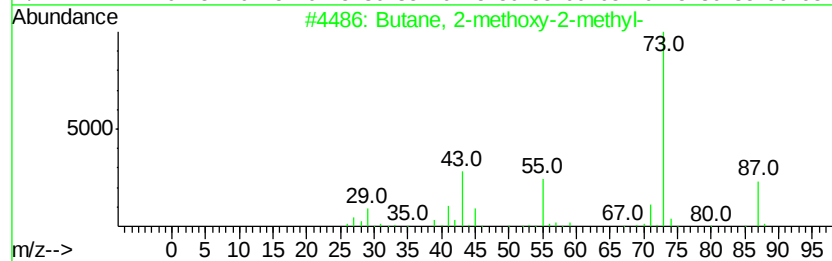
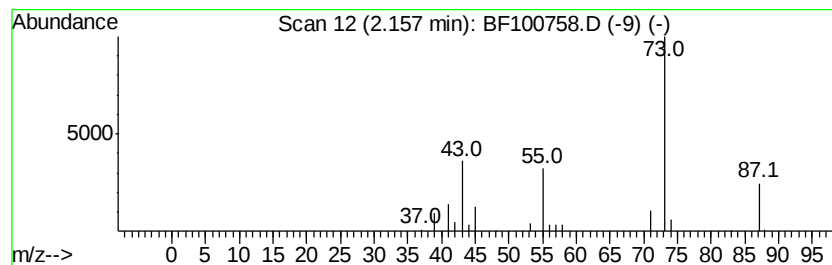
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	5.69 ng	136468	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	47
3		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
4		1,4-Butanediamine	88	C4H12N2	000110-60-1	9
5		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9



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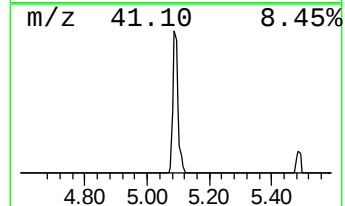
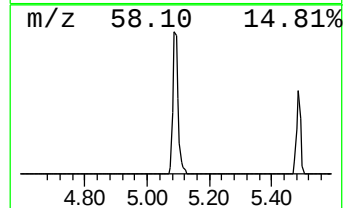
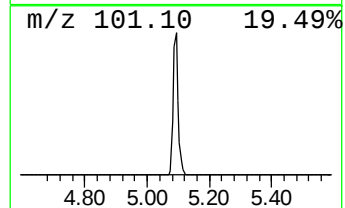
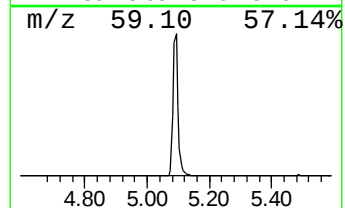
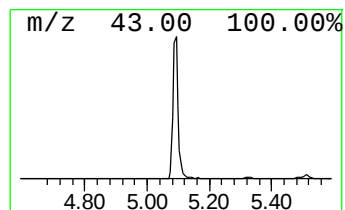
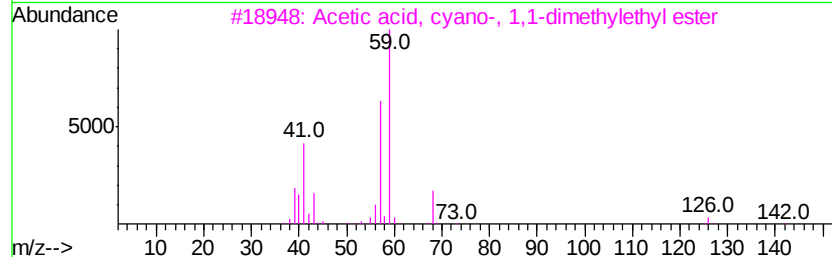
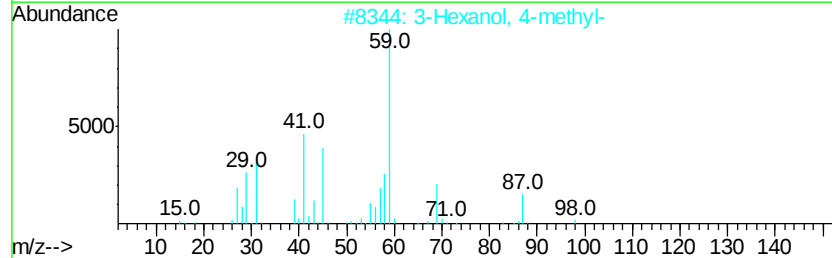
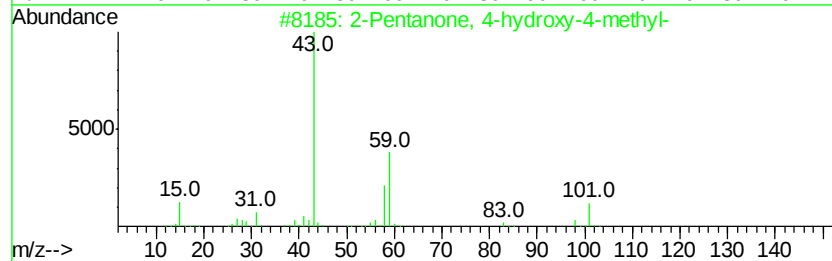
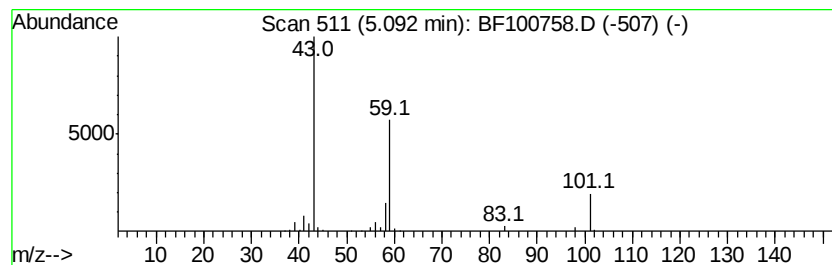
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	9.87 ng	236411	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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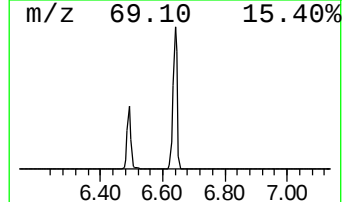
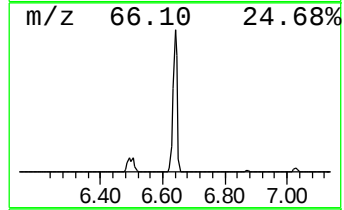
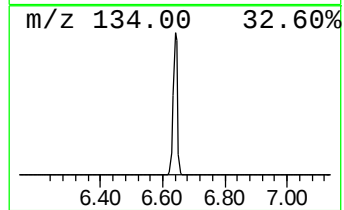
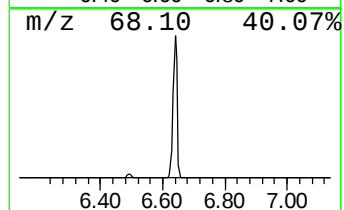
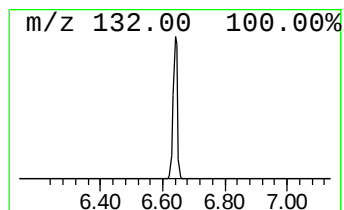
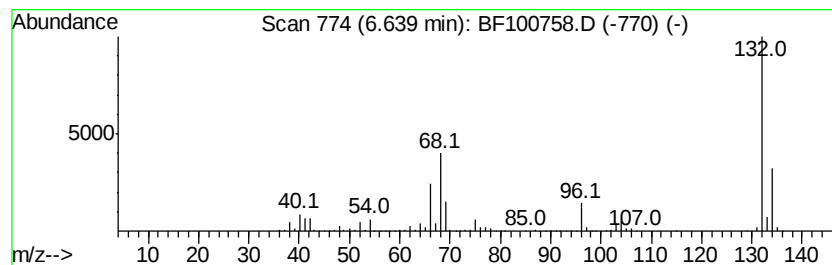
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Peak Number 3 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	71.37 ng	1710210	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	1-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-59-9	9



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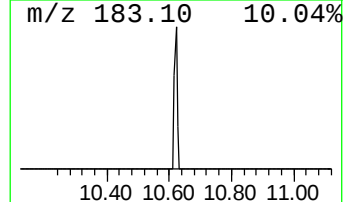
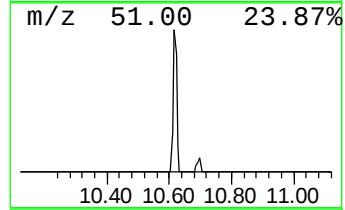
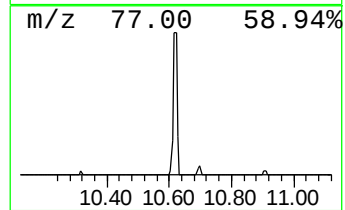
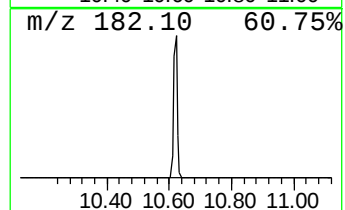
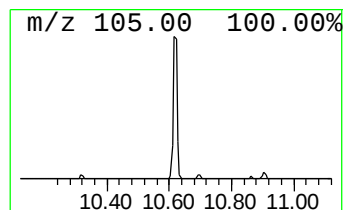
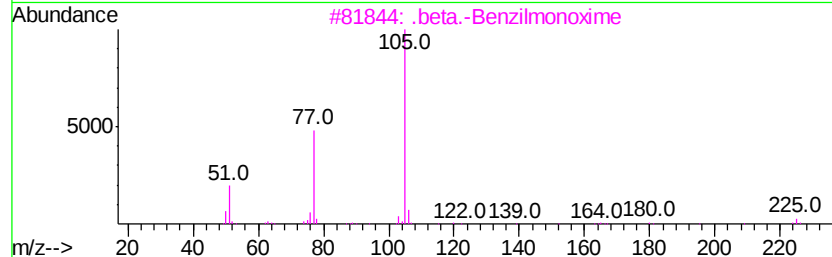
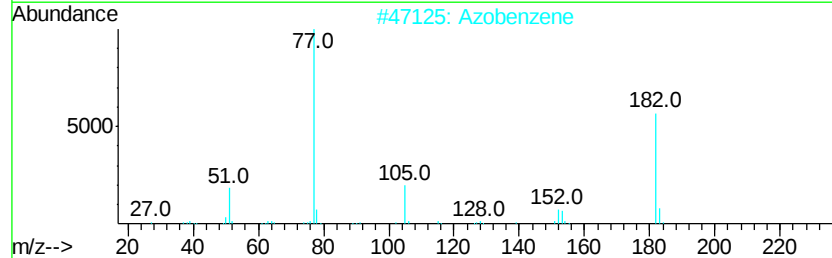
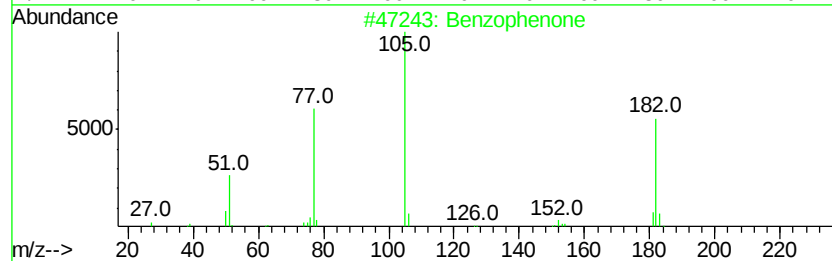
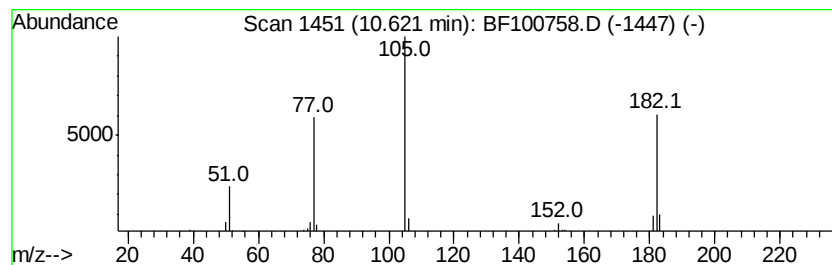
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	2.15 ng	60027	Acenaphthene-d10	9.91
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 95
2		Azobenzene	182 C12H10N2	000103-33-3 59
3		.beta.-Benzilmonoxime	225 C14H11N02	014090-77-8 43
4		N-Methoxy-N-methylbenzamide	165 C9H11N02	006919-61-5 43
5		Benzenebutanoic acid, .gamma.-oxo-	178 C10H10O3	002051-95-8 43



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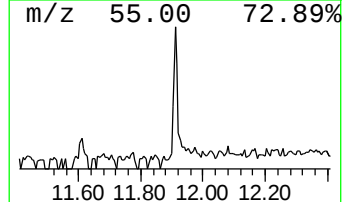
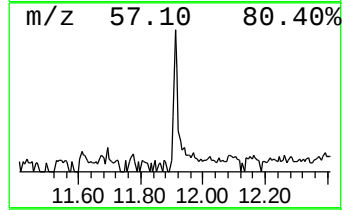
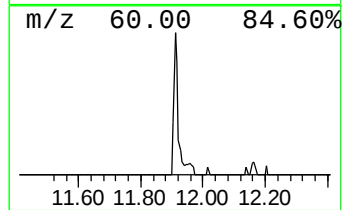
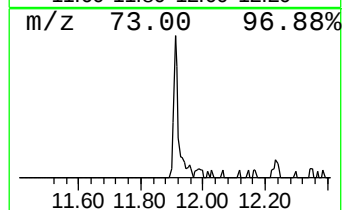
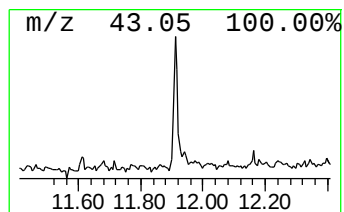
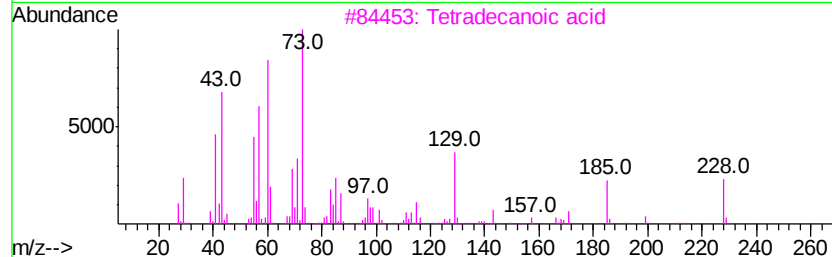
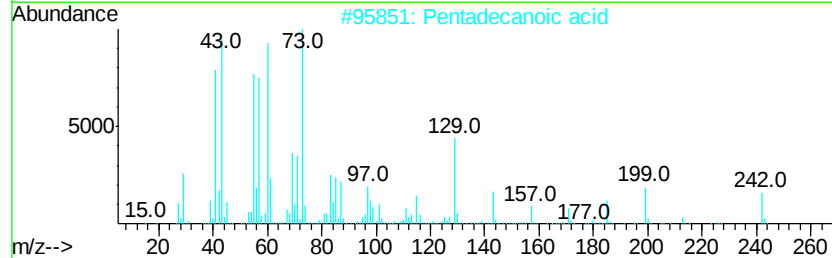
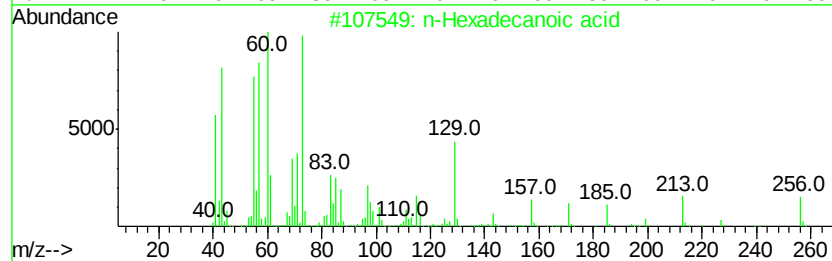
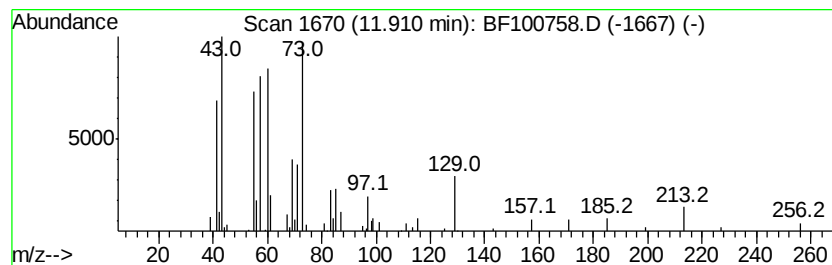
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	2.93 ng	66103	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59



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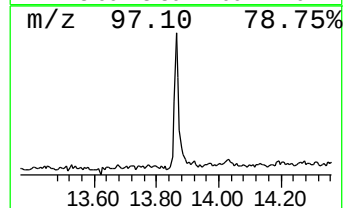
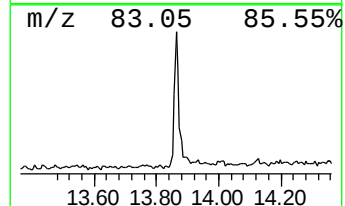
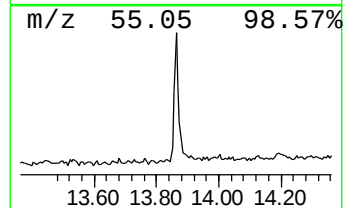
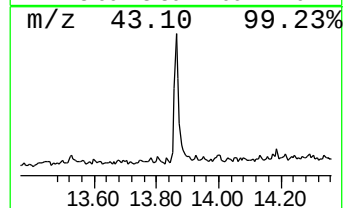
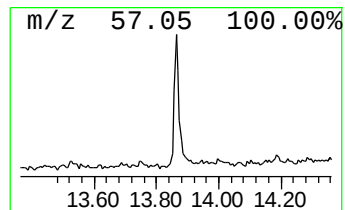
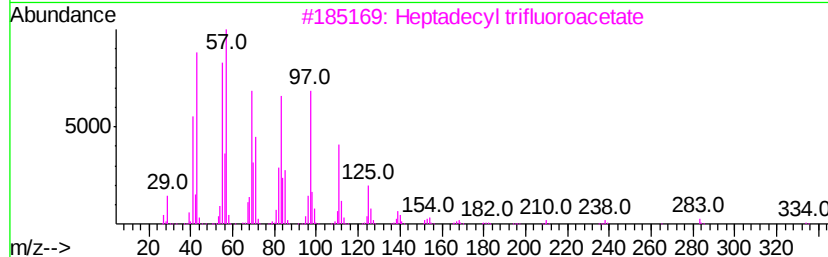
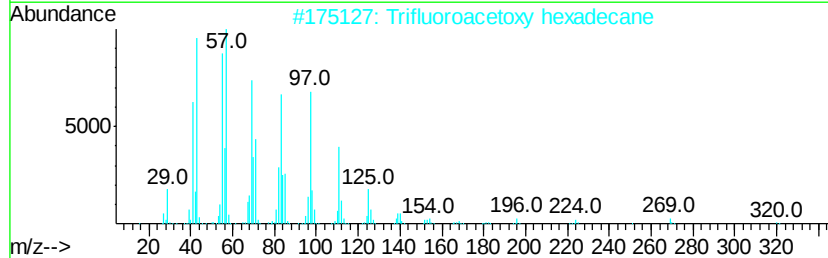
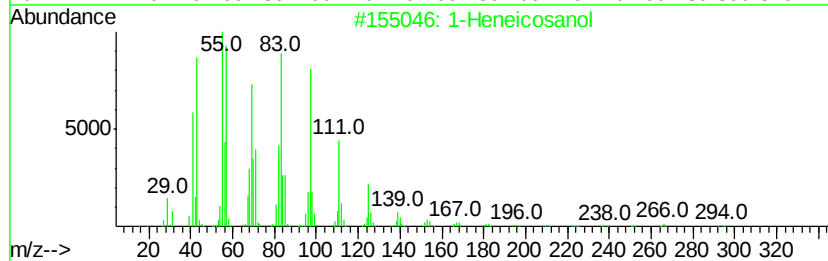
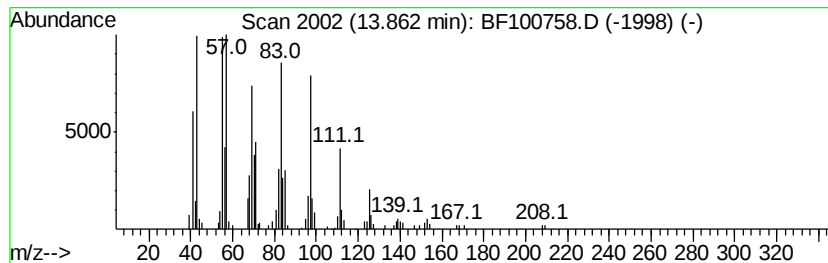
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TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.86	6.47 ng	166666	Chrysene-d12	14.03	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112017\
Data File : BF100758.D
Acq On : 21 Nov 2017 3:55
Operator : SJ/JU
Sample : I6535-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-4252-RT-3025-RT-2342

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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
Butane, 2-methoxy...	2.16	5.7	ng	136468	1	6.87	479259	20.0
2-Pentanone, 4-hy...	5.09	9.9	ng	236411	1	6.87	479259	20.0
unknown6.64	6.64	71.4	ng	1710210	1	6.87	479259	20.0
Benzophenone	10.62	2.1	ng	60027	3	9.91	559339	20.0
n-Hexadecanoic acid	11.91	2.9	ng	66103	4	11.39	451271	20.0
1-Heneicosanol	13.86	6.5	ng	166666	5	14.03	515191	20.0