

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102817\
 Data File : BF099944.D
 Acq On : 29 Oct 2017 5:36
 Operator : SJ/JU
 Sample : I6059-03
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 101817-TIDO-F-U-B

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-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	5.004	493	496	507	rBV	76468	115583	4.18%	0.712%
2	5.410	562	565	593	rBV	646174	836564	30.22%	5.155%
3	6.428	735	738	753	rBV	518866	646188	23.35%	3.982%
4	6.557	757	760	780	rVB	1624535	1496252	54.06%	9.220%
5	6.787	796	799	809	rBV	647294	564808	20.41%	3.480%
6	6.939	821	825	841	rBV	2085423	2014036	72.77%	12.411%
7	7.357	892	896	916	rBV	1457690	1518137	54.85%	9.355%
8	8.069	1013	1017	1034	rBV	851946	746623	26.98%	4.601%
9	8.628	1109	1112	1121	rBV	113474	100887	3.65%	0.622%
10	9.145	1195	1200	1203	rBV	3008357	2767789	100.00%	17.056%
11	9.539	1264	1267	1277	rBB	98464	79564	2.87%	0.490%
12	9.822	1308	1315	1326	rBB2	823149	734382	26.53%	4.525%
13	10.492	1426	1429	1433	rVB	56367	45272	1.64%	0.279%
14	10.533	1433	1436	1445	rVB	411498	318853	11.52%	1.965%
15	10.616	1446	1450	1460	rBV	782272	703409	25.41%	4.335%
16	11.310	1565	1568	1576	rBV	573703	533343	19.27%	3.287%
17	12.704	1801	1805	1808	rBV	164021	148635	5.37%	0.916%
18	12.898	1833	1838	1841	rBV	1865603	1734452	62.67%	10.688%
19	13.404	1921	1924	1928	rVB	117152	95140	3.44%	0.586%
20	13.774	1984	1987	1997	rBV	46242	55991	2.02%	0.345%
21	13.963	2015	2019	2029	rBV	560208	490130	17.71%	3.020%
22	15.421	2263	2267	2279	rVB2	364251	481843	17.41%	2.969%

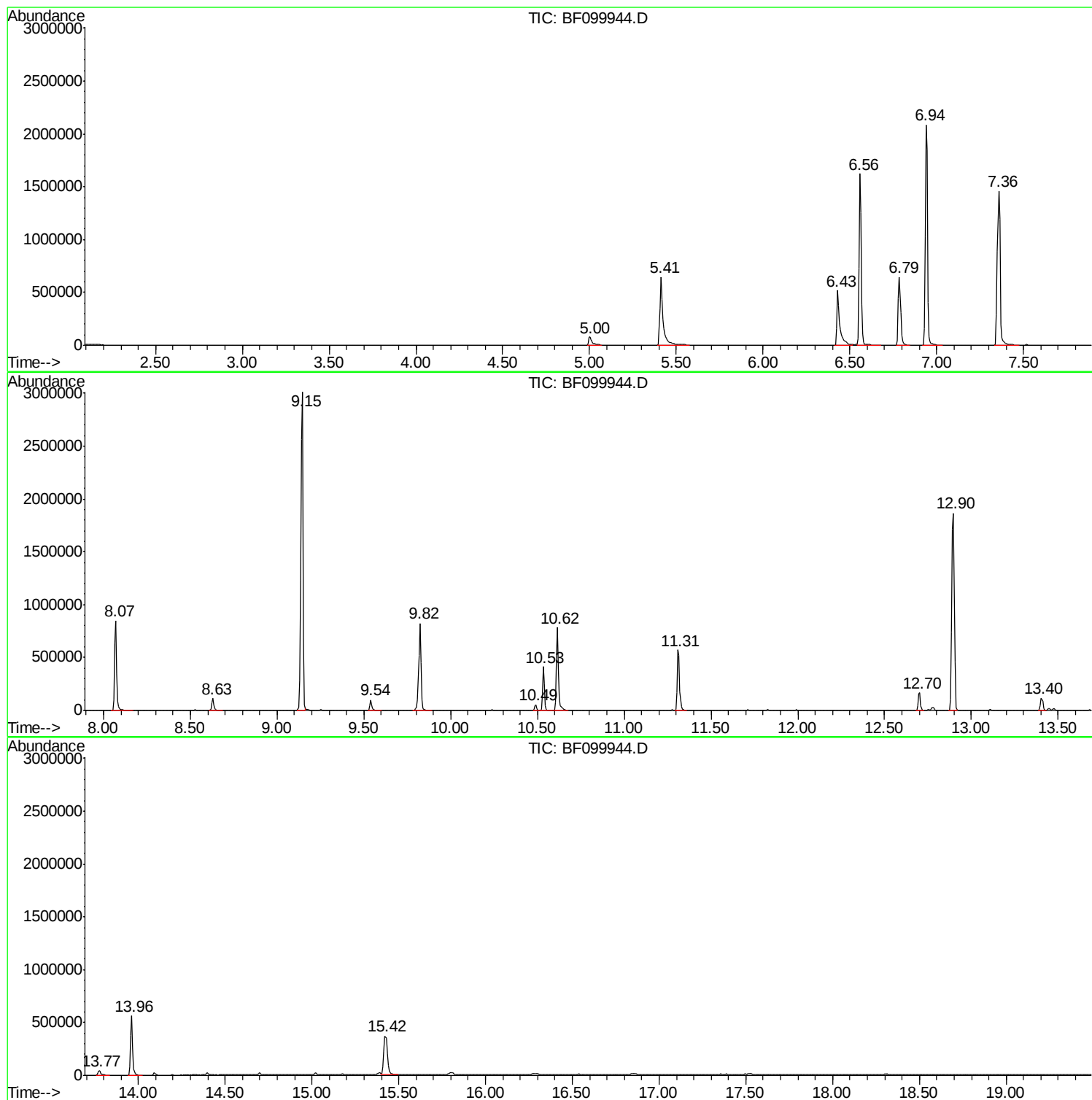
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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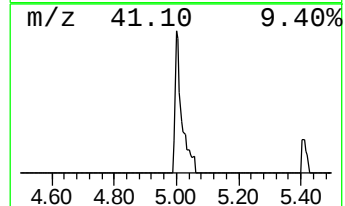
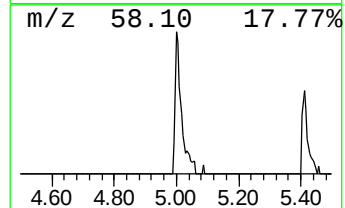
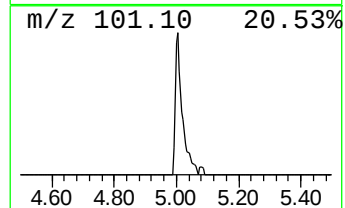
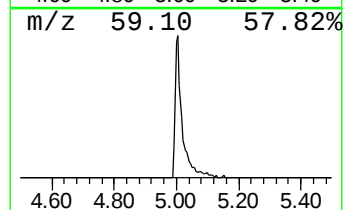
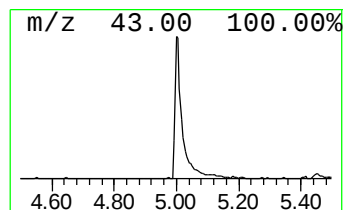
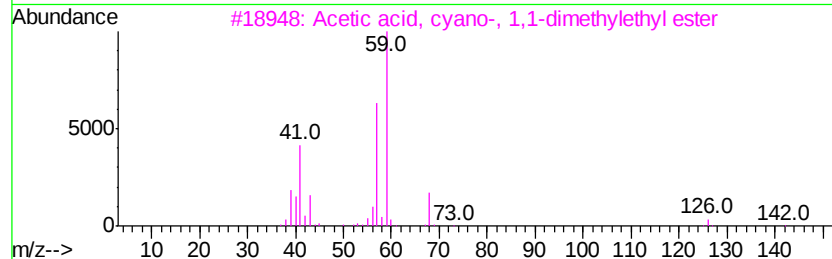
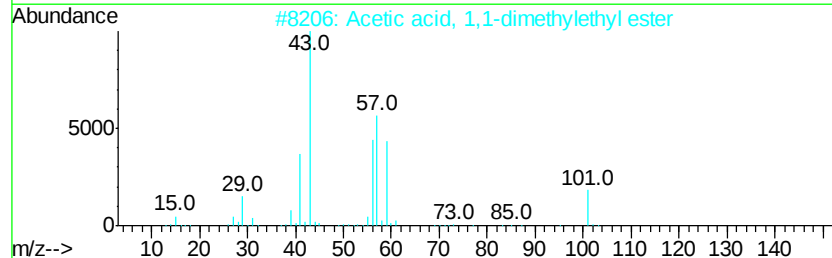
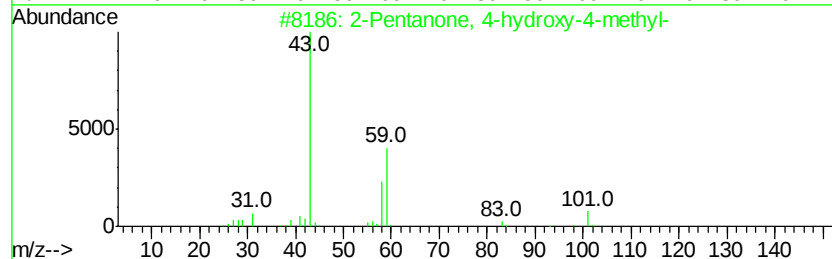
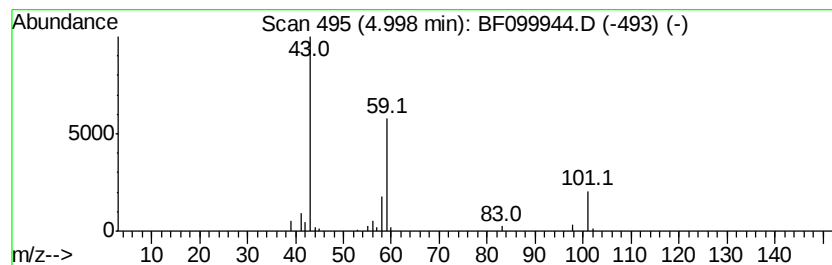
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	4.09 ng	115583	1,4-Dichlorobenzene-d4	6.79

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	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Acetone	58	C3H6O	000067-64-1	9



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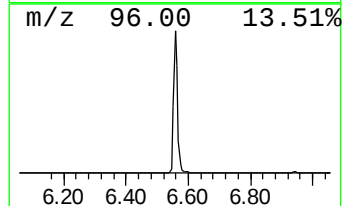
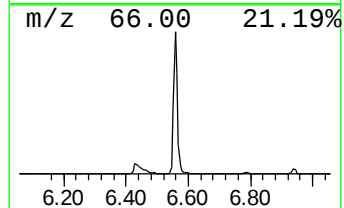
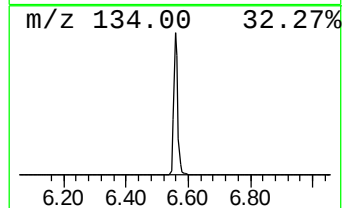
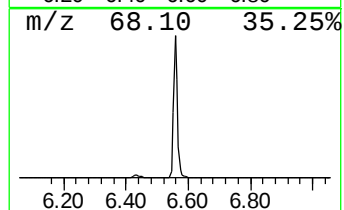
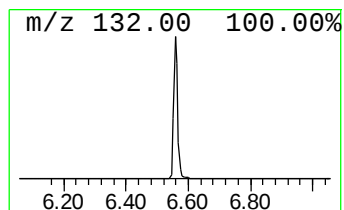
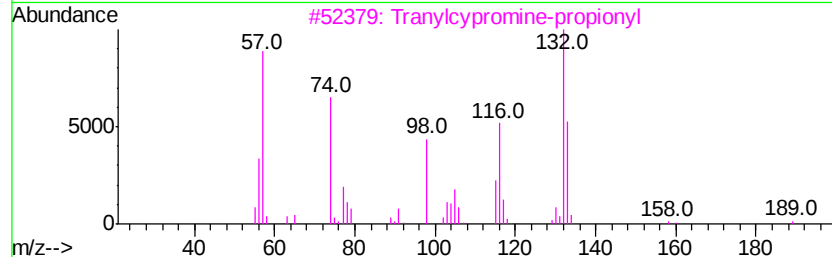
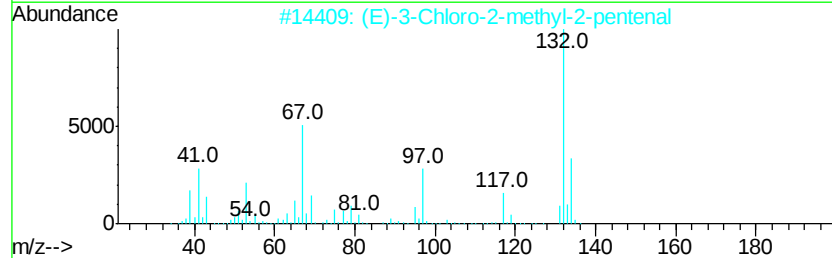
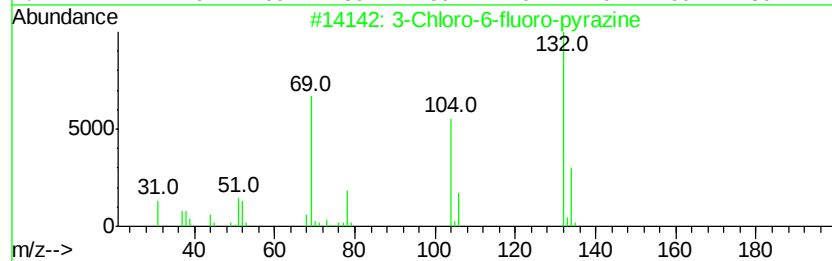
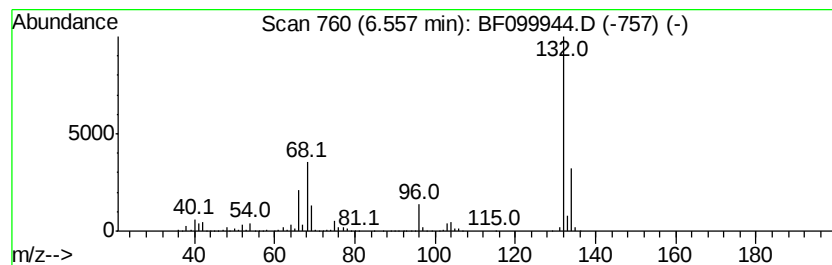
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	52.98 ng	1496250	1,4-Dichlorobenzene-d4	6.79

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	35
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12
4		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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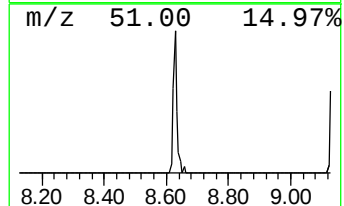
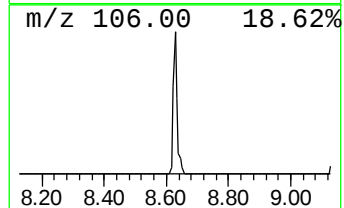
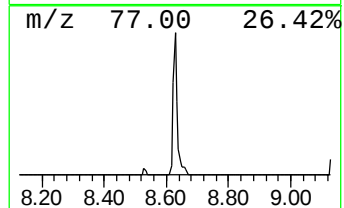
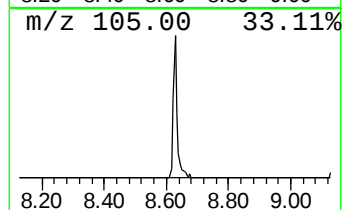
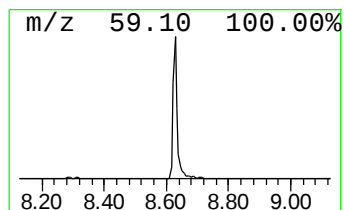
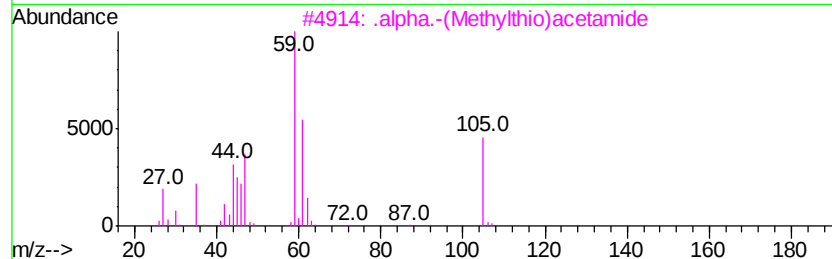
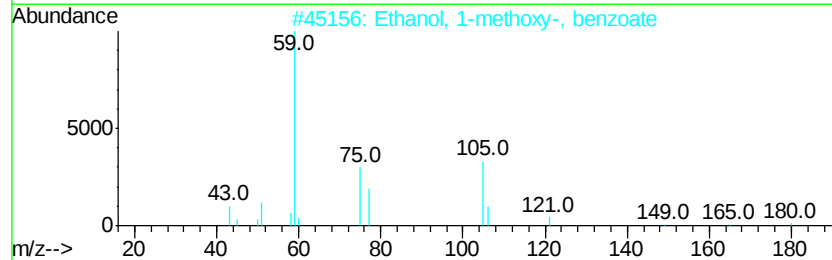
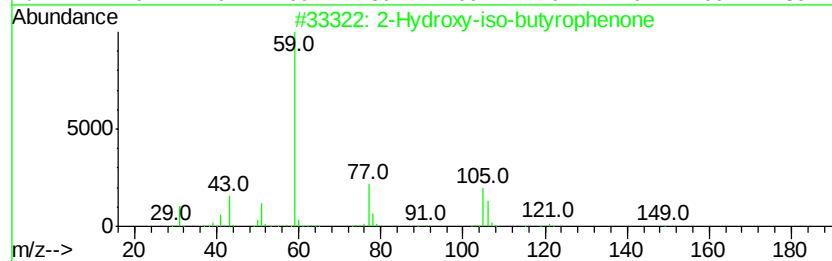
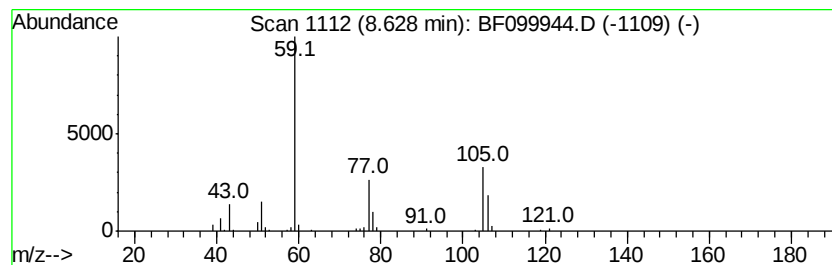
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.63	2.70 ng	100887	Napthalene-d8	8.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	86
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	64
3		.alpha.-(Methylthio)acetamide	105	C3H7NOS	022551-24-2	7
4		Guanidine	59	CH5N3	000113-00-8	7
5		Formamide, N-methyl-	59	C2H5NO	000123-39-7	5



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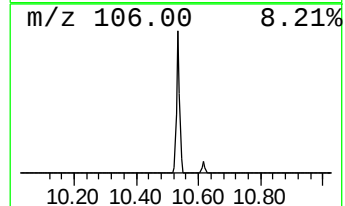
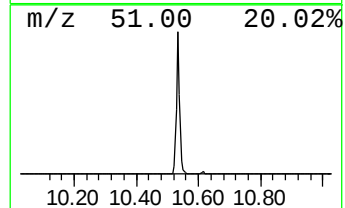
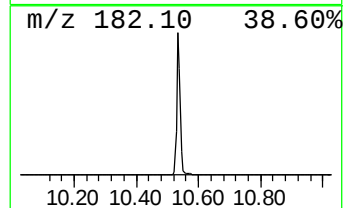
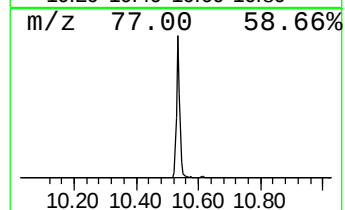
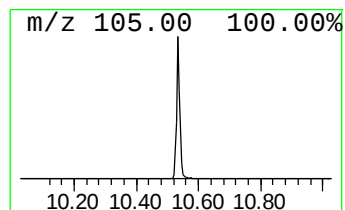
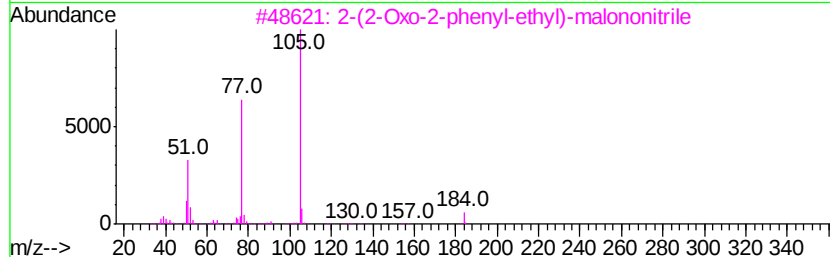
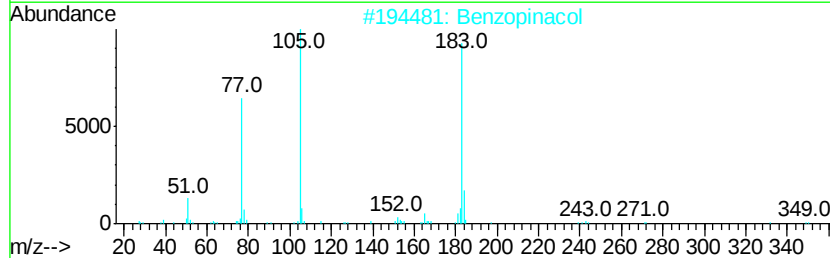
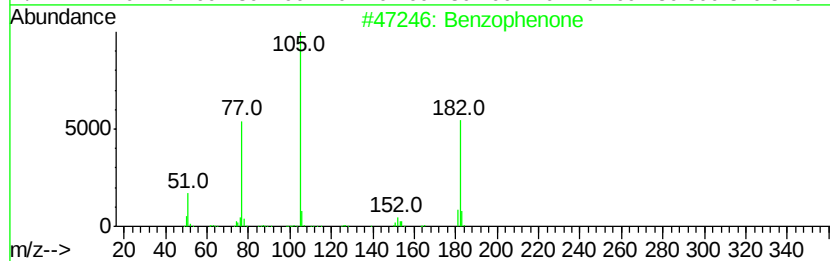
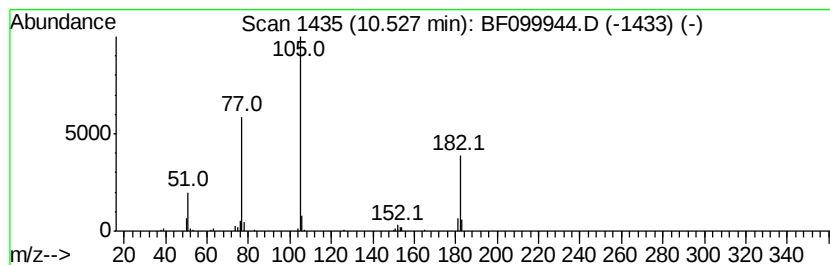
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Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	8.68 ng	318853	Acenaphthene-d10	9.82
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 96
2		Benzopinacol	366 C26H22O2	000464-72-2 50
3		2-(2-Oxo-2-phenyl-ethyl)-malonon...	184 C11H8N2O	1000296-76-9 47
4		Vinyl benzoate	148 C9H8O2	000769-78-8 43
5		Pentanediamide, N,N'-di-benzoyloxy-	370 C19H18N2O6	1000253-26-3 43



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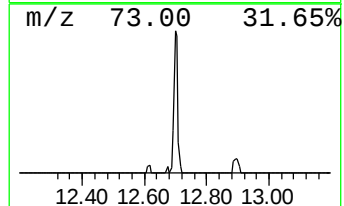
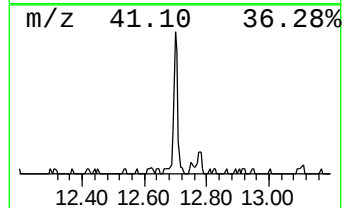
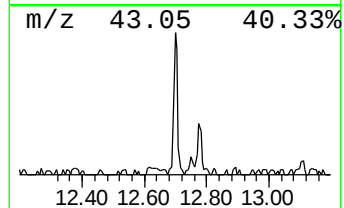
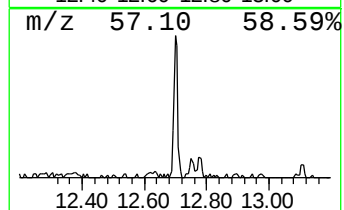
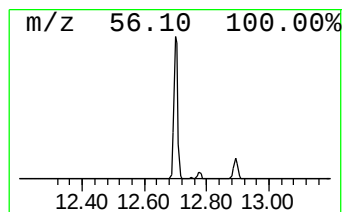
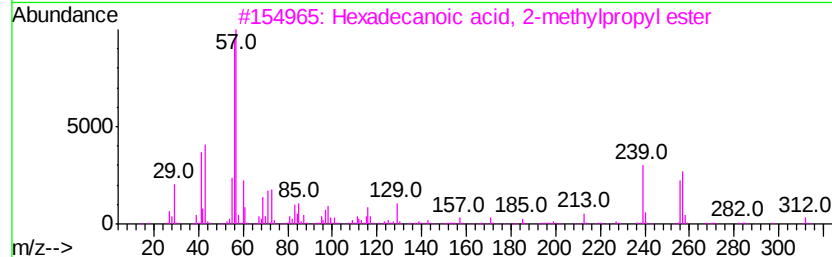
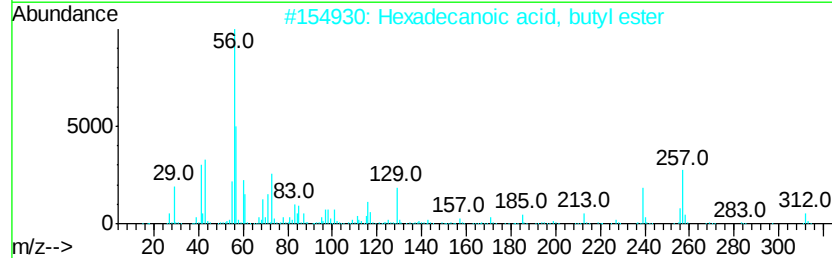
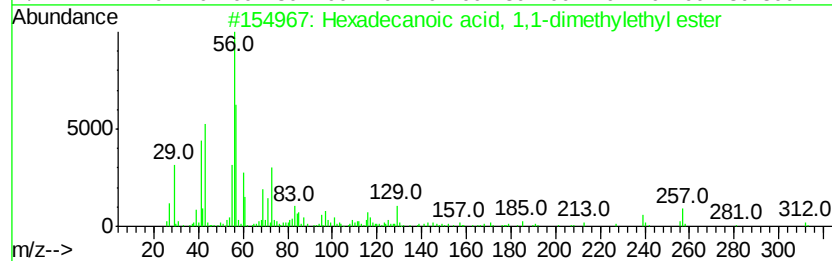
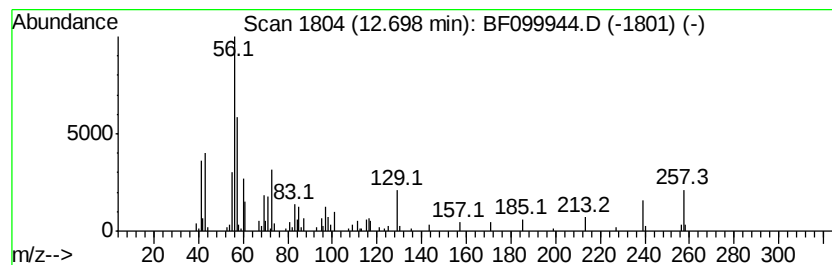
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	6.07 ng	148635	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	95
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	64
4		Nipecotic acid	129	C6H11NO2	000498-95-3	47
5		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38



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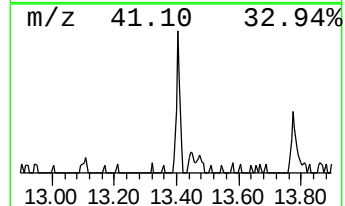
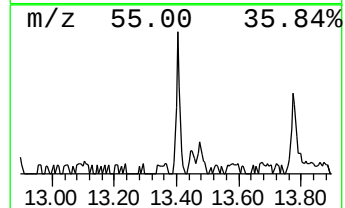
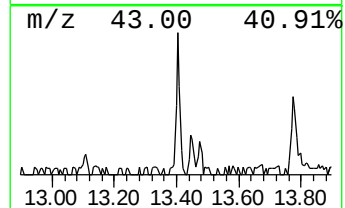
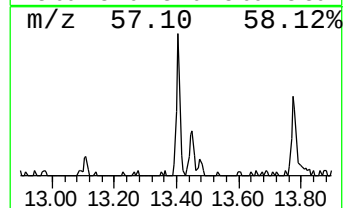
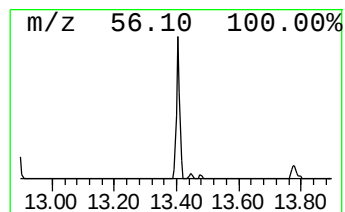
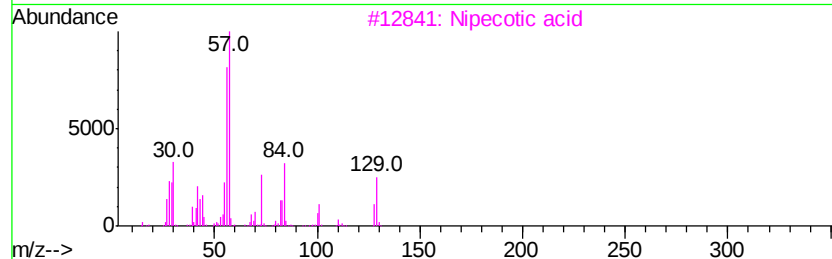
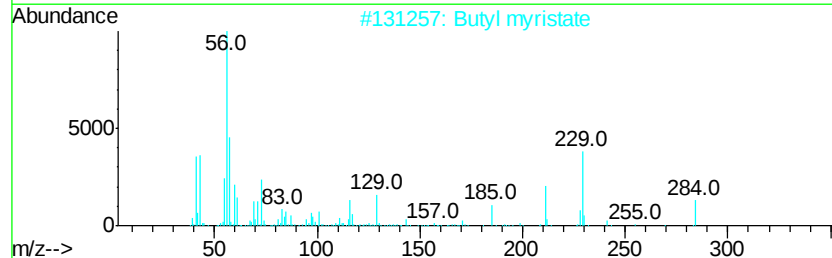
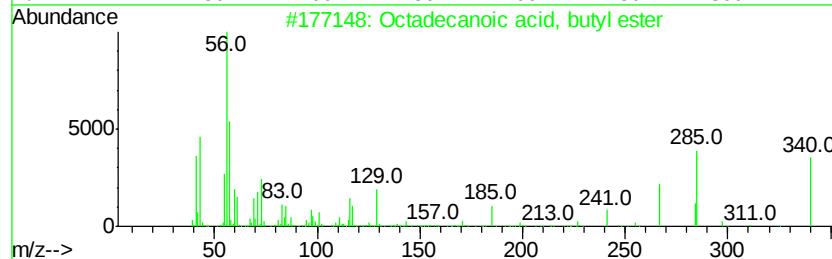
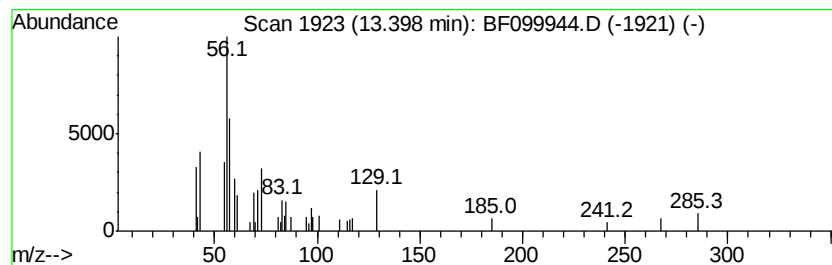
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	3.88 ng	95140	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2		Butyl myristate	284	C18H36O2	000110-36-1	64
3		Nipecotic acid	129	C6H11NO2	000498-95-3	50
4		Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	43
5		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102817\
Data File : BF099944.D
Acq On : 29 Oct 2017 5:36
Operator : SJ/JU
Sample : I6059-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

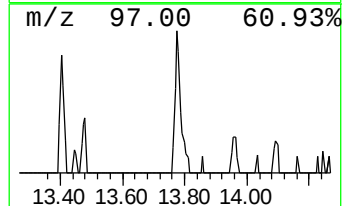
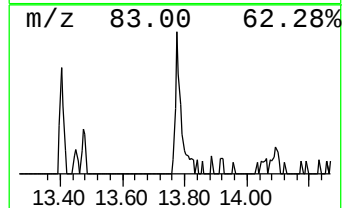
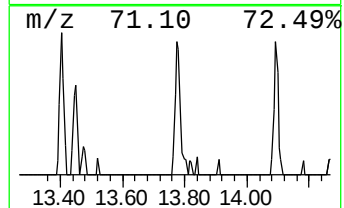
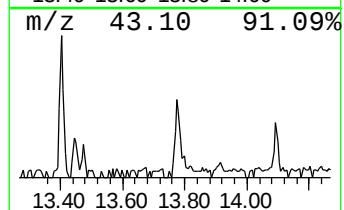
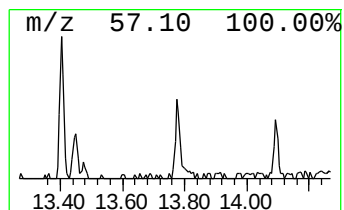
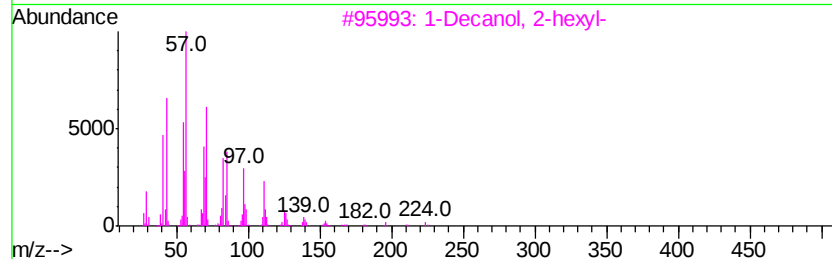
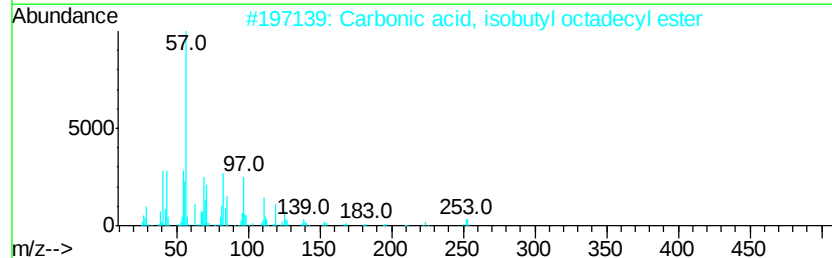
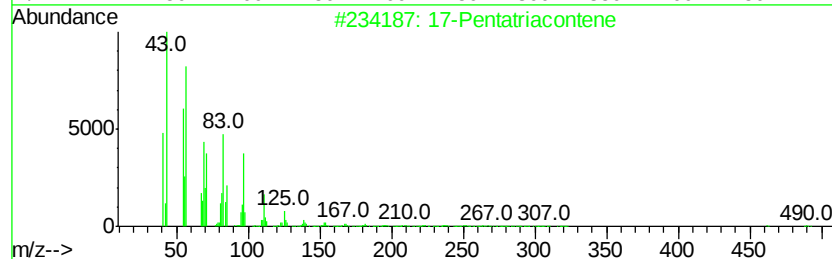
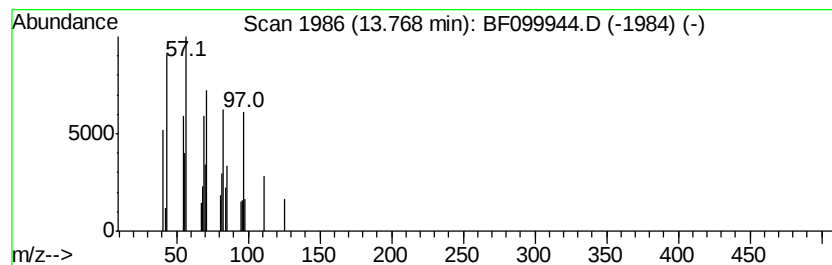
Instrument :
BNA_F
ClientSampleId :
101817-TIDO-F-U-B

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 8 17-Pentatriacontene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	2.28 ng	55991	Chrysene-d12	13.96
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	17-Pentatriacontene	491 C35H70	006971-40-0	72
2	Carbonic acid, isobutyl octadecyl...	370 C23H46O3	1000314-61-5	72
3	1-Decanol, 2-hexyl-	242 C16H34O	002425-77-6	58
4	3-Eicosene, (E)-	280 C20H40	074685-33-9	58
5	5-Eicosene, (E)-	280 C20H40	074685-30-6	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102817\
Data File : BF099944.D
Acq On : 29 Oct 2017 5:36
Operator : SJ/JU
Sample : I6059-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
101817-TIDO-F-U-B

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	4.1 ng		115583	1	6.79	564808	20.0
unknown6.56	6.56	53.0 ng		1496250	1	6.79	564808	20.0
2-Hydroxy-iso-but...	8.63	2.7 ng		100887	2	8.07	746623	20.0
Benzophenone	10.53	8.7 ng		318853	3	9.82	734382	20.0
Hexadecanoic acid...	12.70	6.1 ng		148635	5	13.96	490130	20.0
Octadecanoic acid...	13.40	3.9 ng		95140	5	13.96	490130	20.0
17-Pentatriacontene	13.77	2.3 ng		55991	5	13.96	490130	20.0