

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102617\
 Data File : BF099872.D
 Acq On : 26 Oct 2017 20:43
 Operator : SJ/JU
 Sample : I6111-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MARION-26KV-3-WATER

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	4.999	492	495	510	rBV	108850	141745	6.68%	0.919%
2	5.410	562	565	592	rBV	754504	966161	45.54%	6.262%
3	6.440	736	740	758	rBV	506667	651851	30.72%	4.225%
4	6.569	758	762	769	rBV	1752173	1561865	73.61%	10.123%
5	6.793	797	800	809	rBV	426606	364122	17.16%	2.360%
6	6.951	823	827	840	rBV	1630430	1401306	66.05%	9.082%
7	7.363	893	897	914	rBV	1083289	1075959	50.71%	6.973%
8	8.075	1015	1018	1034	rBV	541438	509309	24.00%	3.301%
9	8.639	1111	1114	1123	rBV	70419	62502	2.95%	0.405%
10	9.157	1198	1202	1205	rBV	2515044	2121740	100.00%	13.751%
11	9.551	1263	1269	1273	rBV	89410	96151	4.53%	0.623%
12	9.839	1314	1318	1321	rBV	675362	545327	25.70%	3.534%
13	9.986	1339	1343	1346	rBV5	16611	26451	1.25%	0.171%
14	10.081	1357	1359	1363	rBV4	40463	43713	2.06%	0.283%
15	10.198	1376	1379	1382	rBV4	23244	27206	1.28%	0.176%
16	10.239	1382	1386	1388	rBV2	58817	61736	2.91%	0.400%
17	10.381	1407	1410	1412	rBV3	21963	24293	1.14%	0.157%
18	10.481	1424	1427	1429	rVB	50107	43799	2.06%	0.284%
19	10.557	1437	1440	1443	rBV	277856	235577	11.10%	1.527%
20	10.639	1450	1454	1457	rBV	1158044	1131888	53.35%	7.336%
21	10.745	1468	1472	1475	rBV	162037	179772	8.47%	1.165%
22	10.804	1480	1482	1484	rBV	36369	34056	1.61%	0.221%
23	11.210	1549	1551	1557	rVB	101666	108414	5.11%	0.703%
24	11.333	1569	1572	1576	rBV	667760	550323	25.94%	3.567%
25	12.804	1818	1822	1830	rVB	149607	213032	10.04%	1.381%
26	12.922	1838	1842	1846	rVB	2038333	2091243	98.56%	13.554%
27	13.804	1989	1992	1997	rVB3	44268	46337	2.18%	0.300%
28	13.986	2019	2023	2027	rBV	650831	581218	27.39%	3.767%
29	15.468	2271	2275	2283	rVB	425626	532260	25.09%	3.450%

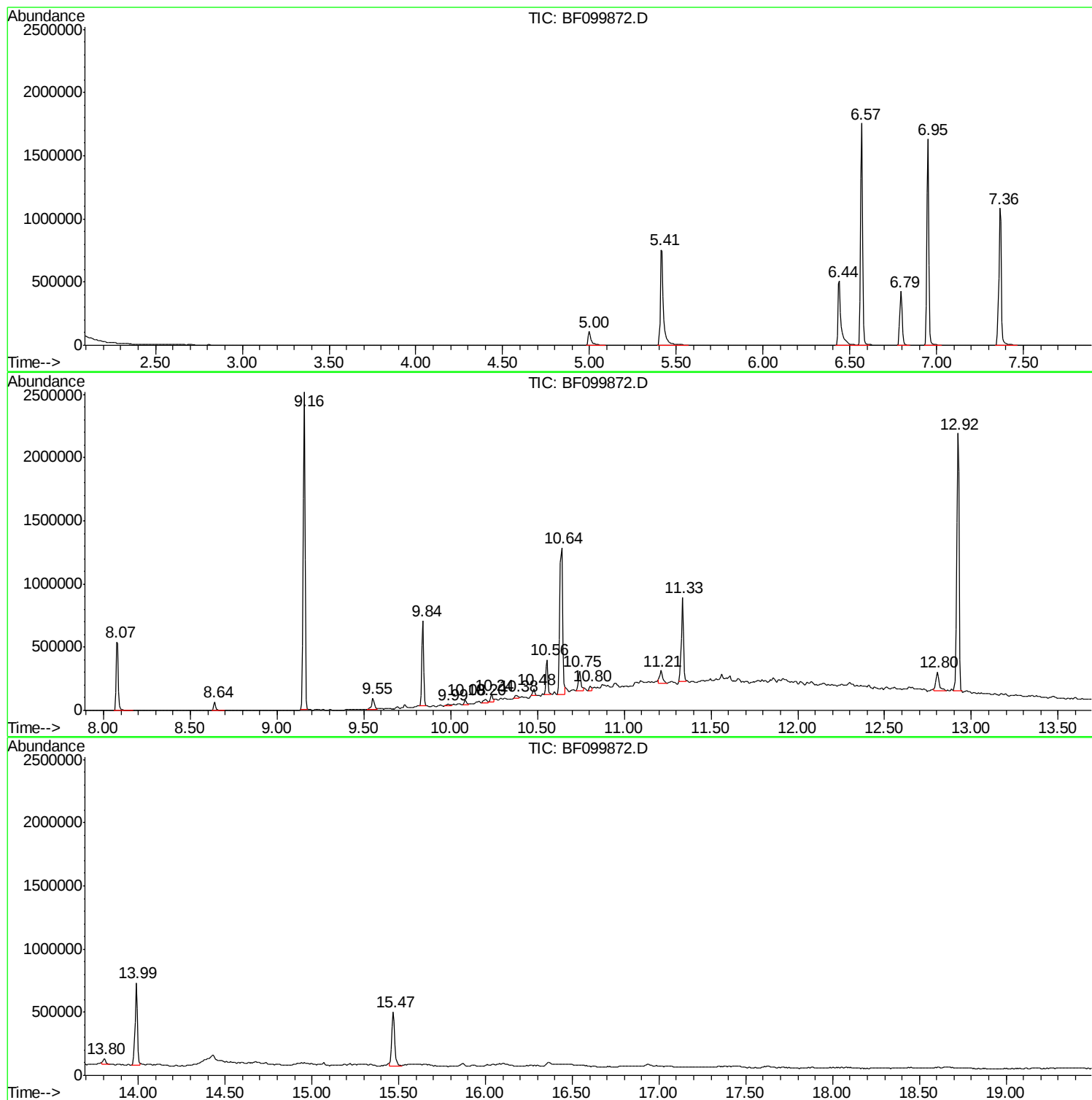
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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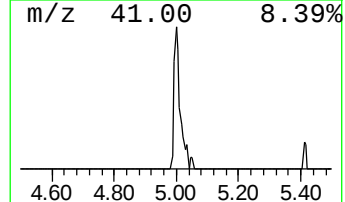
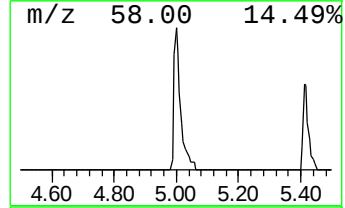
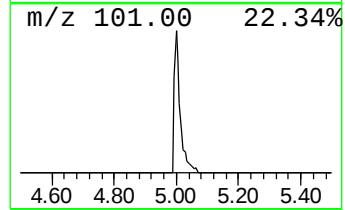
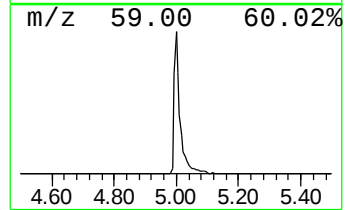
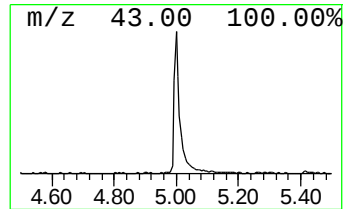
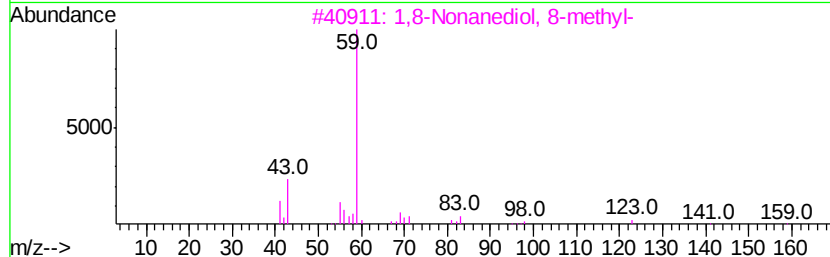
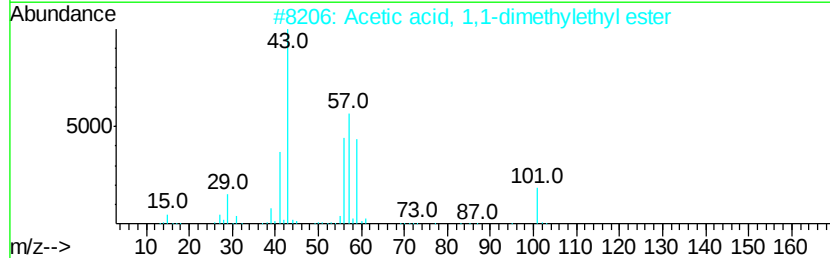
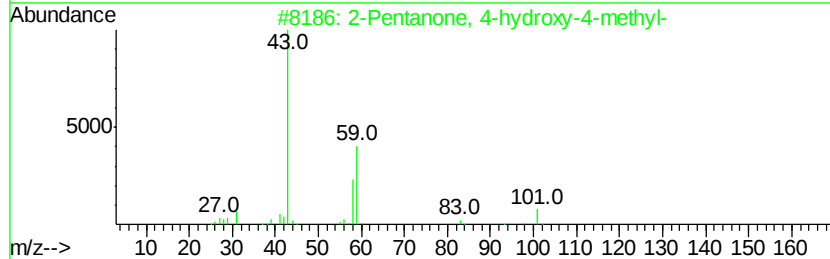
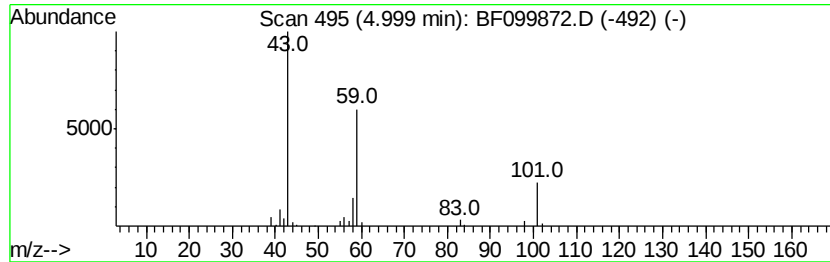
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	7.79 ng	141745	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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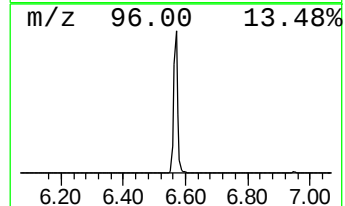
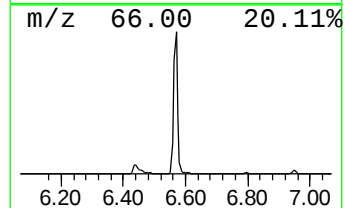
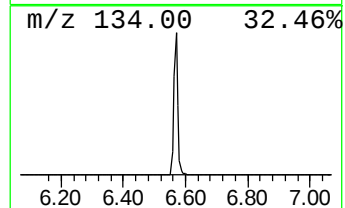
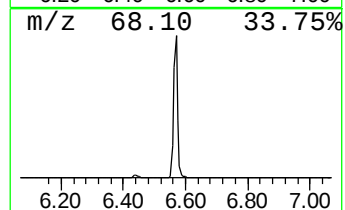
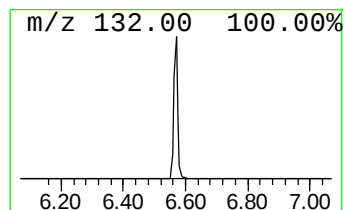
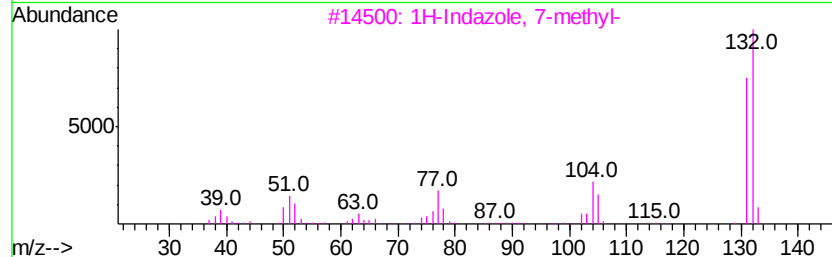
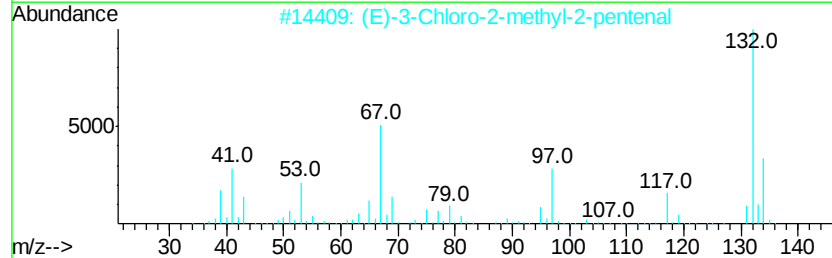
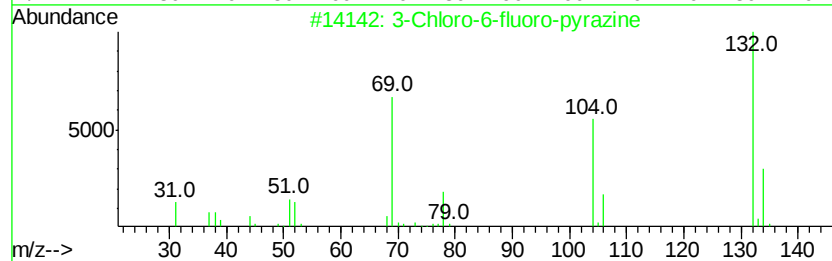
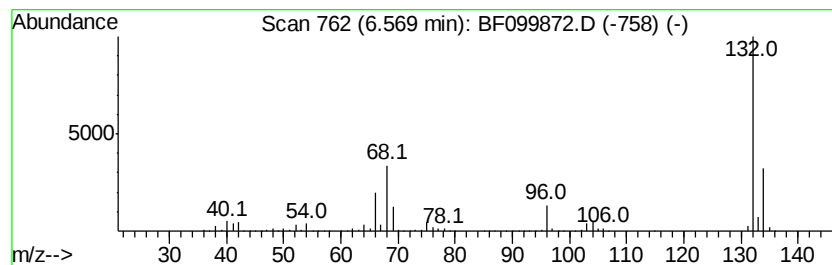
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	85.79 ng	1561870	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	17
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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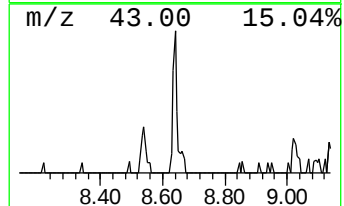
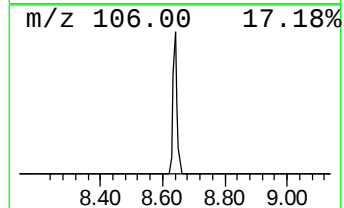
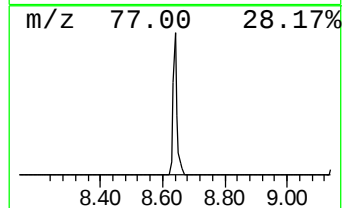
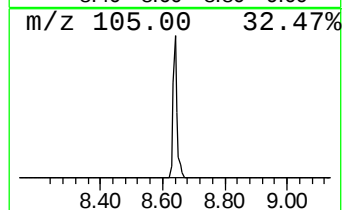
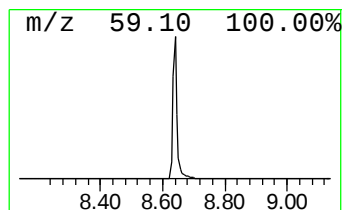
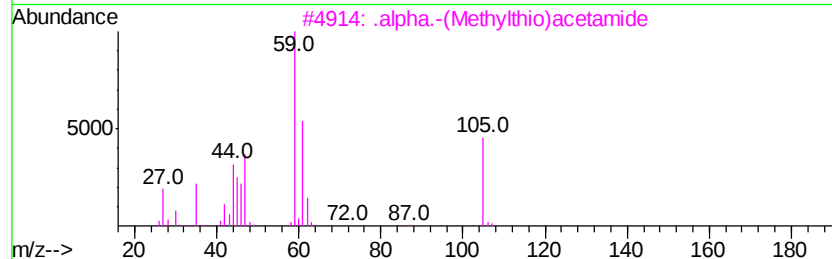
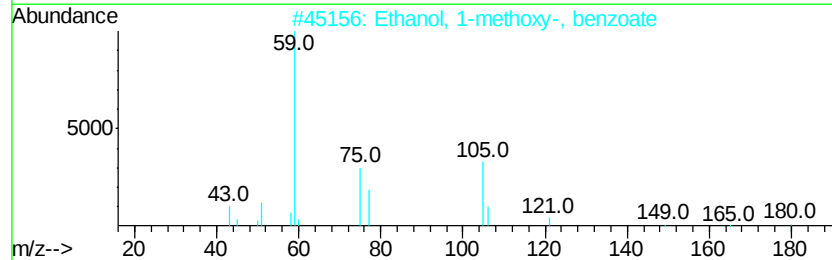
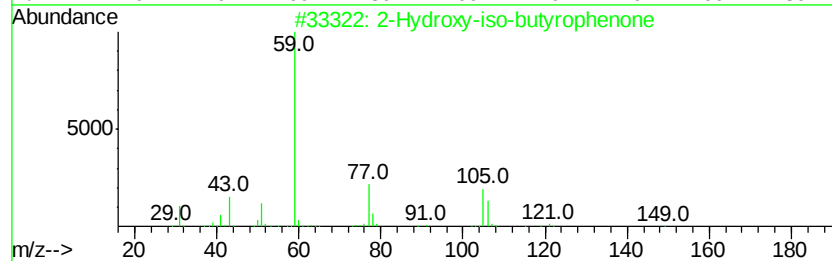
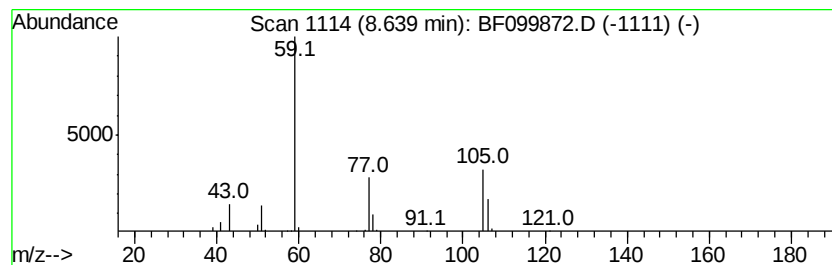
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.64	2.45 ng	62502	Napthalene-d8	8.08

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		Acetamide	59	C2H5NO	000060-35-5	5



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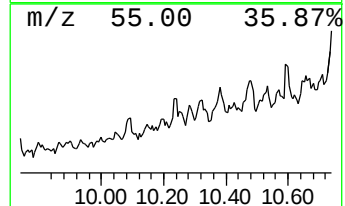
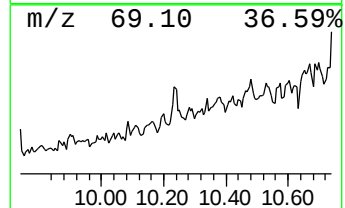
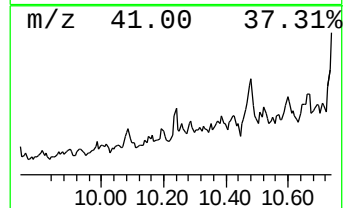
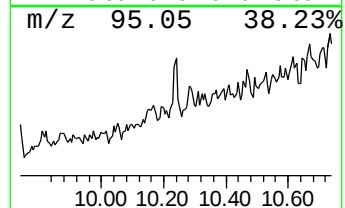
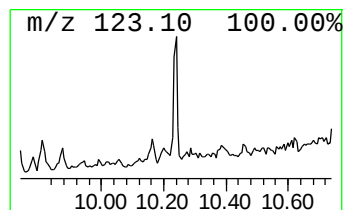
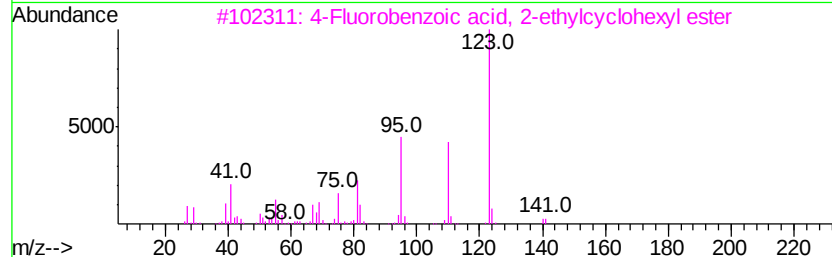
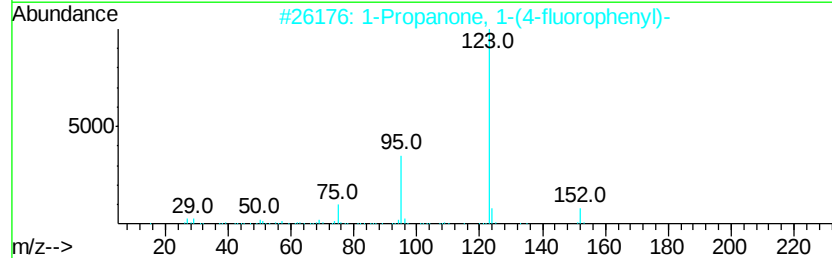
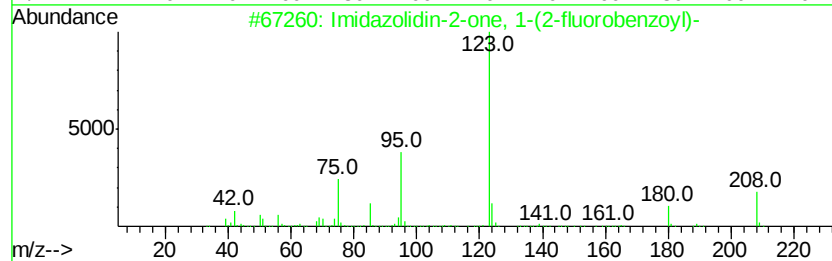
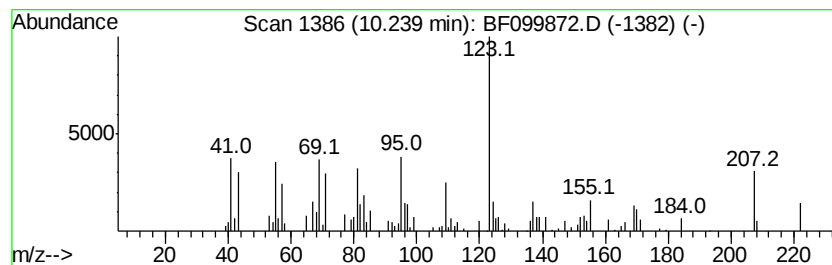
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Peak Number 5 unknown10.24 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.24	2.26 ng	61736	Acenaphthene-d10	9.84
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Imidazolidin-2-one, 1-(2-fluorob...	208 C10H9FN2O2	1000310-62-2 47
2		1-Propanone, 1-(4-fluorophenyl)-	152 C9H9FO	000456-03-1 46
3		4-Fluorobenzoic acid, 2-ethylcyc...	250 C15H19FO2	1000279-06-0 43
4		3-Fluorobenzoic acid, 2-ethylcyc...	250 C15H19FO2	1000279-04-9 43
5		3-Fluorobenzoic acid, 2-pentadec...	350 C22H35FO2	1000280-60-7 43



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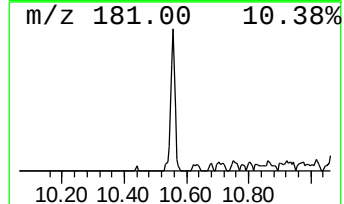
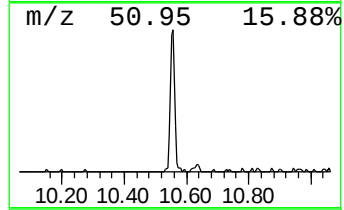
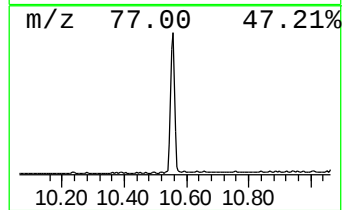
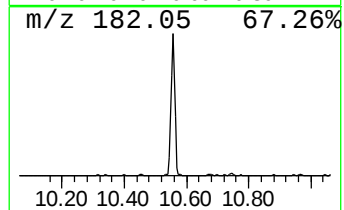
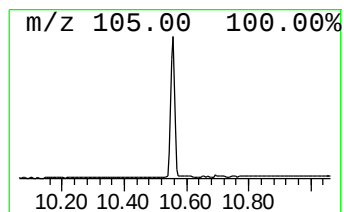
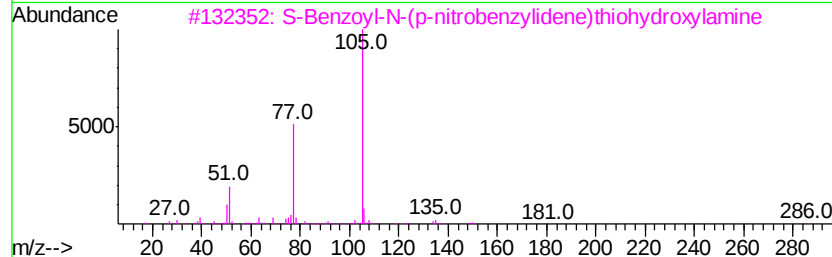
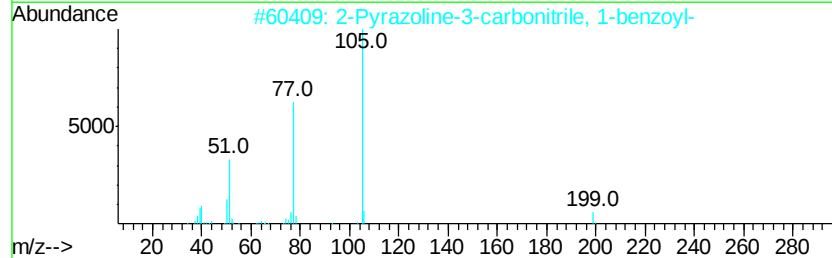
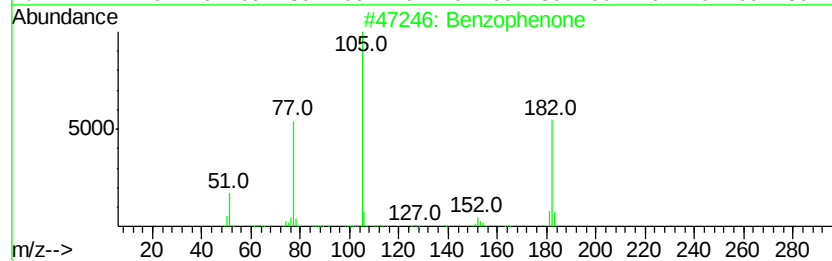
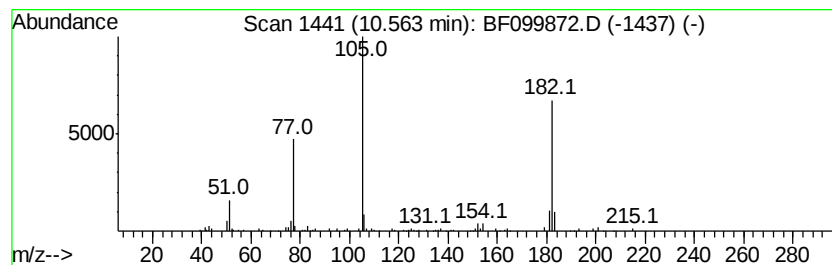
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Peak Number 6 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.56	8.64 ng	235577	Acenaphthene-d10	9.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	2-Pyrazoline-3-carbonitrile, 1-b...	199	C11H9N3O	067872-68-8	47
3	S-Benzoyl-N-(p-nitrobenzylidene)...	286	C14H10N2O3S	139776-09-3	47
4	Glyoxylohydroximoyl chloride, 2-...	183	C8H6ClN02	004937-87-5	47
5	Hippuric acid, methyl ester	193	C10H11N03	001205-08-9	47



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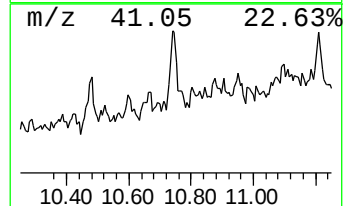
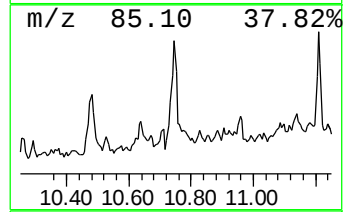
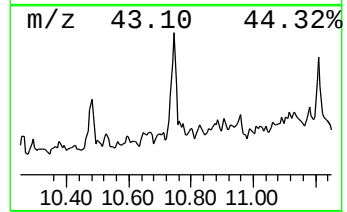
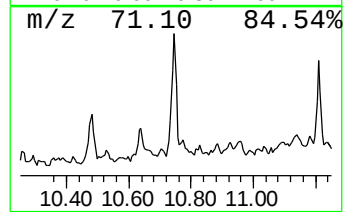
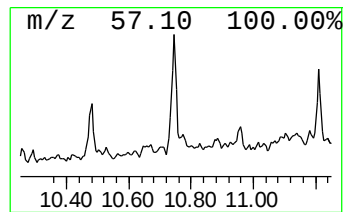
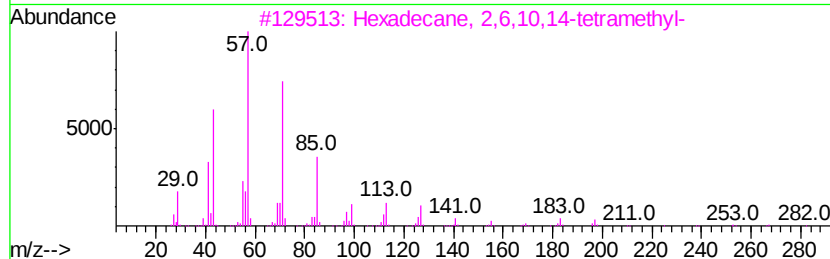
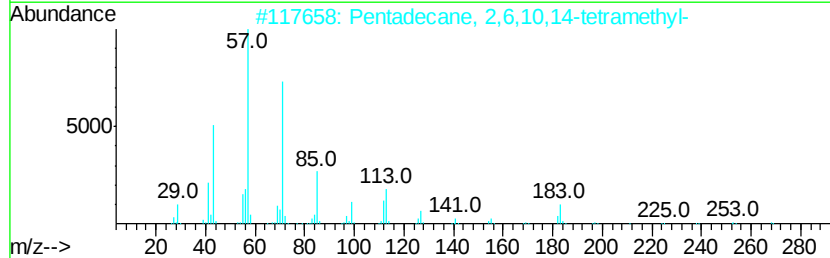
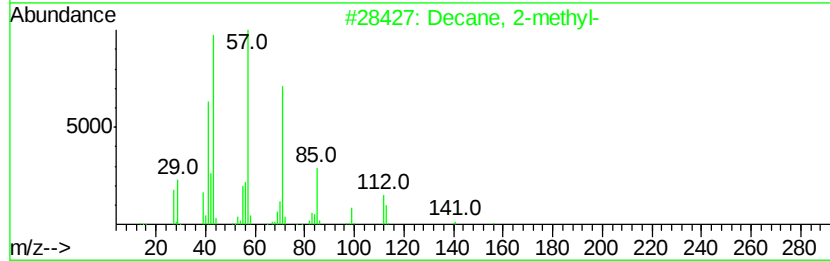
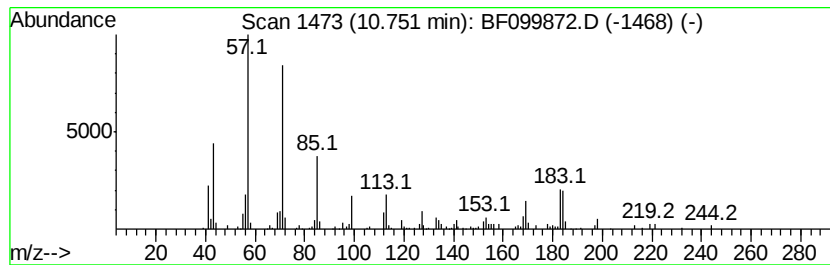
Instrument :
BNA_F
ClientSampleId :
MARION-26KV-3-WATER

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 7 Decane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.75	6.53 ng	179772	Phenanthrene-d10	11.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2-methyl-	156	C11H24	006975-98-0	74
2	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	72
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72
4	Pentadecane, 4-methyl-	226	C16H34	002801-87-8	72
5	Undecane, 6-ethyl-	184	C13H28	017312-60-6	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102617\
Data File : BF099872.D
Acq On : 26 Oct 2017 20:43
Operator : SJ/JU
Sample : I6111-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

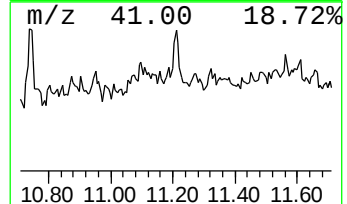
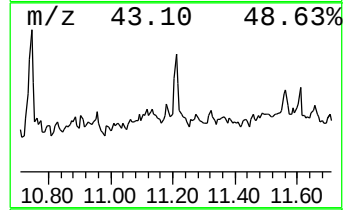
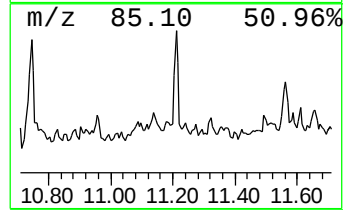
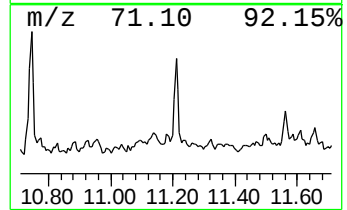
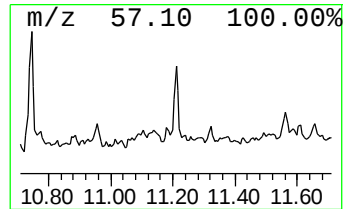
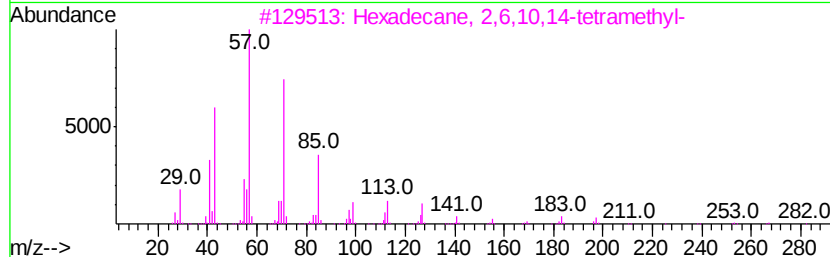
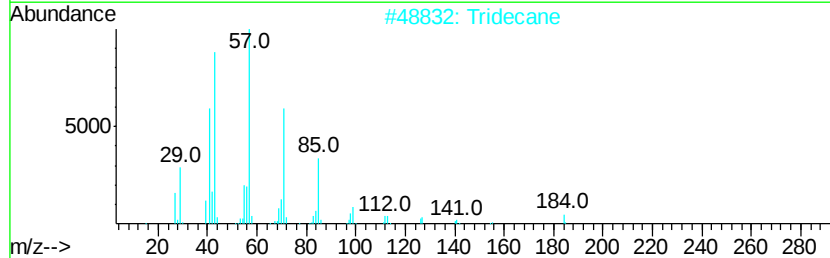
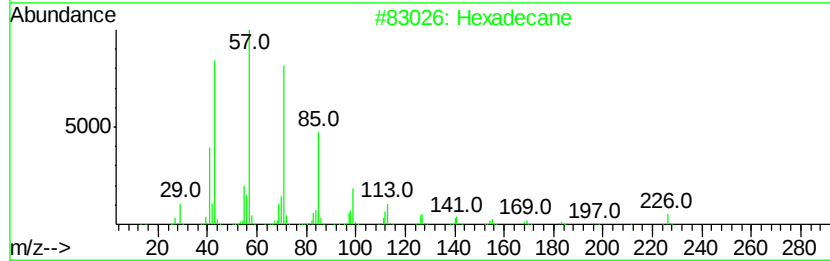
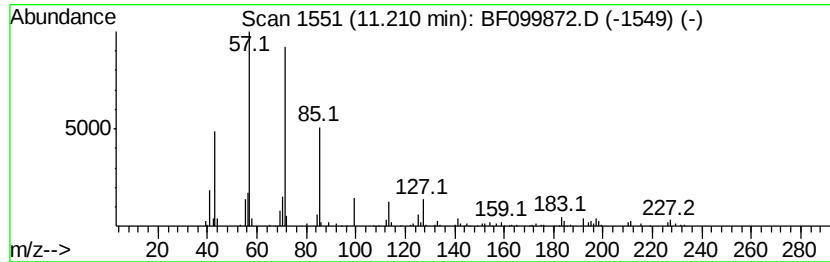
Instrument :
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ClientSampleId :
MARION-26KV-3-WATER

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 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.21	3.94 ng	108414	Phenanthrene-d10	11.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Tridecane	184	C13H28	000629-50-5	86
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
4	Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	64
5	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102617\
Data File : BF099872.D
Acq On : 26 Oct 2017 20:43
Operator : SJ/JU
Sample : I6111-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

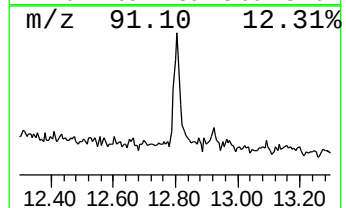
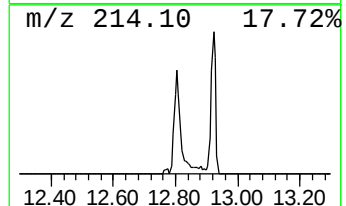
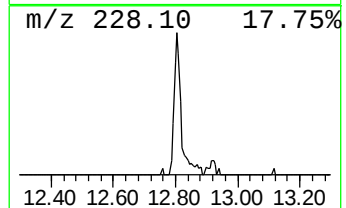
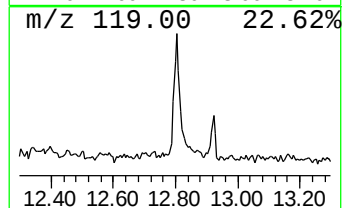
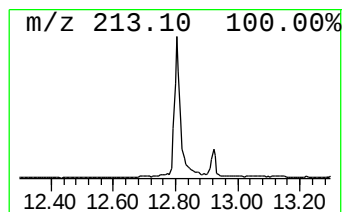
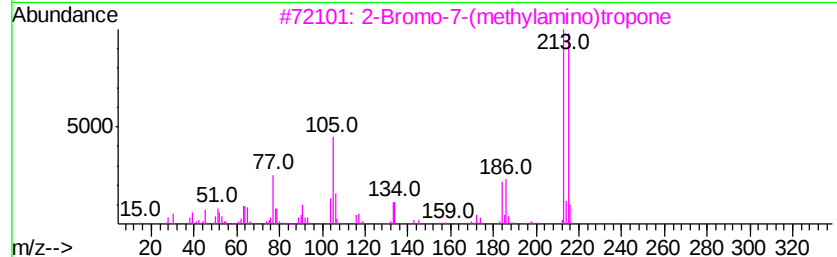
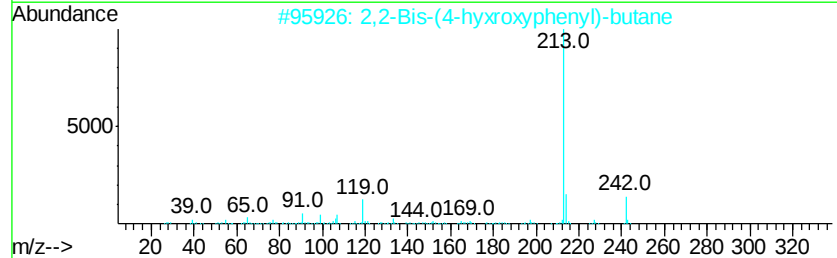
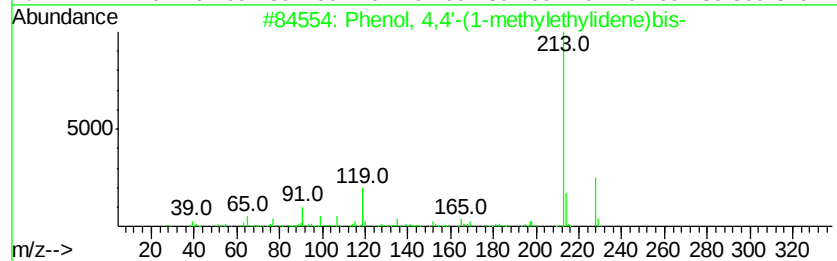
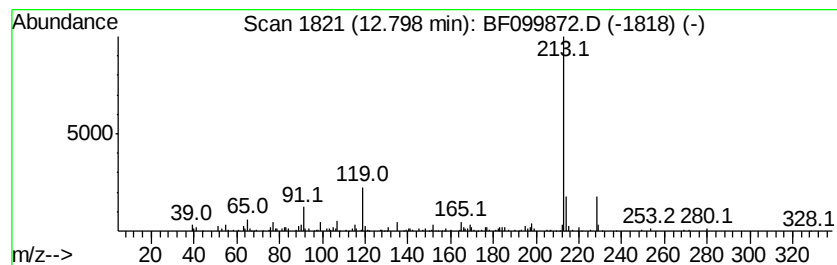
Instrument :
BNA_F
ClientSampleId :
MARION-26KV-3-WATER

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 9 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.80	7.33 ng	213032	Chrysene-d12	13.99	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	91
2	2,2-Bis-(4-hydroxyphenyl)-butane	242	C16H18O2	000077-40-7	59
3	2-Bromo-7-(methylamino)tropon	213	C8H8BrNO	103539-25-9	53
4	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	53
5	Decanedioic acid, diethyl ester	258	C14H26O4	000110-40-7	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102617\
Data File : BF099872.D
Acq On : 26 Oct 2017 20:43
Operator : SJ/JU
Sample : I6111-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MARION-26KV-3-WATER

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	7.8	ng	141745	1	6.79	364122	20.0
unknown6.57	6.57	85.8	ng	1561870	1	6.79	364122	20.0
2-Hydroxy-iso-but...	8.64	2.5	ng	62502	2	8.08	509309	20.0
unknown10.24	10.24	2.3	ng	61736	3	9.84	545327	20.0
Benzophenone	10.56	8.6	ng	235577	3	9.84	545327	20.0
Decane, 2-methyl-	10.75	6.5	ng	179772	4	11.33	550323	20.0
Hexadecane	11.21	3.9	ng	108414	4	11.33	550323	20.0
Phenol, 4,4'-(1-m...	12.80	7.3	ng	213032	5	13.99	581218	20.0