

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
 Data File : BG032245.D
 Acq On : 24 Jan 2018 4:18
 Operator : SJ/JU
 Sample : J1239-14
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-53-01

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_G\METHODS\8270-BG011218.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	3.504	31	37	44	rBV	371179	646612	13.82%	2.867%
2	5.672	397	406	413	rBV	62223	104647	2.24%	0.464%
3	6.178	485	492	501	rBV	628737	1080070	23.08%	4.789%
4	7.858	770	778	789	rBV	600165	1081425	23.11%	4.795%
5	8.258	838	846	859	rVB	736408	1372739	29.33%	6.087%
6	8.745	919	929	937	rBV	140418	258659	5.53%	1.147%
7	9.080	976	986	993	rBV	618391	1151208	24.60%	5.105%
8	9.298	1017	1023	1032	rVB	84676	155129	3.32%	0.688%
9	9.944	1124	1133	1143	rBV	432588	826738	17.67%	3.666%
10	11.624	1411	1419	1422	rBV	190006	365656	7.81%	1.621%
11	11.671	1422	1427	1437	rVV	578782	1085048	23.19%	4.811%
12	11.795	1441	1448	1460	rVB	100823	188695	4.03%	0.837%
13	12.958	1639	1646	1654	rBV	46075	77796	1.66%	0.345%
14	13.234	1685	1693	1700	rBV	130533	220836	4.72%	0.979%
15	13.340	1704	1711	1718	rBV2	60271	105044	2.24%	0.466%
16	13.446	1718	1729	1738	rVB2	115044	229537	4.91%	1.018%
17	13.998	1816	1823	1831	rBV	1684790	2697806	57.65%	11.962%
18	14.533	1902	1914	1924	rBV8	24900	65042	1.39%	0.288%
19	15.097	2002	2010	2016	rBV	101617	170125	3.64%	0.754%
20	15.373	2050	2057	2063	rBV2	330377	573425	12.25%	2.543%
21	15.432	2063	2067	2072	rVB	31311	50008	1.07%	0.222%
22	16.407	2227	2233	2242	rVB	73542	128559	2.75%	0.570%
23	16.842	2299	2307	2315	rBV	1143622	1858581	39.72%	8.241%
24	17.923	2485	2491	2496	rVB2	30613	49510	1.06%	0.220%
25	18.099	2513	2521	2526	rBV2	493419	808515	17.28%	3.585%
26	18.140	2526	2528	2534	rVB	133987	185717	3.97%	0.823%
27	18.493	2579	2588	2593	rBV	119804	186646	3.99%	0.828%
28	18.998	2670	2674	2680	rVB3	33877	55814	1.19%	0.247%
29	20.637	2947	2953	2962	rBV	3430235	4679567	100.00%	20.749%
30	22.435	3251	3259	3270	rVB2	559688	1074643	22.96%	4.765%
31	26.131	3875	3888	3904	rBV3	262857	1018957	21.77%	4.518%

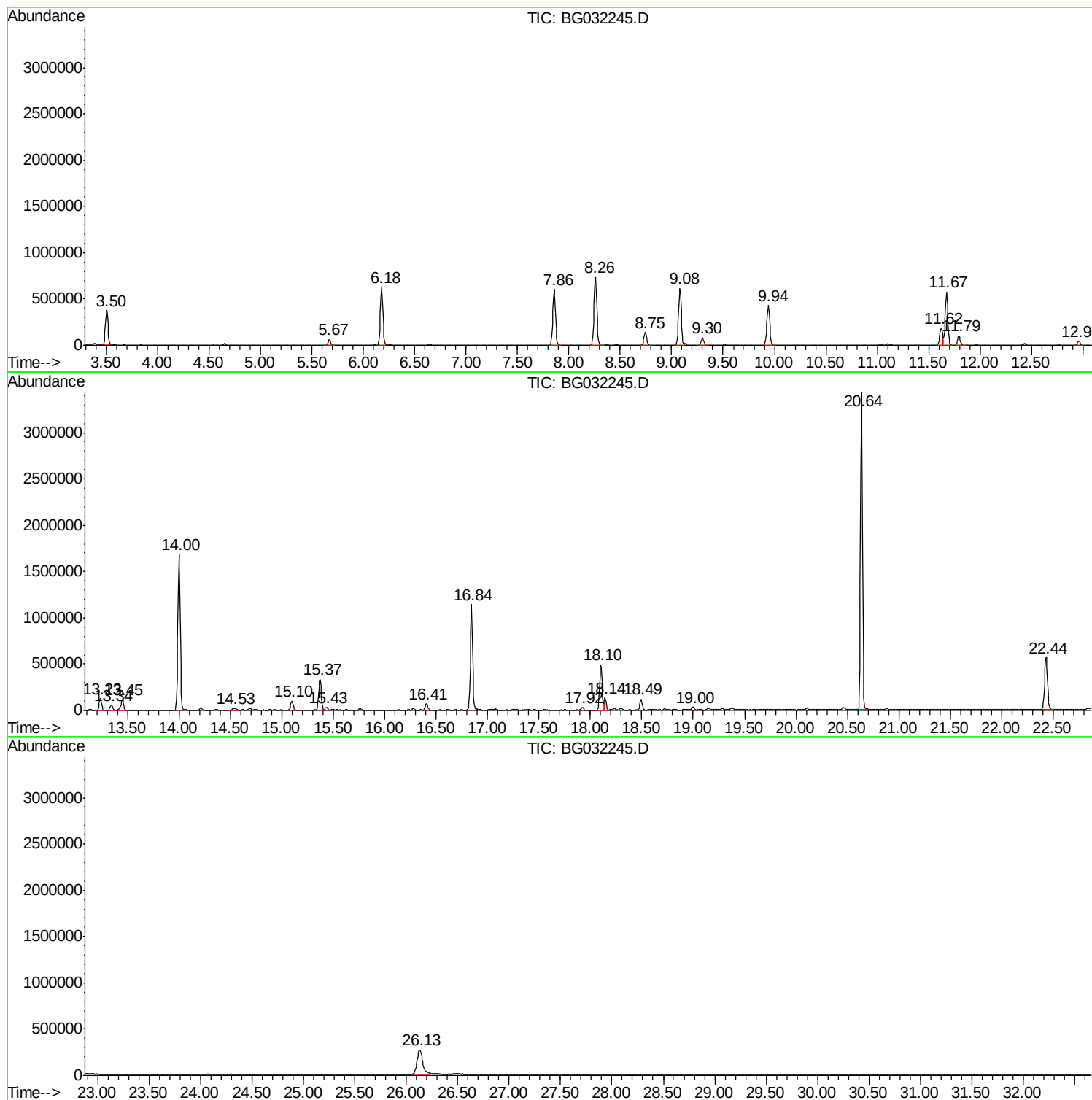
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BNA_G
ClientSampleId :
WC-53-01

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG011218.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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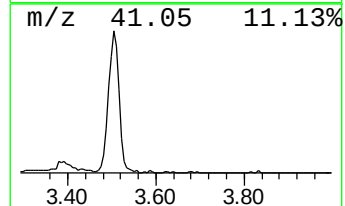
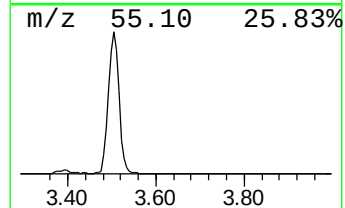
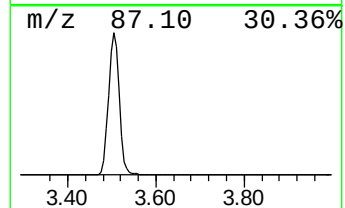
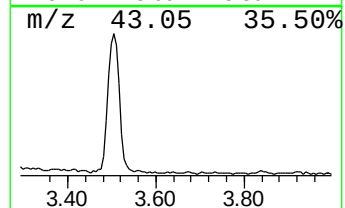
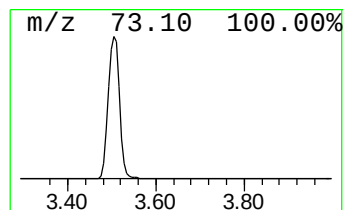
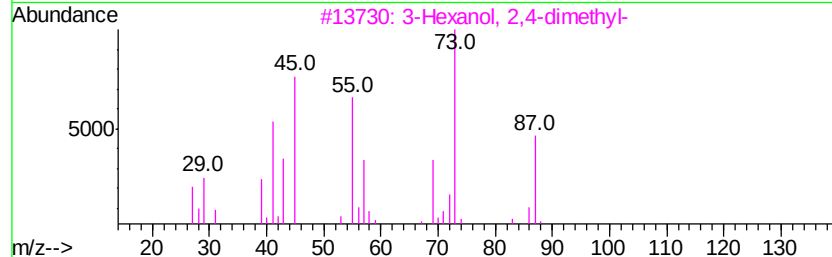
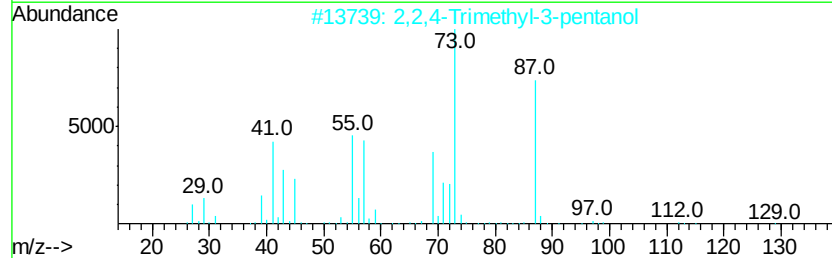
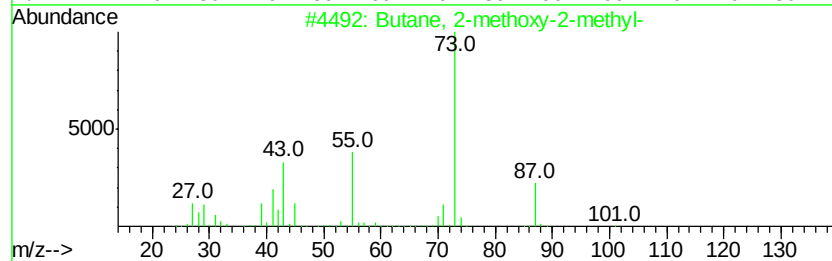
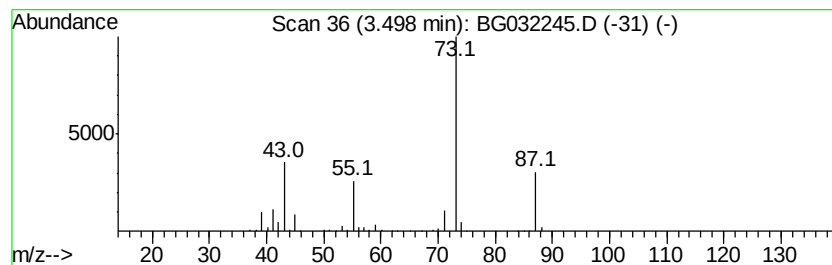
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.50	50.00 ng	646612	1,4-Dichlorobenzene-d4	8.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3		3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	36
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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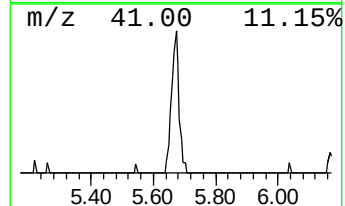
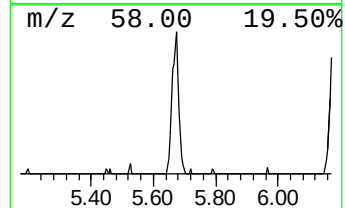
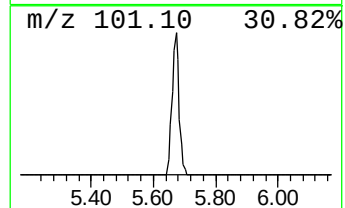
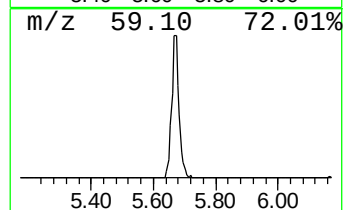
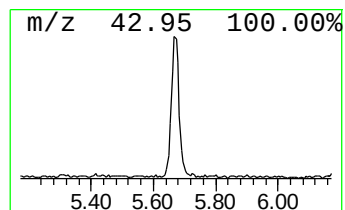
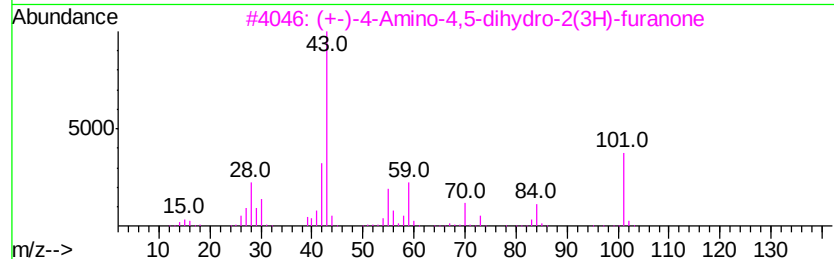
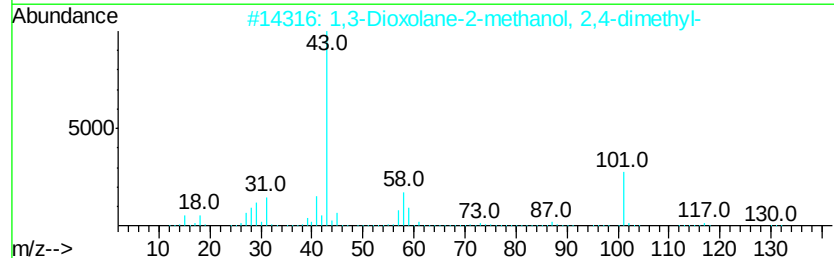
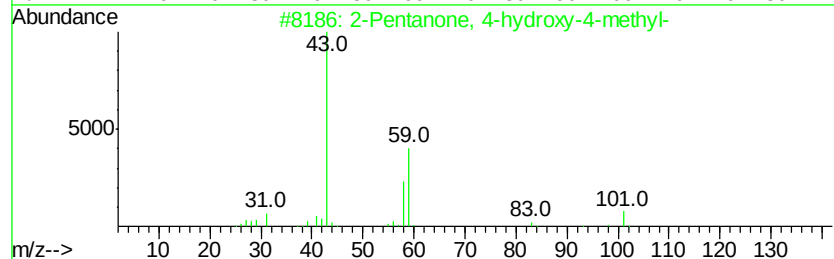
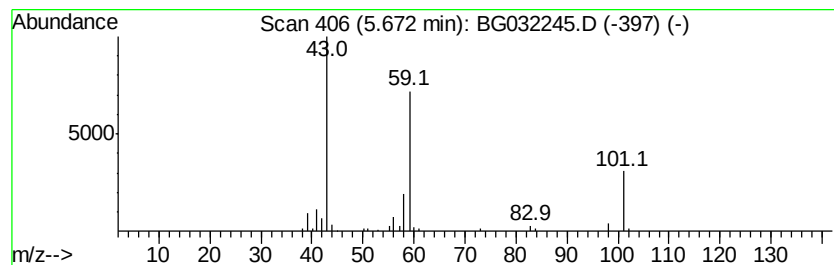
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.67	8.09 ng	104647	1,4-Dichlorobenzene-d4	8.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	38
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	38
4		3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	28
5		5-Ethyl-3-methylhept-1-en-4-ol	156	C10H20O	286424-80-4	25



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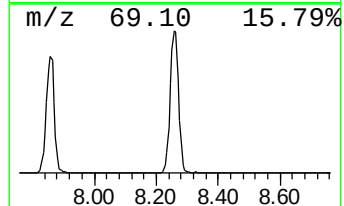
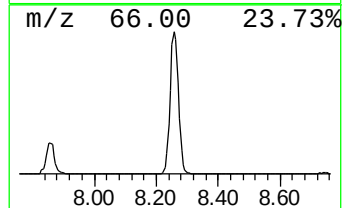
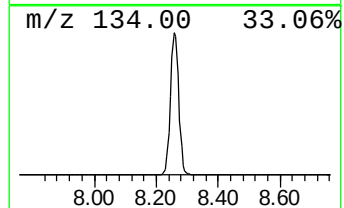
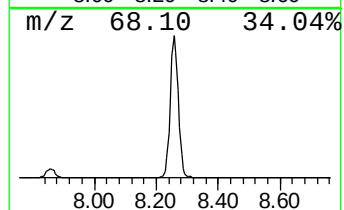
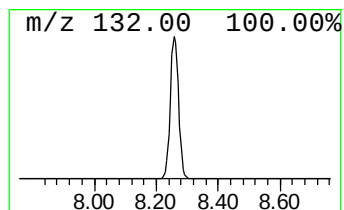
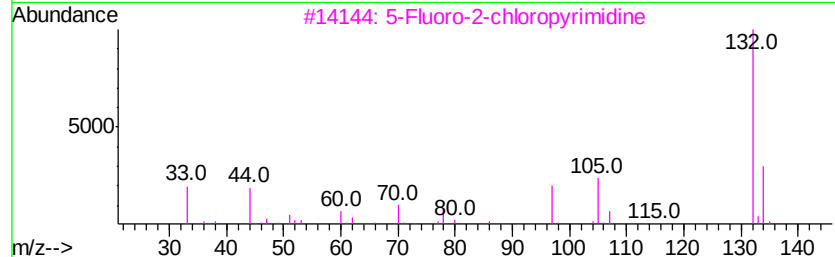
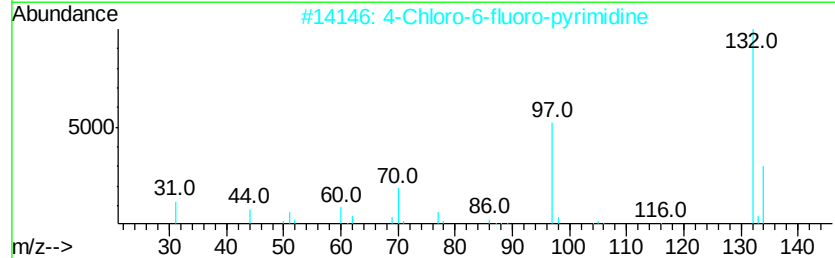
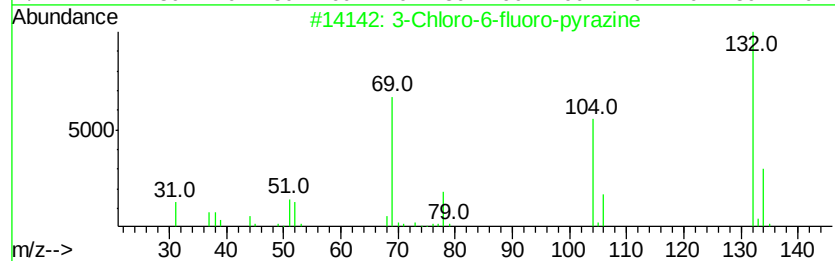
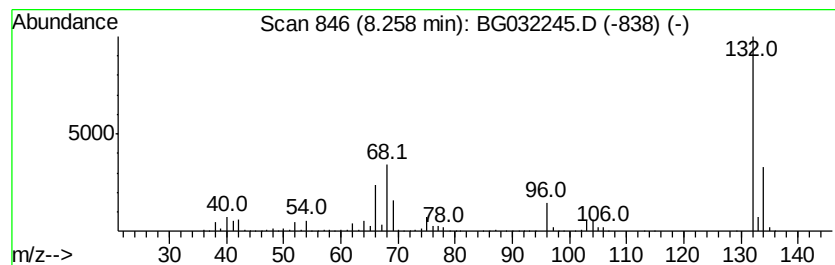
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Peak Number 3 unknown8.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.26	106.14 ng	1372740	1,4-Dichlorobenzene-d4	8.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	35
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10



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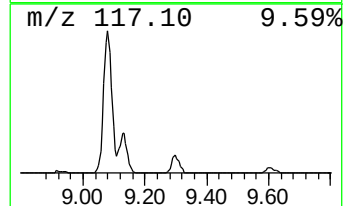
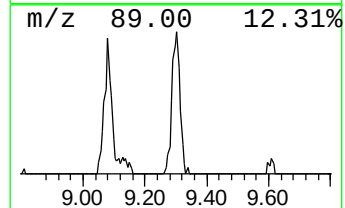
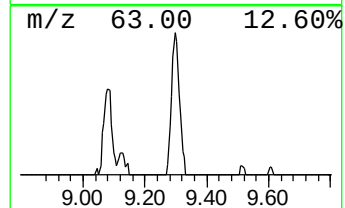
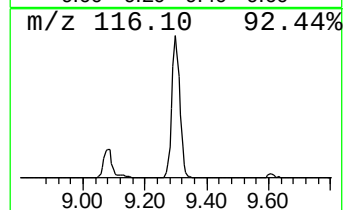
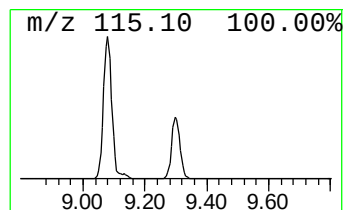
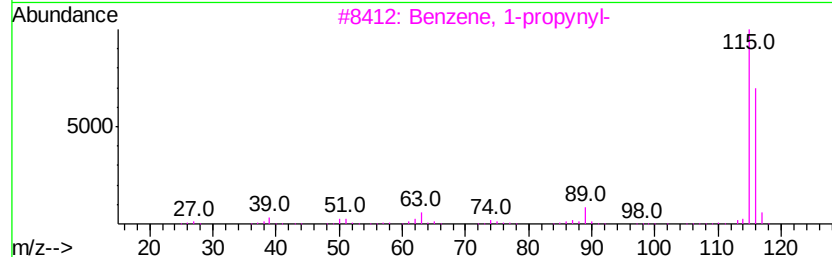
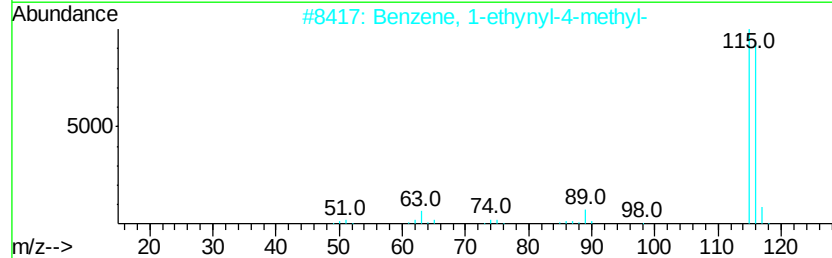
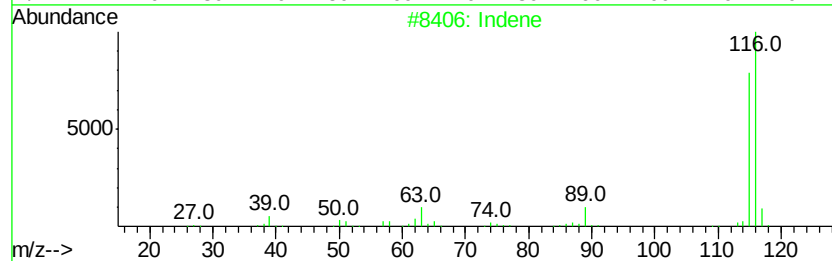
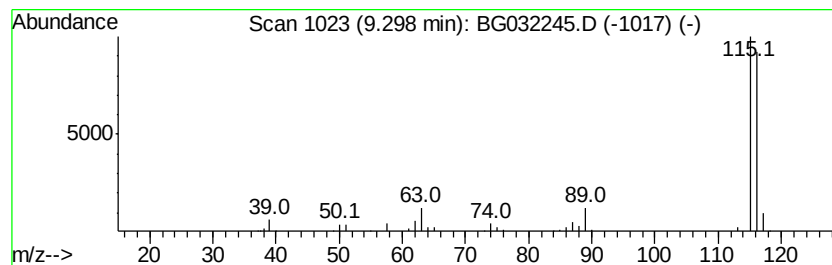
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Peak Number 5 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.30	11.99 ng	155129	1,4-Dichlorobenzene-d4	8.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indene	116	C9H8	000095-13-6	91
2		Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
3		Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4		3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5		Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	90



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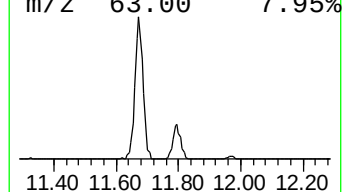
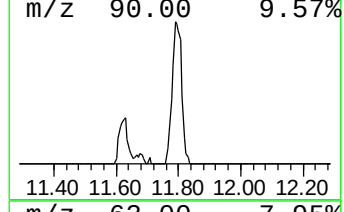
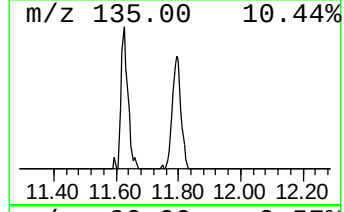
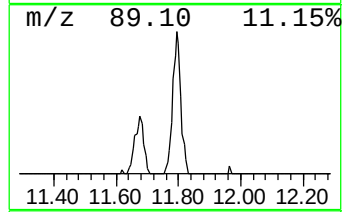
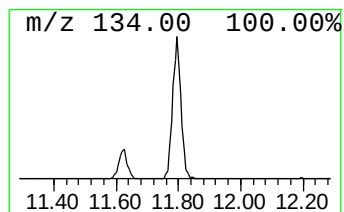
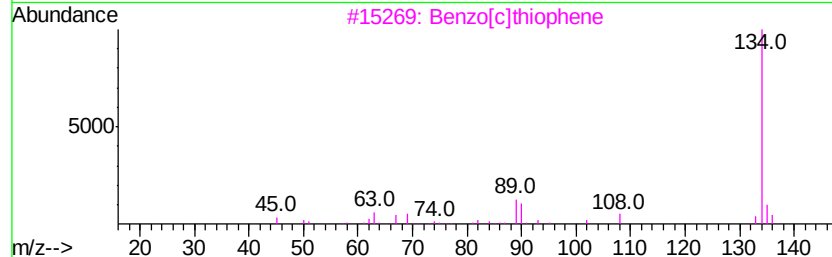
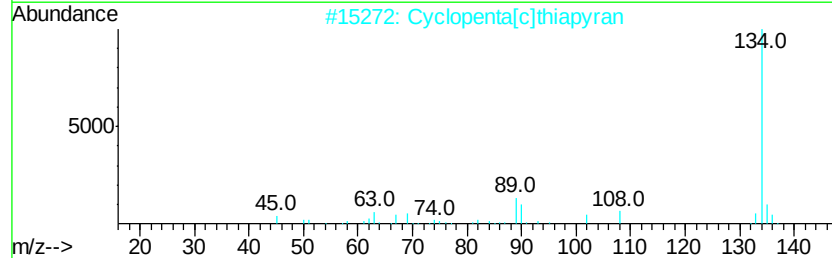
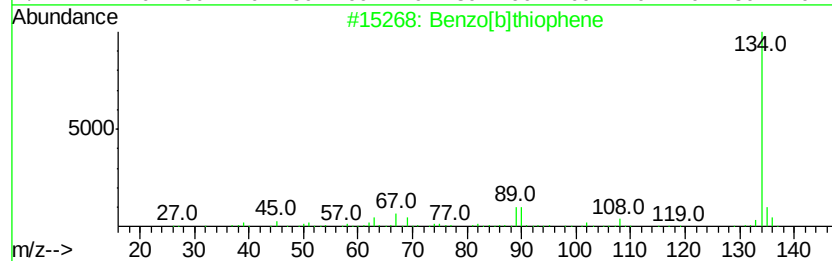
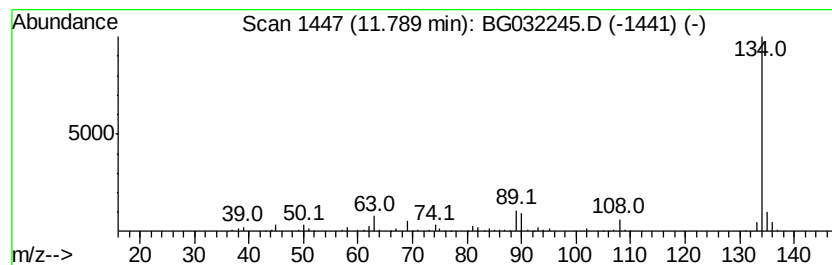
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Peak Number 6 Benzo[b]thiophene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.79	10.32 ng	188695	Napthalene-d8	11.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]thiophene	134	C8H6S	000095-15-8	94
2	Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	91
3	Benzo[c]thiophene	134	C8H6S	000270-82-6	91
4	Benzo[b]cyclobuta[d]thiophene-1,...	264	C13H12O4S	034244-75-2	83
5	3-(2'-Methyl benzenaminomethyl),...	324	C18H16N2O2S	312926-67-3	78



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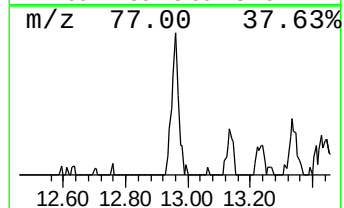
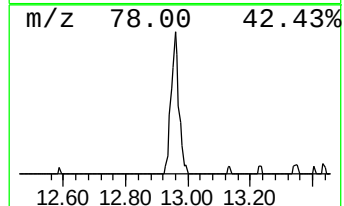
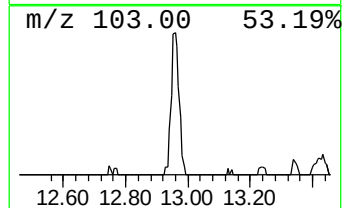
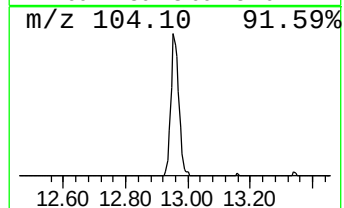
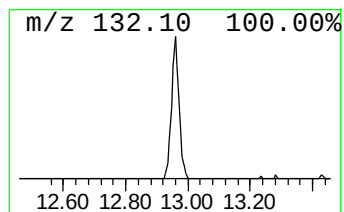
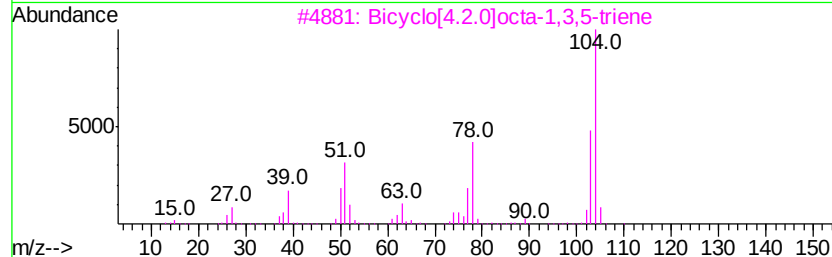
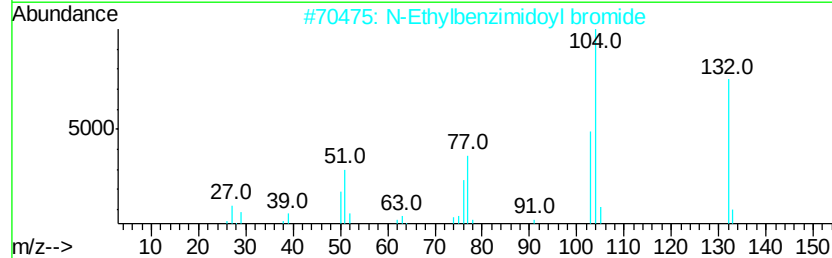
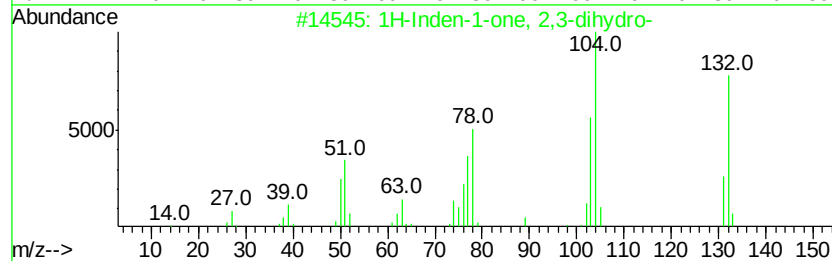
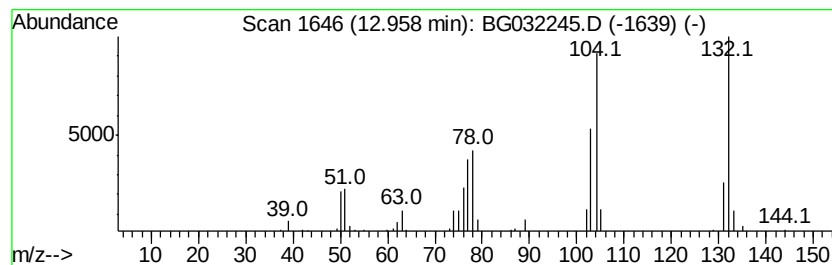
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1H-Inden-1-one, 2,3-dihydro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	4.26 ng	77796	Naphthalene-d8	11.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	95
2		N-Ethylbenzimidoyl bromide	211	C9H10BrN	041182-87-0	64
3		Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	55
4		Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	53
5		2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	52



Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032245.D
Acq On : 24 Jan 2018 4:18
Operator : SJ/JU
Sample : J1239-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-53-01

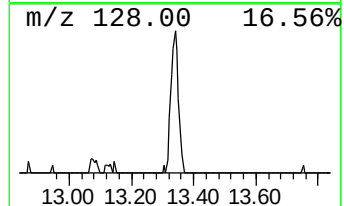
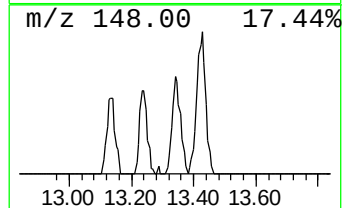
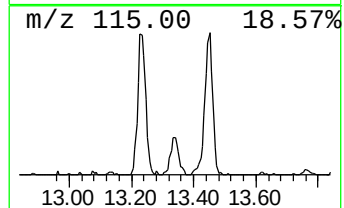
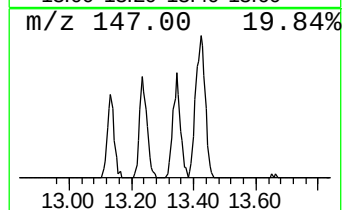
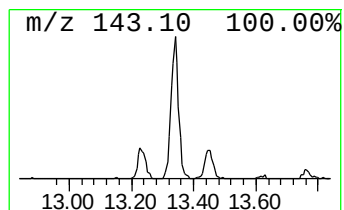
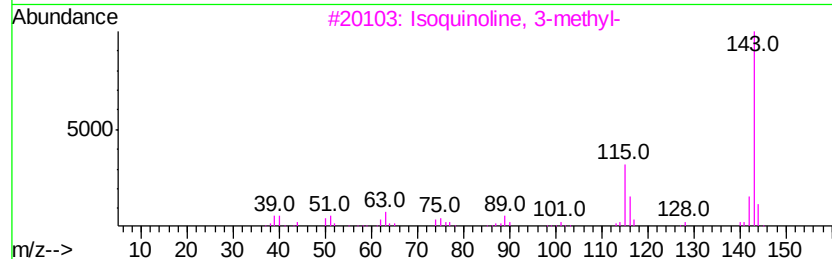
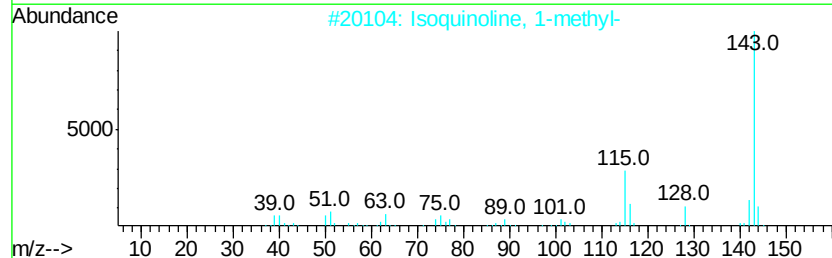
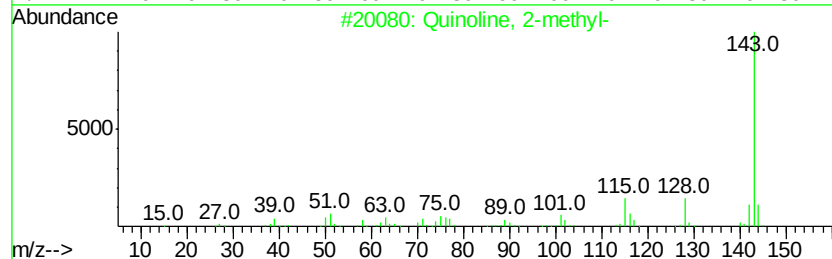
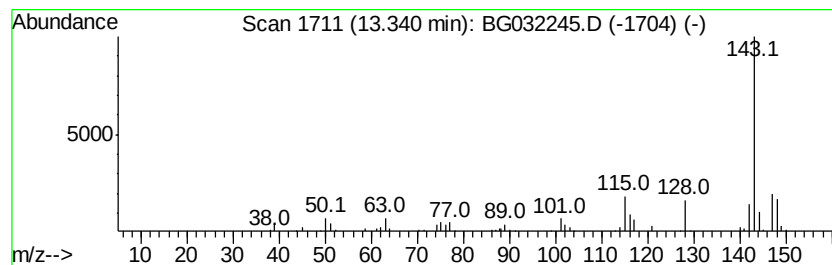
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Quinoline, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	5.75 ng	105044	Naphthalene-d8	11.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Quinoline, 2-methyl-	143	C10H9N	000091-63-4	94
2		Isoquinoline, 1-methyl-	143	C10H9N	001721-93-3	76
3		Isoquinoline, 3-methyl-	143	C10H9N	001125-80-0	76
4		Quinoline, 4-methyl-	143	C10H9N	000491-35-0	76
5		1-Naphthalenamine	143	C10H9N	000134-32-7	64



Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032245.D
Acq On : 24 Jan 2018 4:18
Operator : SJ/JU
Sample : J1239-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-53-01

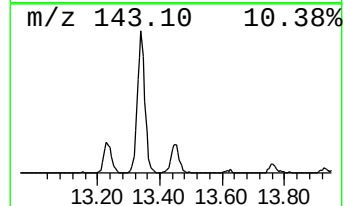
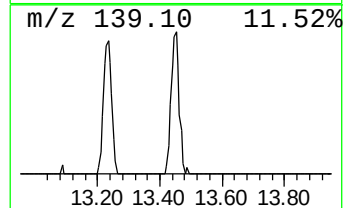
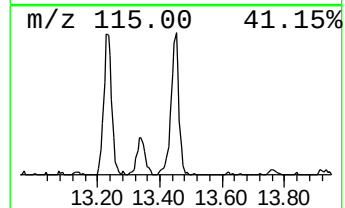
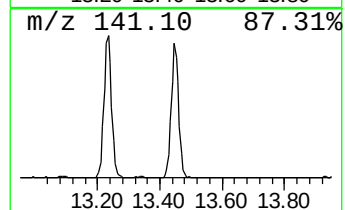
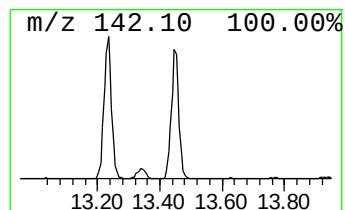
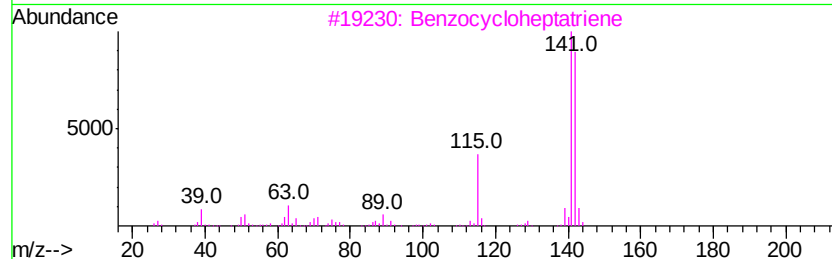
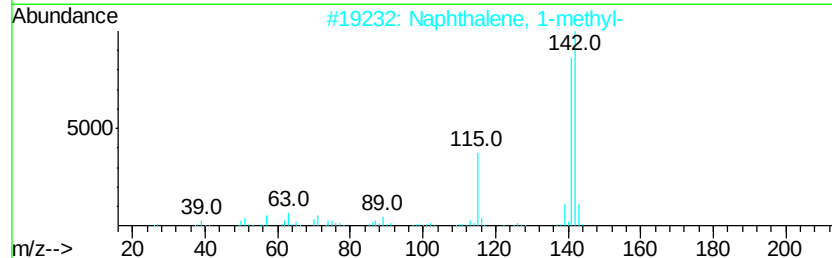
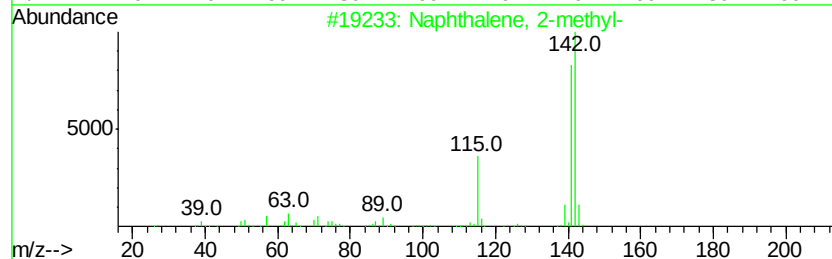
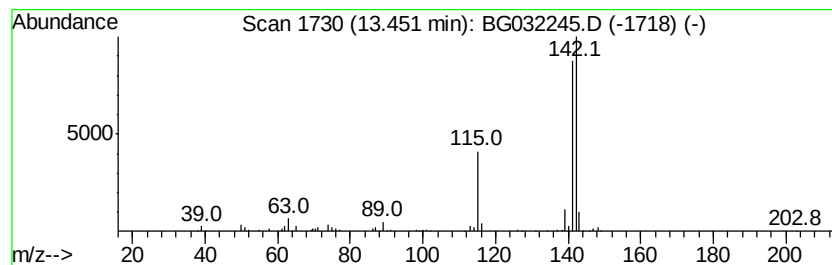
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Naphthalene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	12.55 ng	229537	Naphthalene-d8	11.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3		Benzocycloheptatriene	142	C11H10	000264-09-5	91
4		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032245.D
Acq On : 24 Jan 2018 4:18
Operator : SJ/JU
Sample : J1239-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

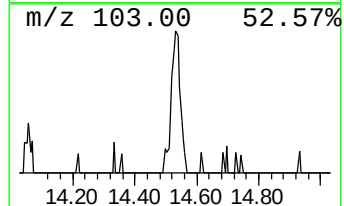
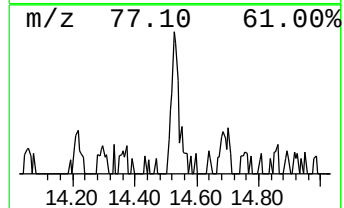
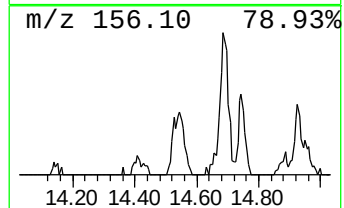
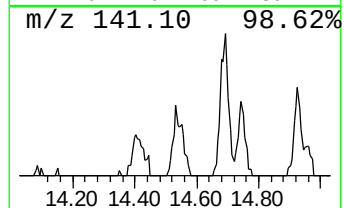
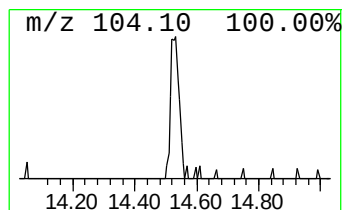
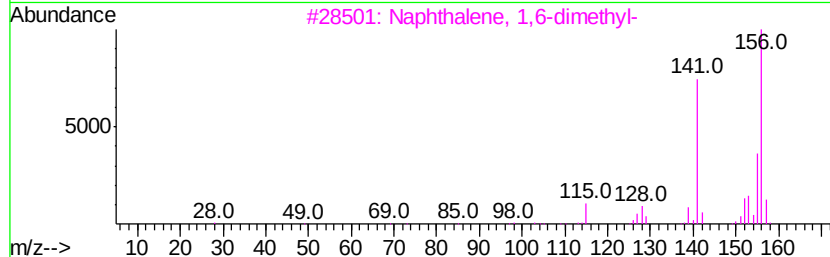
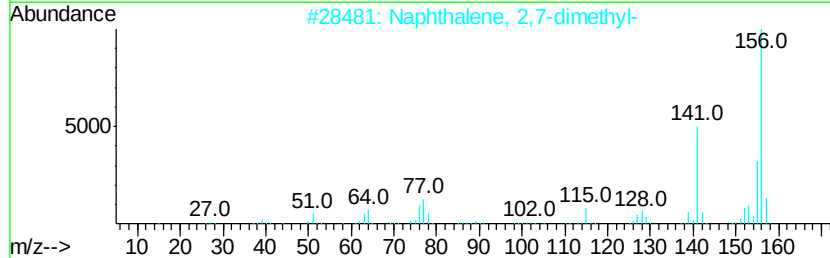
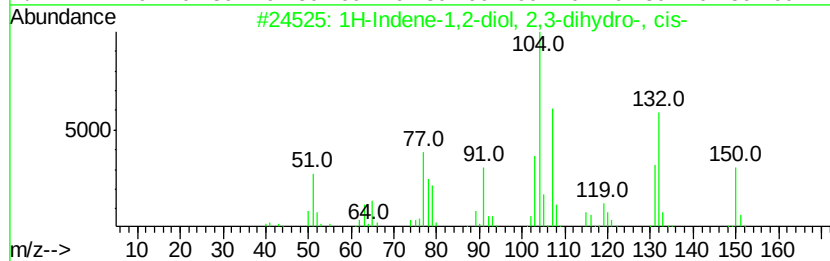
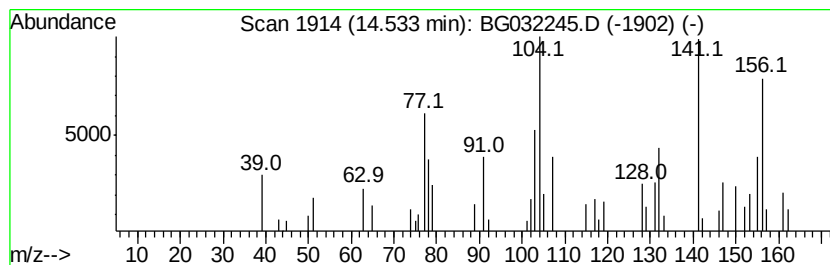
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.53 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.27 ng	65042	Acenaphthene-d10	15.37
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1H-Indene-1,2-diol, 2,3-dihydro-...	150 C9H10O2	004647-42-1 38
2		Naphthalene, 2,7-dimethyl-	156 C12H12	000582-16-1 38
3		Naphthalene, 1,6-dimethyl-	156 C12H12	000575-43-9 38
4		Naphthalene, 2,6-dimethyl-	156 C12H12	000581-42-0 38
5		Benzene, (1,4-cyclohexadien-1-yl)-	156 C12H12	013703-52-1 35



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012318\
Data File : BG032245.D
Acq On : 24 Jan 2018 4:18
Operator : SJ/JU
Sample : J1239-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.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...	3.50	50.0	ng	646612	1	8.75	258659	20.0
2-Pentanone, 4-hy...	5.67	8.1	ng	104647	1	8.75	258659	20.0
unknown8.26	8.26	106.1	ng	1372740	1	8.75	258659	20.0
Indene	9.30	12.0	ng	155129	1	8.75	258659	20.0
Benzo[b]thiophene	11.79	10.3	ng	188695	2	11.62	365656	20.0
1H-Inden-1-one, 2...	12.96	4.3	ng	77796	2	11.62	365656	20.0
Quinoline, 2-methyl-	13.34	5.8	ng	105044	2	11.62	365656	20.0
Naphthalene, 2-me...	13.45	12.6	ng	229537	2	11.62	365656	20.0
unknown14.53	14.53	2.3	ng	65042	3	15.37	573425	20.0