

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
 Data File : BG052522.D
 Acq On : 1 Mar 2022 17:01
 Operator : CG/JU
 Sample : N1688-17
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-34

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:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG052522.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.834	55	59	69	rVB2	29249	45466	1.87%	0.446%
2	4.574	175	185	191	rBV4	15863	34598	1.42%	0.339%
3	5.755	377	386	395	rBV	259879	425508	17.49%	4.171%
4	7.370	653	661	672	rBV	160075	319635	13.14%	3.133%
5	7.864	740	745	750	rVB2	18327	29111	1.20%	0.285%
6	8.222	799	806	812	rBV	101002	174728	7.18%	1.713%
7	8.498	848	853	864	rBV2	38576	91385	3.76%	0.896%
8	8.598	864	870	882	rVB	53362	102531	4.22%	1.005%
9	9.238	964	979	986	rBV7	48879	184251	7.57%	1.806%
10	9.314	986	992	1000	rVV4	87368	288993	11.88%	2.833%
11	9.391	1000	1005	1022	rVB	375348	758998	31.20%	7.440%
12	9.867	1081	1086	1091	rVB2	16792	25879	1.06%	0.254%
13	9.925	1091	1096	1102	rVB	18477	28093	1.15%	0.275%
14	10.025	1102	1113	1120	rBV6	26121	65463	2.69%	0.642%
15	10.448	1179	1185	1191	rVB2	31907	57405	2.36%	0.563%
16	11.059	1276	1289	1295	rBV	137251	267782	11.01%	2.625%
17	11.106	1295	1297	1303	rVV3	15743	25180	1.04%	0.247%
18	11.647	1383	1389	1397	rBV9	8355	26062	1.07%	0.255%
19	12.921	1596	1606	1614	rBV4	23238	57080	2.35%	0.560%
20	13.485	1693	1702	1709	rBV	975427	1501484	61.73%	14.718%
21	13.879	1764	1769	1778	rBV7	13582	32265	1.33%	0.316%
22	14.672	1900	1904	1913	rVB5	11129	25172	1.03%	0.247%
23	14.866	1926	1937	1944	rBV	224359	362293	14.89%	3.551%
24	16.352	2183	2190	2203	rBV	812414	1289887	53.03%	12.644%
25	17.615	2397	2405	2411	rBV	297779	446816	18.37%	4.380%
26	18.555	2562	2565	2570	rVB	19794	26200	1.08%	0.257%
27	20.211	2841	2847	2855	rVB	1878690	2432526	100.00%	23.844%
28	21.539	3069	3073	3082	rVB	13517	28325	1.16%	0.278%
29	21.933	3132	3140	3149	rBV	292878	522538	21.48%	5.122%
30	25.393	3719	3729	3744	rVB	178975	526129	21.63%	5.157%

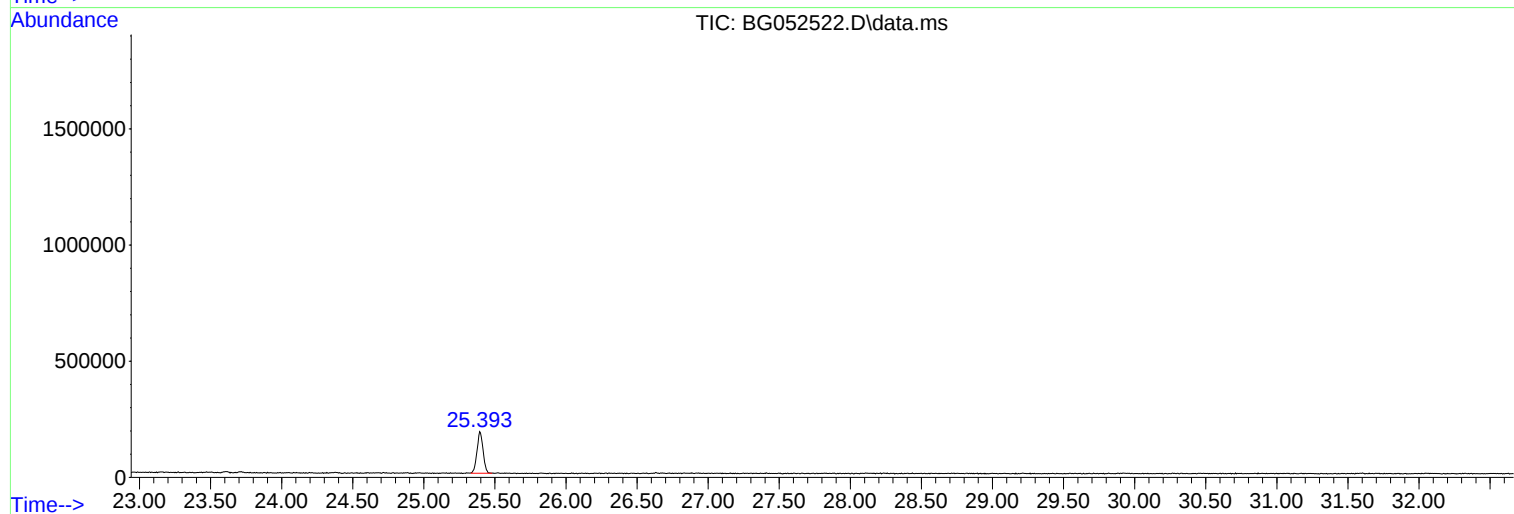
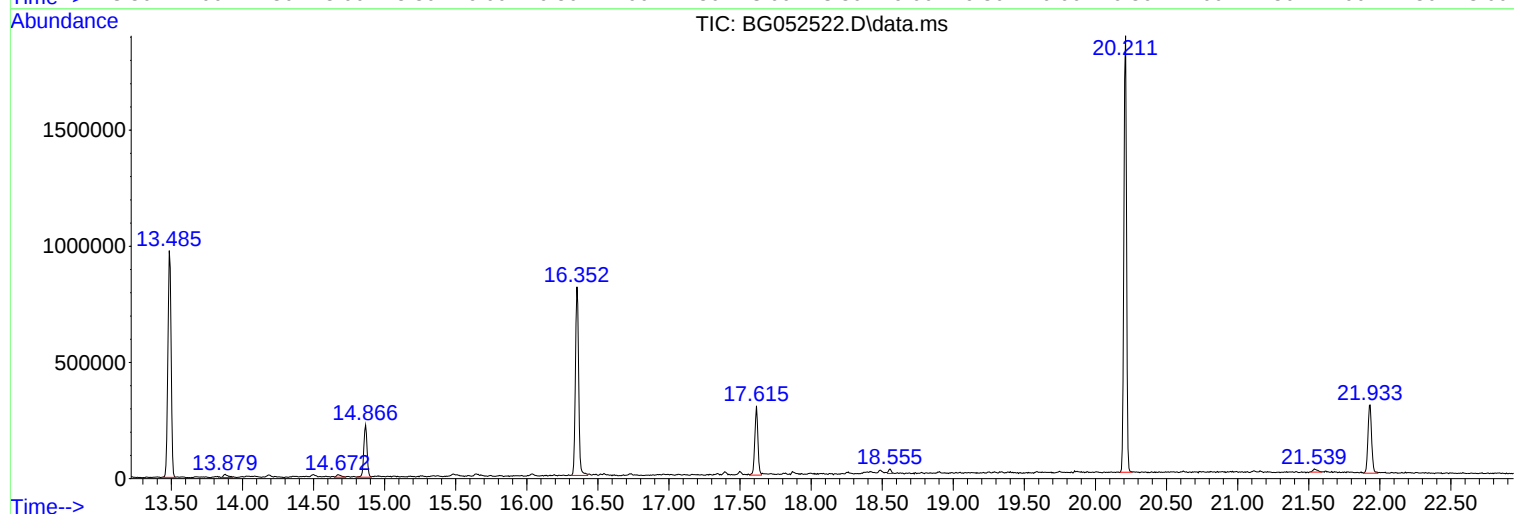
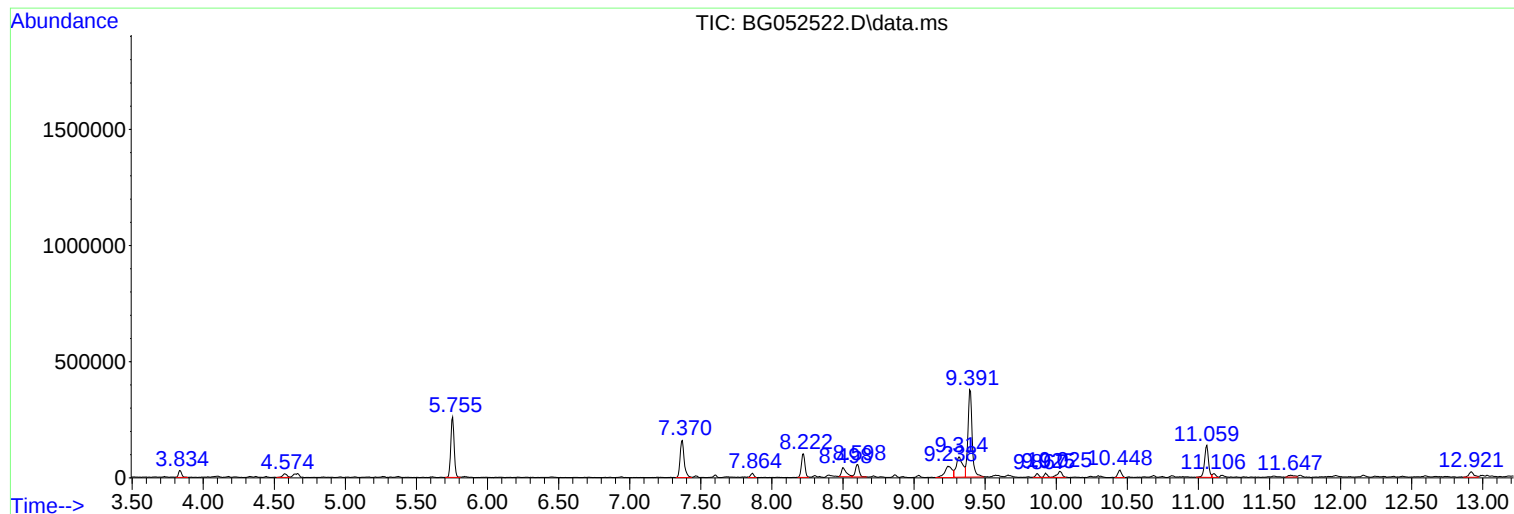
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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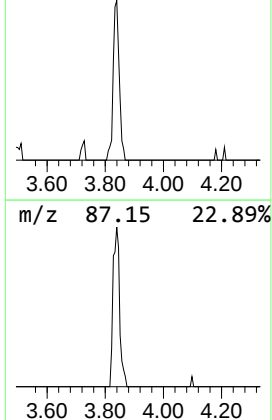
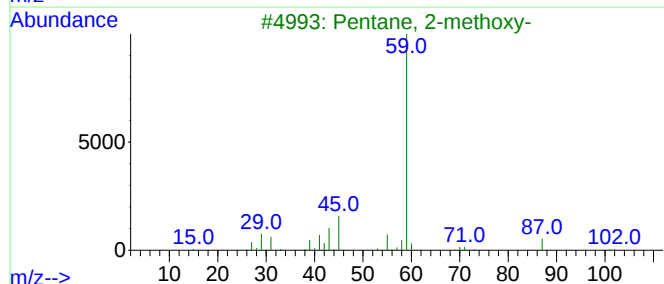
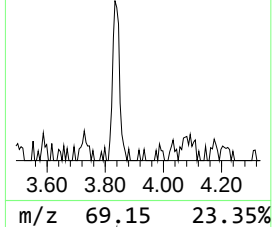
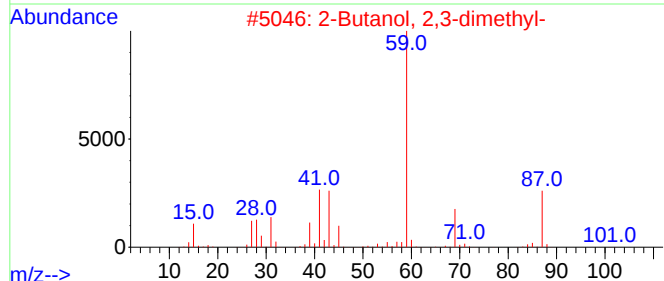
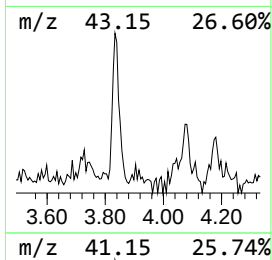
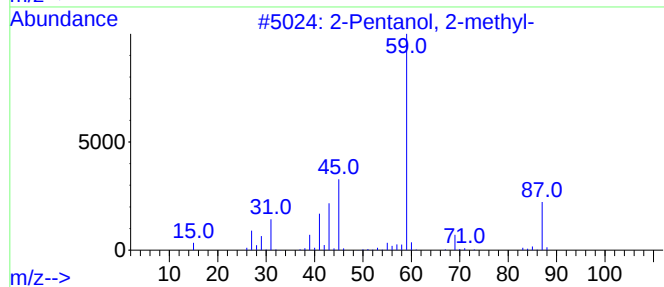
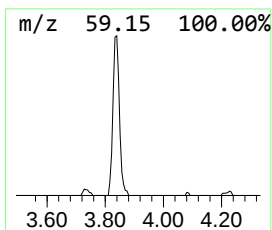
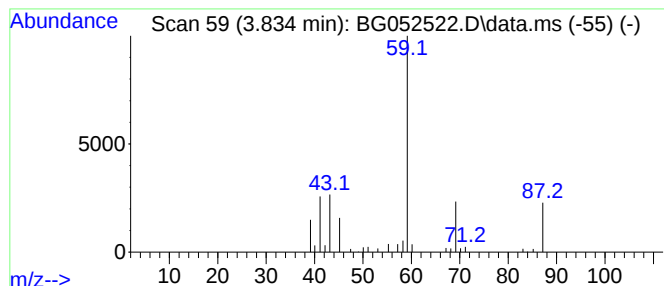
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.834	5.20 ng	45466	1,4-Dichlorobenzene-d4	8.222

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	83
2		2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	78
3		Pentane, 2-methoxy-	102	C6H14O	006795-88-6	56
4		4-O-Acetyl-2,5-di-O-methyl-3,6-d...	215	C10H17NO4	1010101-80-3	42
5		3-Pentanol	88	C5H12O	000584-02-1	42



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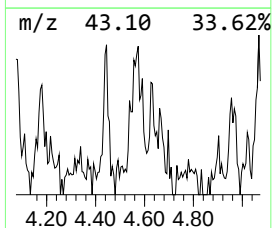
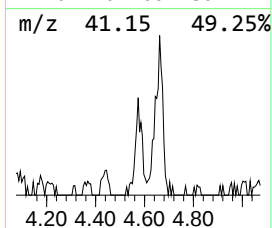
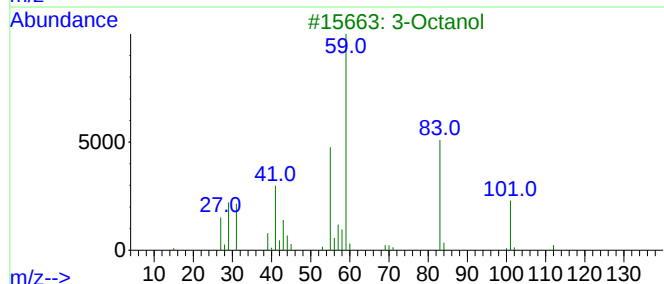
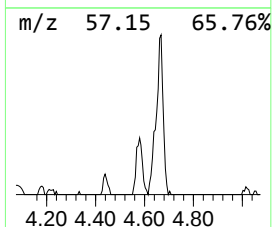
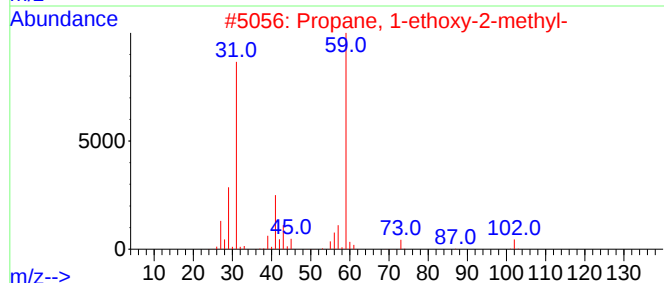
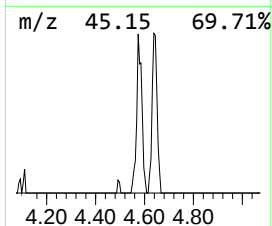
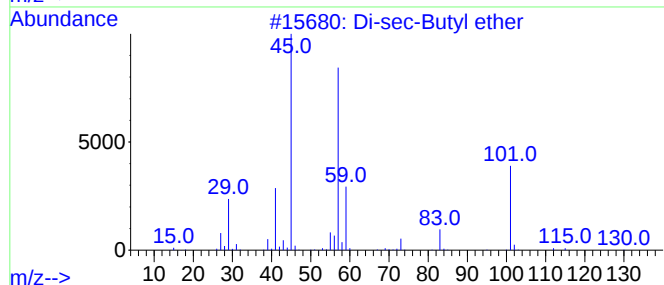
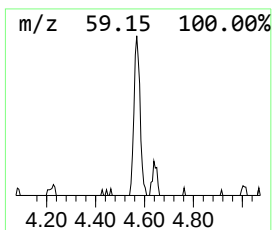
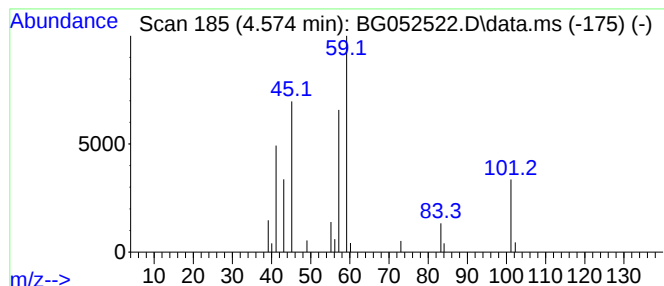
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown4.574 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.574	3.96 ng	34598	1,4-Dichlorobenzene-d4	8.222

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	37
2			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	37
3			3-Octanol	130	C8H18O	000589-98-0	33
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	25
5			2-Hydroxy-3-pentanone	102	C5H10O2	005704-20-1	9



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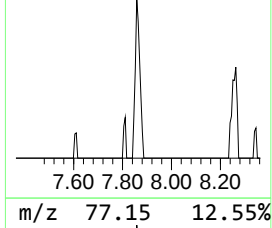
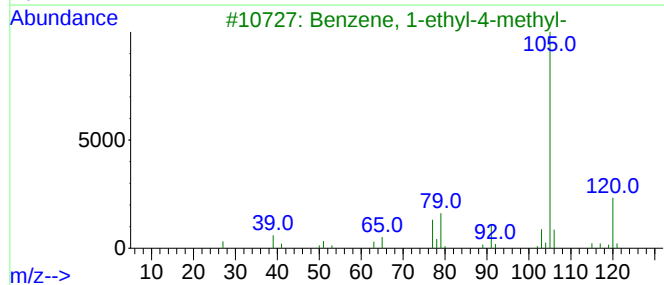
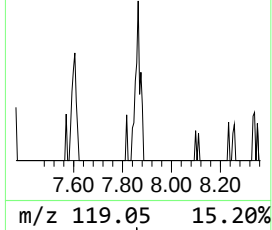
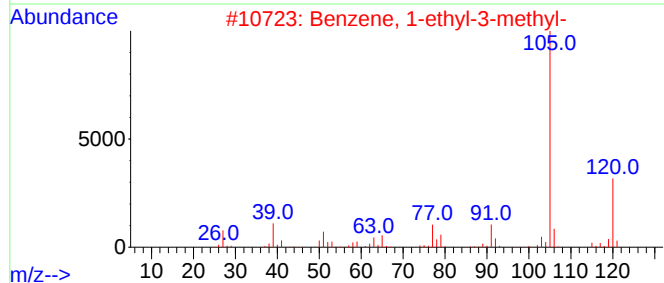
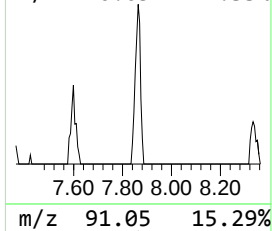
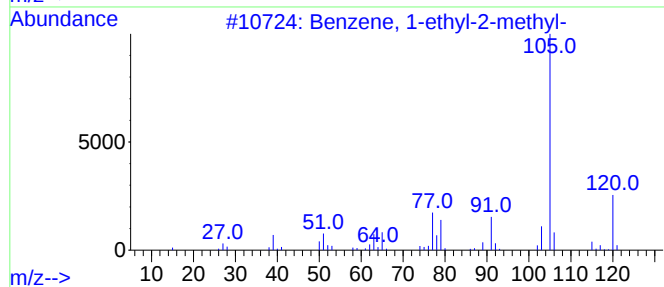
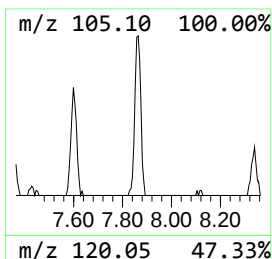
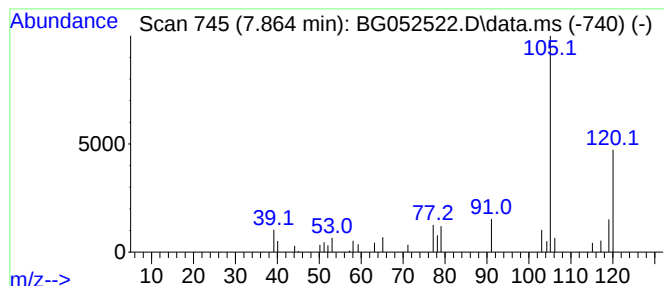
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	3.33 ng	29111	1,4-Dichlorobenzene-d4	8.222

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	86
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	72
4			2,4-Nonadiyne	120	C9H12	063621-15-8	59
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	59



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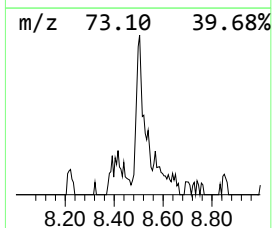
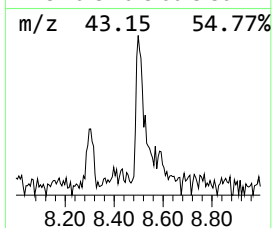
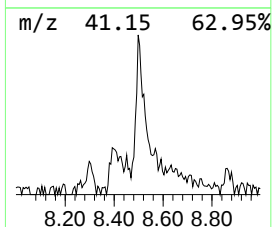
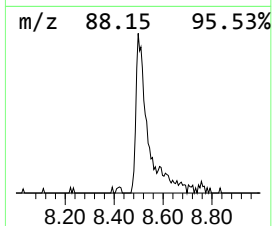
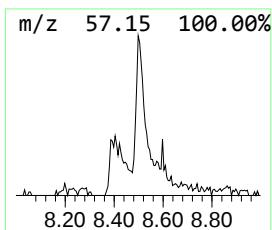
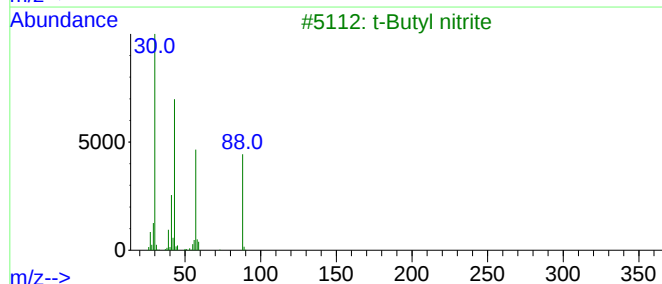
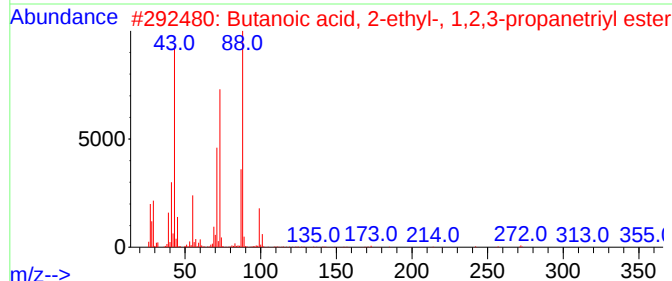
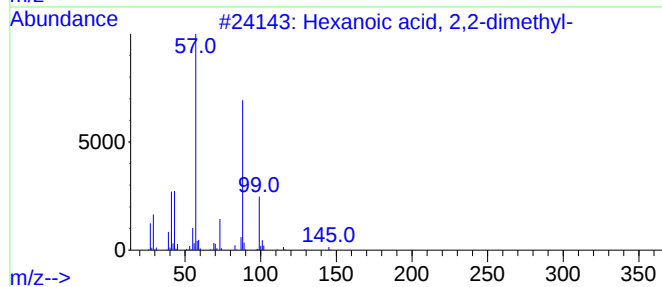
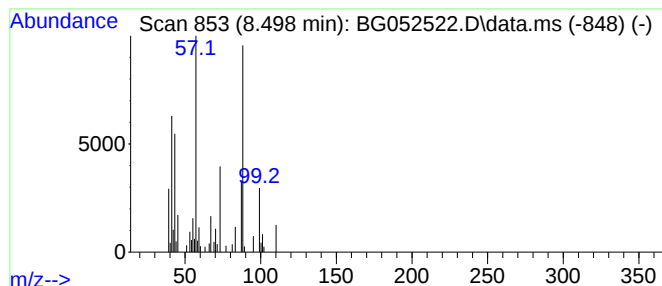
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Hexanoic acid, 2,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.498	10.46 ng	91385	1,4-Dichlorobenzene-d4	8.222

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2,2-dimethyl-	144	C8H16O2	000813-72-9	64
2			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	40
3			t-Butyl nitrite	103	C4H9NO2	000540-80-7	38
4			Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	38
5			Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	28



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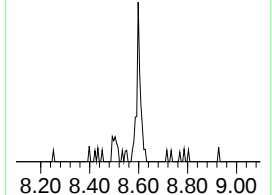
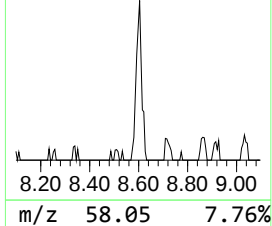
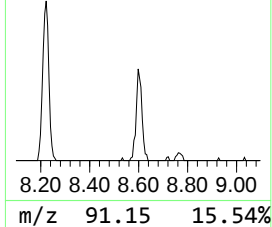
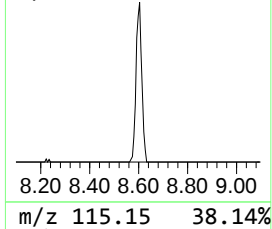
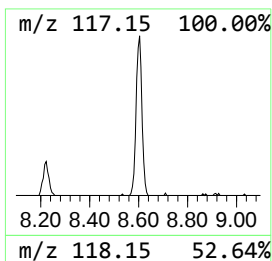
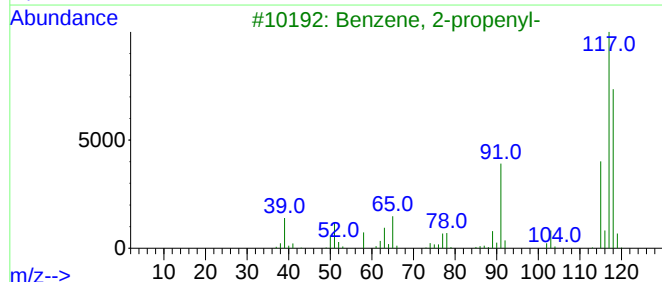
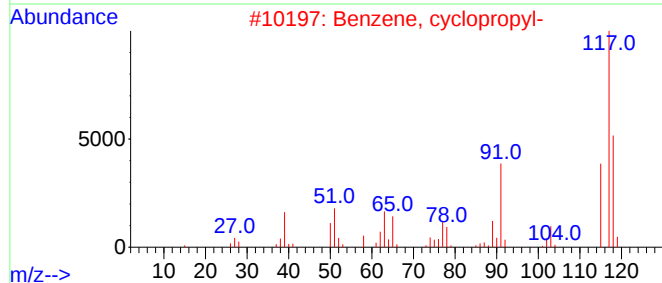
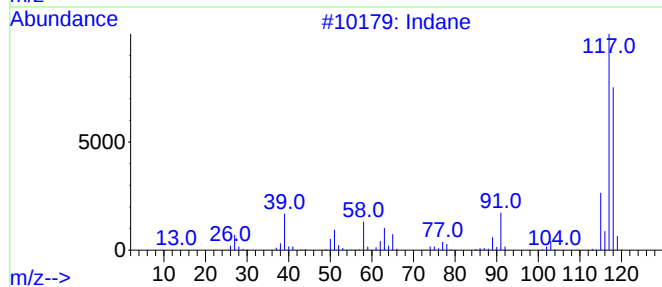
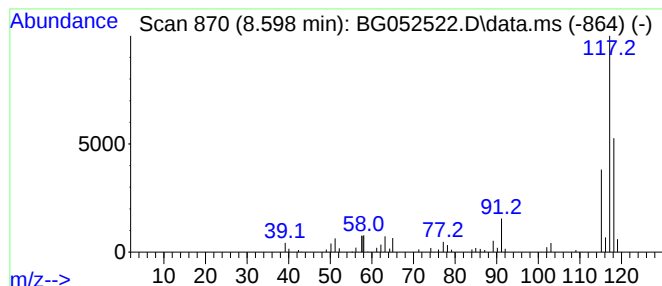
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.598	11.74 ng	102531	1,4-Dichlorobenzene-d4	8.222

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	96
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	93
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
4			Delatacyclene	118	C9H10	007785-10-6	64
5			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	62



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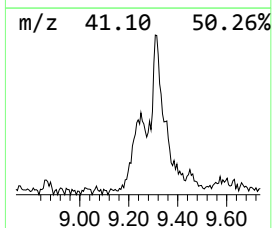
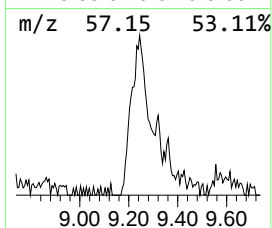
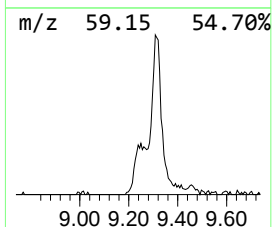
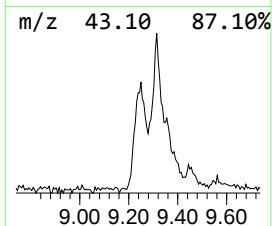
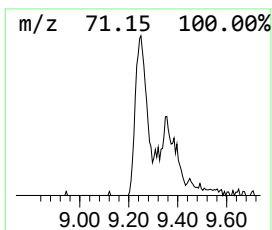
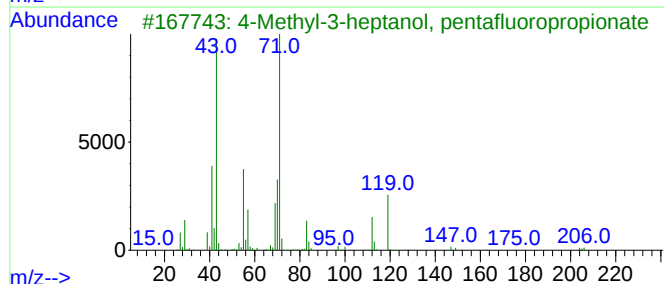
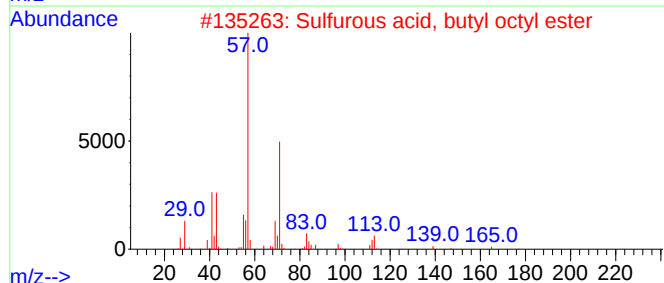
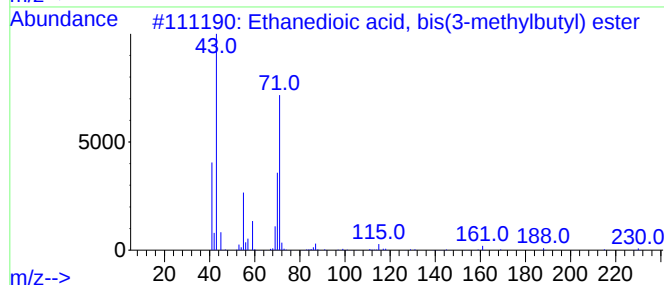
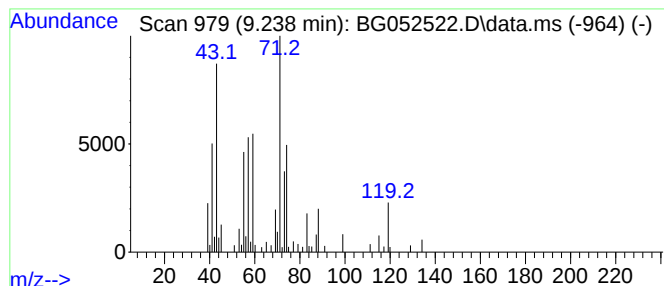
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown9.238 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.238	21.09 ng	184251	1,4-Dichlorobenzene-d4	8.222

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	27
2			Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	22
3			4-Methyl-3-heptanol, pentafluoro...	276	C11H17F5O2	1000365-51-7	16
4			Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	14
5			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052522.D
Acq On : 1 Mar 2022 17:01
Operator : CG/JU
Sample : N1688-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-34

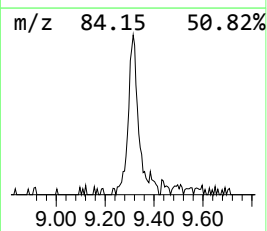
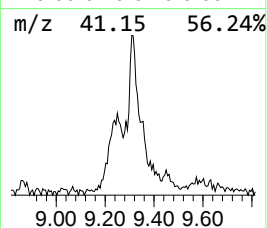
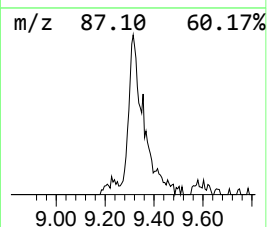
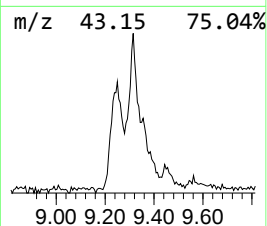
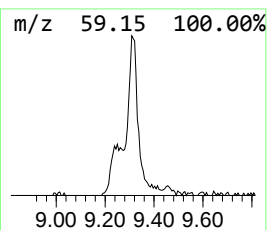
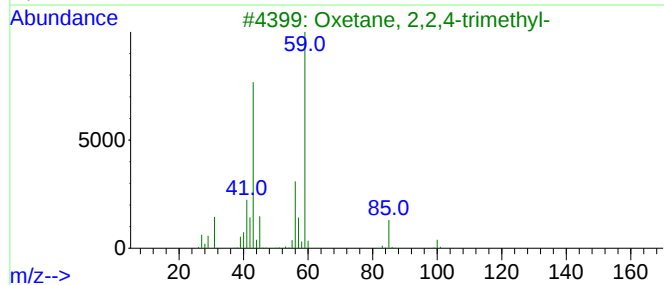
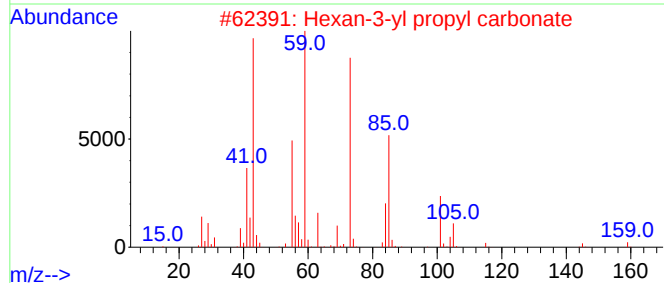
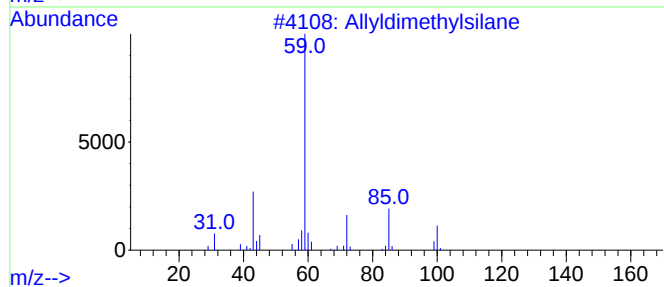
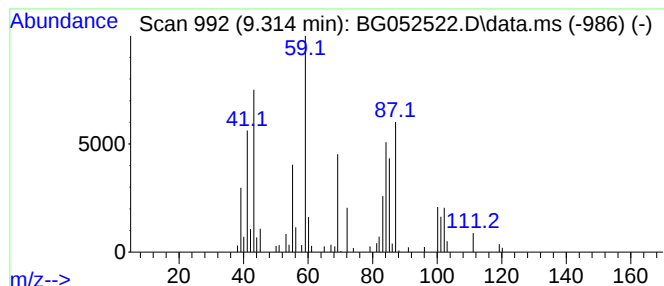
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown9.314 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.314	33.08 ng	288993	1,4-Dichlorobenzene-d4	8.222

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Allyldimethylsilane	100	C5H12Si	003937-30-2	38
2			Hexan-3-yl propyl carbonate	188	C10H20O3	1000372-82-0	35
3			Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	35
4			Methyl 2-(hydroxymethyl)acrylate	116	C5H8O3	015484-46-5	25
5			Oxirane, 2,2-dimethyl-3-propyl-	114	C7H14O	017612-35-0	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052522.D
Acq On : 1 Mar 2022 17:01
Operator : CG/JU
Sample : N1688-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-34

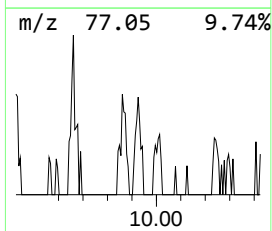
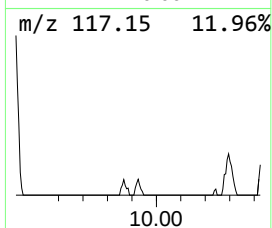
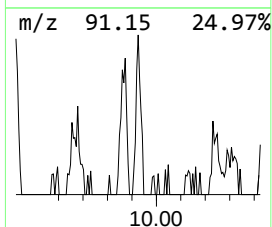
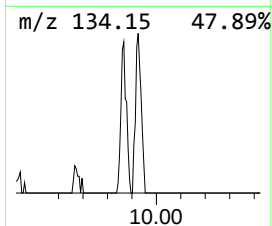
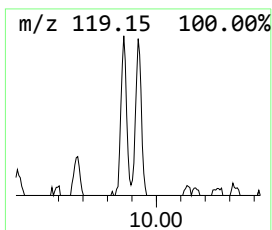
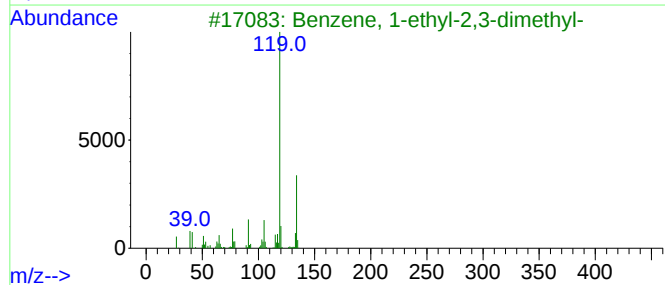
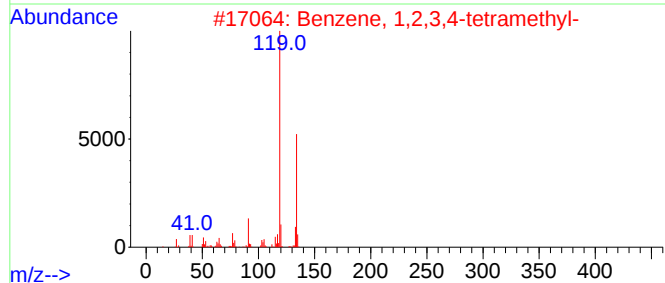
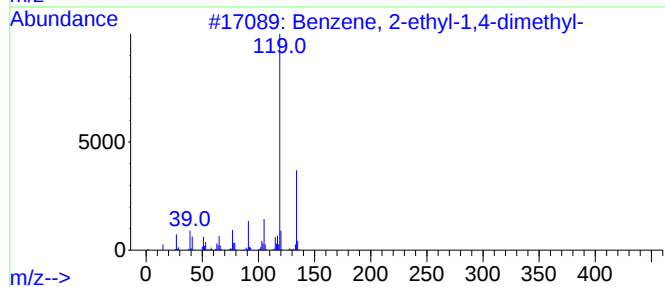
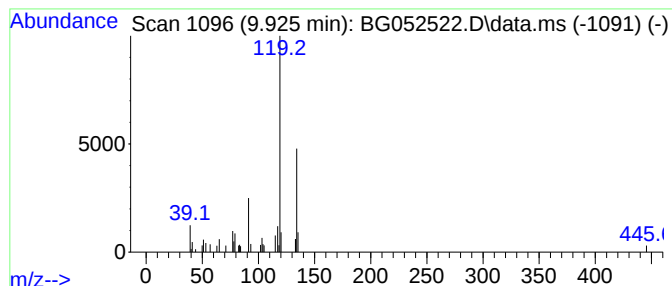
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.925	2.10 ng	28093	Naphthalene-d8	11.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
4			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052522.D
Acq On : 1 Mar 2022 17:01
Operator : CG/JU
Sample : N1688-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-34

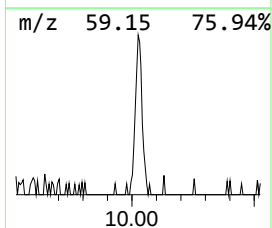
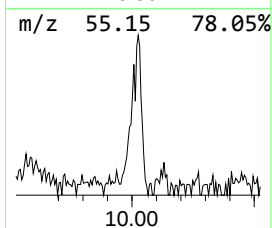
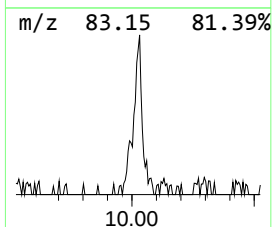
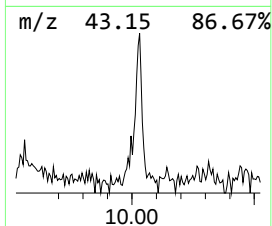
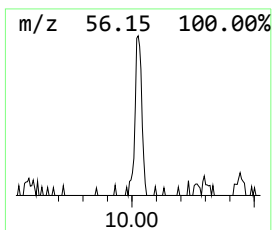
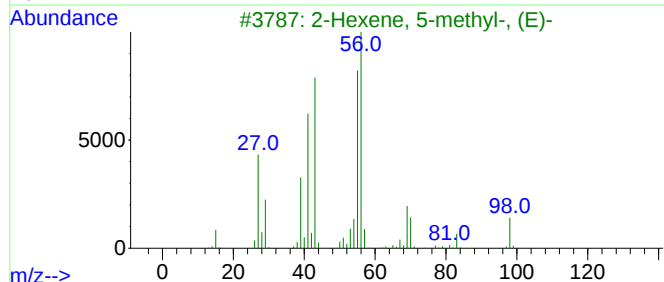
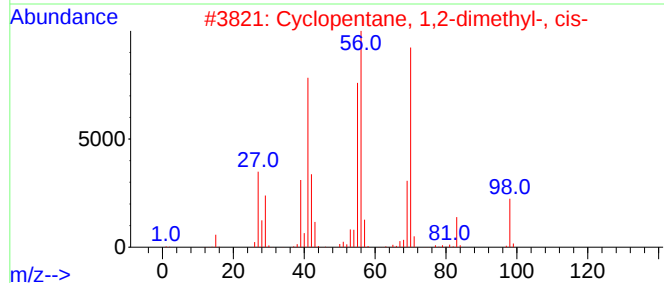
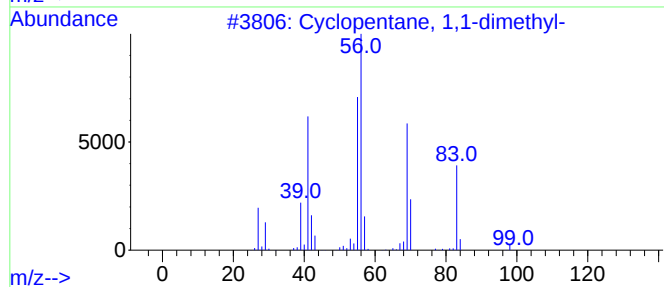
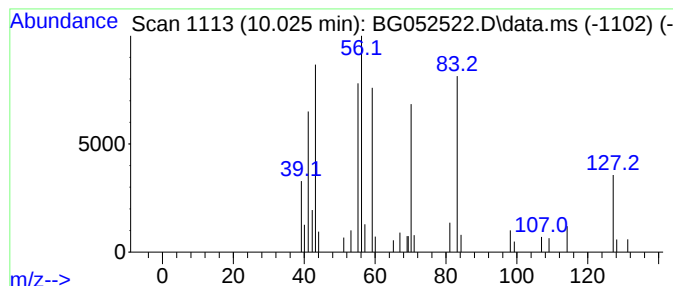
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown10.025 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.025	4.89 ng	65463	Naphthalene-d8	11.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	47
2			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	38
3			2-Hexene, 5-methyl-, (E)-	98	C7H14	007385-82-2	25
4			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	25
5			Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052522.D
Acq On : 1 Mar 2022 17:01
Operator : CG/JU
Sample : N1688-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-34

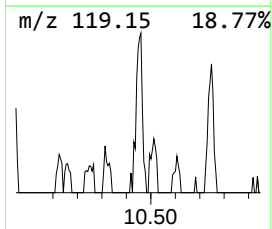
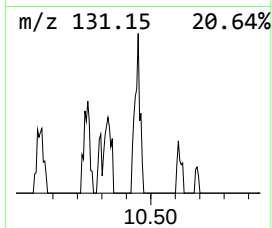
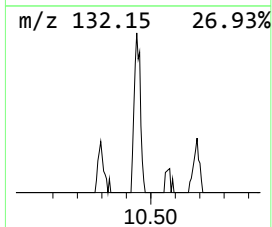
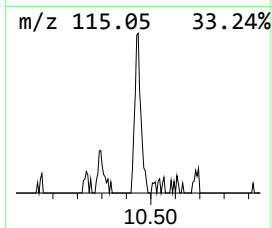
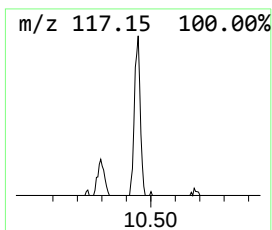
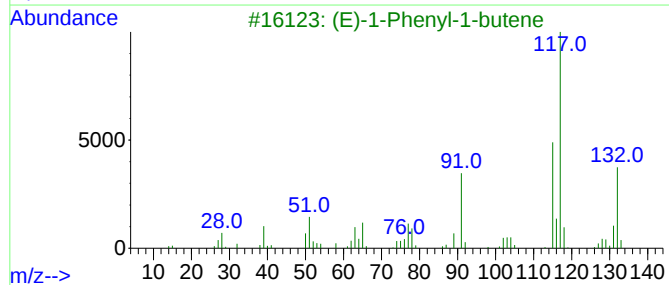
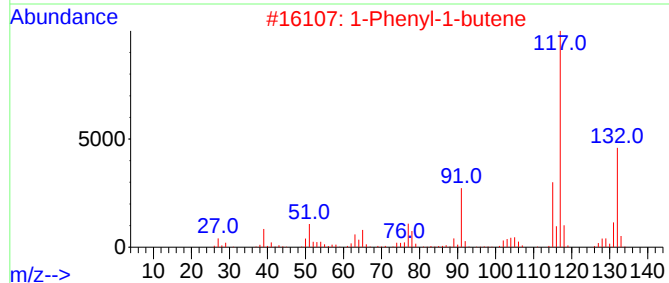
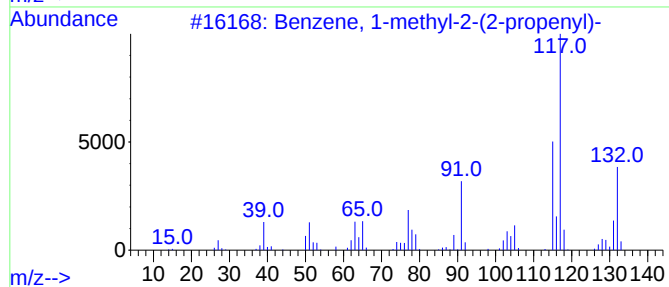
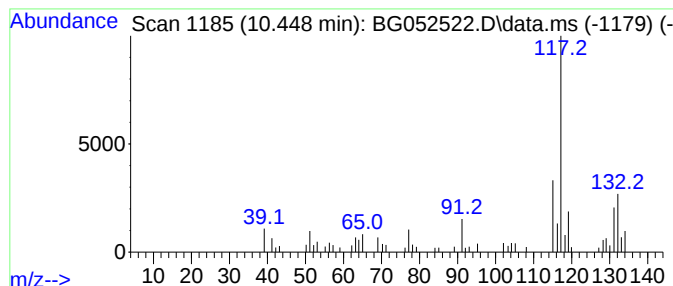
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzene, 1-methyl-2-(2-prop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.448	4.29 ng	57405	Naphthalene-d8	11.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	68
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	68
3			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	64
4			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	64
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052522.D
Acq On : 1 Mar 2022 17:01
Operator : CG/JU
Sample : N1688-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-34

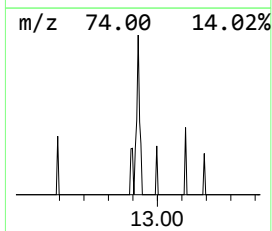
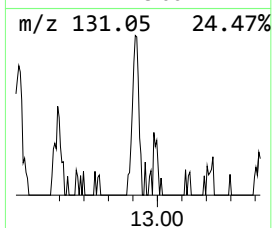
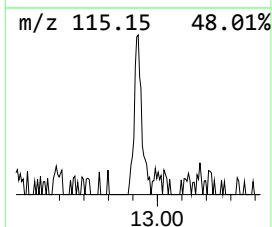
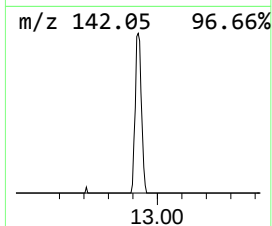
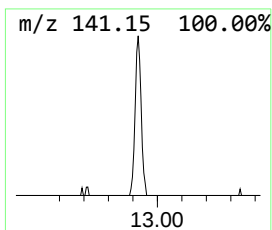
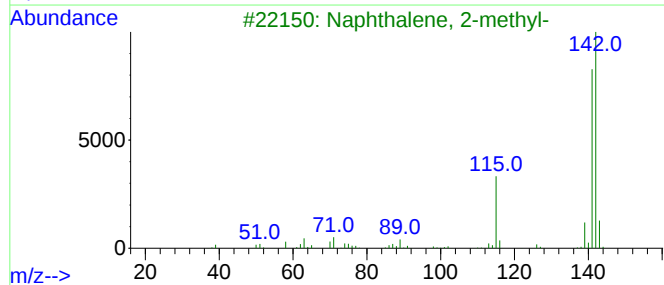
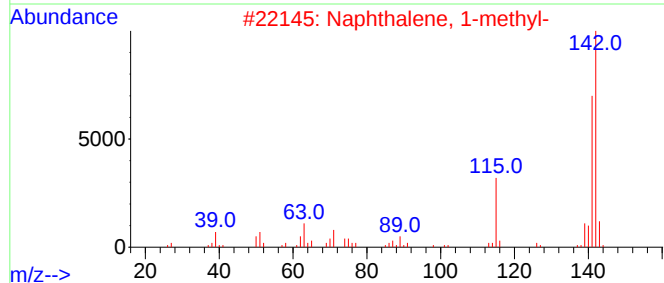
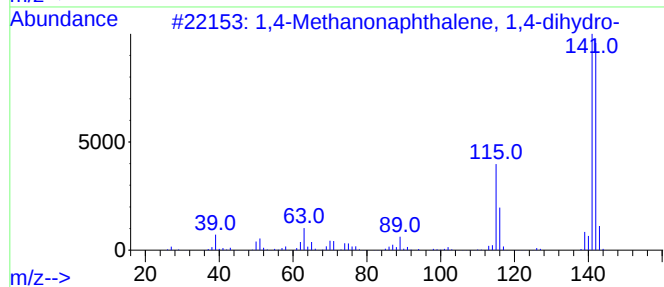
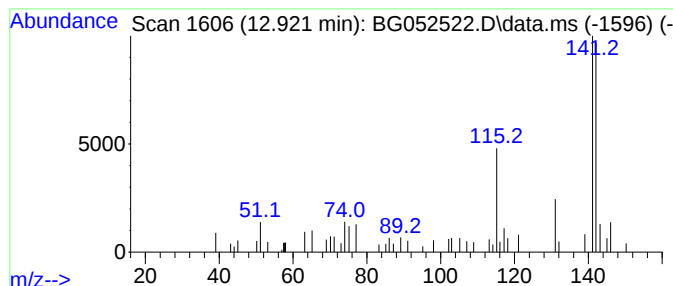
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 1,4-Methanonaphthalene, 1,4... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.921	4.26 ng	57080	Naphthalene-d8	11.059

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	81
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	81
3		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	74
4		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	74
5		Benzocycloheptatriene	142	C11H10	000264-09-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030122\
Data File : BG052522.D
Acq On : 1 Mar 2022 17:01
Operator : CG/JU
Sample : N1688-17
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-34

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanol, 2-m...	3.834	5.2	ng	45466	1	8.222	174728	20.0
unknown4.574	4.574	4.0	ng	34598	1	8.222	174728	20.0
Benzene, 1-ethy...	7.864	3.3	ng	29111	1	8.222	174728	20.0
Hexanoic acid, ...	8.498	10.5	ng	91385	1	8.222	174728	20.0
Indane	8.598	11.7	ng	102531	1	8.222	174728	20.0
unknown9.238	9.238	21.1	ng	184251	1	8.222	174728	20.0
unknown9.314	9.314	33.1	ng	288993	1	8.222	174728	20.0
Benzene, 2-ethy...	9.925	2.1	ng	28093	2	11.059	267782	20.0
unknown10.025	10.025	4.9	ng	65463	2	11.059	267782	20.0
Benzene, 1-meth...	10.448	4.3	ng	57405	2	11.059	267782	20.0
1,4-Methanonaph...	12.921	4.3	ng	57080	2	11.059	267782	20.0