

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
 Data File : BG055197.D
 Acq On : 17 Oct 2022 18:04
 Operator : CG/JU
 Sample : N5145-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-7-101322

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-BG101322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055197.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.325	3	6	21	rVB	587808	889491	38.94%	7.751%
2	5.341	343	349	356	rBV2	40847	63477	2.78%	0.553%
3	5.822	423	431	442	rVB	252160	410957	17.99%	3.581%
4	7.438	699	706	715	rVB	160755	273873	11.99%	2.387%
5	8.302	841	853	860	rBV	100069	173540	7.60%	1.512%
6	8.813	933	940	946	rBV	19018	33778	1.48%	0.294%
7	9.477	1045	1053	1060	rBV	376252	694965	30.43%	6.056%
8	9.553	1060	1066	1074	rVB	44529	81350	3.56%	0.709%
9	9.929	1119	1130	1140	rBV	61858	144714	6.34%	1.261%
10	10.388	1202	1208	1217	rBV7	19878	52395	2.29%	0.457%
11	10.535	1225	1233	1239	rBV	144551	256565	11.23%	2.236%
12	10.670	1248	1256	1261	rBV8	15315	32011	1.40%	0.279%
13	11.128	1327	1334	1341	rBV	143119	260134	11.39%	2.267%
14	11.428	1371	1385	1388	rBV6	25228	60309	2.64%	0.526%
15	11.639	1413	1421	1423	rBV4	12257	23502	1.03%	0.205%
16	12.215	1513	1519	1525	rVB5	20000	36113	1.58%	0.315%
17	13.202	1683	1687	1697	rVB6	17501	36313	1.59%	0.316%
18	13.543	1738	1745	1751	rVB	1030737	1644619	72.00%	14.331%
19	13.784	1783	1786	1791	rVB2	21771	30929	1.35%	0.270%
20	13.919	1803	1809	1812	rBV7	14934	30593	1.34%	0.267%
21	14.430	1892	1896	1902	rBV5	20199	32935	1.44%	0.287%
22	14.706	1936	1943	1945	rBV6	16791	38158	1.67%	0.333%
23	14.747	1945	1950	1958	rVB	91362	143473	6.28%	1.250%
24	14.912	1968	1978	1983	rBV	233064	399954	17.51%	3.485%
25	15.170	2019	2022	2029	rVB6	19986	35794	1.57%	0.312%
26	15.306	2040	2045	2049	rVB	28401	41935	1.84%	0.365%
27	15.922	2147	2150	2156	rVB9	16740	29084	1.27%	0.253%
28	16.081	2175	2177	2181	rVB	21619	24802	1.09%	0.216%
29	16.387	2223	2229	2236	rBV	851980	1303487	57.07%	11.359%
30	16.569	2256	2260	2264	rBV2	28343	42755	1.87%	0.373%
31	17.644	2438	2443	2448	rVB	283126	407802	17.85%	3.554%
32	18.290	2550	2553	2557	rVB5	35983	47294	2.07%	0.412%
33	18.502	2586	2589	2597	rVB4	38926	58347	2.55%	0.508%
34	19.765	2800	2804	2816	rVB2	55315	123302	5.40%	1.074%
35	20.035	2846	2850	2856	rVB	97363	140508	6.15%	1.224%
36	20.217	2876	2881	2887	rBV	1699711	2284047	100.00%	19.903%

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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-BG101322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.746	2968	2971	2975	rVB	62074	75125	3.29%	0.655%
38	21.927	3167	3172	3181	rVB2	277763	500956	21.93%	4.365%
39	25.358	3747	3756	3770	rVB2	166218	516448	22.61%	4.500%

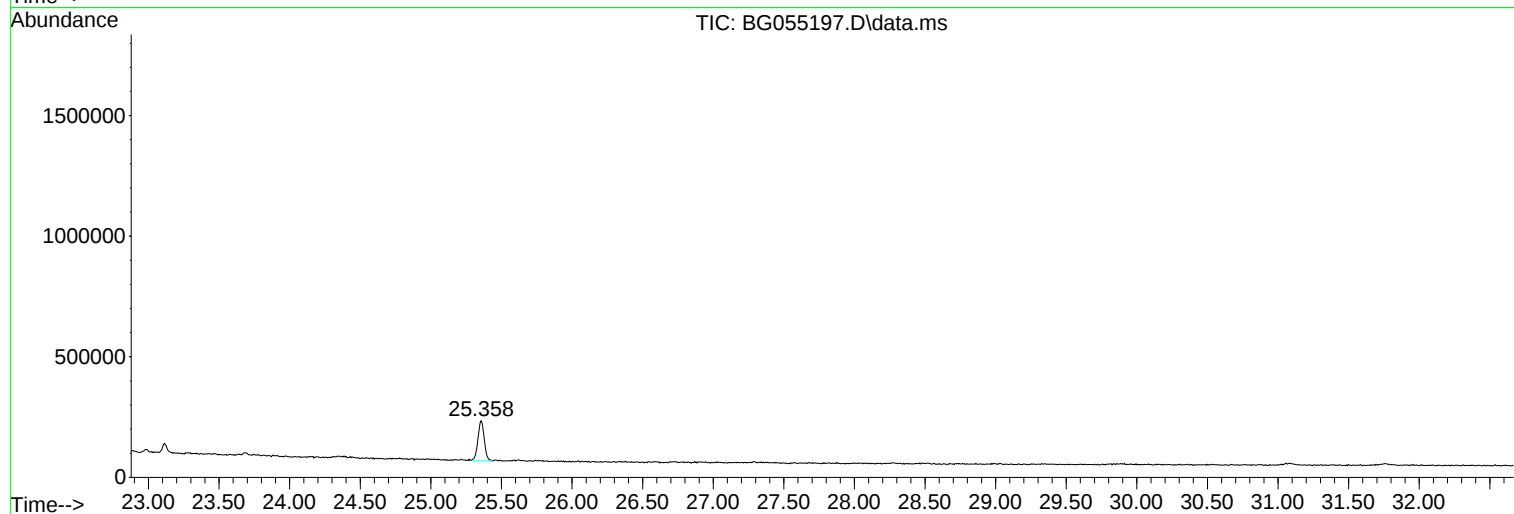
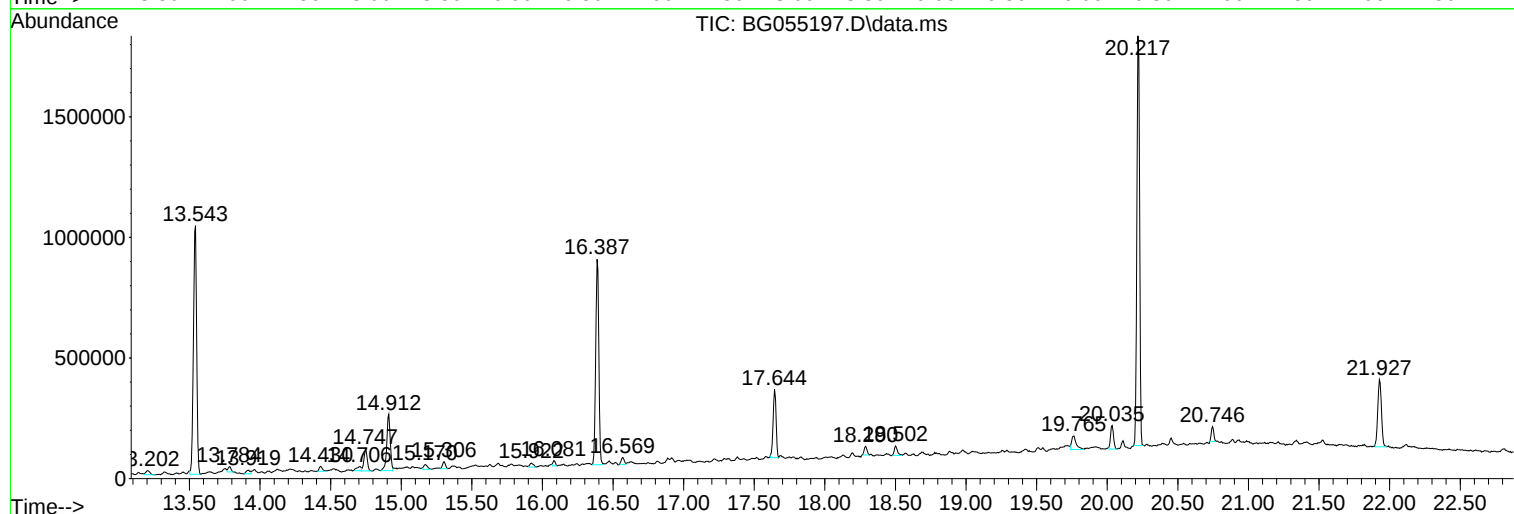
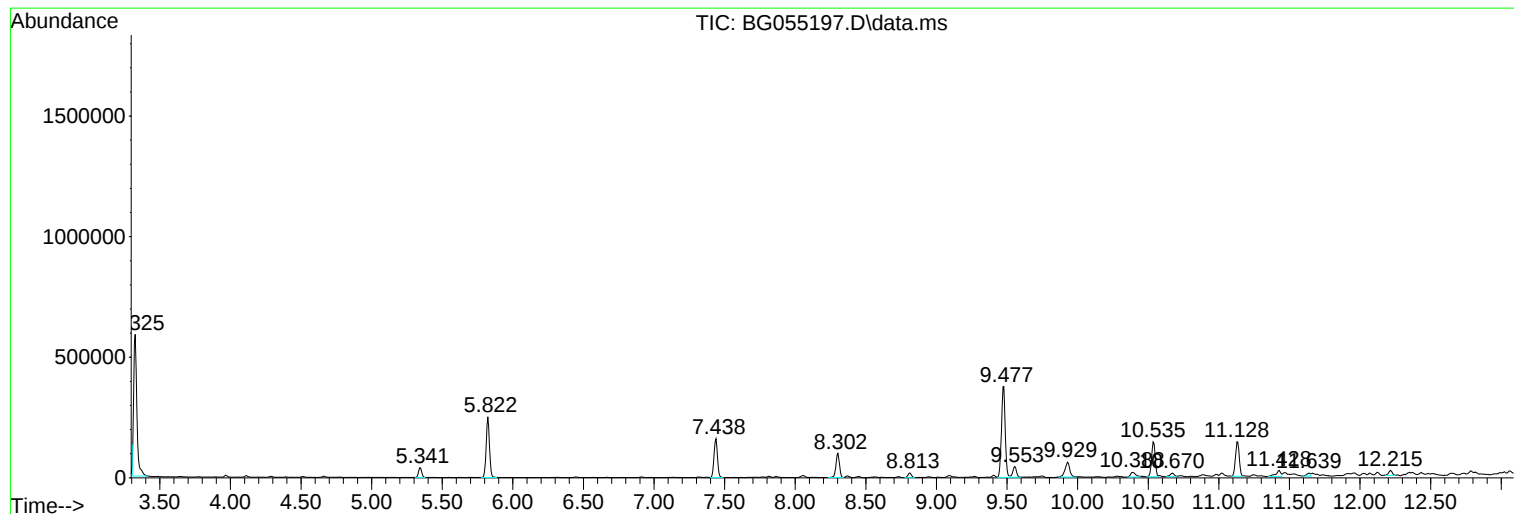
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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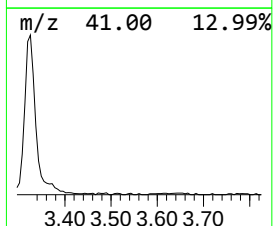
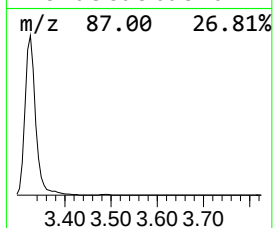
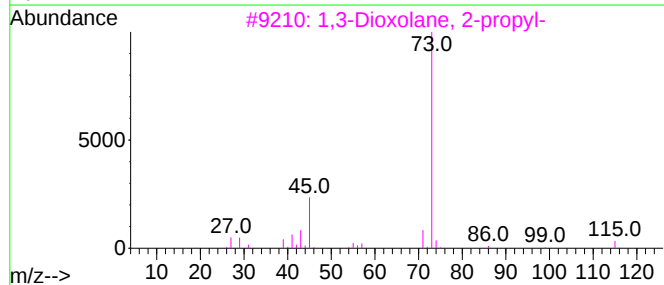
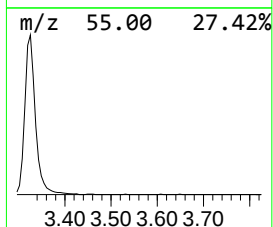
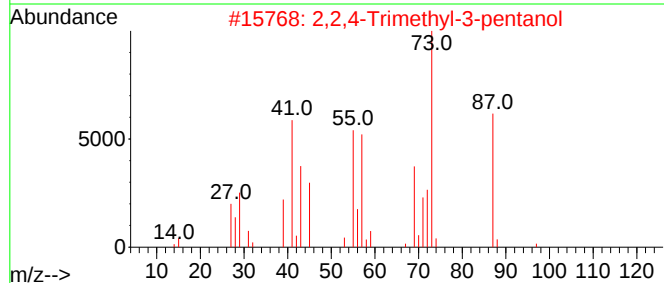
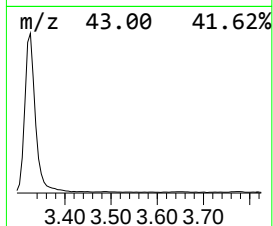
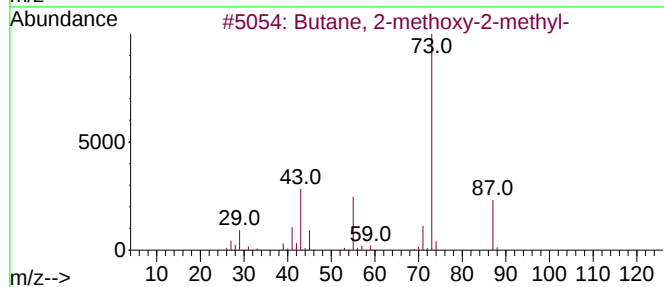
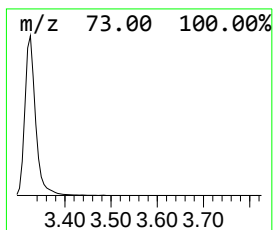
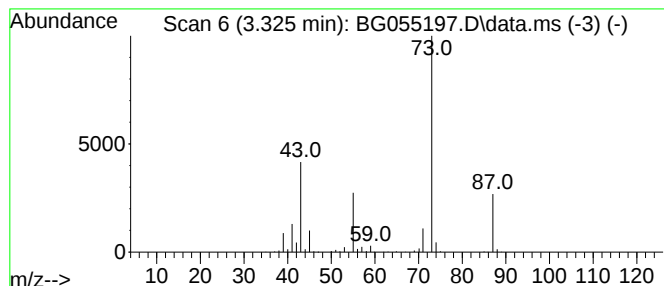
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.325	102.51 ng	889491	1,4-Dichlorobenzene-d4	8.302

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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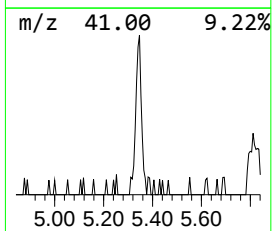
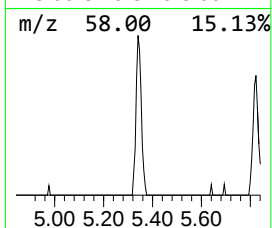
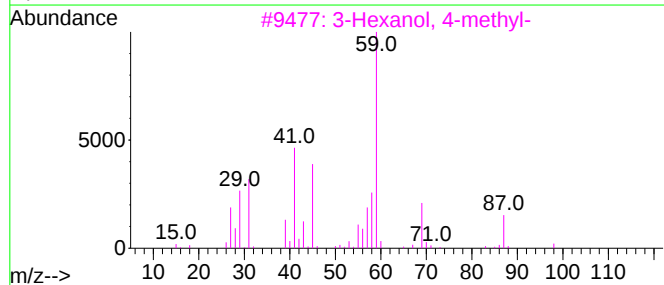
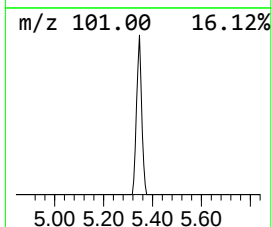
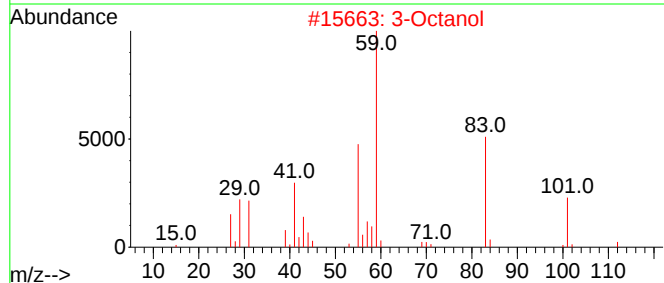
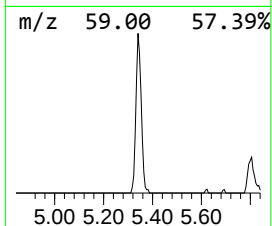
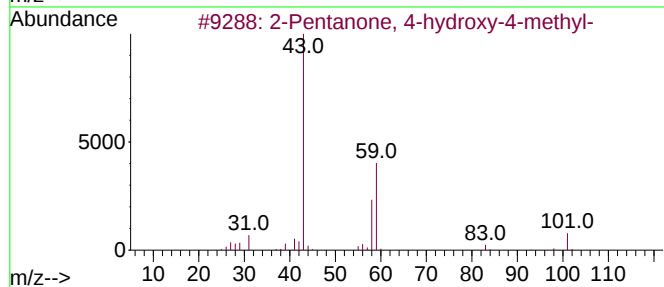
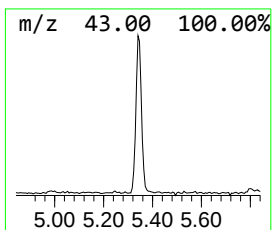
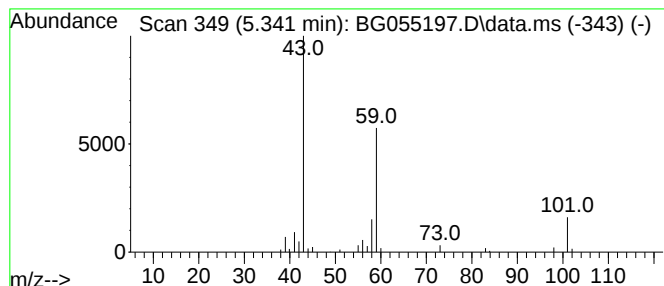
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.341	7.32 ng	63477	1,4-Dichlorobenzene-d4	8.302

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		3-Octanol	130	C8H18O	000589-98-0	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Propenoic acid, 3-methoxybutyl...	158	C8H14O3	002768-07-2	25
5		1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	23



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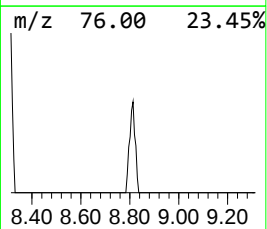
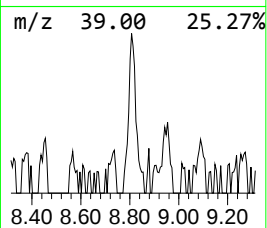
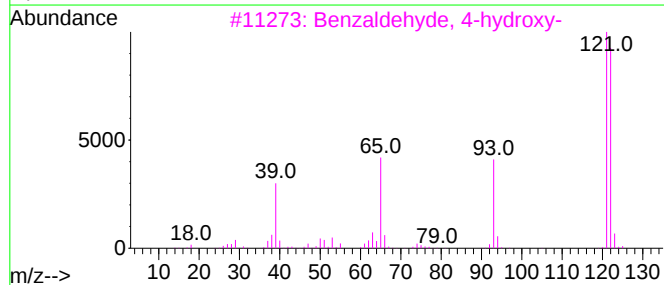
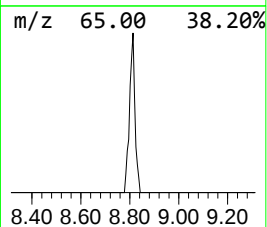
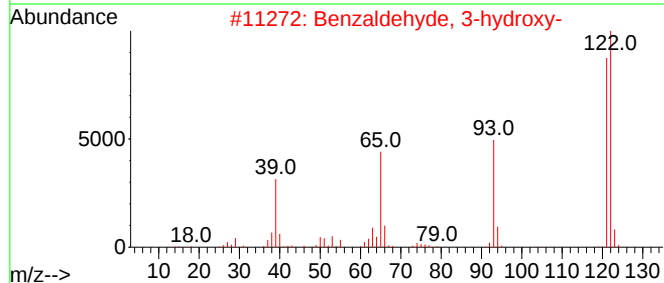
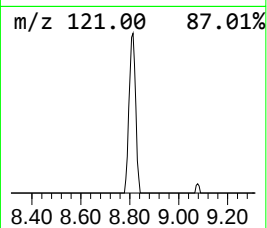
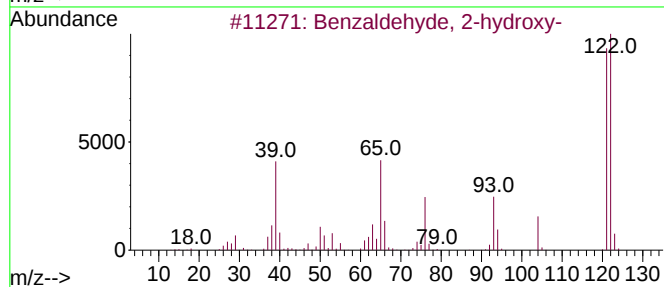
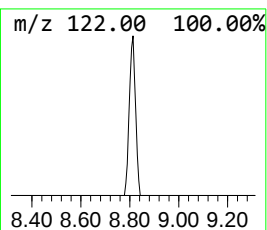
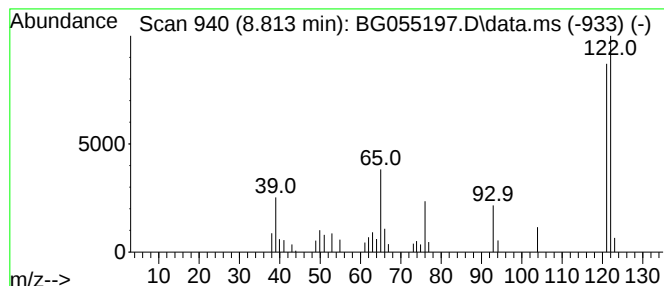
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzaldehyde, 2-hydroxy- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.813	3.89 ng	33778	1,4-Dichlorobenzene-d4	8.302

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 2-hydroxy-	122	C7H6O2	000090-02-8	94
2			Benzaldehyde, 3-hydroxy-	122	C7H6O2	000100-83-4	90
3			Benzaldehyde, 4-hydroxy-	122	C7H6O2	000123-08-0	90
4			Propanoic acid, 3-chloro-, 4-for...	212	C10H9ClO3	1010142-41-5	56
5			1,3-Benzodioxole	122	C7H6O2	000274-09-9	35



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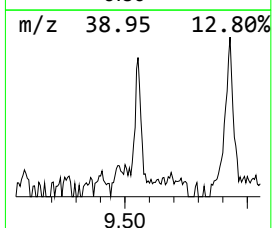
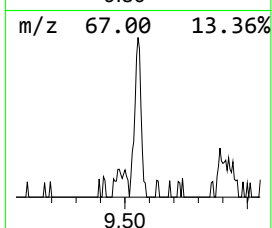
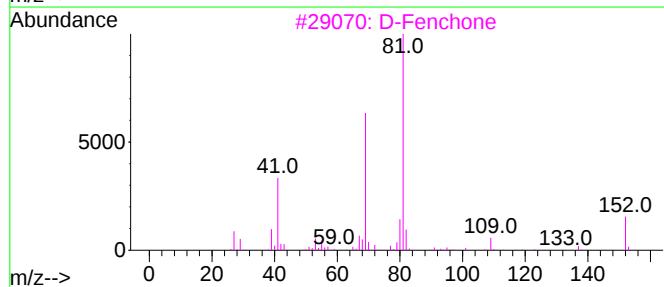
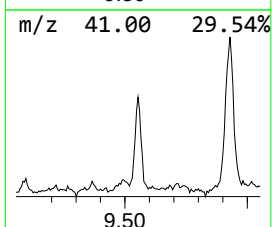
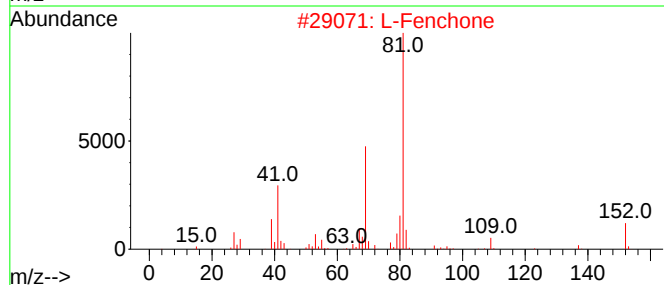
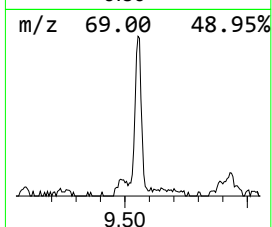
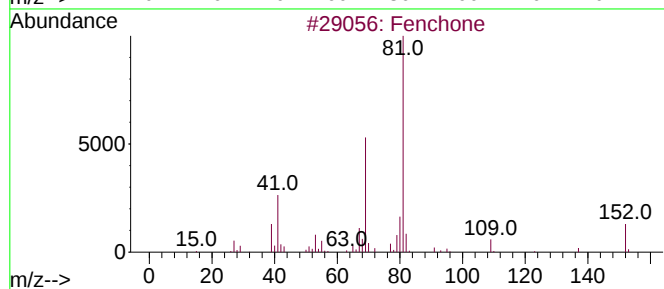
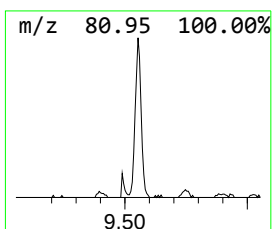
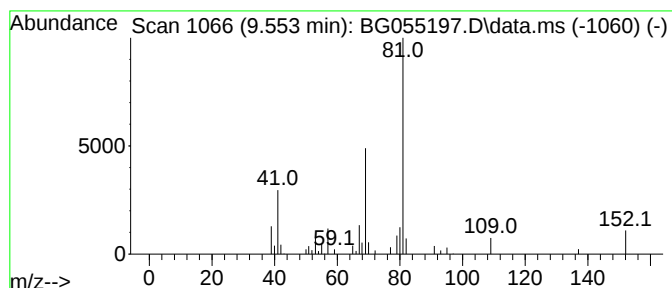
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Fenchone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.553	9.38 ng	81350	1,4-Dichlorobenzene-d4	8.302

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchone	152	C10H16O	001195-79-5	90
2			L-Fenchone	152	C10H16O	007787-20-4	90
3			D-Fenchone	152	C10H16O	004695-62-9	83
4			Cyclohexane, 1,3-dichloro-, cis-	152	C6H10Cl2	024955-63-3	50
5			1-[4-(4-tert-Butyl-spirocyclohex...	371	C20H28F3NO2	1000301-43-3	42



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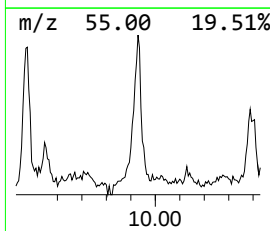
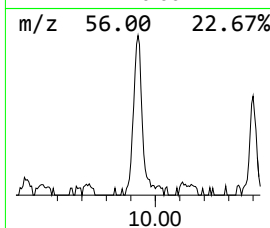
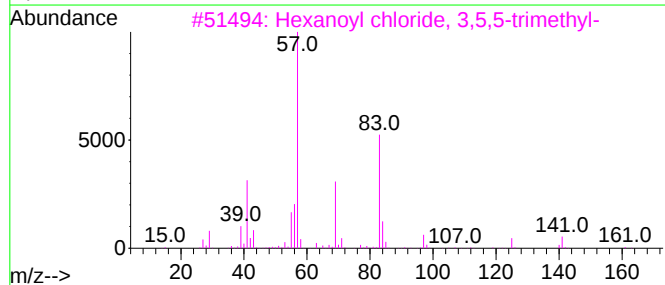
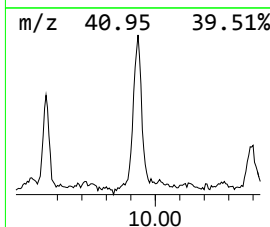
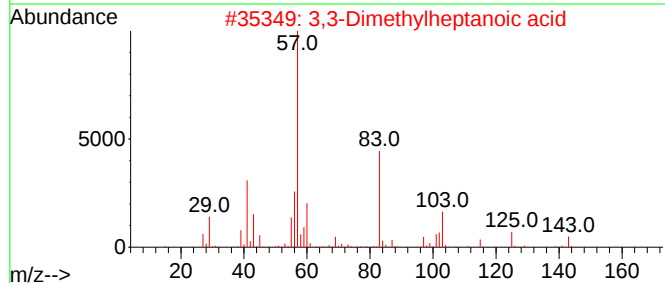
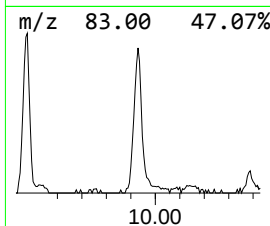
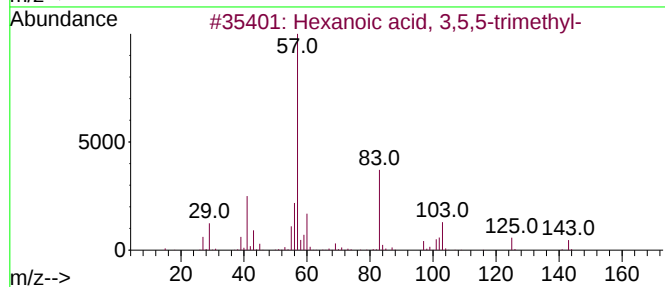
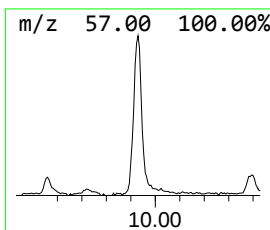
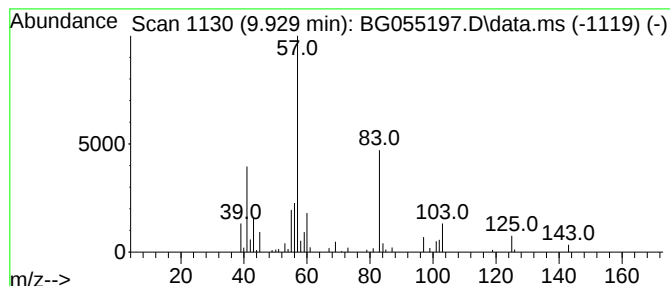
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexanoic acid, 3,5,5-trimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.929	11.13 ng	144714	Naphthalene-d8	11.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	90
2			3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	59
3			Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	42
4			4,4-Dimethyl-2-pentanol, chlorod...	228	C9H15ClF2O2	1000376-27-0	38
5			Propanoic acid, 2,2-dimethyl-, c...	184	C11H20O2	029878-49-7	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055197.D
Acq On : 17 Oct 2022 18:04
Operator : CG/JU
Sample : N5145-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-7-101322

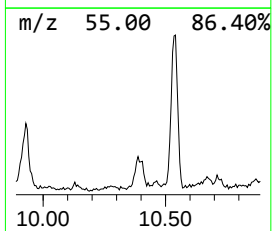
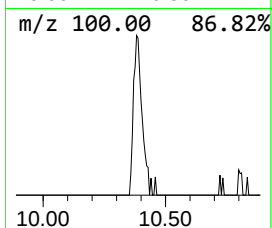
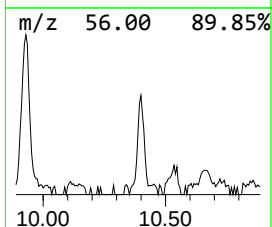
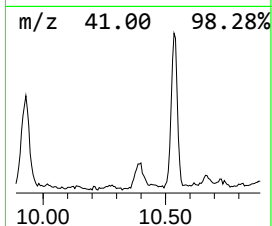
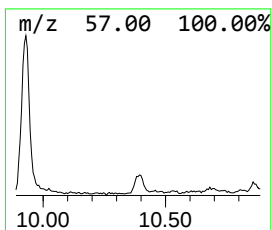
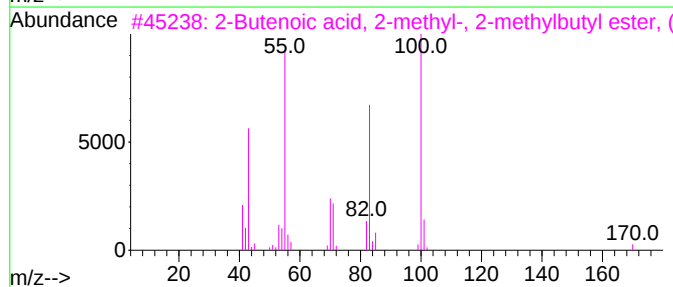
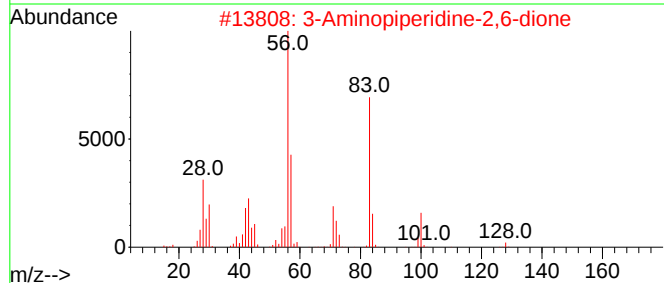
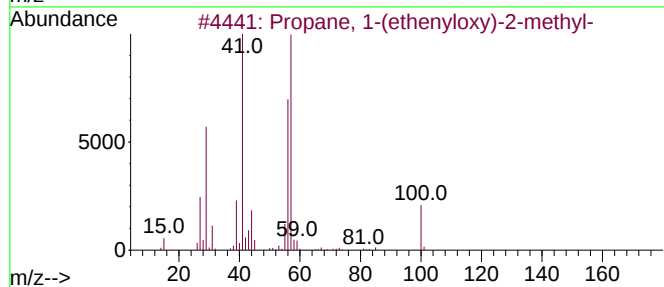
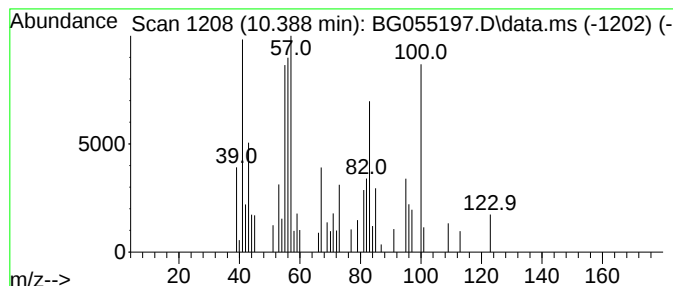
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown10.388 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.388	4.03 ng	52395	Naphthalene-d8	11.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1-(ethenyloxy)-2-methyl-	100	C6H12O	000109-53-5	35
2			3-Aminopiperidine-2,6-dione	128	C5H8N2O2	002353-44-8	22
3			2-Butenoic acid, 2-methyl-, 2-me...	170	C10H18O2	061692-77-1	22
4			1-Propoxypropan-2-yl 2-methylbut...	200	C11H20O3	1000367-10-6	22
5			Oxirane, decyl-	184	C12H24O	002855-19-8	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055197.D
Acq On : 17 Oct 2022 18:04
Operator : CG/JU
Sample : N5145-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

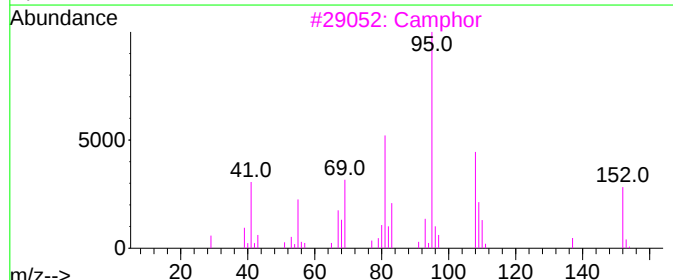
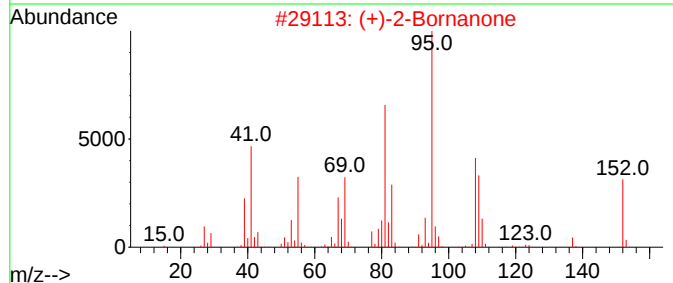
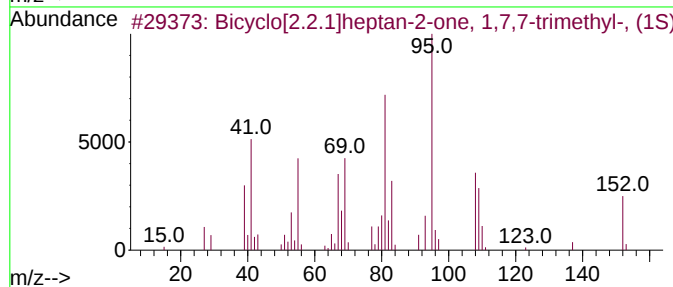
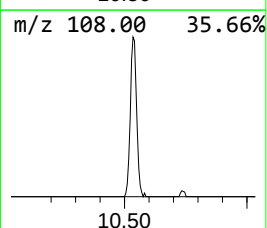
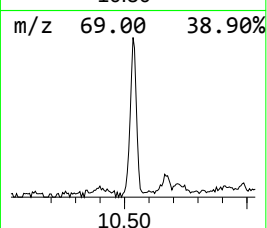
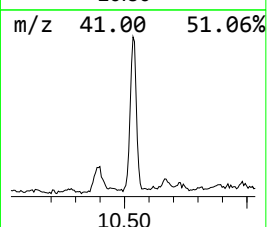
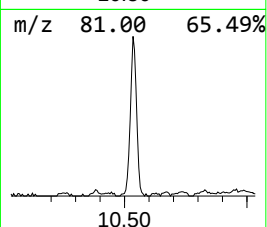
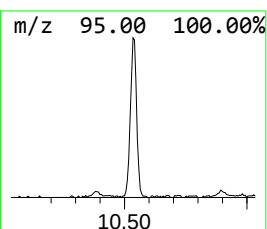
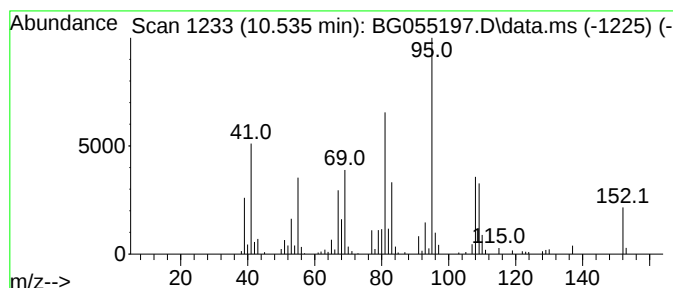
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.535	19.73 ng	256565	Naphthalene-d8	11.128	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
2	(+)-2-Bornanone	152	C10H16O	000464-49-3	97
3	Camphor	152	C10H16O	000076-22-2	93
4	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	52
5	Cycloheptane, 1-chloro-3-iodo-	258	C7H12ClI	1000337-09-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055197.D
Acq On : 17 Oct 2022 18:04
Operator : CG/JU
Sample : N5145-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

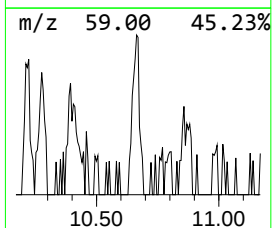
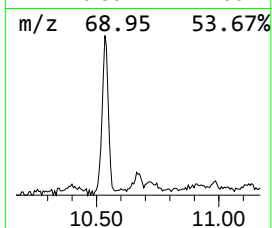
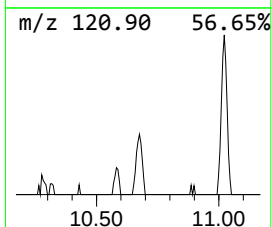
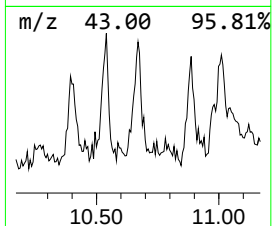
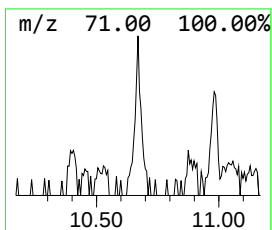
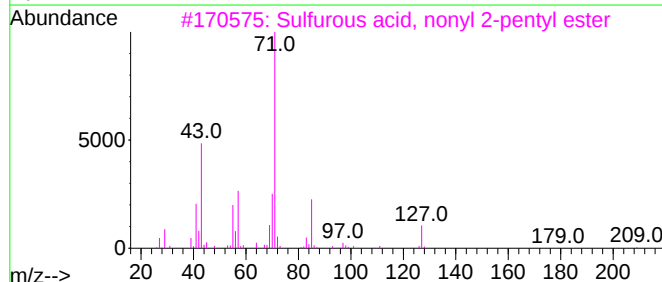
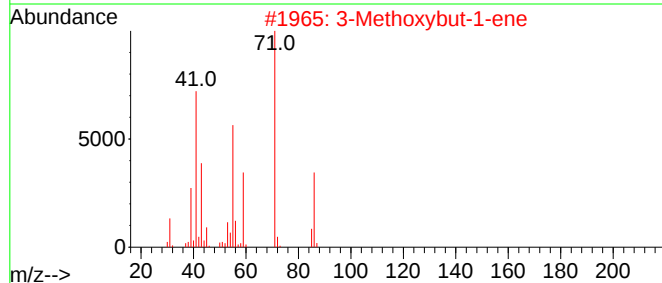
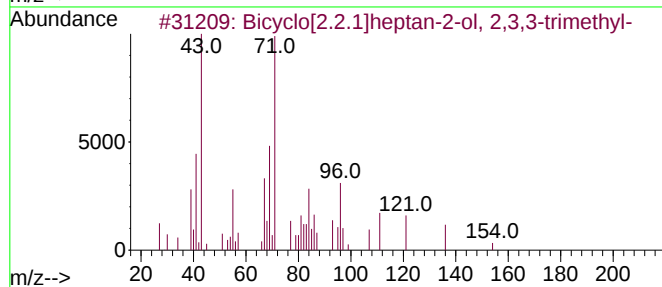
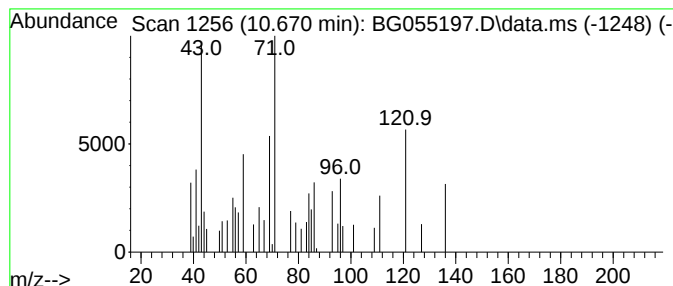
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Bicyclo[2.2.1]heptan-2-ol, ... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.670	2.46 ng	32011	Naphthalene-d8	11.128	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-ol, 2,3,3...	154	C10H18O	000465-31-6	53
2	3-Methoxybut-1-ene	86	C5H10O	017351-24-5	43
3	Sulfurous acid, nonyl 2-pentyl e...	278	C14H30O3S	1010309-15-8	35
4	trans-1-Methoxy-1-butene	86	C5H10O	010034-13-6	30
5	2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055197.D
Acq On : 17 Oct 2022 18:04
Operator : CG/JU
Sample : N5145-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

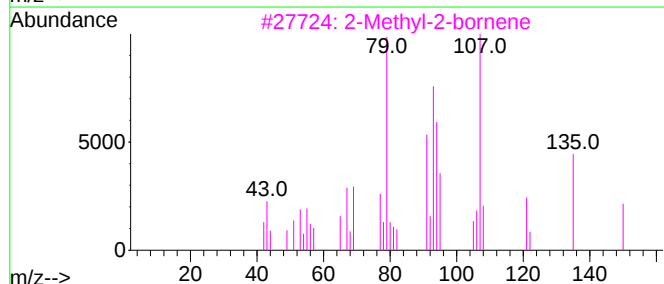
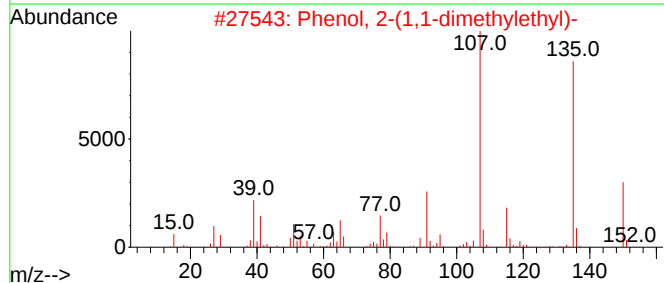
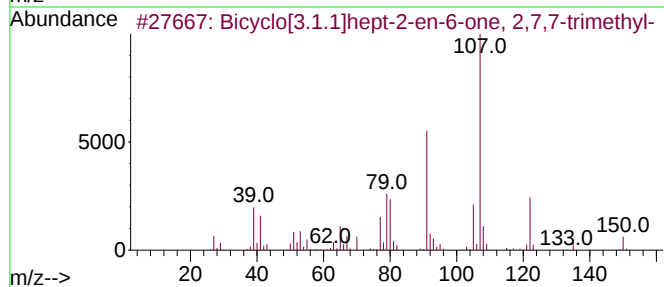
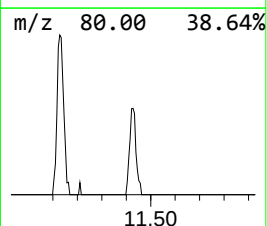
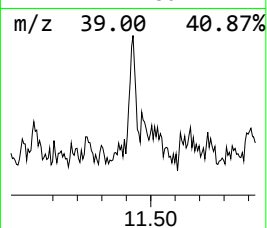
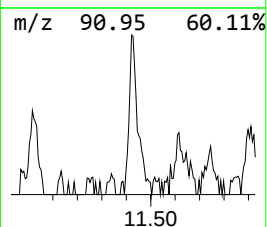
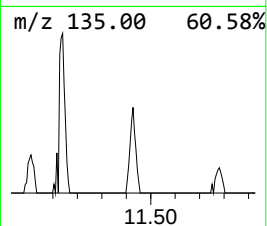
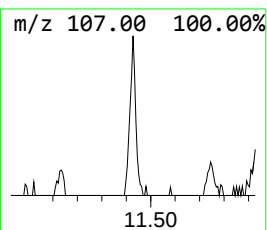
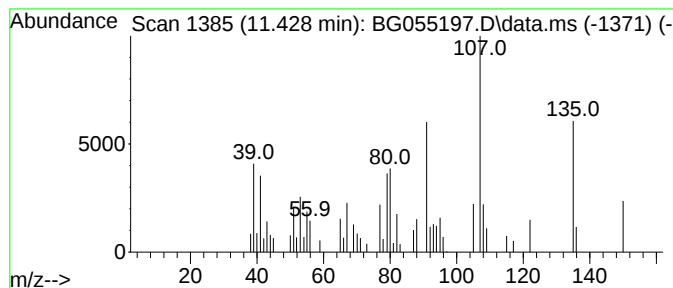
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ClientSampleId :
MW-7-101322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Bicyclo[3.1.1]hept-2-en-6-o... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.428	4.64 ng	60309	Naphthalene-d8	11.128	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]hept-2-en-6-one, 2...	150	C10H14O	000473-06-3	52
2	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	49
3	2-Methyl-2-bornene	150	C11H18	072540-93-3	47
4	1,3-Cyclopentadiene, 1,3-bis(1-m...	150	C11H18	123278-27-3	47
5	2-Methylenebornane	150	C11H18	027538-47-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055197.D
Acq On : 17 Oct 2022 18:04
Operator : CG/JU
Sample : N5145-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-7-101322

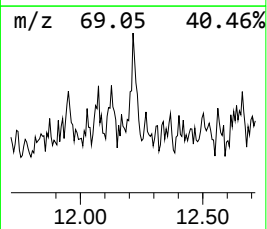
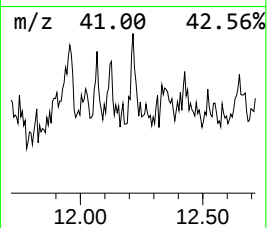
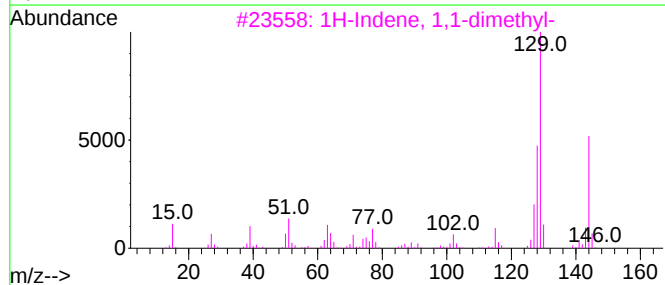
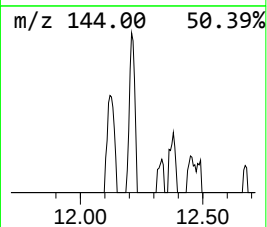
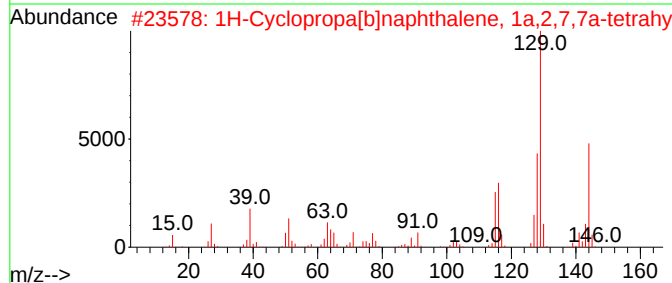
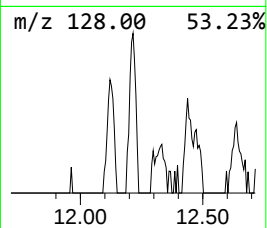
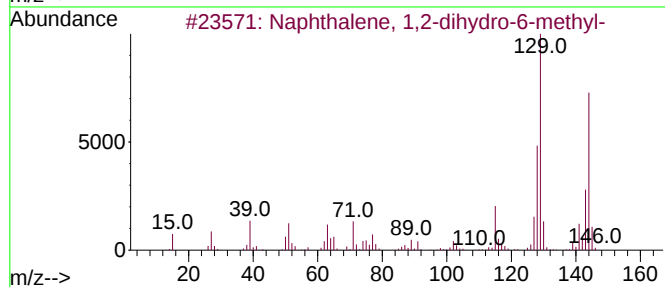
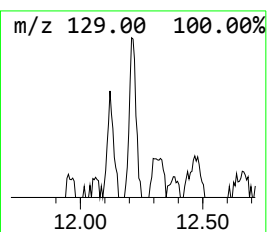
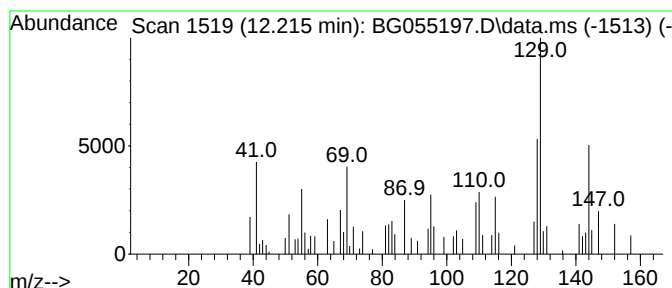
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Naphthalene, 1,2-dihydro-6-... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.215	2.78 ng	36113	Naphthalene-d8	11.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2-dihydro-6-methyl-	144	C11H12	002717-47-7	60
2			1H-Cyclopropa[b]naphthalene, 1a,...	144	C11H12	006571-72-8	60
3			1H-Indene, 1,1-dimethyl-	144	C11H12	018636-55-0	60
4			1H-Indene, 1,3-dimethyl-	144	C11H12	002177-48-2	53
5			Naphthalene, 1,2-dihydro-3-methyl-	144	C11H12	002717-44-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055197.D
Acq On : 17 Oct 2022 18:04
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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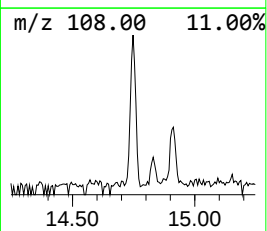
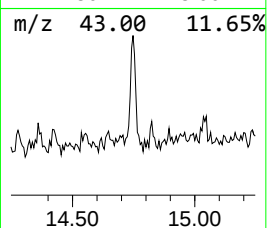
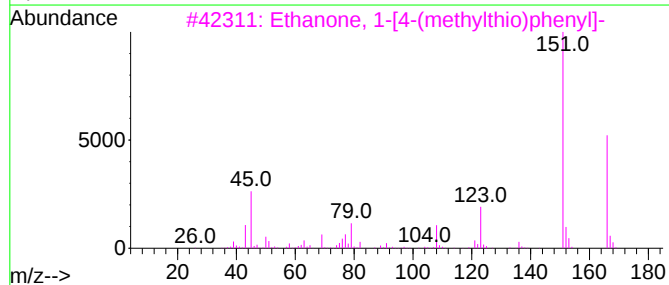
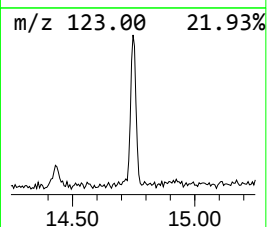
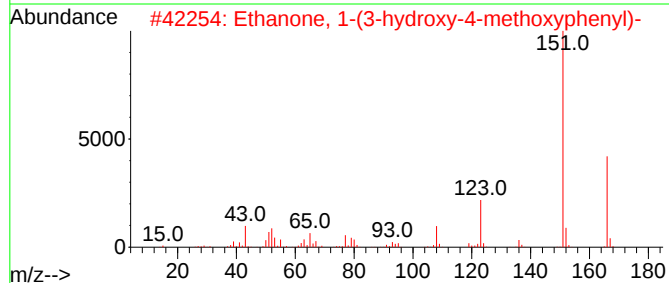
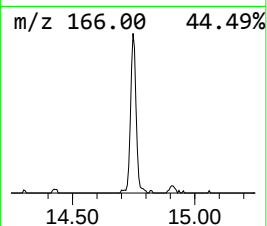
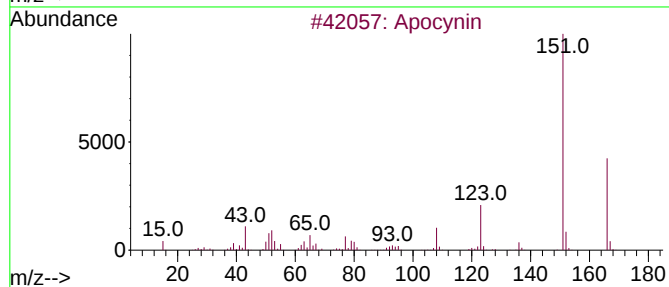
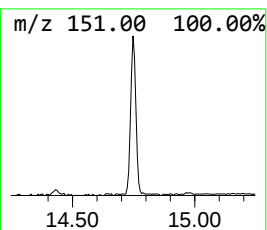
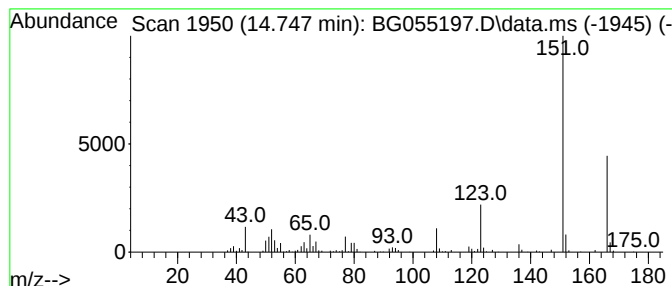
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Apocynin Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.747	7.17 ng	143473	Acenaphthene-d10	14.912

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Apocynin			166	C9H10O3	000498-02-2	97
2	Ethanone, 1-(3-hydroxy-4-methoxy...			166	C9H10O3	006100-74-9	94
3	Ethanone, 1-[4-(methylthio)phenyl]-			166	C9H10OS	001778-09-2	80
4	Stibine, trimethyl-			166	C3H9Sb	000594-10-5	78
5	Ethanone, 1-(2-hydroxy-4-methoxy...			166	C9H10O3	000552-41-0	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055197.D
Acq On : 17 Oct 2022 18:04
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Sample : N5145-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

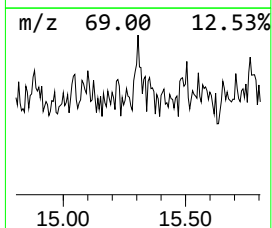
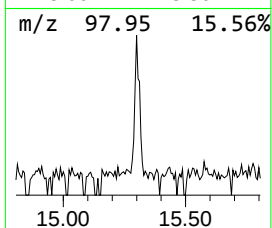
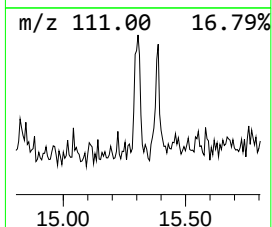
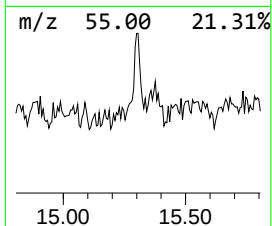
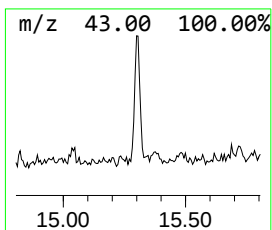
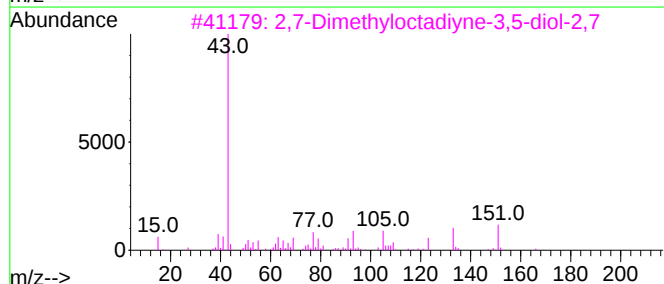
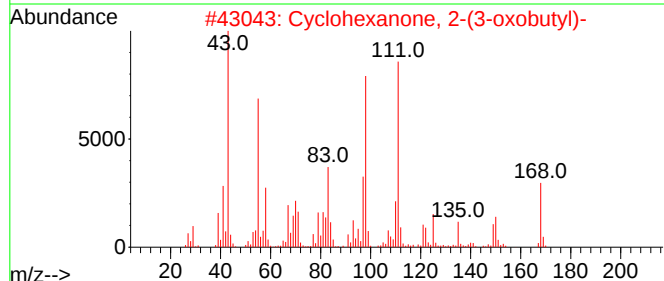
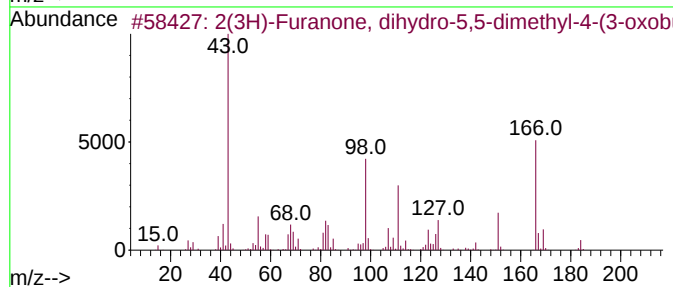
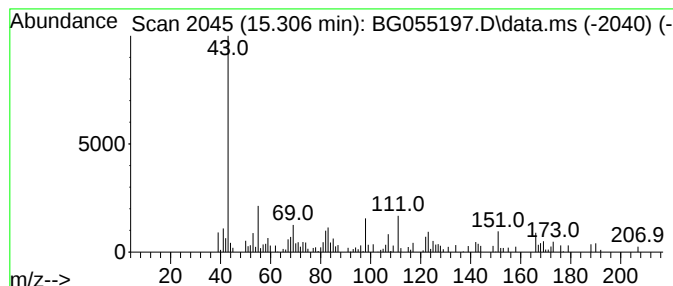
Instrument :
BNA_G
ClientSampleId :
MW-7-101322

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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 12 unknown15.306 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.306	2.10 ng	41935	Acenaphthene-d10	14.912	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, dihydro-5,5-dime...	184	C10H16O3	004436-81-1	32
2	Cyclohexanone, 2-(3-oxobutyl)-	168	C10H16O2	026942-62-1	14
3	2,7-Dimethyloctadiyne-3,5-diol-2,7	166	C10H14O2	005929-72-6	10
4	Ethanone, 1-(2,6,6-trimethyl-1-c...	166	C11H18O	001197-92-8	10
5	3-Acetyl-2,6-dimethyl-2,5-heptad...	166	C11H18O	1000432-11-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055197.D
Acq On : 17 Oct 2022 18:04
Operator : CG/JU
Sample : N5145-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

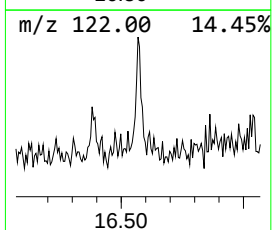
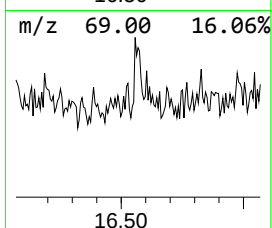
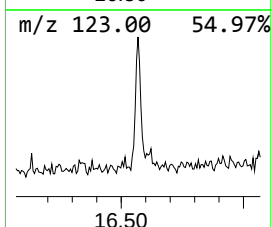
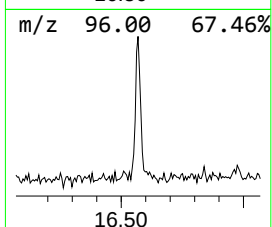
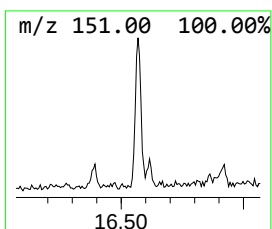
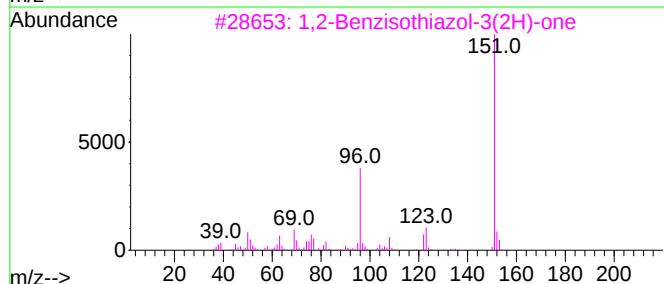
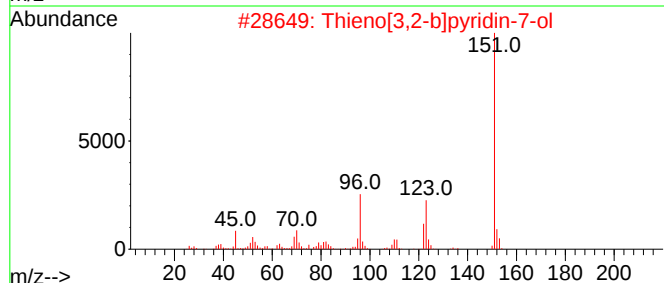
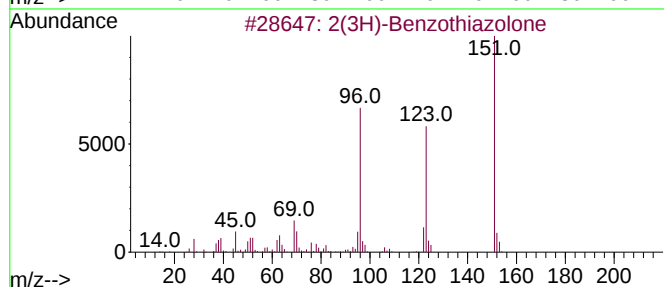
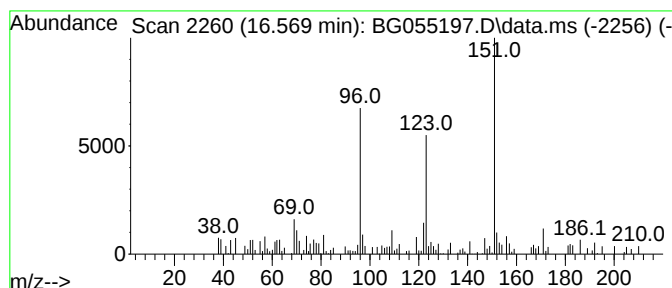
Instrument :
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ClientSampleId :
MW-7-101322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2(3H)-Benzothiazolone Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.569	2.10 ng	42755	Phenanthrene-d10	17.644
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		2(3H)-Benzothiazolone	151 C7H5NOS	000934-34-9 87
2		Thieno[3,2-b]pyridin-7-ol	151 C7H5NOS	107818-20-2 64
3		1,2-Benzisothiazol-3(2H)-one	151 C7H5NOS	002634-33-5 59
4		3-Isopropoxy-4-methoxybenzamide	209 C11H15NO3	1000267-17-1 38
5		4-Mercaptobenzoic acid, S-methyl...	182 C9H10O2S	003795-79-7 38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055197.D
Acq On : 17 Oct 2022 18:04
Operator : CG/JU
Sample : N5145-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-7-101322

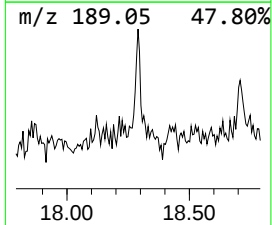
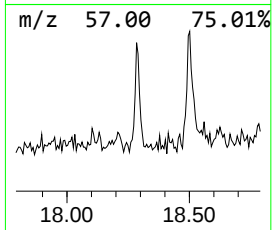
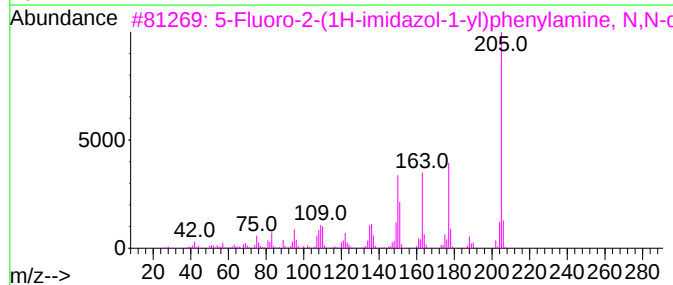
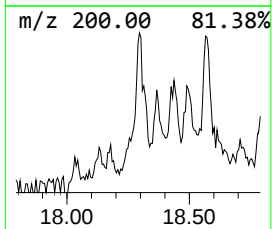
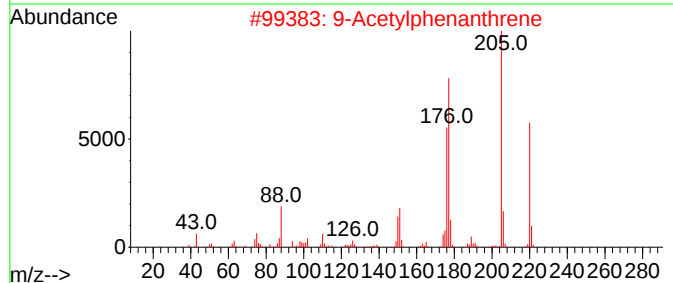
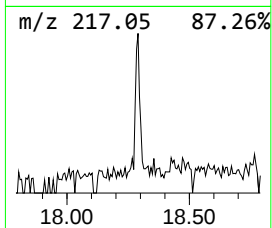
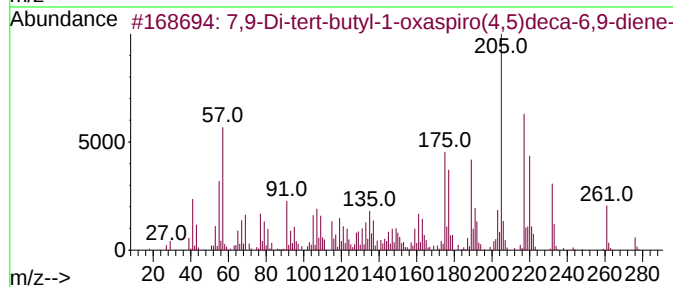
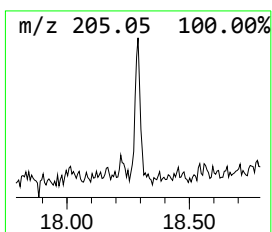
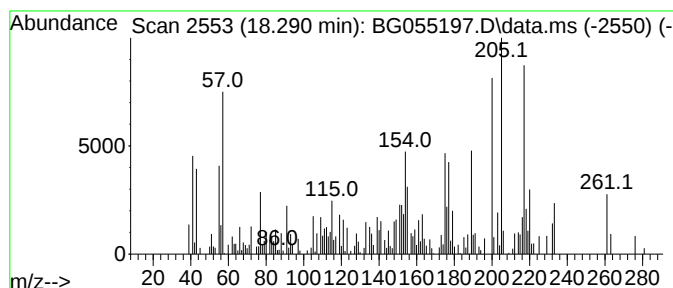
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown18.290 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.290	2.32 ng	47294	Phenanthrene-d10	17.644

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	46		
2	9-Acetylphenanthrene	220	C16H12O	002039-77-2	25		
3	5-Fluoro-2-(1H-imidazol-1-yl)phe...	205	C11H12FN3	1000512-19-0	25		
4	4,6-di-tert-Butyl-m-cresol	220	C15H24O	000497-39-2	25		
5	3,4,7,8,9,10-Hexahydrobenzo[c]ci...	217	C12H15N3O	184021-60-1	22		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055197.D
Acq On : 17 Oct 2022 18:04
Operator : CG/JU
Sample : N5145-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

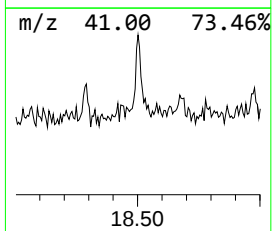
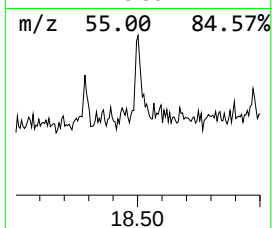
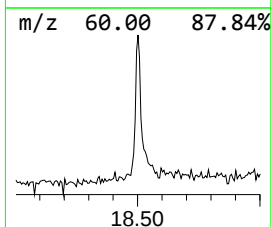
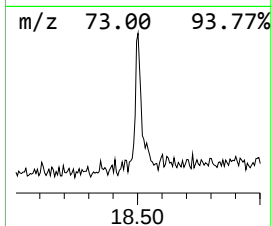
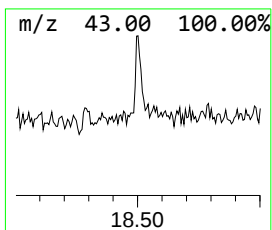
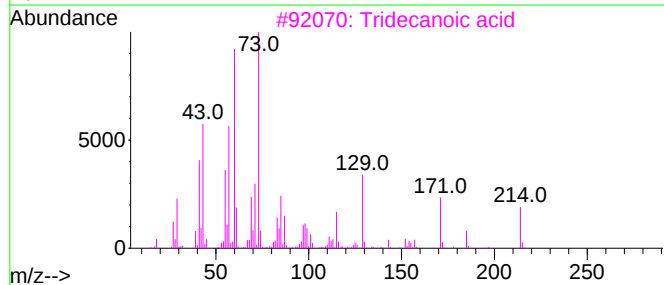
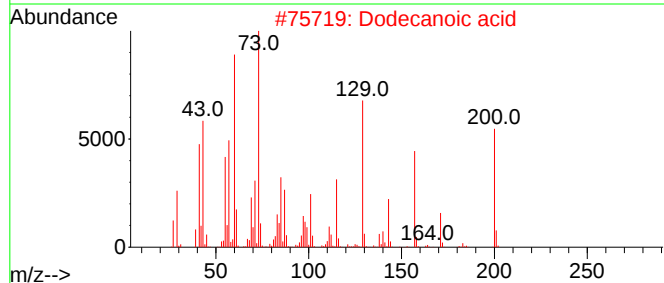
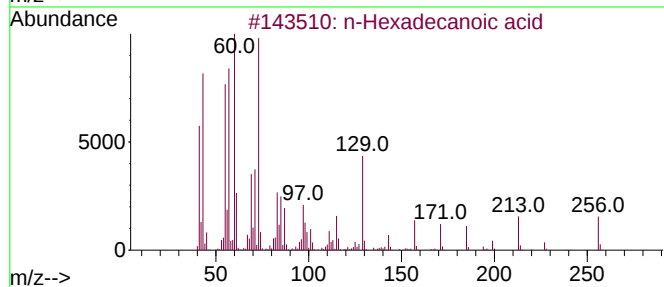
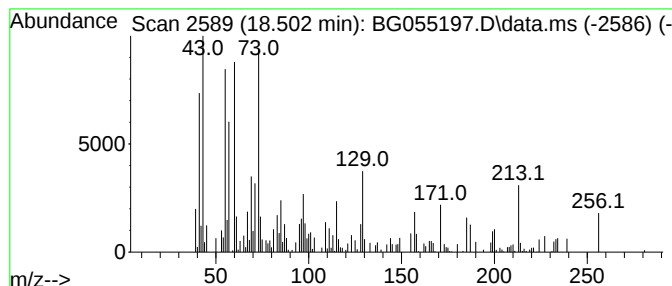
Instrument :
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ClientSampleId :
MW-7-101322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.502	2.86 ng	58347	Phenanthrene-d10		17.644	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	94
2	Dodecanoic acid		200	C12H24O2	000143-07-7	83
3	Tridecanoic acid		214	C13H26O2	000638-53-9	64
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	58
5	Nonanoic acid		158	C9H18O2	000112-05-0	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055197.D
Acq On : 17 Oct 2022 18:04
Operator : CG/JU
Sample : N5145-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

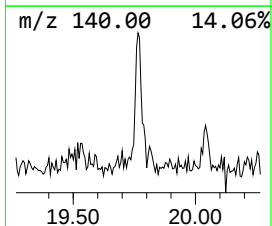
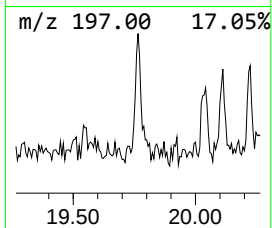
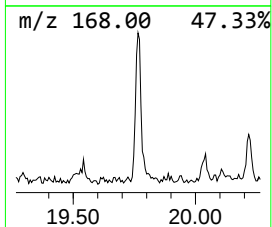
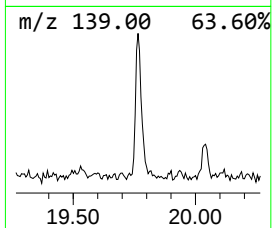
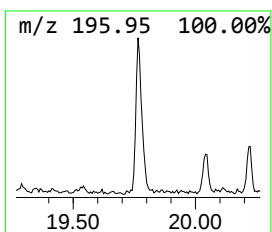
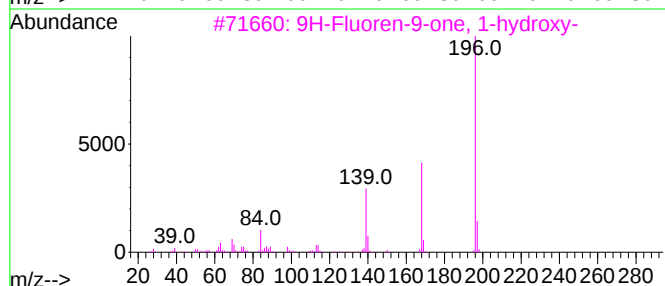
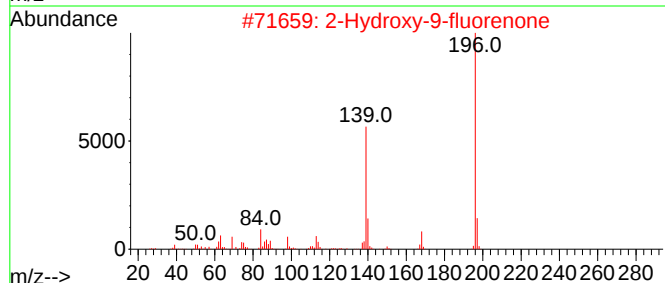
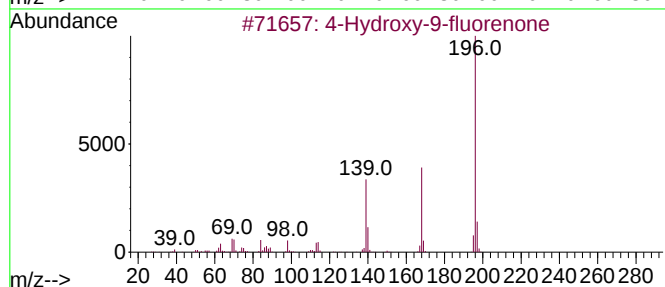
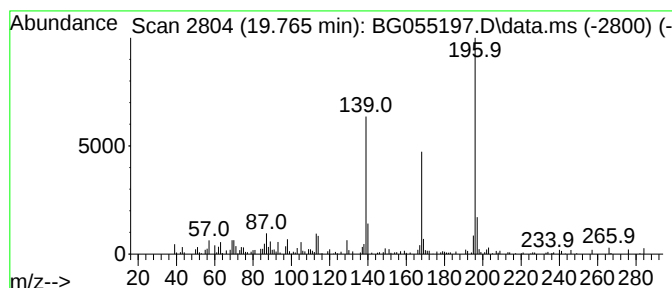
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ClientSampleId :
MW-7-101322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 4-Hydroxy-9-fluorenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.765	6.05 ng	123302	Phenanthrene-d10	17.644	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Hydroxy-9-fluorenone	196	C13H8O2	001986-00-1	93
2	2-Hydroxy-9-fluorenone	196	C13H8O2	006949-73-1	89
3	9H-Fluoren-9-one, 1-hydroxy-	196	C13H8O2	006344-60-1	87
4	Xanthone	196	C13H8O2	000090-47-1	78
5	2-Hydroxyfluorenone, trimethylac...	280	C18H16O3	1621187-12-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055197.D
Acq On : 17 Oct 2022 18:04
Operator : CG/JU
Sample : N5145-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-7-101322

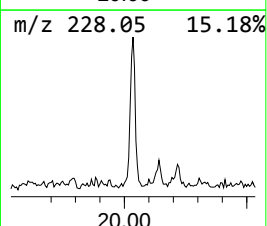
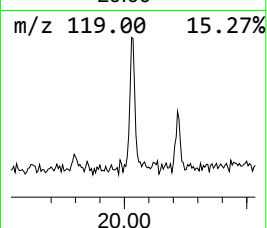
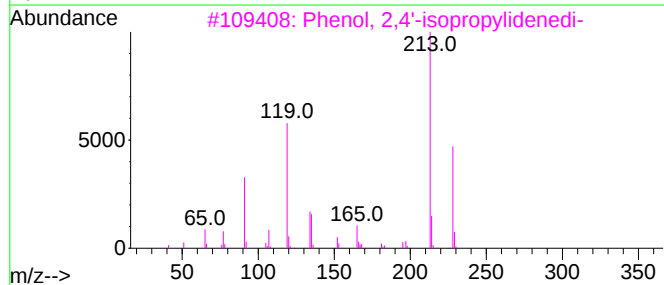
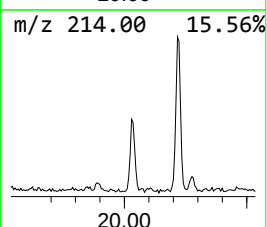
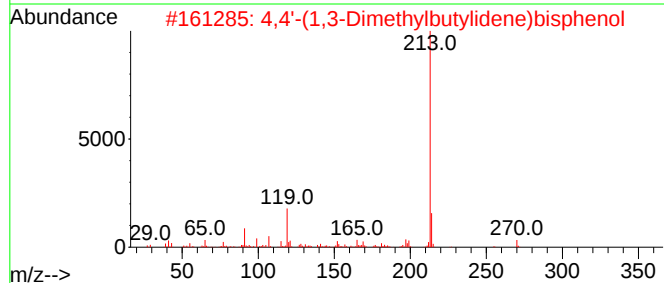
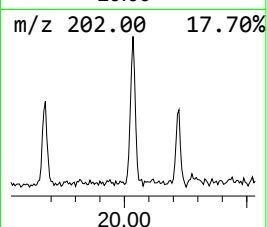
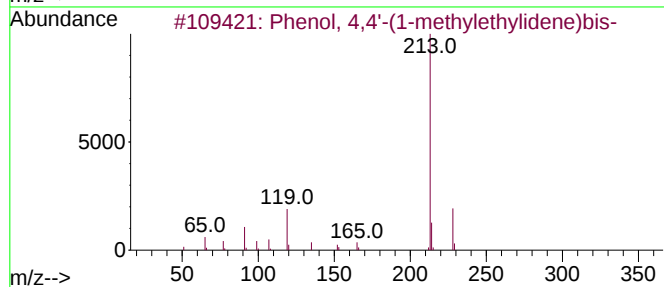
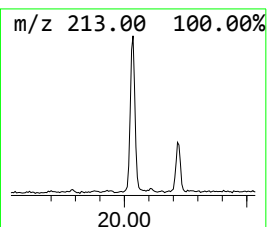
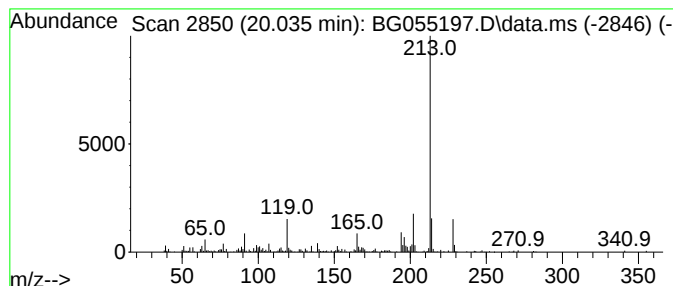
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Phenol, 4,4'-(1-methylethyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.035	5.61 ng	140508	Chrysene-d12	21.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	86
2			4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	58
3			Phenol, 2,4'-isopropylidenedi-	228	C15H16O2	000837-08-1	53
4			2,2-Bis-(4-hydroxyphenyl)-butane	242	C16H18O2	000077-40-7	53
5			Pyridine, 2-(5-trifluoromethyl-3...	213	C9H6F3N3	003974-71-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055197.D
Acq On : 17 Oct 2022 18:04
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-7-101322

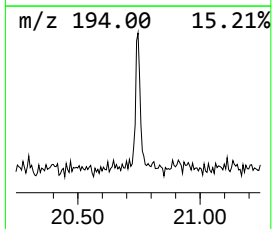
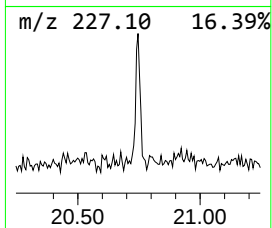
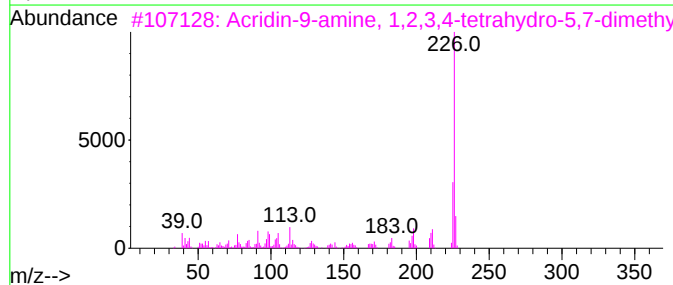
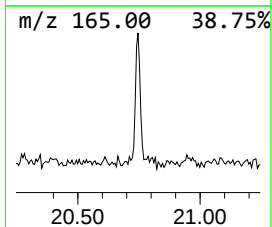
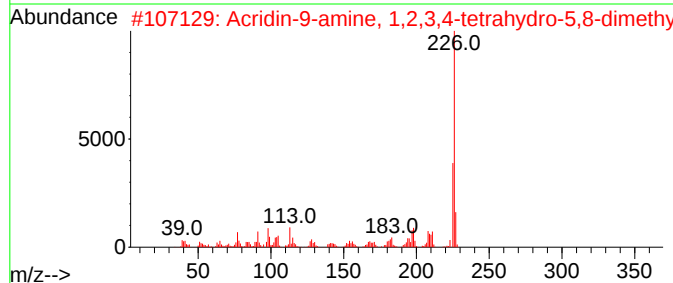
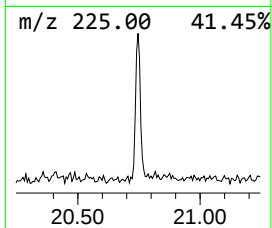
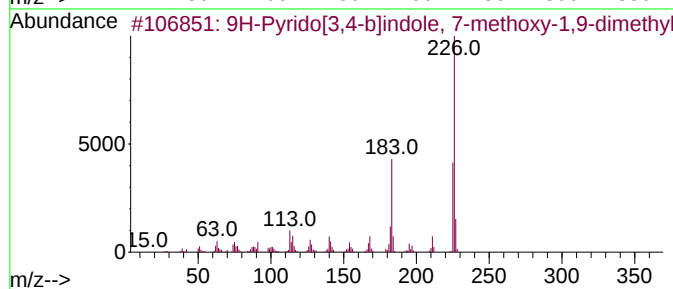
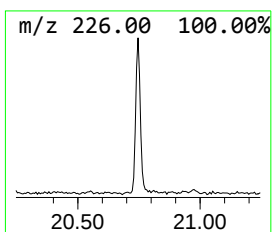
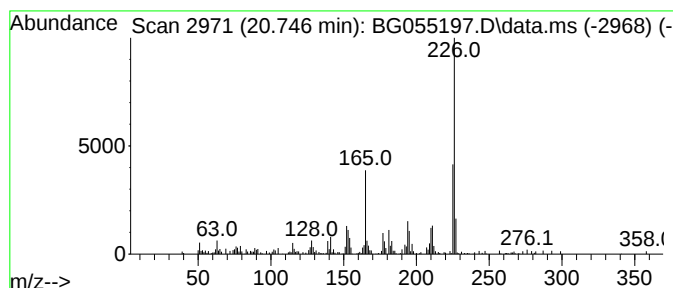
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 9H-Pyrido[3,4-b]indole, 7-m... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.746	3.00 ng	75125	Chrysene-d12	21.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9H-Pyrido[3,4-b]indole, 7-methox...	226	C14H14N2O	143502-37-8	62
2			Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	297758-19-1	59
3			Acridin-9-amine, 1,2,3,4-tetrahy...	226	C15H18N2	1000300-57-6	58
4			Benzenamine, N-[(4-nitrophenyl)m...	226	C13H10N2O2	000785-80-8	53
5			Benzenamine, 4,4'-methylenebis[2...	226	C15H18N2	000838-88-0	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101722\
Data File : BG055197.D
Acq On : 17 Oct 2022 18:04
Operator : CG/JU
Sample : N5145-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-7-101322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.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
Butane, 2-metho...	3.325	102.5	ng	889491	1	8.302	173540	20.0
2-Pentanone, 4-...	5.341	7.3	ng	63477	1	8.302	173540	20.0
Benzaldehyde, 2...	8.813	3.9	ng	33778	1	8.302	173540	20.0
Fenchone	9.553	9.4	ng	81350	1	8.302	173540	20.0
Hexanoic acid, ...	9.929	11.1	ng	144714	2	11.128	260134	20.0
unknown10.388	10.388	4.0	ng	52395	2	11.128	260134	20.0
Bicyclo[2.2.1]h...	10.535	19.7	ng	256565	2	11.128	260134	20.0
Bicyclo[2.2.1]h...	10.670	2.5	ng	32011	2	11.128	260134	20.0
Bicyclo[3.1.1]h...	11.428	4.6	ng	60309	2	11.128	260134	20.0
Naphthalene, 1,...	12.215	2.8	ng	36113	2	11.128	260134	20.0
Apocynin	14.747	7.2	ng	143473	3	14.912	399954	20.0
unknown15.306	15.306	2.1	ng	41935	3	14.912	399954	20.0
2(3H)-Benzothia...	16.569	2.1	ng	42755	4	17.644	407802	20.0
unknown18.290	18.290	2.3	ng	47294	4	17.644	407802	20.0
n-Hexadecanoic ...	18.502	2.9	ng	58347	4	17.644	407802	20.0
4-Hydroxy-9-flu...	19.765	6.0	ng	123302	4	17.644	407802	20.0
Phenol, 4,4'-(1...	20.035	5.6	ng	140508	5	21.927	500956	20.0
9H-Pyrido[3,4-b...	20.746	3.0	ng	75125	5	21.927	500956	20.0