

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042822\
 Data File : BG053364.D
 Acq On : 28 Apr 2022 13:33
 Operator : CG/JU
 Sample : N2482-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 2

Instrument :
 BNA_G
 ClientSampleId :
 MW-7R

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-BG040822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053364.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.551	192	198	207	rVB	72982	125046	5.09%	1.029%
2	5.192	301	307	315	rBB	29744	46240	1.88%	0.381%
3	5.668	382	388	399	rVB	279684	477952	19.45%	3.934%
4	7.265	653	660	668	rBV	196823	356404	14.50%	2.934%
5	7.630	715	722	726	rBV	51668	81778	3.33%	0.673%
6	7.677	726	730	737	rVB	52034	79897	3.25%	0.658%
7	7.870	756	763	771	rBV	86259	144235	5.87%	1.187%
8	8.100	791	802	808	rBV	186704	331932	13.51%	2.732%
9	8.158	808	812	821	rVB	53471	86120	3.50%	0.709%
10	9.263	992	1000	1008	rBV	326528	586185	23.85%	4.825%
11	10.673	1234	1240	1249	rBV5	13373	27610	1.12%	0.227%
12	10.913	1273	1281	1293	rVB	241905	441792	17.98%	3.636%
13	11.266	1334	1341	1347	rBV2	12384	25164	1.02%	0.207%
14	11.818	1427	1435	1442	rBV5	15467	33564	1.37%	0.276%
15	13.087	1645	1651	1659	rBV	69312	117304	4.77%	0.966%
16	13.351	1686	1696	1703	rBV	829471	1462858	59.53%	12.041%
17	13.569	1725	1733	1739	rBV	258717	402431	16.38%	3.312%
18	14.726	1923	1930	1937	rVB	403962	624391	25.41%	5.139%
19	15.525	2060	2066	2072	rVB	40593	62378	2.54%	0.513%
20	16.065	2151	2158	2165	rBV	41153	65571	2.67%	0.540%
21	16.212	2176	2183	2195	rBV	732524	1153235	46.93%	9.492%
22	17.469	2390	2397	2405	rBV	503622	799128	32.52%	6.578%
23	18.127	2505	2509	2513	rBV3	29651	36568	1.49%	0.301%
24	19.760	2782	2787	2792	rVB	44181	49757	2.02%	0.410%
25	20.077	2834	2841	2846	rBV	1864366	2457522	100.00%	20.228%
26	20.800	2960	2964	2969	rVB3	30338	36831	1.50%	0.303%
27	21.752	3120	3126	3134	rVB2	566069	978070	39.80%	8.050%
28	22.551	3257	3262	3267	rBV3	20155	32702	1.33%	0.269%
29	24.084	3519	3523	3528	rVB6	14504	25658	1.04%	0.211%
30	25.053	3677	3688	3700	rVB2	339285	1001004	40.73%	8.239%

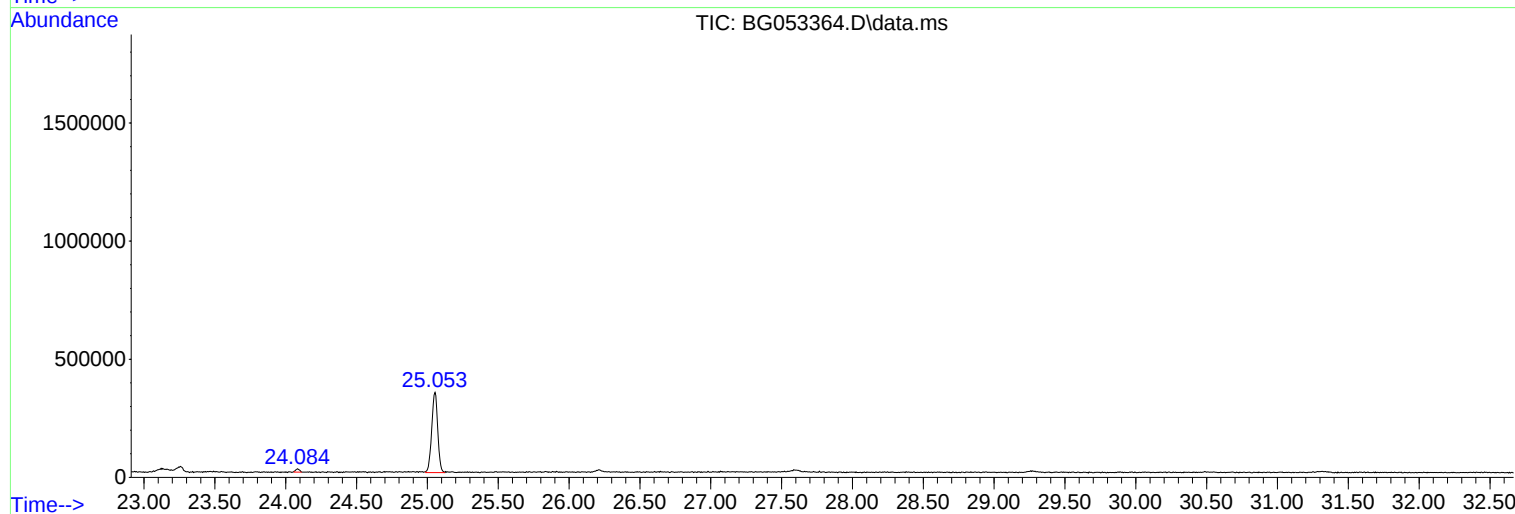
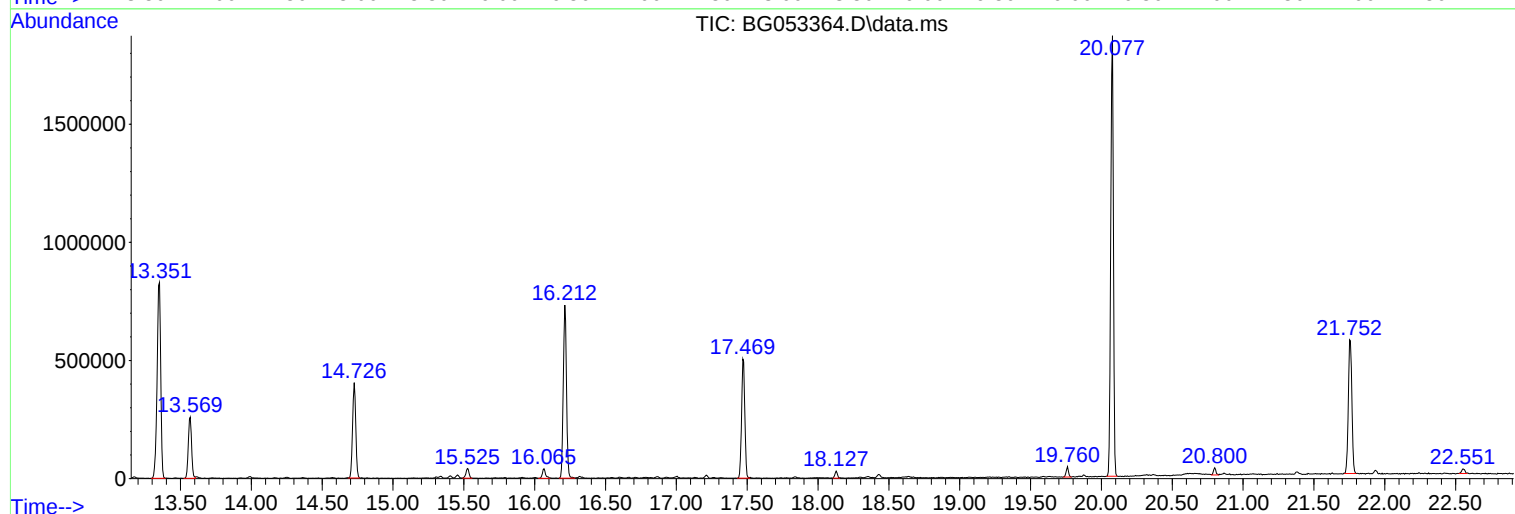
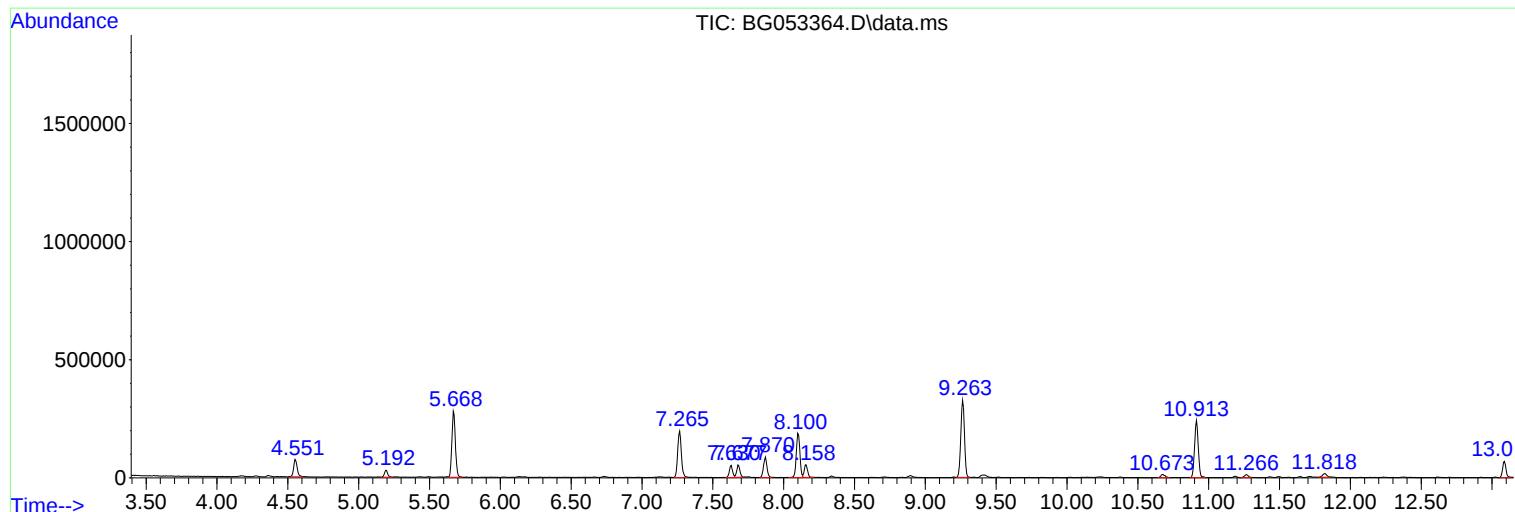
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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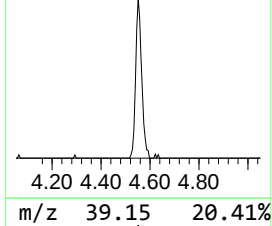
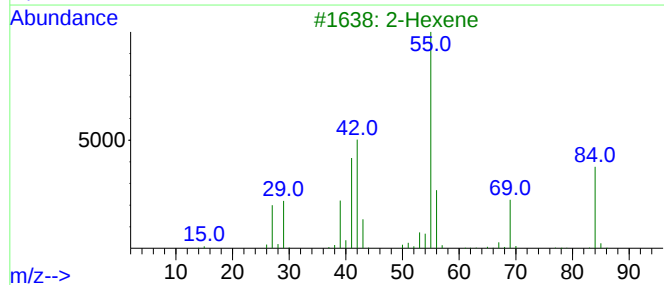
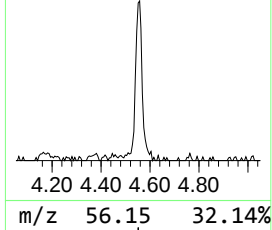
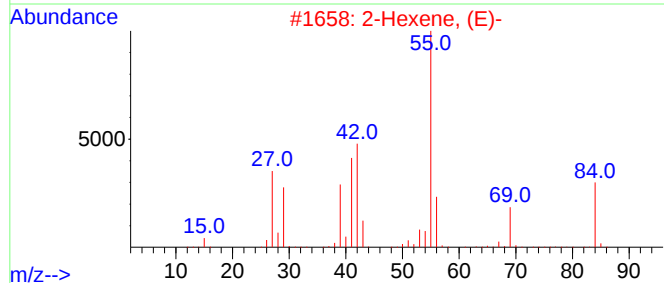
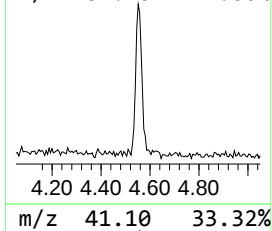
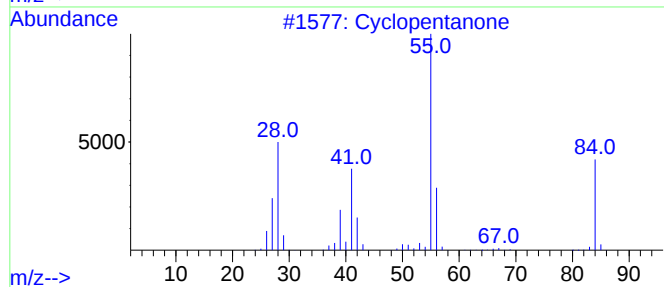
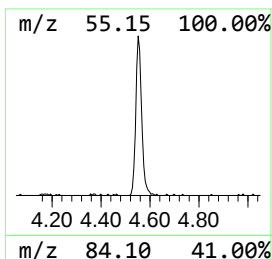
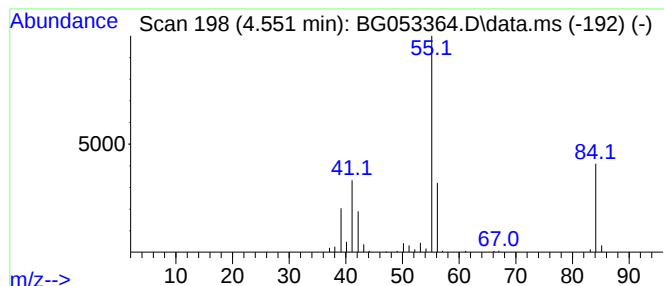
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.551	7.53 ng	125046	1,4-Dichlorobenzene-d4	8.100

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentanone	84	C5H8O	000120-92-3	91
2		2-Hexene, (E)-	84	C6H12	004050-45-7	53
3		2-Hexene	84	C6H12	000592-43-8	53
4		2-Hexene, (Z)-	84	C6H12	007688-21-3	50
5		1H-Imidazole, 4,5-dihydro-2-methyl-	84	C4H8N2	000534-26-9	40



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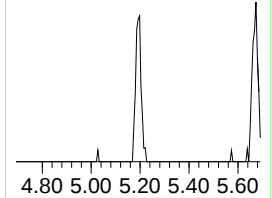
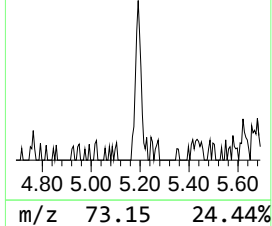
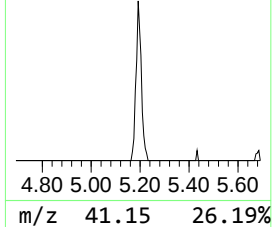
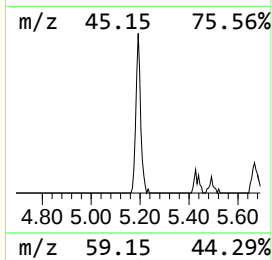
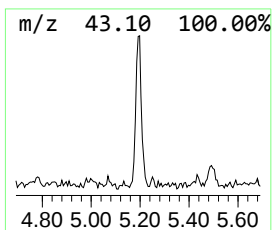
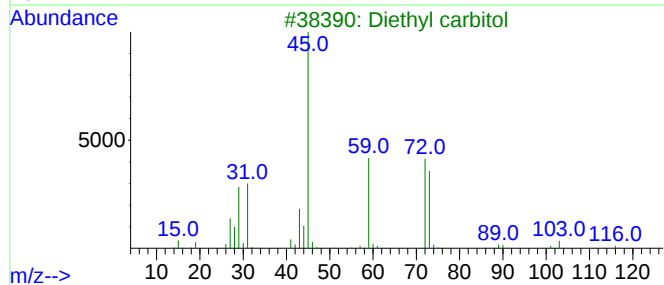
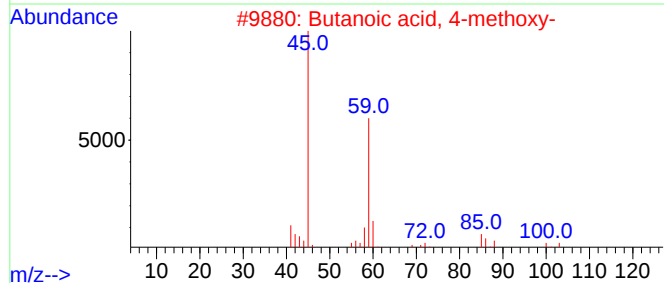
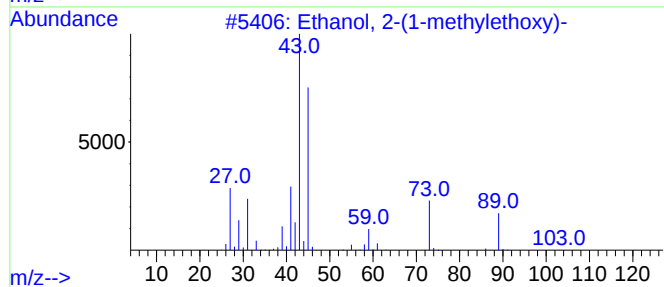
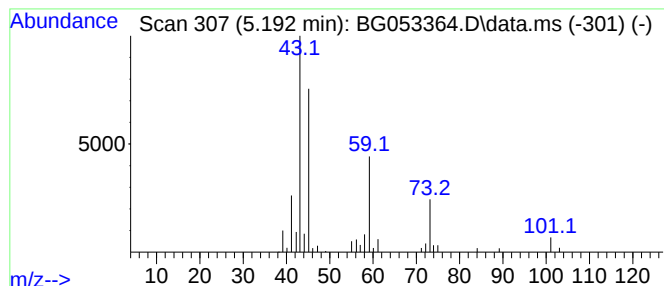
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(1-methylethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.192	2.79 ng	46240	1,4-Dichlorobenzene-d4	8.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	59
2			Butanoic acid, 4-methoxy-	118	C5H10O3	029006-02-8	53
3			Diethyl carbitol	162	C8H18O3	000112-36-7	50
4			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	45
5			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45



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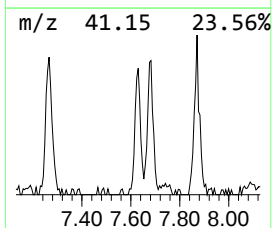
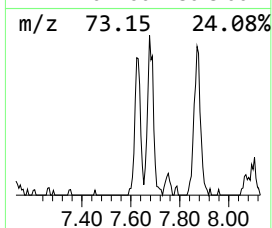
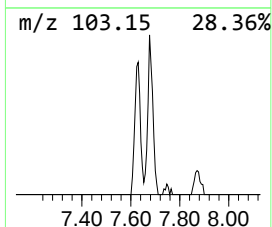
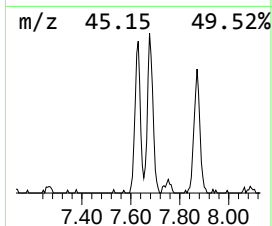
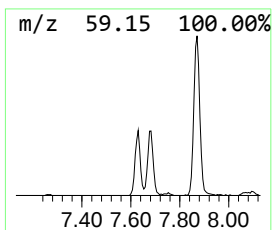
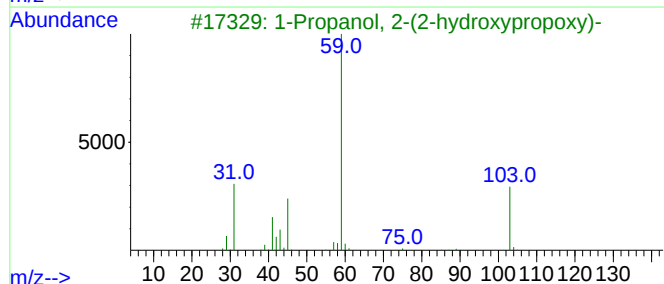
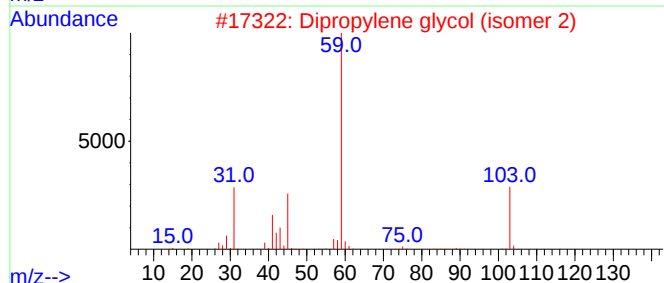
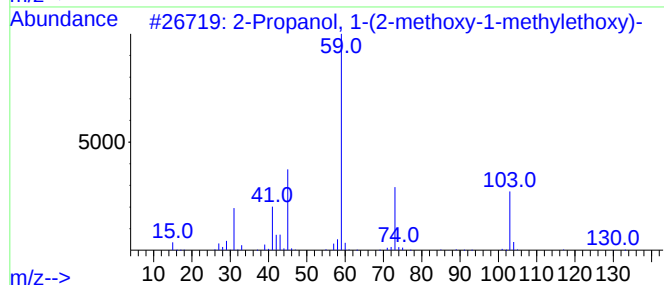
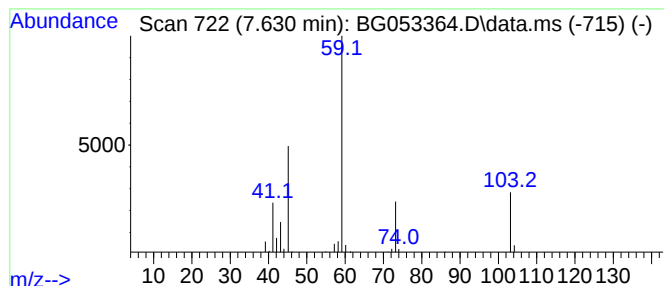
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.630	4.93 ng	81778	1,4-Dichlorobenzene-d4	8.100

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2		Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	53
3		1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
4		1-Propanol, 3,3'-oxybis-	134	C6H14O3	002396-61-4	50
5		1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	42



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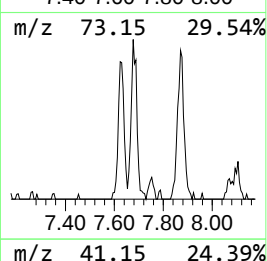
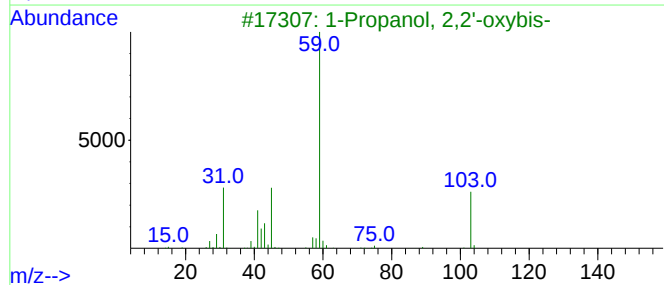
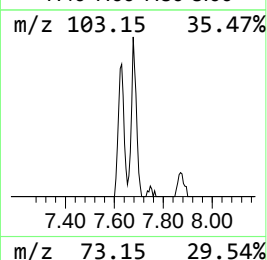
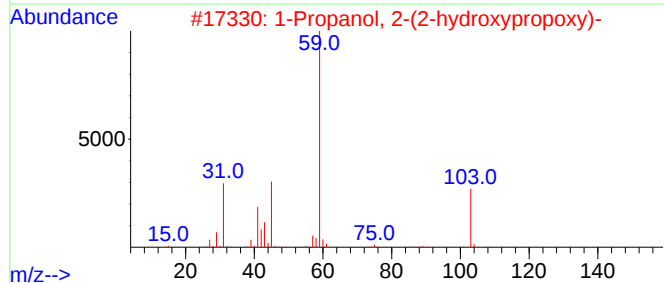
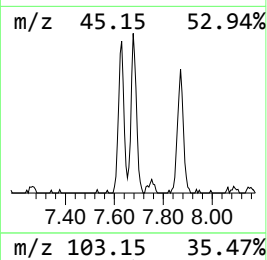
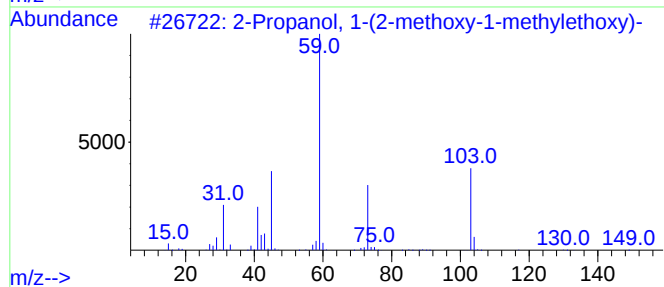
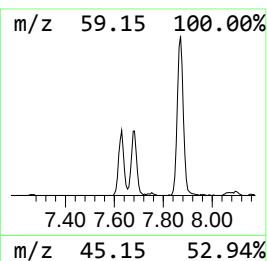
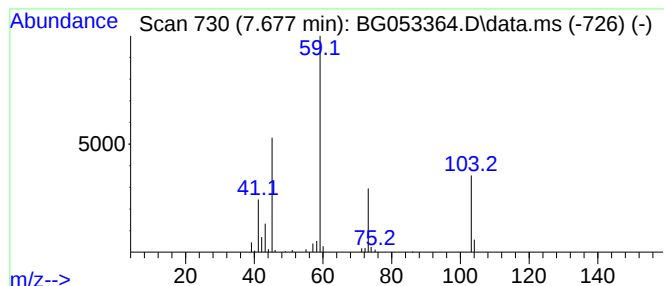
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Propanol, 2-(2-hydroxypro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.
7.677	4.81 ng	79897	1,4-Dichlorobenzene-d4			8.100

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol,	1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	80
2	1-Propanol,	2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	50
3	1-Propanol,	2,2'-oxybis-	134	C6H14O3	000108-61-2	50
4	Dipropylene glycol (isomer 2)		134	C6H14O3	1000506-25-4	50
5	Dipropylene glycol (isomer 3)		134	C6H14O3	1000506-25-5	50



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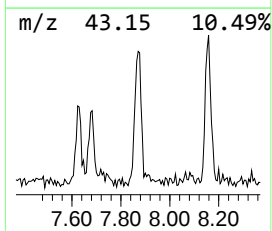
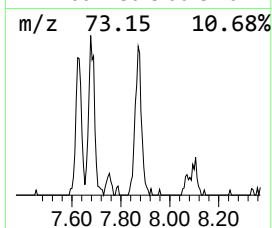
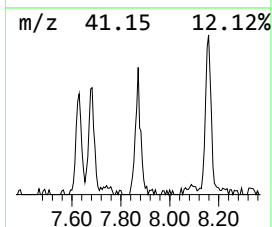
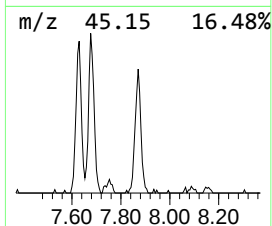
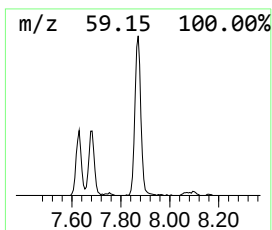
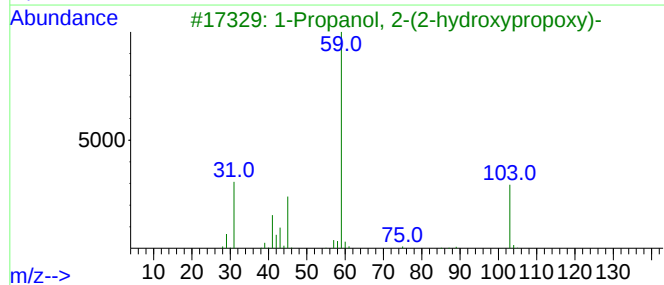
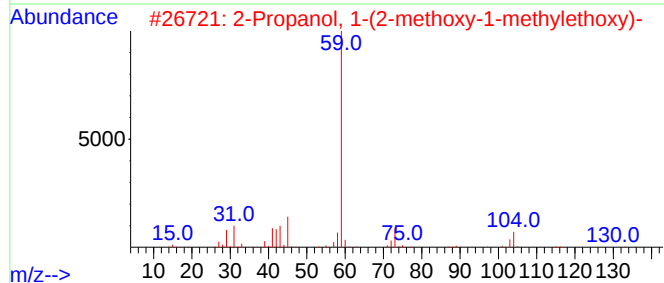
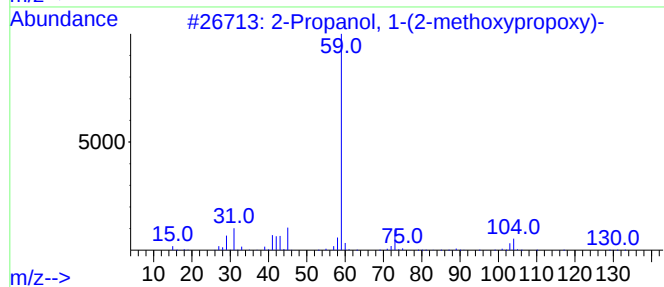
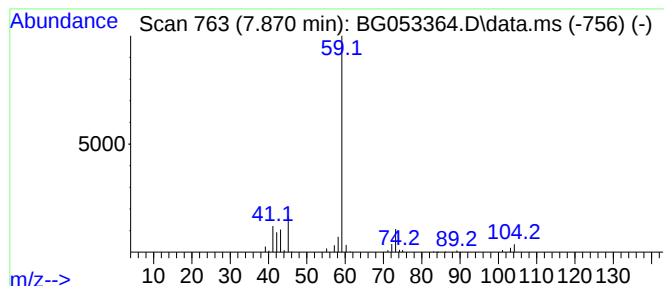
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Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.870	8.69 ng	144235	1,4-Dichlorobenzene-d4	8.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
2			2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	74
3			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
4			Butanal, 3-methyl-, oxime	101	C5H11NO	000626-90-4	64
5			Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	59



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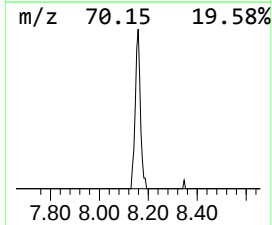
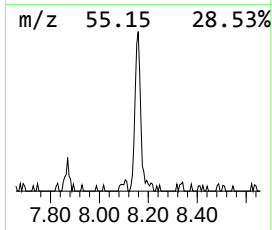
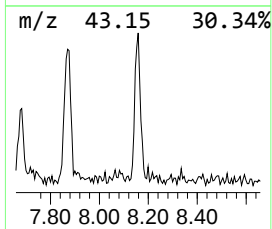
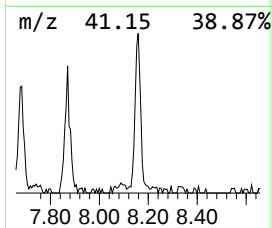
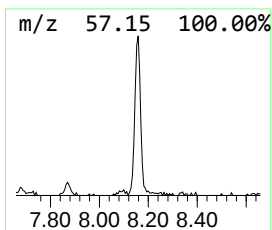
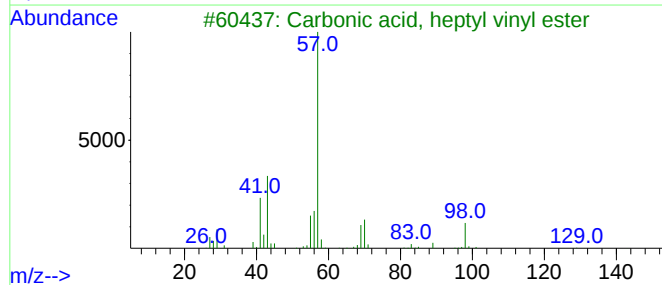
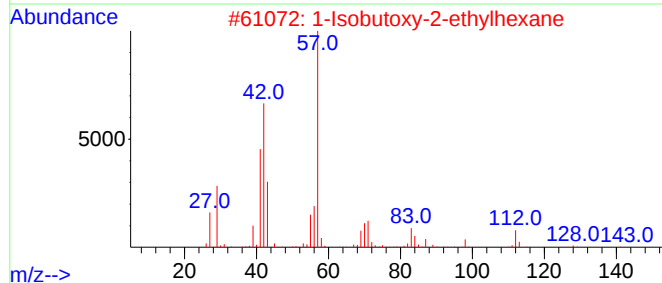
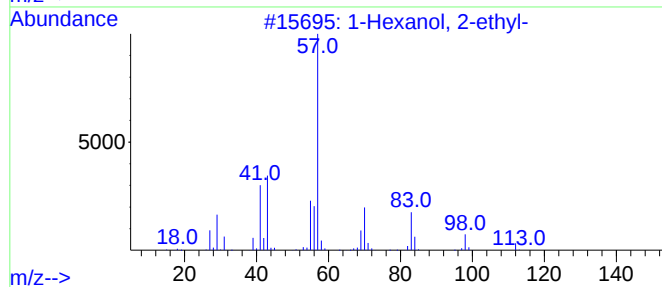
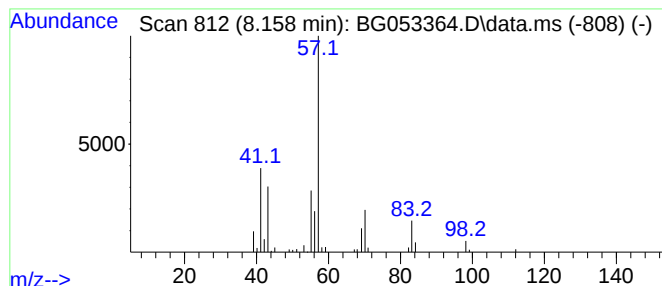
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.158	5.19 ng	86120	1,4-Dichlorobenzene-d4	8.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	72
3			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	50
4			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	47
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042822\
Data File : BG053364.D
Acq On : 28 Apr 2022 13:33
Operator : CG/JU
Sample : N2482-03
Misc :
ALS Vial : 6 Sample Multiplier: 2

Instrument :
BNA_G
ClientSampleId :
MW-7R

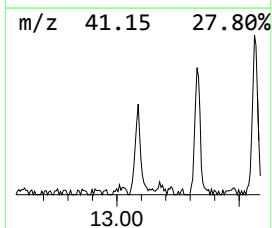
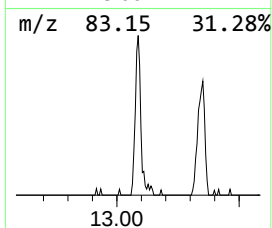
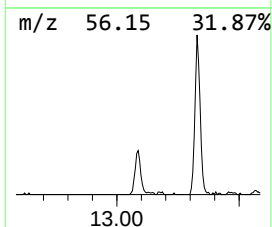
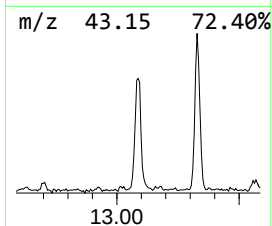
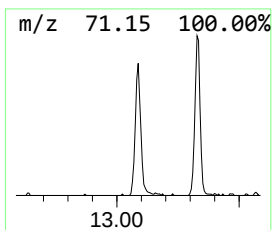
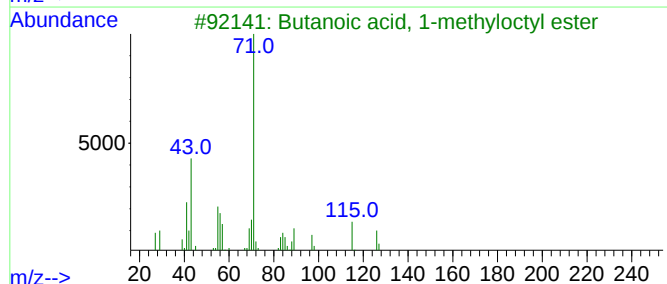
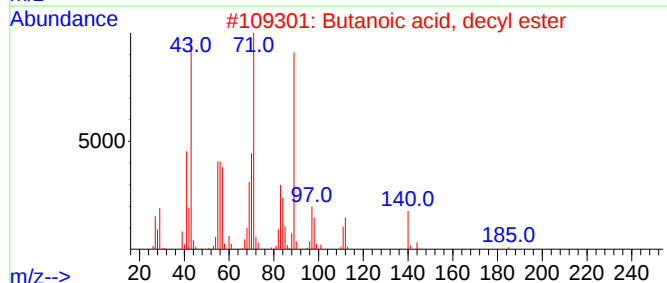
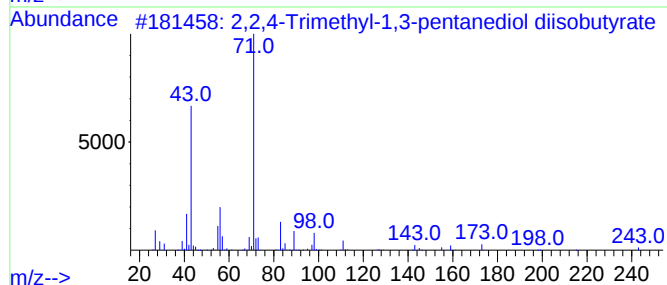
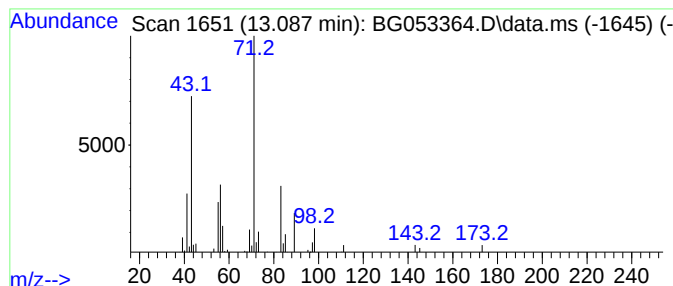
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.087	3.76 ng	117304	Acenaphthene-d10	14.726

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	64	
2	Butanoic acid, decyl ester	228	C14H28O2	005454-09-1	50	
3	Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	50	
4	Sulfurous acid, decyl 2-pentyl e...	292	C15H32O3S	1000309-15-9	43	
5	Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	42	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042822\
Data File : BG053364.D
Acq On : 28 Apr 2022 13:33
Operator : CG/JU
Sample : N2482-03
Misc :
ALS Vial : 6 Sample Multiplier: 2

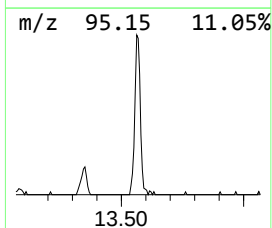
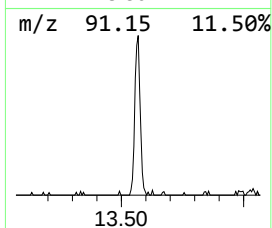
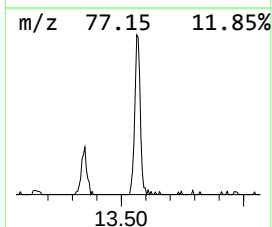
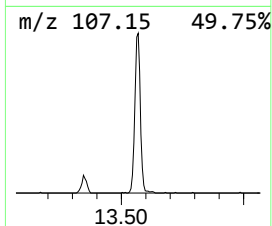
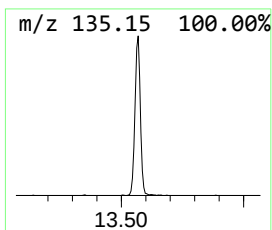
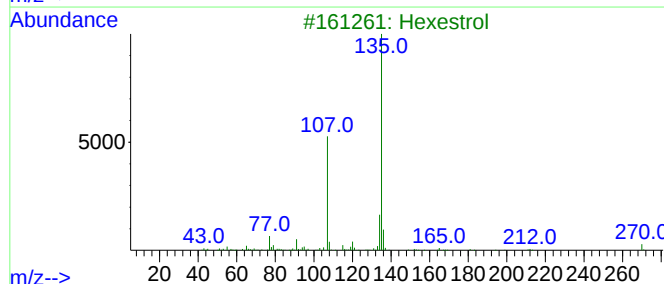
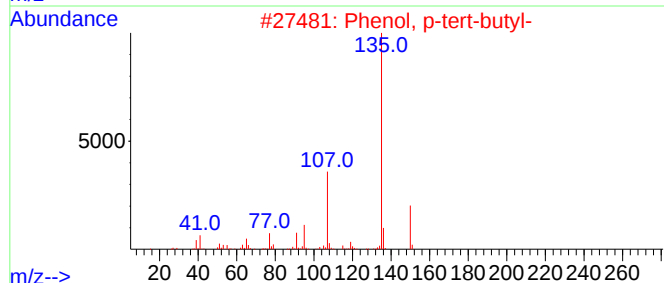
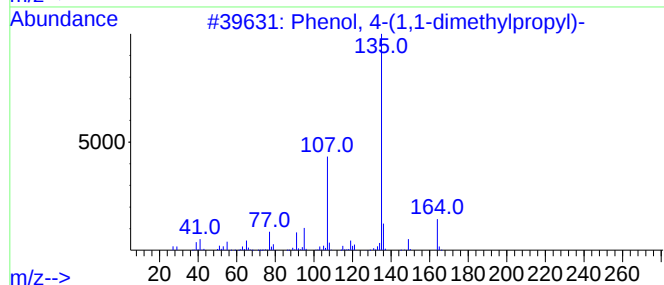
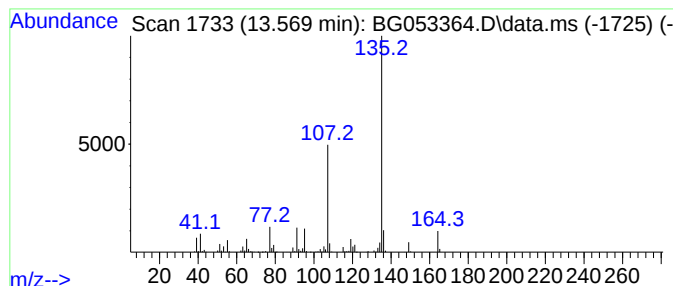
Instrument :
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ClientSampleId :
MW-7R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.569	12.89 ng	402431	Acenaphthene-d10		14.726	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-		164	C11H16O	000080-46-6	94
2	Phenol, p-tert-butyl-		150	C10H14O	000098-54-4	80
3	Hexestrol		270	C18H22O2	000084-16-2	64
4	Imidazo[1,2-c]pyrimidin-5-ol		135	C6H5N3O	055662-66-3	64
5	Phenol, 2-(1,1,3,3-tetramethylbu...		206	C14H22O	003884-95-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042822\
Data File : BG053364.D
Acq On : 28 Apr 2022 13:33
Operator : CG/JU
Sample : N2482-03
Misc :
ALS Vial : 6 Sample Multiplier: 2

Instrument :
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ClientSampleId :
MW-7R

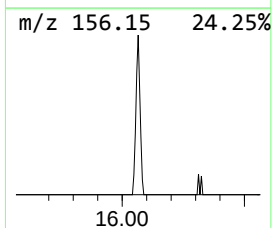
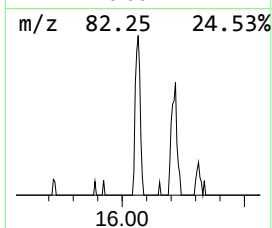
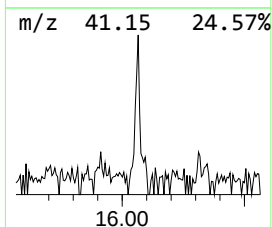
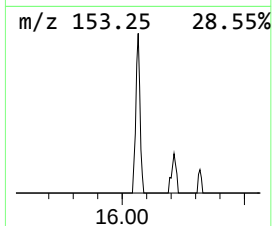
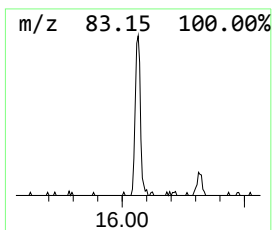
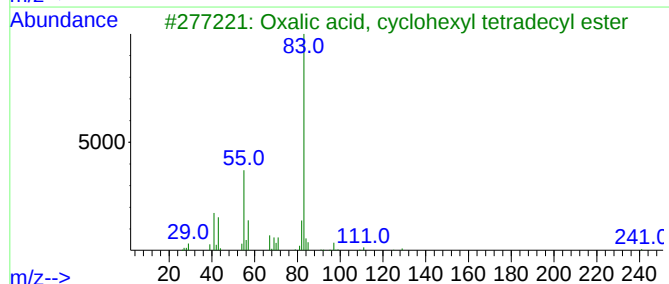
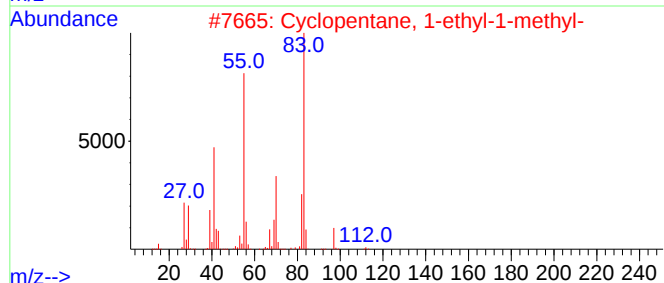
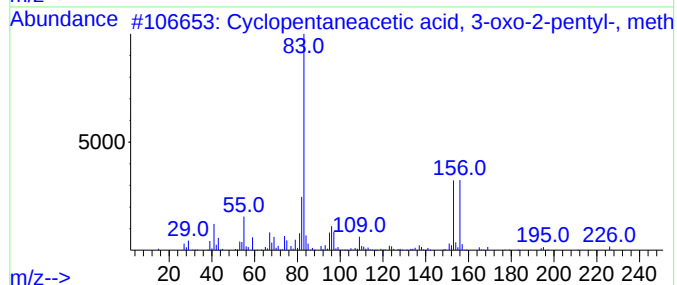
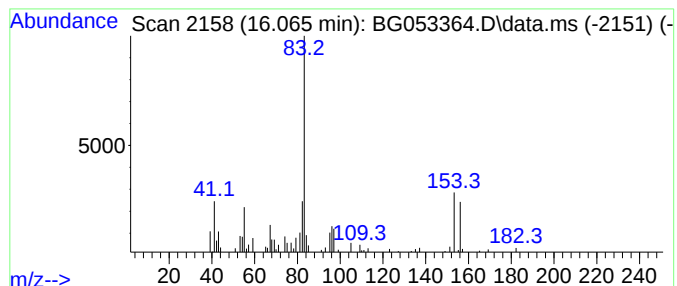
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclopentaneacetic acid, 3-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.065	2.10 ng	65571	Acenaphthene-d10	14.726

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	90
2			Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	47
3			Oxalic acid, cyclohexyl tetradec...	368	C22H40O4	1000309-31-5	43
4			Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	43
5			6-Hydroxy-10a-methyl-4,7-dimethy...	376	C20H24O7	1798297-60-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042822\
Data File : BG053364.D
Acq On : 28 Apr 2022 13:33
Operator : CG/JU
Sample : N2482-03
Misc :
ALS Vial : 6 Sample Multiplier: 2

Instrument :
BNA_G
ClientSampleId :
MW-7R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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
Cyclopentanone	4.551	7.5	ng	125046	1	8.100	331932	20.0
Ethanol, 2-(1-m...	5.192	2.8	ng	46240	1	8.100	331932	20.0
2-Propanol, 1-(...	7.630	4.9	ng	81778	1	8.100	331932	20.0
1-Propanol, 2-(...	7.677	4.8	ng	79897	1	8.100	331932	20.0
2-Propanol, 1-(...	7.870	8.7	ng	144235	1	8.100	331932	20.0
1-Hexanol, 2-et...	8.158	5.2	ng	86120	1	8.100	331932	20.0
2,2,4-Trimethyl...	13.087	3.8	ng	117304	3	14.726	624391	20.0
Phenol, 4-(1,1-...	13.569	12.9	ng	402431	3	14.726	624391	20.0
Cyclopentaneace...	16.065	2.1	ng	65571	3	14.726	624391	20.0