

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
 Data File : BG053354.D
 Acq On : 28 Apr 2022 00:40
 Operator : CG/JU
 Sample : N2482-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-22R

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: BG053354.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	190	198	209	rBV	68766	116114	3.61%	0.997%
2	5.192	301	307	315	rBV	45188	71819	2.24%	0.617%
3	5.668	382	388	397	rBV	314560	516495	16.08%	4.436%
4	7.260	652	659	669	rBV	217131	398812	12.41%	3.426%
5	7.630	715	722	726	rBV	37219	59649	1.86%	0.512%
6	7.677	726	730	739	rVB	38307	59549	1.85%	0.511%
7	7.871	756	763	770	rBV	58259	102360	3.19%	0.879%
8	8.106	794	803	807	rBV	98753	169573	5.28%	1.457%
9	8.158	807	812	819	rVB	95843	152609	4.75%	1.311%
10	8.476	860	866	872	rBV2	42426	72740	2.26%	0.625%
11	9.263	994	1000	1011	rVB	413545	747739	23.28%	6.423%
12	10.913	1273	1281	1287	rBV	125480	230913	7.19%	1.983%
13	11.730	1415	1420	1428	rBV3	18252	42717	1.33%	0.367%
14	13.087	1645	1651	1661	rBV	57760	95444	2.97%	0.820%
15	13.351	1686	1696	1705	rBV	1043183	1754898	54.63%	15.073%
16	13.569	1727	1733	1739	rBV	165926	250892	7.81%	2.155%
17	14.732	1924	1931	1937	rBV	213624	338812	10.55%	2.910%
18	15.531	2059	2067	2072	rVB	44733	66272	2.06%	0.569%
19	16.065	2153	2158	2168	rVB	47182	67299	2.09%	0.578%
20	16.218	2177	2184	2195	rBV	912456	1435654	44.69%	12.331%
21	17.475	2391	2398	2403	rBV	290863	447366	13.93%	3.843%
22	18.133	2504	2510	2515	rBV3	28804	38378	1.19%	0.330%
23	20.078	2835	2841	2847	rBV	2383531	3212426	100.00%	27.592%
24	21.758	3120	3127	3133	rBV	337084	562421	17.51%	4.831%
25	23.261	3374	3383	3391	rBV6	18123	47546	1.48%	0.408%
26	25.053	3677	3688	3702	rVB2	195682	583948	18.18%	5.016%

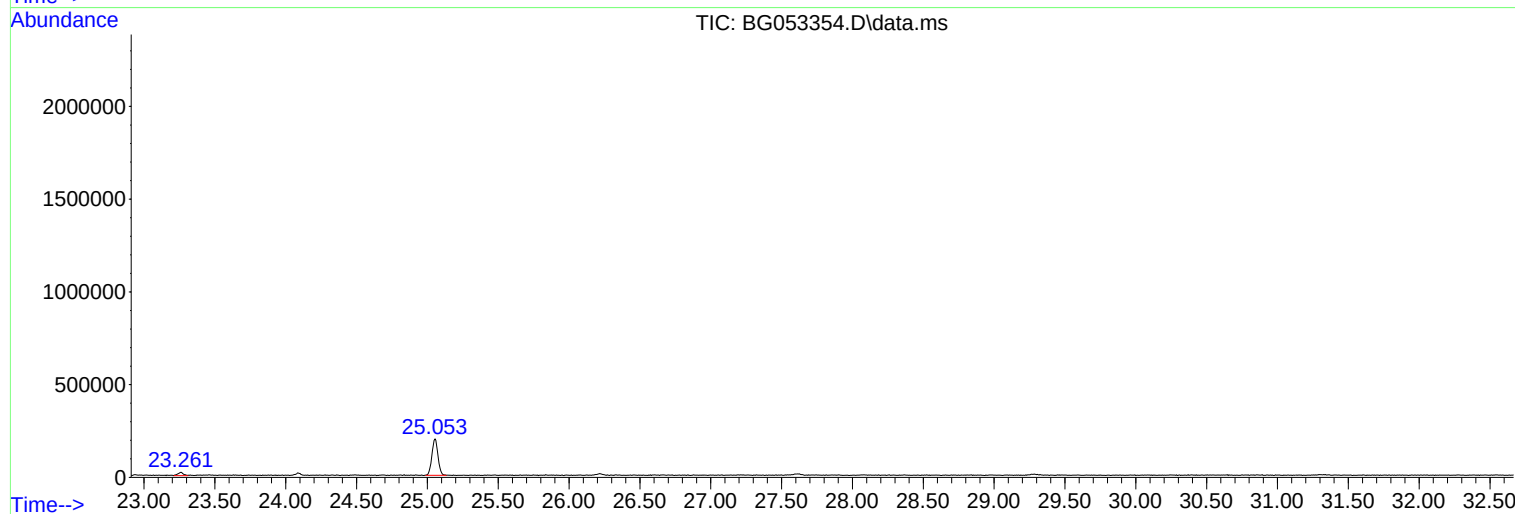
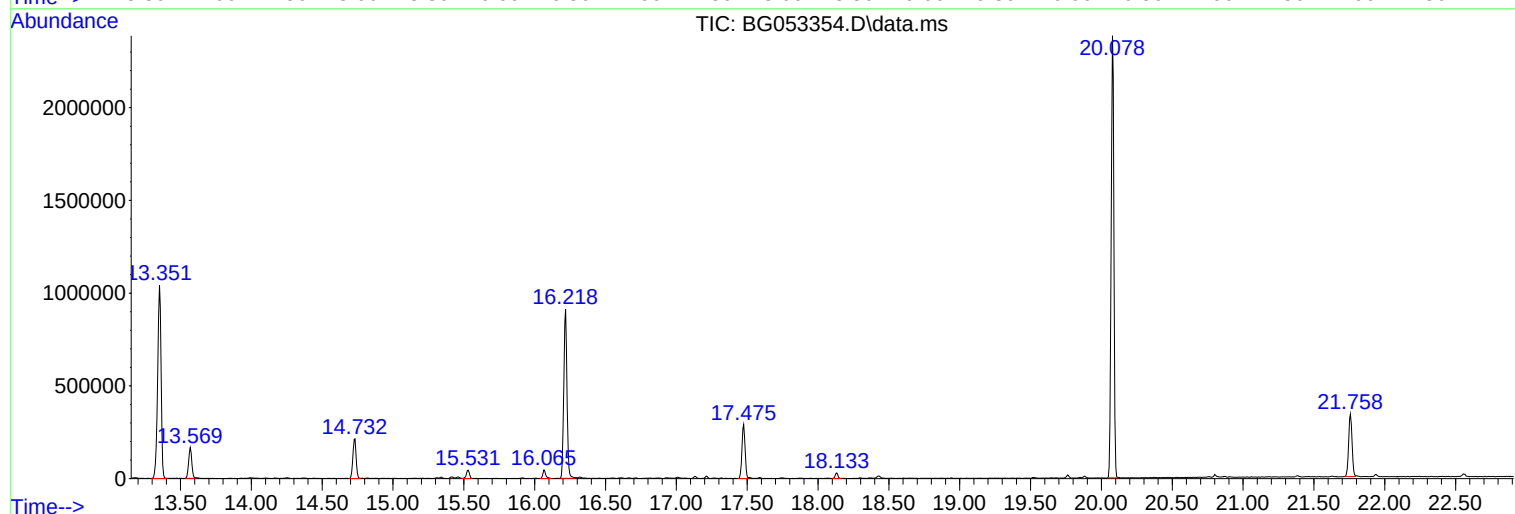
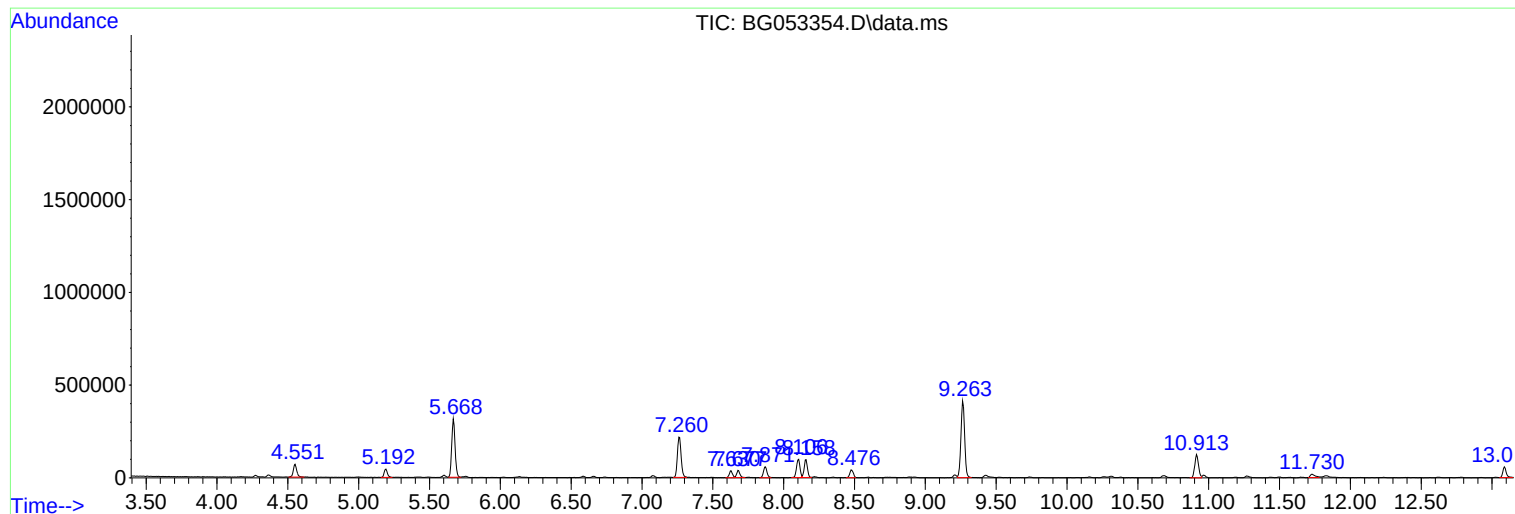
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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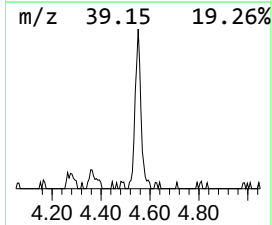
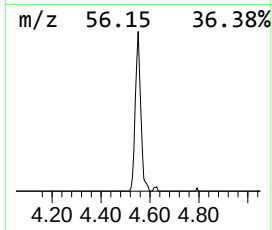
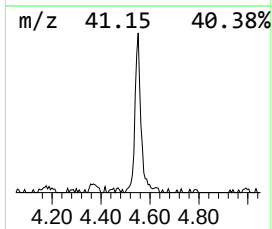
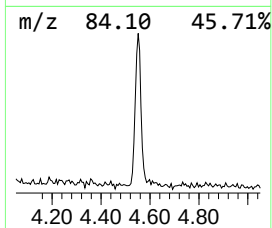
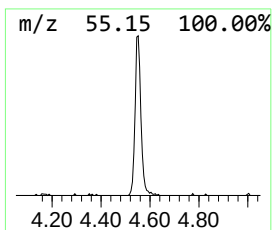
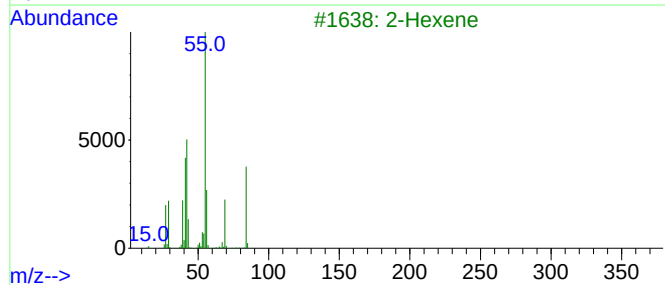
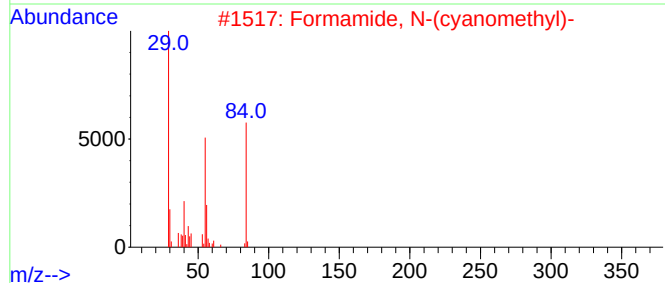
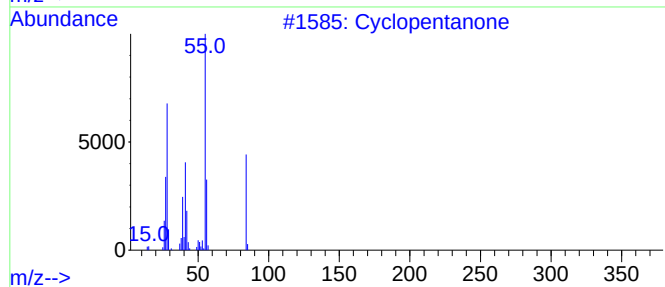
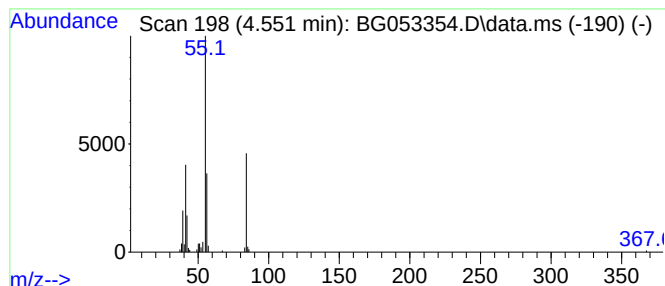
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	13.69 ng	116114	1,4-Dichlorobenzene-d4	8.105

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone	84	C5H8O	000120-92-3	91
2			Formamide, N-(cyanomethyl)-	84	C3H4N2O	005018-27-9	64
3			2-Hexene	84	C6H12	000592-43-8	64
4			2-Hexene, (E)-	84	C6H12	004050-45-7	50
5			2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	50



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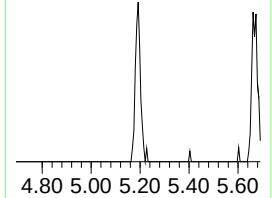
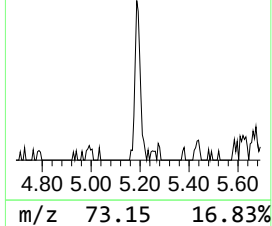
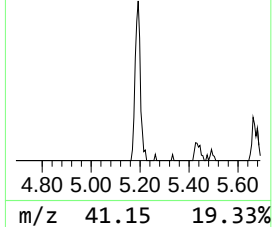
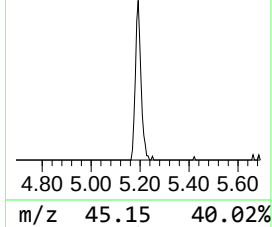
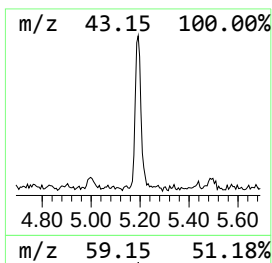
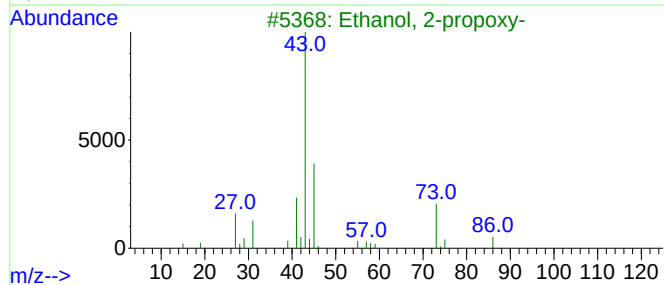
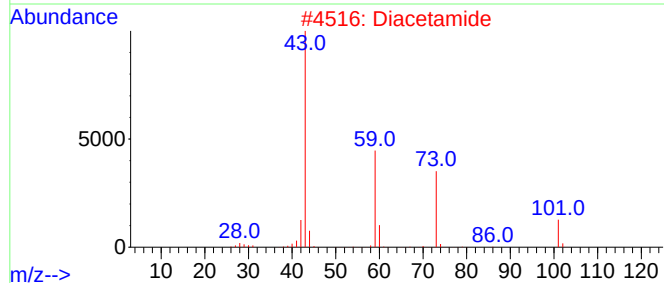
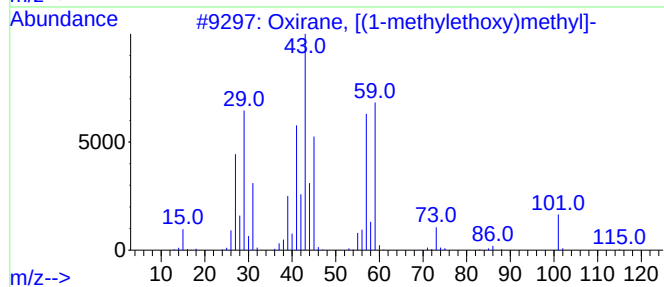
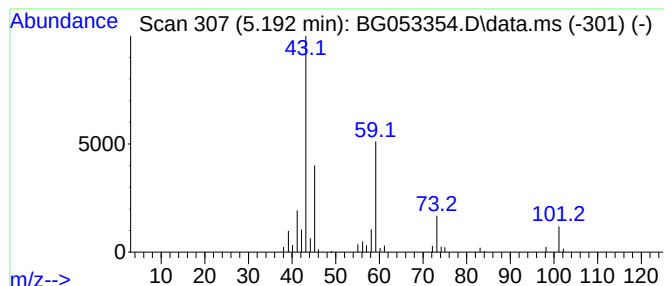
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Oxirane, [(1-methylethoxy)m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.192	8.47 ng	71819	1,4-Dichlorobenzene-d4	8.105

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	56
2			Diacetamide	101	C4H7NO2	000625-77-4	43
3			Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	43
4			Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	38
5			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38



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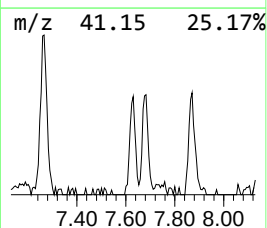
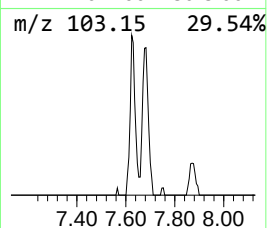
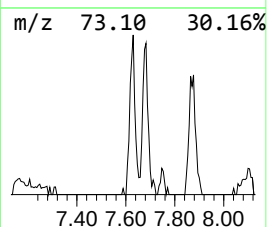
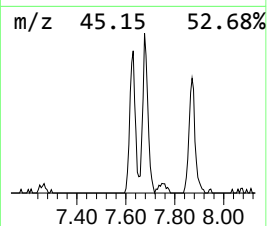
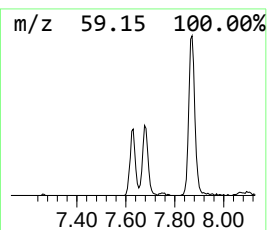
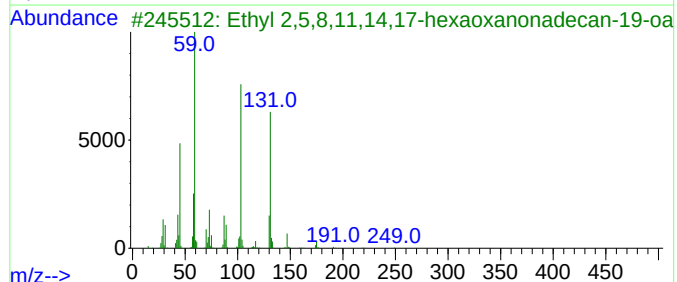
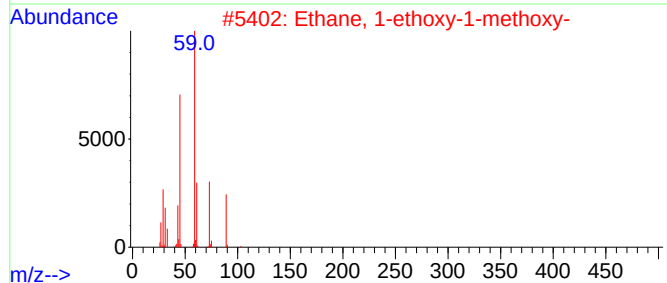
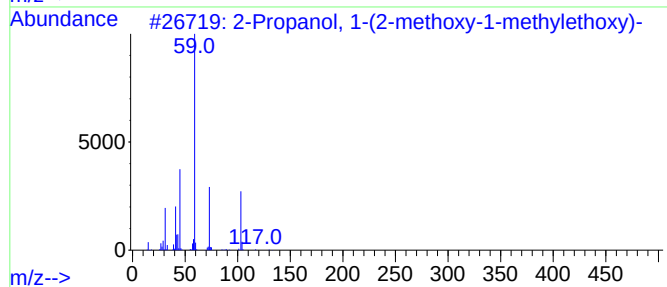
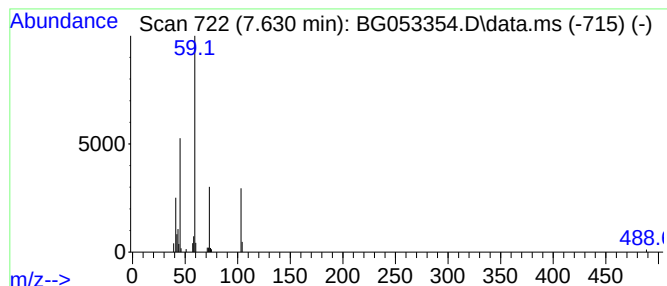
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.630	7.04 ng	59649	1,4-Dichlorobenzene-d4	8.105

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83		
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	64		
3	Ethyl 2,5,8,11,14,17-hexaoxanona...	338	C15H30O8	1000366-80-6	56		
4	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	56		
5	Ethyl 2,5,8,11,14,17,20-heptaoxa...	382	C17H34O9	1000366-80-5	56		



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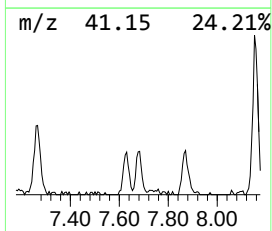
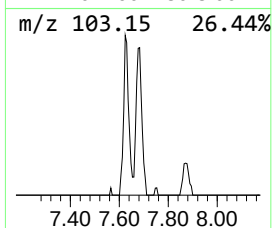
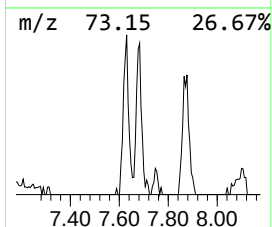
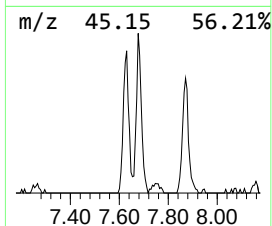
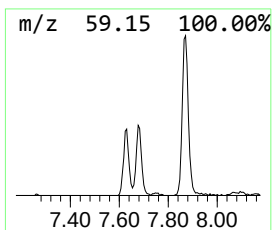
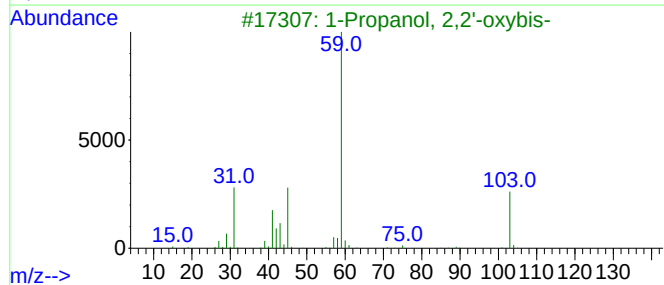
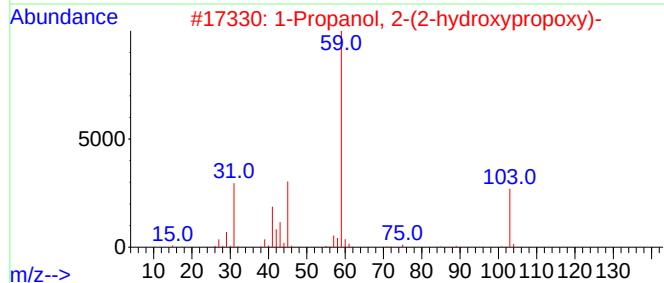
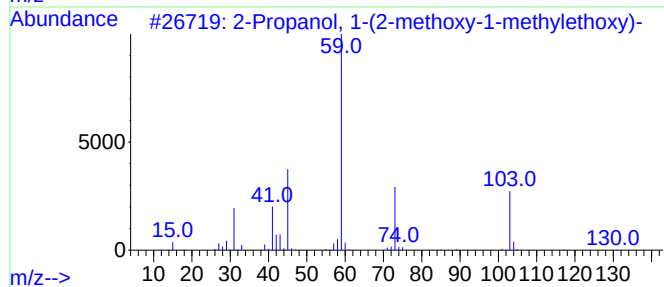
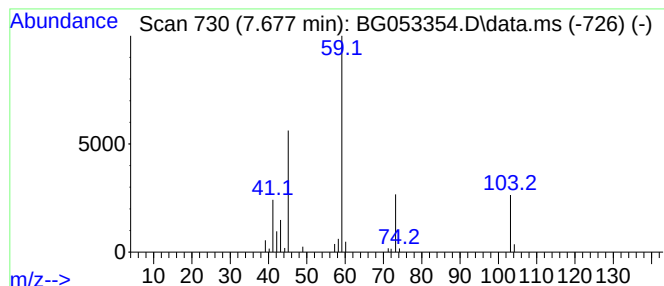
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Peak Number 4 1-Propanol, 2-(2-hydroxypro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.677	7.02 ng	59549	1,4-Dichlorobenzene-d4	8.105

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72		
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59		
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	59		
4	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	45		
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	42		



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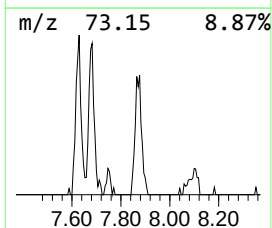
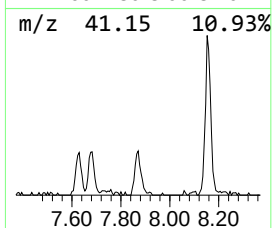
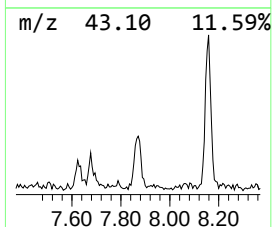
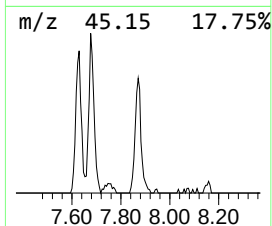
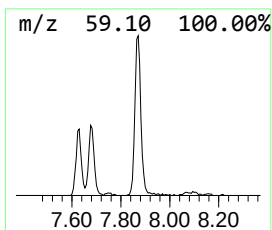
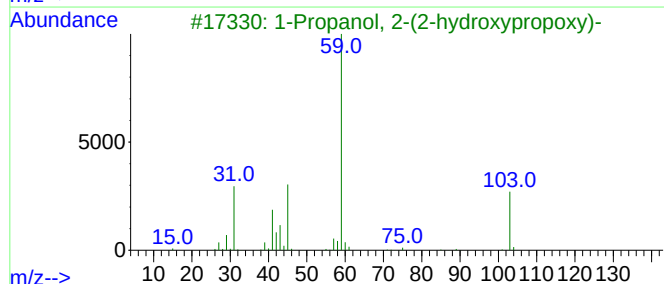
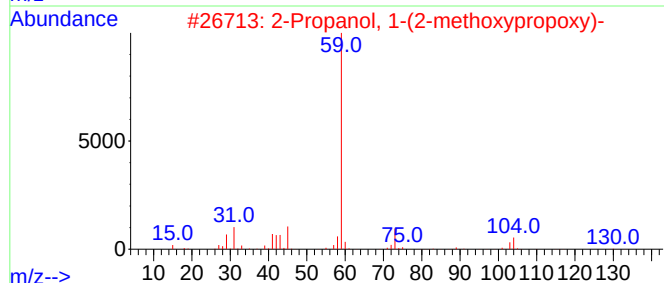
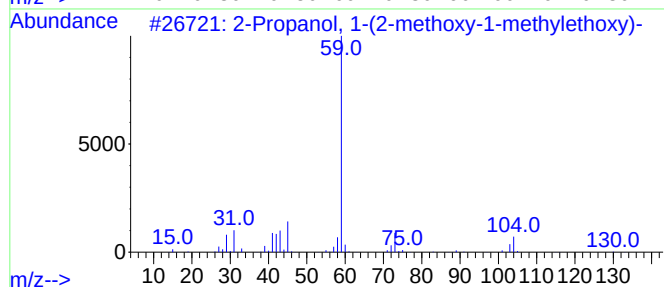
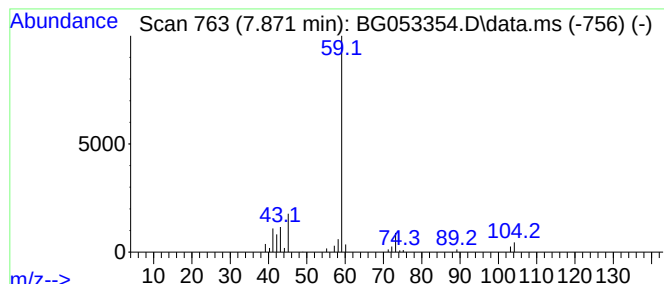
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.871	12.07 ng	102360	1,4-Dichlorobenzene-d4	8.105

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
2			2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
3			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	56
4			Propane, 2-methoxy-	74	C4H10O	000598-53-8	50
5			2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	43



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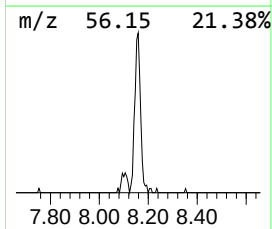
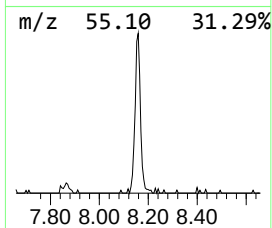
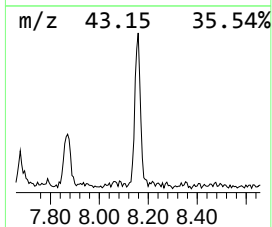
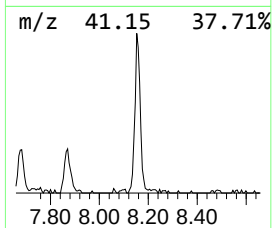
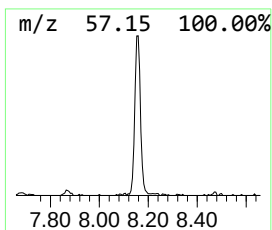
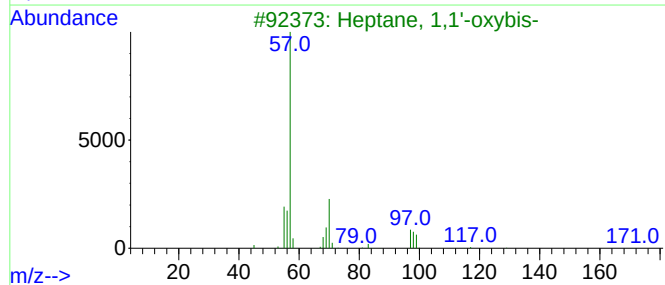
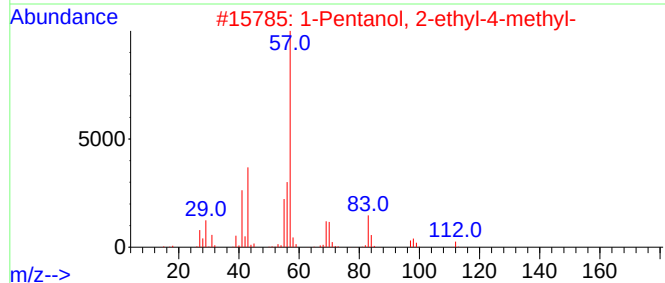
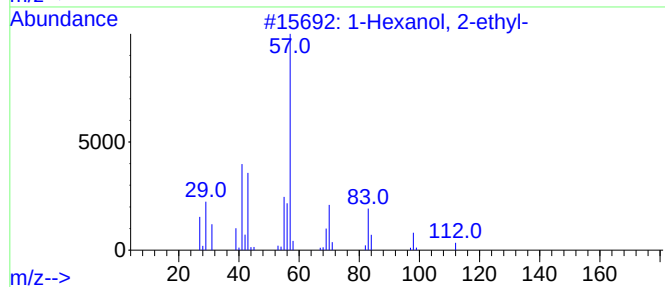
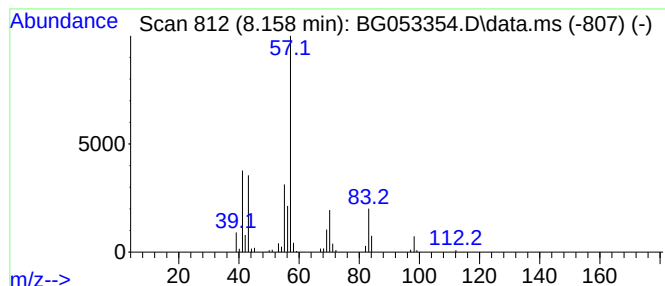
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.158	18.00 ng	152609	1,4-Dichlorobenzene-d4	8.105

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	72
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
4			Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	50
5			1-Hexene, 4-methyl-	98	C7H14	003769-23-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053354.D
Acq On : 28 Apr 2022 00:40
Operator : CG/JU
Sample : N2482-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-22R

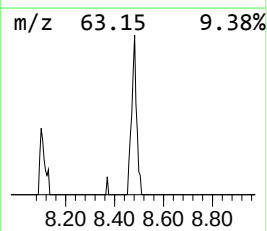
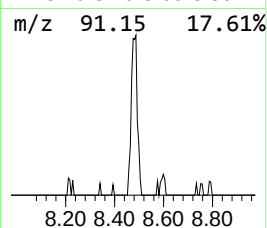
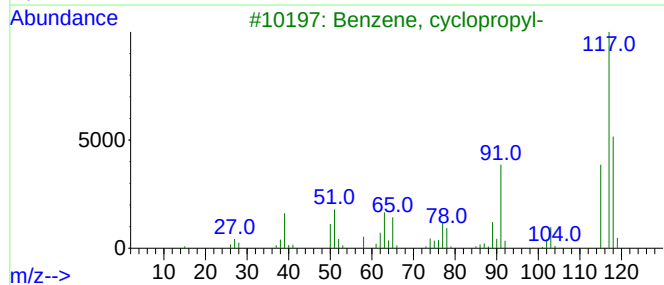
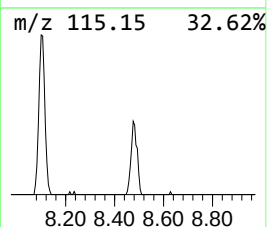
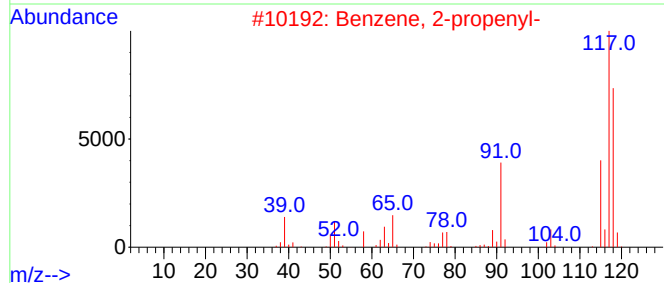
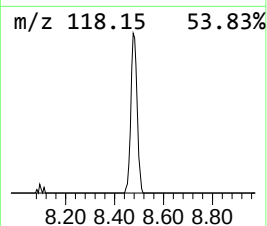
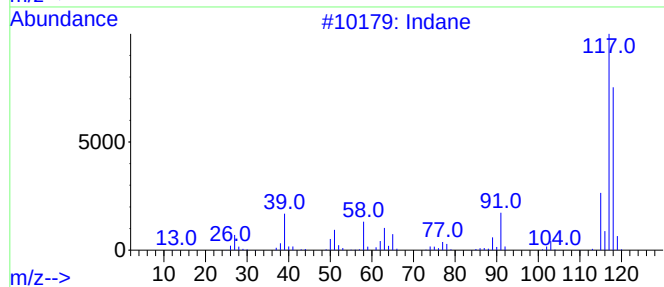
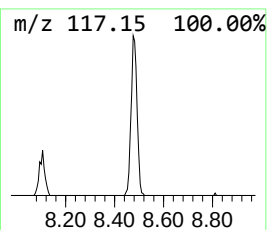
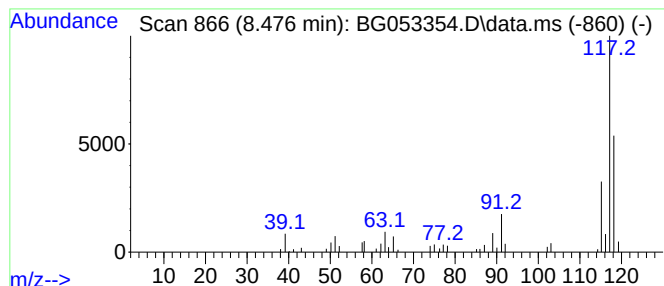
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.476	8.58 ng	72740	1,4-Dichlorobenzene-d4	8.105

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Indane	118	C9H10	000496-11-7	95
2		Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
3		Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	74
5		Deltacyclene	118	C9H10	007785-10-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053354.D
Acq On : 28 Apr 2022 00:40
Operator : CG/JU
Sample : N2482-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

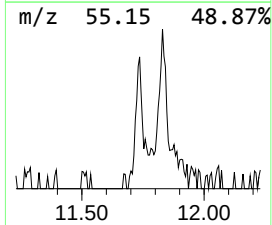
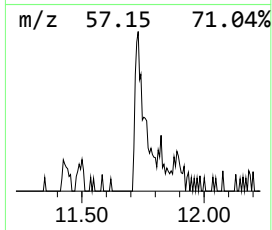
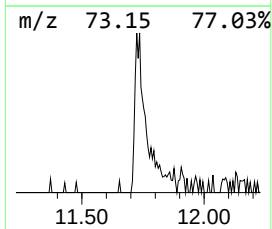
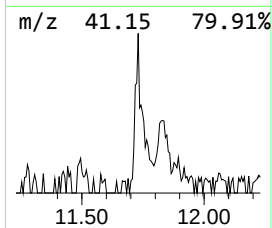
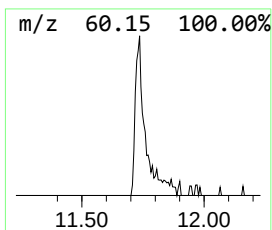
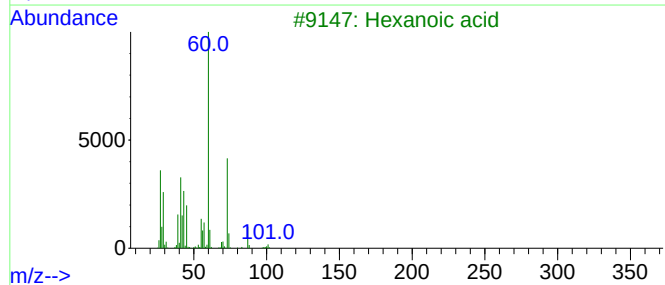
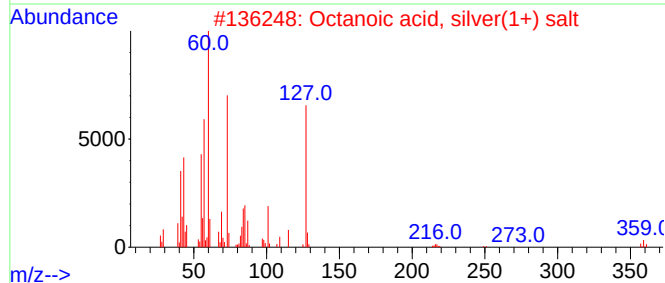
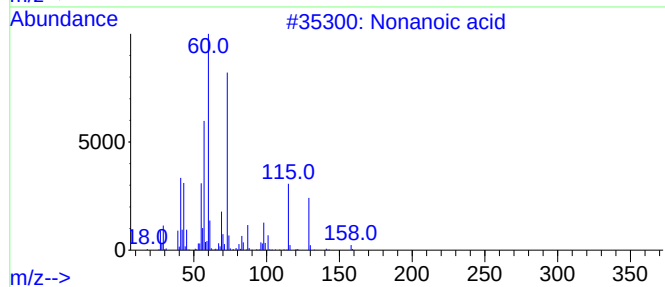
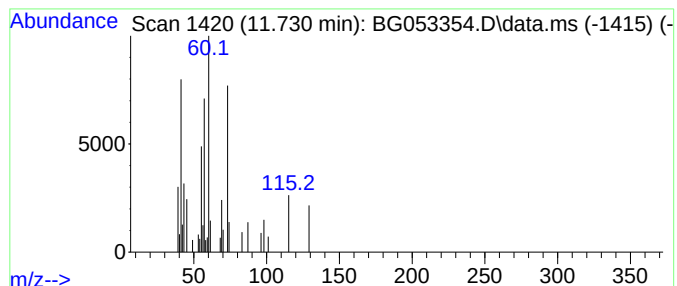
Instrument :
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ClientSampleId :
MW-22R

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 Nonanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.730	3.70 ng	42717	Naphthalene-d8	10.914	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	80
2	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	47
3	Hexanoic acid	116	C6H12O2	000142-62-1	42
4	Octanoic acid	144	C8H16O2	000124-07-2	42
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053354.D
Acq On : 28 Apr 2022 00:40
Operator : CG/JU
Sample : N2482-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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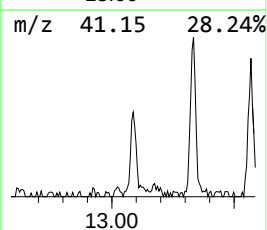
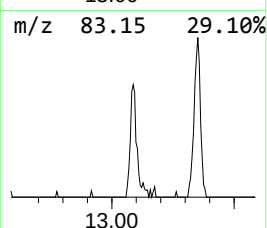
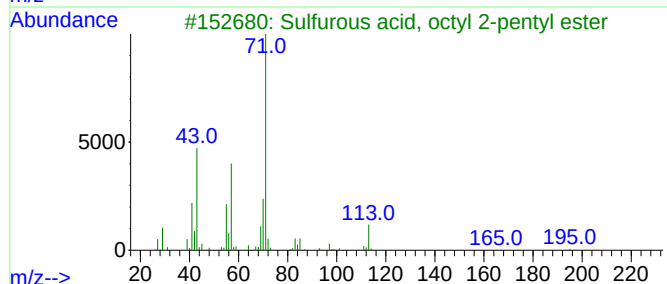
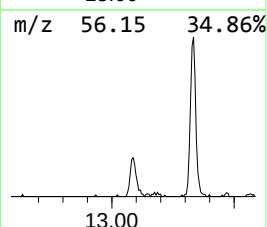
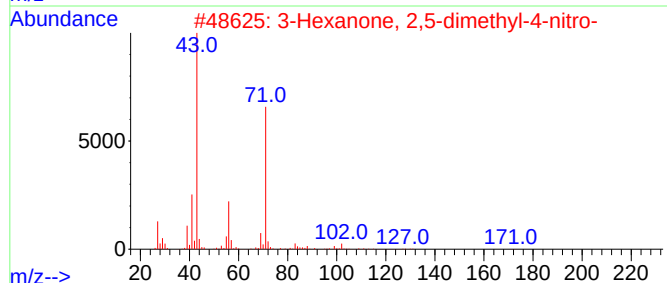
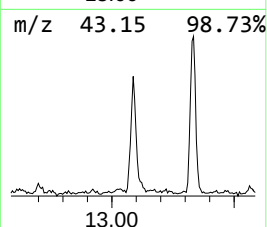
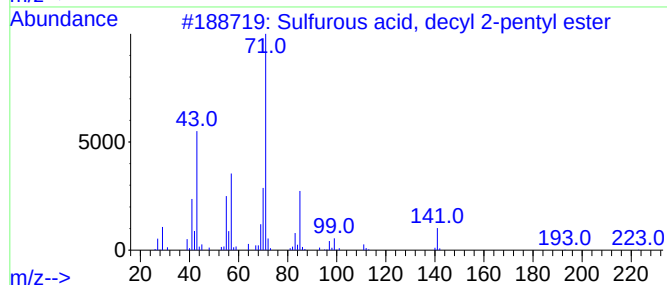
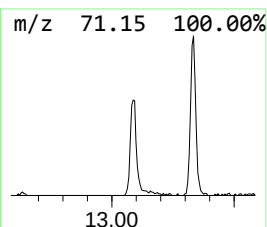
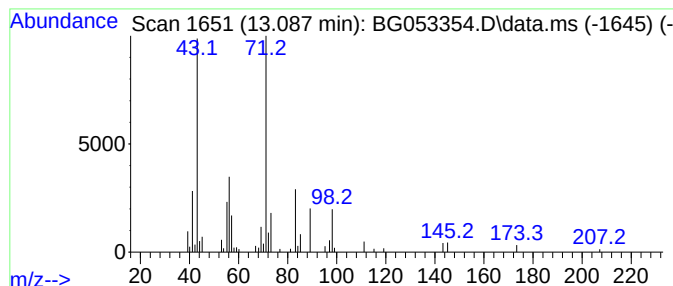
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.087 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.087	5.63 ng	95444	Acenaphthene-d10	14.726

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, decyl 2-pentyl e...	292	C15H32O3S	1000309-15-9	43
2			3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	43
3			Sulfurous acid, octyl 2-pentyl e...	264	C13H28O3S	1000309-15-7	43
4			Sulfurous acid, 2-pentyl undecyl...	306	C16H34O3S	1000309-16-0	43
5			Pentanoic acid, 2,2,4-trimethyl...	216	C12H24O3	244074-78-0	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053354.D
Acq On : 28 Apr 2022 00:40
Operator : CG/JU
Sample : N2482-02
Misc :
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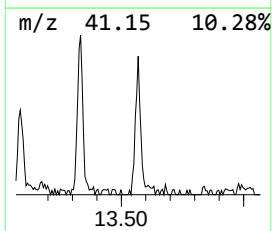
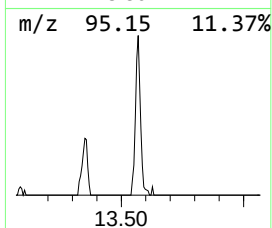
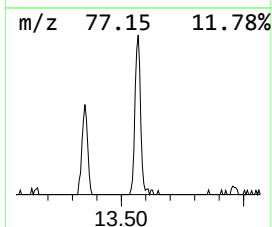
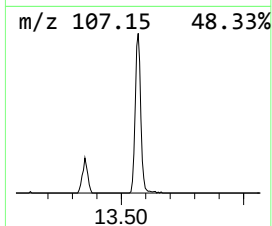
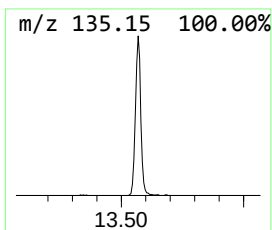
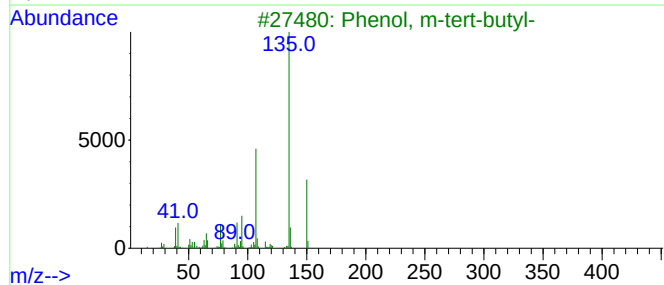
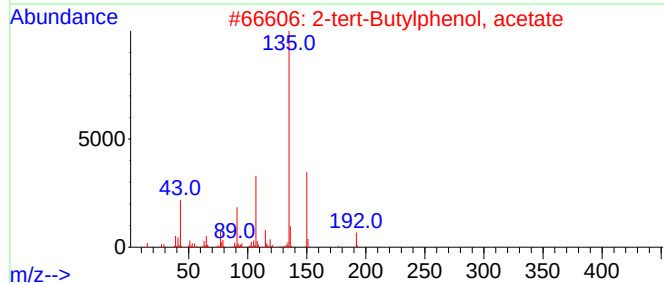
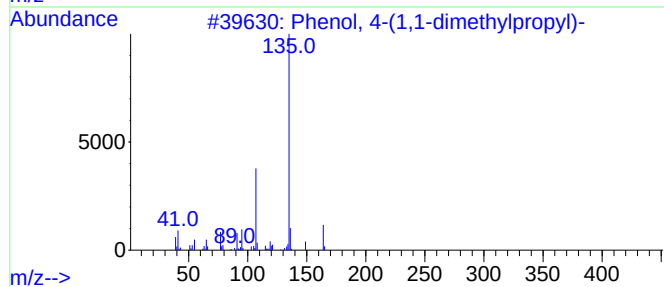
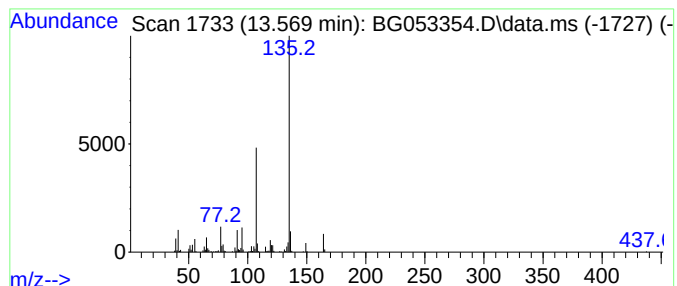
Instrument :
BNA_G
ClientSampleId :
MW-22R

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 10 Phenol, 4-(1,1-dimethylprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
13.569	14.81 ng	250892	Acenaphthene-d10			14.726
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-		164	C11H16O	000080-46-6	96
2	2-tert-Butylphenol, acetate		192	C12H16O2	003245-25-8	72
3	Phenol, m-tert-butyl-		150	C10H14O	000585-34-2	72
4	meso-Hexestrol, 0,0'-bis(n-propy...		442	C26H34O6	1000487-65-0	64
5	Phenol, p-tert-butyl-		150	C10H14O	000098-54-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
Data File : BG053354.D
Acq On : 28 Apr 2022 00:40
Operator : CG/JU
Sample : N2482-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-22R

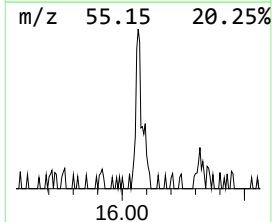
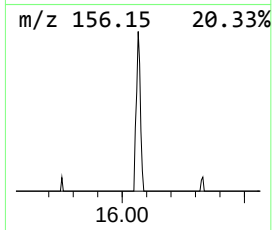
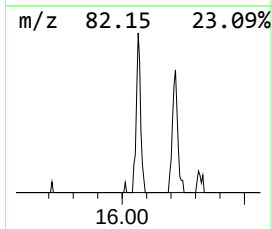
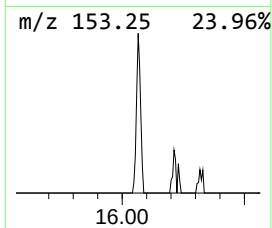
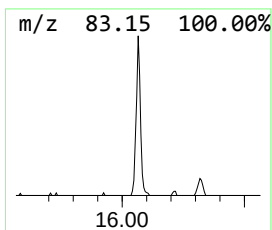
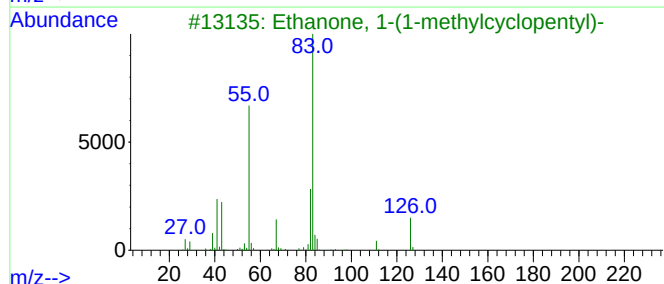
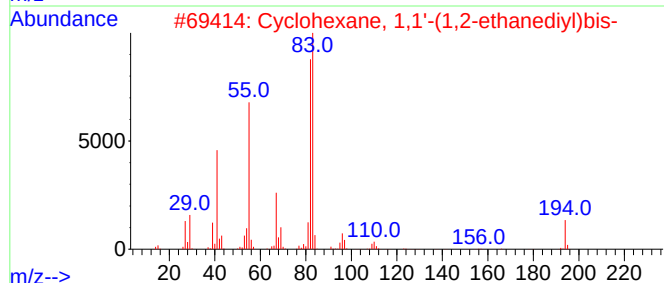
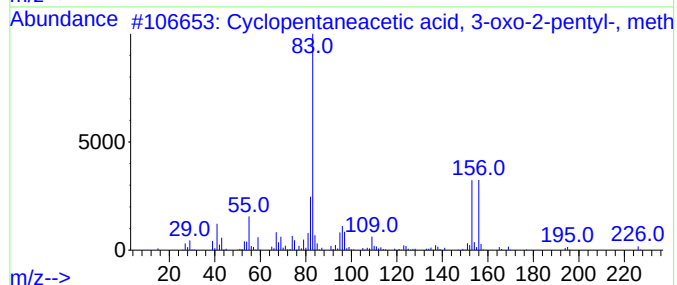
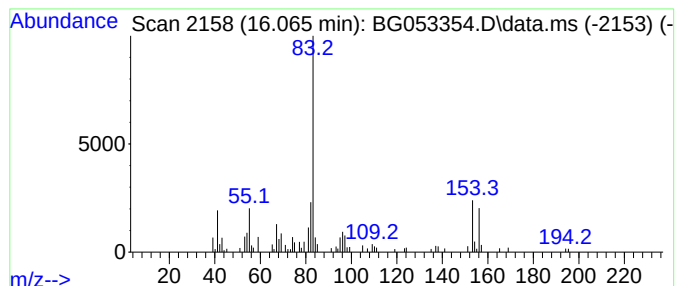
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclopentaneacetic acid, 3-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.065	3.97 ng	67299	Acenaphthene-d10	14.726

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	50
2		Cyclohexane, 1,1'-(1,2-ethanediyl...	194	C14H26	003321-50-4	43
3		Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	43
4		trans-4,4-Dimethyl-2-hexene	112	C8H16	019550-83-5	38
5		Nonenyl tiglate, 2Z-	224	C14H24O2	1000383-61-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
 Data File : BG053354.D
 Acq On : 28 Apr 2022 00:40
 Operator : CG/JU
 Sample : N2482-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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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\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Oxirane, [(1-me...	5.192	8.5	ng	71819	1	8.105	169573	20.0
2-Propanol, 1-(...	7.630	7.0	ng	59649	1	8.105	169573	20.0
1-Propanol, 2-(...	7.677	7.0	ng	59549	1	8.105	169573	20.0
2-Propanol, 1-(...	7.871	12.1	ng	102360	1	8.105	169573	20.0
1-Hexanol, 2-et...	8.158	18.0	ng	152609	1	8.105	169573	20.0
Indane	8.476	8.6	ng	72740	1	8.105	169573	20.0
Nonanoic acid	11.730	3.7	ng	42717	2	10.914	230913	20.0
unknown13.087	13.087	5.6	ng	95444	3	14.726	338812	20.0
Phenol, 4-(1,1-...	13.569	14.8	ng	250892	3	14.726	338812	20.0
Cyclopentaneace...	16.065	4.0	ng	67299	3	14.726	338812	20.0