

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111821\
 Data File : BG051111.D
 Acq On : 18 Nov 2021 18:51
 Operator : CG/JU
 Sample : M4695-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 218

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-BG111321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051111.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.854	57	62	73	rBV	27543	48086	2.83%	0.345%
2	5.758	379	386	398	rBV	547375	912690	53.75%	6.545%
3	7.374	653	661	675	rBV	552458	999075	58.84%	7.165%
4	8.220	798	805	816	rVB	119722	207903	12.24%	1.491%
5	9.395	996	1005	1017	rBV	319139	591627	34.84%	4.243%
6	10.793	1235	1243	1255	rBV	47853	102969	6.06%	0.738%
7	11.046	1277	1286	1295	rBV	176304	314612	18.53%	2.256%
8	13.467	1690	1698	1707	rBV	776562	1210606	71.30%	8.682%
9	13.713	1733	1740	1744	rBV	19876	31511	1.86%	0.226%
10	13.766	1744	1749	1763	rVV	32721	77289	4.55%	0.554%
11	14.753	1911	1917	1926	rBV	22998	51590	3.04%	0.370%
12	14.847	1926	1933	1940	rVB	285095	450901	26.55%	3.234%
13	16.334	2180	2186	2197	rBV	589958	939985	55.36%	6.741%
14	17.221	2333	2337	2346	rBV	49516	103056	6.07%	0.739%
15	17.597	2394	2401	2406	rBV	343476	537666	31.66%	3.856%
16	18.220	2503	2507	2511	rVB2	17399	19537	1.15%	0.140%
17	19.207	2670	2675	2688	rBV	276427	484869	28.56%	3.477%
18	19.377	2701	2704	2709	rVB2	49853	57622	3.39%	0.413%
19	19.506	2723	2726	2731	rVB4	15406	19434	1.14%	0.139%
20	19.636	2744	2748	2755	rVB	50004	70185	4.13%	0.503%
21	20.000	2806	2810	2818	rVB	37413	54886	3.23%	0.394%
22	20.182	2835	2841	2847	rBV	1316507	1697990	100.00%	12.177%
23	20.452	2881	2887	2891	rBV4	21533	42857	2.52%	0.307%
24	20.764	2935	2940	2962	rBV	680754	1117636	65.82%	8.015%
25	21.487	3058	3063	3073	rVB3	48242	106511	6.27%	0.764%
26	21.581	3076	3079	3084	rVB	25188	35342	2.08%	0.253%
27	21.892	3125	3132	3138	rBV	294958	536436	31.59%	3.847%
28	22.327	3199	3206	3224	rBV	632021	1318006	77.62%	9.452%
29	24.471	3563	3571	3597	rBV	312321	984920	58.01%	7.063%
30	25.300	3704	3712	3725	rVB3	164131	490090	28.86%	3.515%
31	27.820	4132	4141	4157	rBV4	64123	328732	19.36%	2.357%

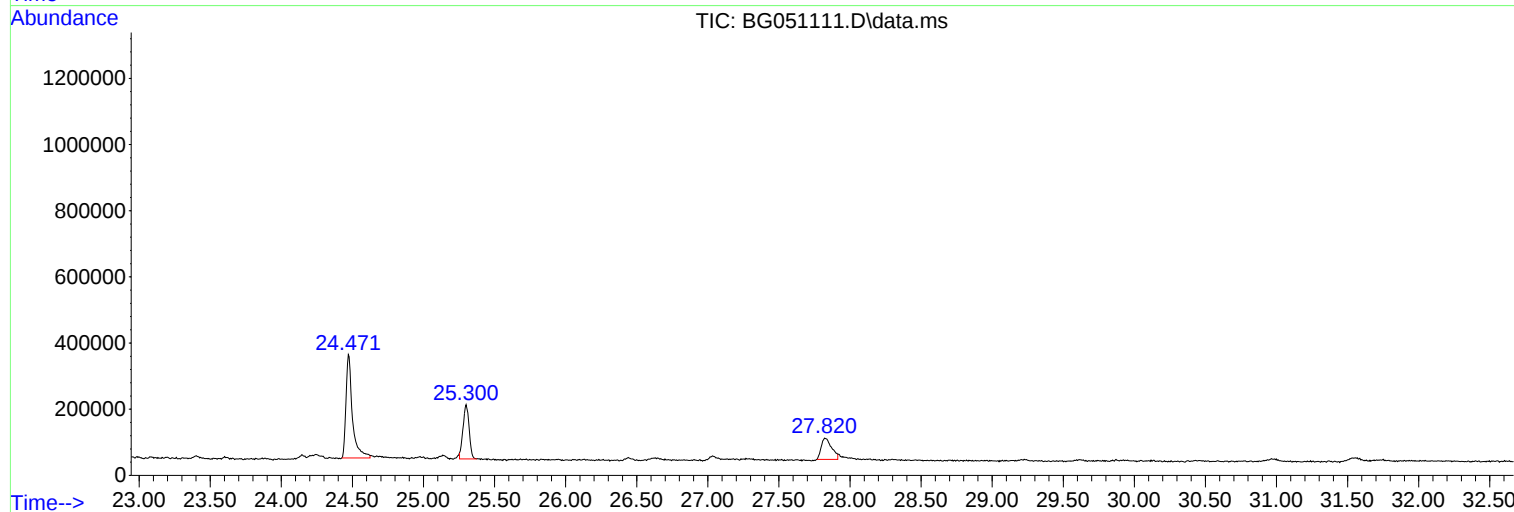
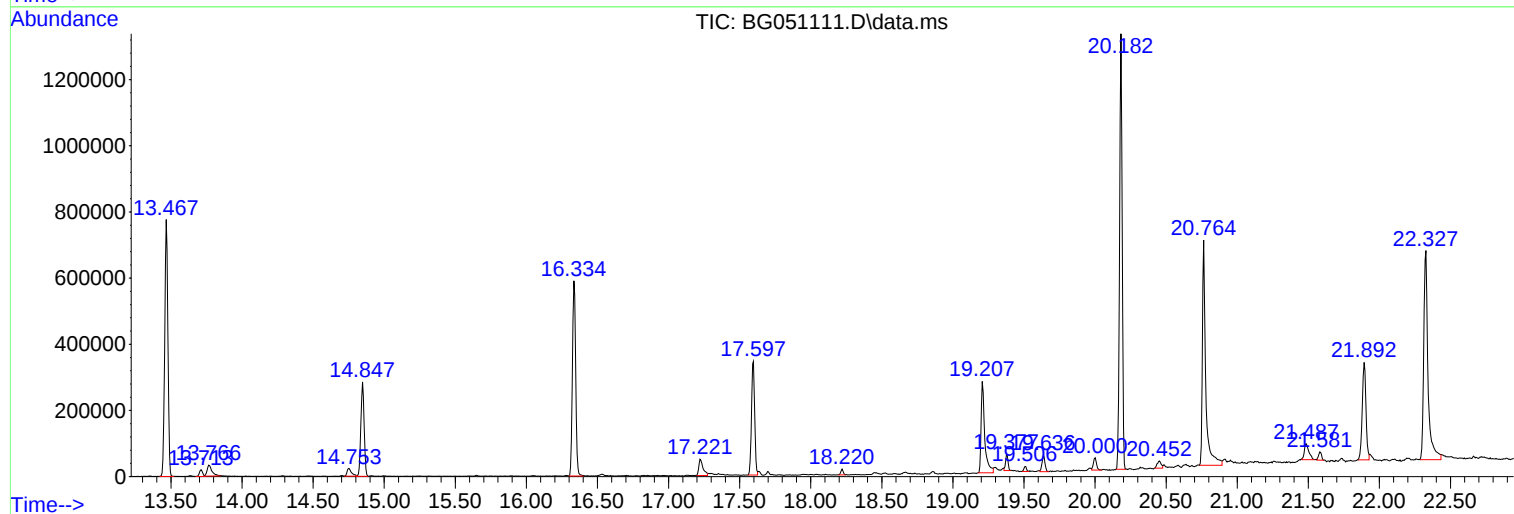
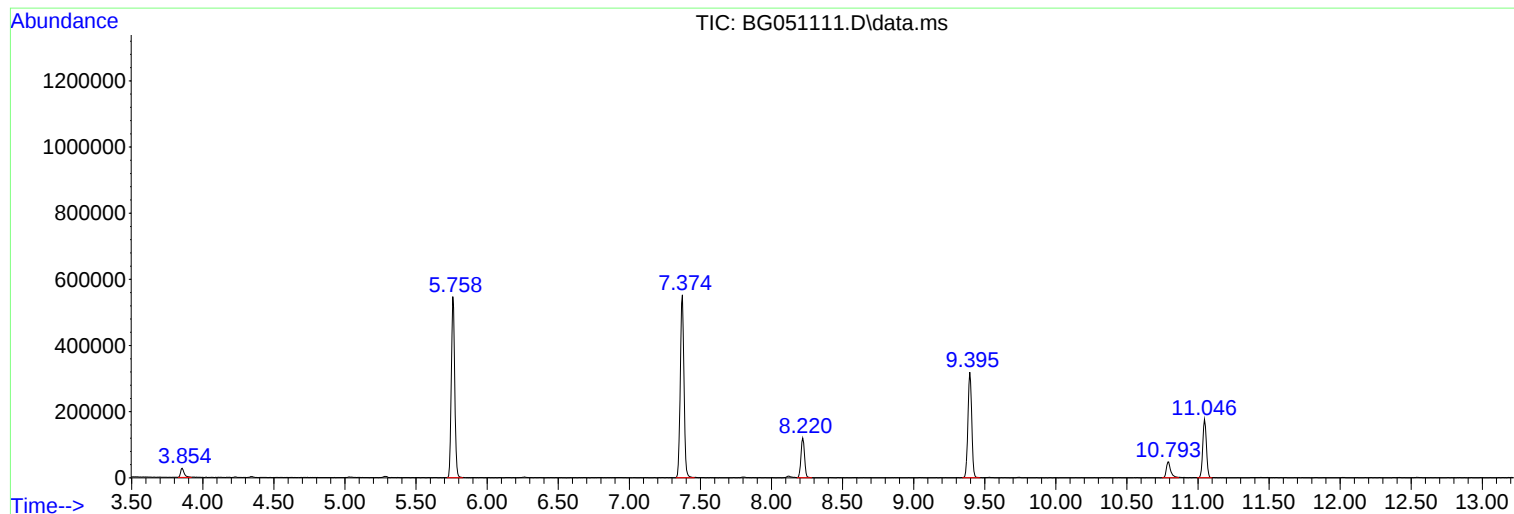
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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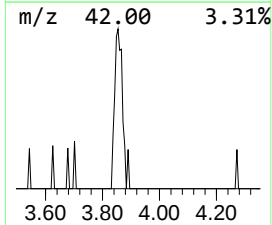
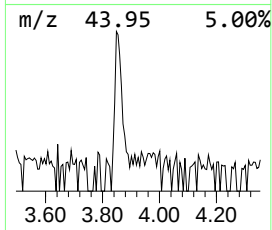
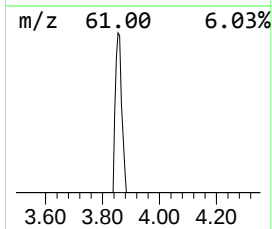
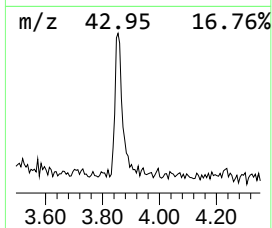
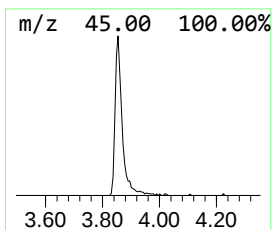
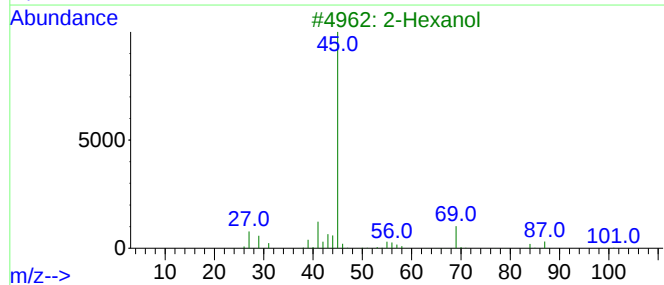
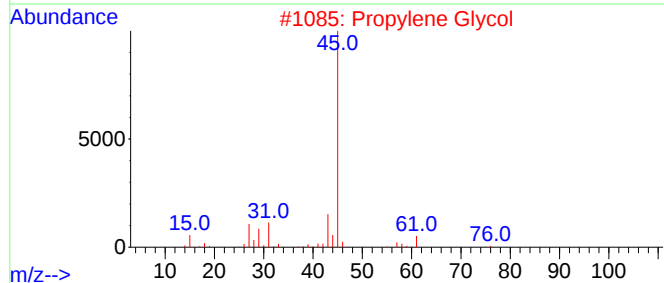
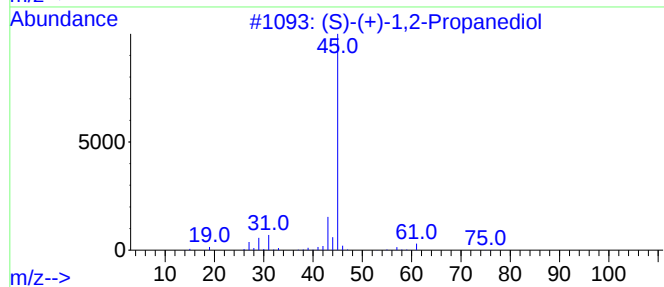
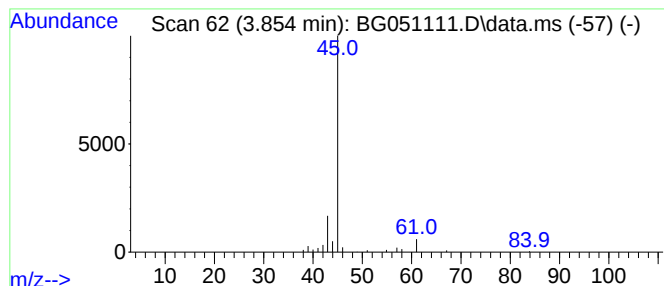
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.854 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.854	4.63 ng	48086	1,4-Dichlorobenzene-d4	8.220

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	43
2	Propylene Glycol			76	C3H8O2	000057-55-6	9
3	2-Hexanol			102	C6H14O	000626-93-7	9
4	Isopropyl Alcohol			60	C3H8O	000067-63-0	9
5	2-Heptanol, (S)-			116	C7H16O	006033-23-4	9



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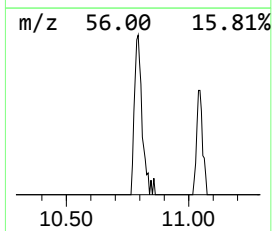
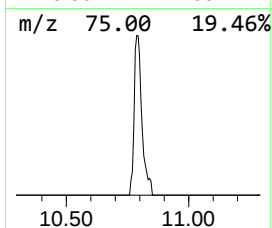
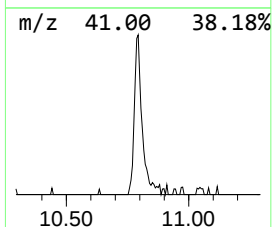
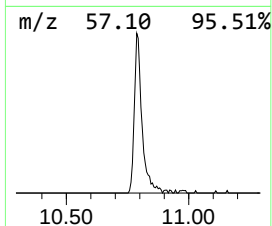
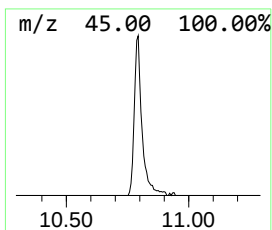
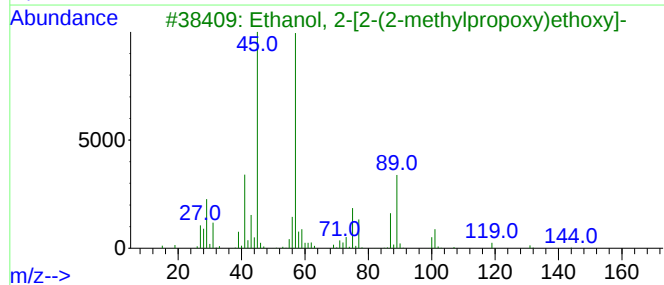
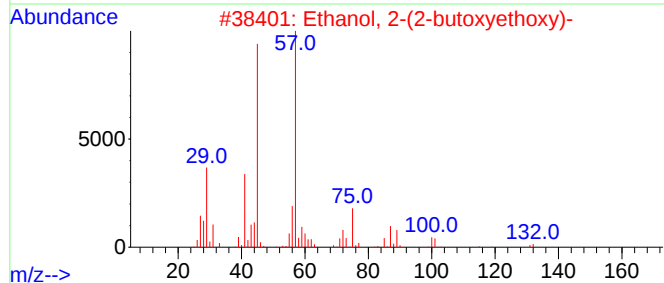
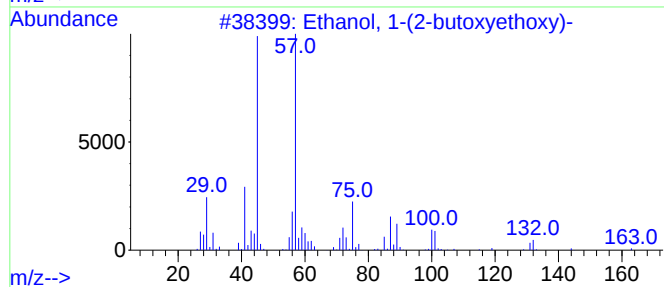
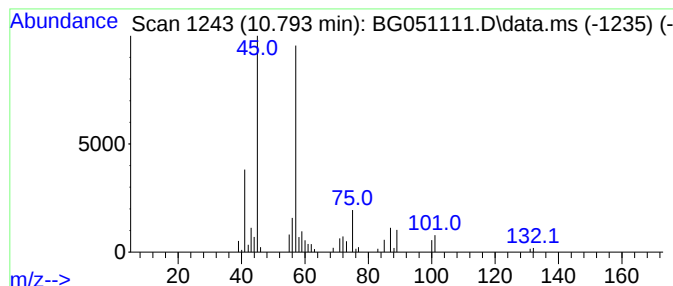
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Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.793	6.55 ng	102969	Naphthalene-d8	11.046

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Tetraethylene glycol	194	C8H18O5	000112-60-7	47
5			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	47



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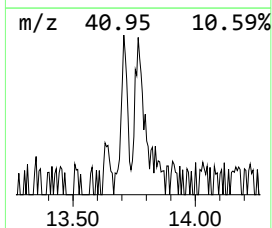
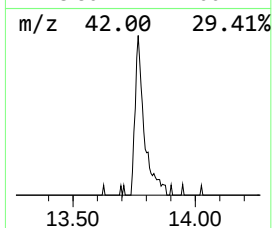
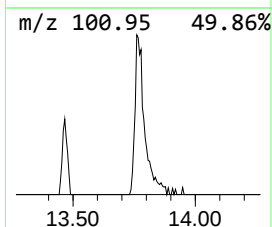
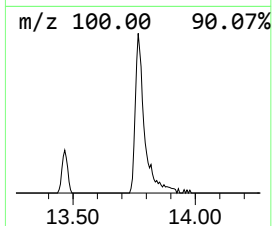
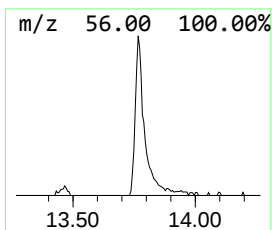
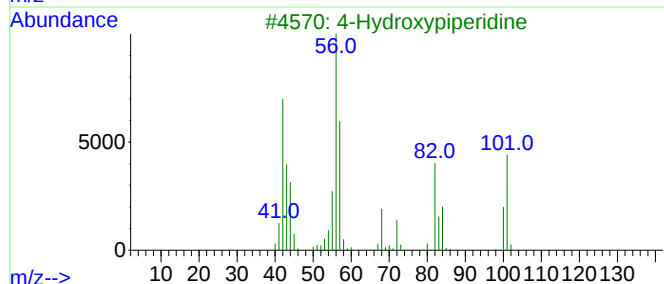
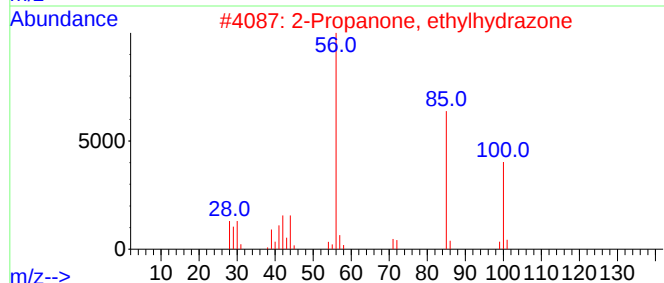
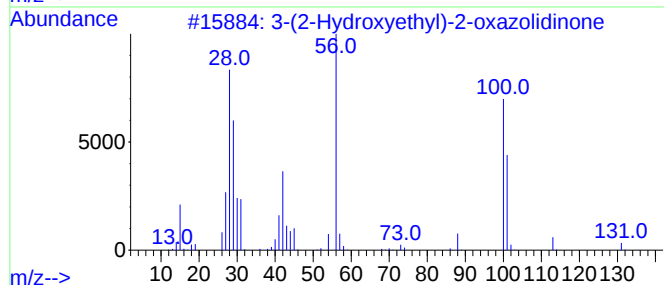
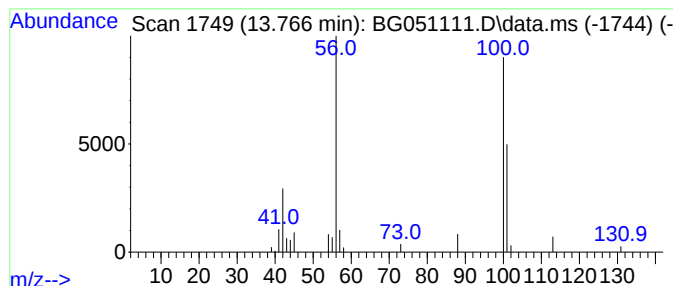
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Peak Number 3 3-(2-Hydroxyethyl)-2-oxazol... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.766	3.43 ng	77289	Acenaphthene-d10	14.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-(2-Hydroxyethyl)-2-oxazolidinone	131	C5H9NO3	003356-88-5	91
2			2-Propanone, ethylhydrazone	100	C5H12N2	007422-99-3	45
3			4-Hydroxypiperidine	101	C5H11NO	005382-16-1	38
4			4-Morpholineethanol	131	C6H13NO2	000622-40-2	32
5			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	25



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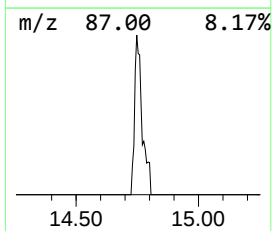
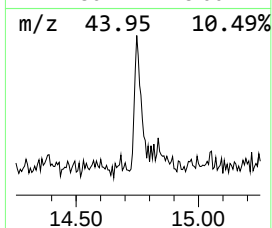
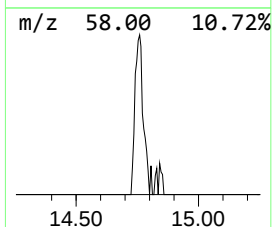
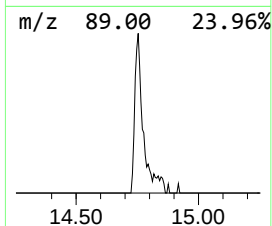
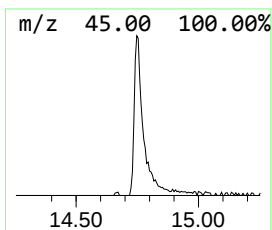
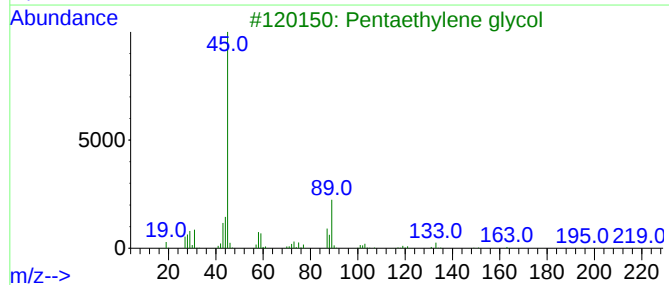
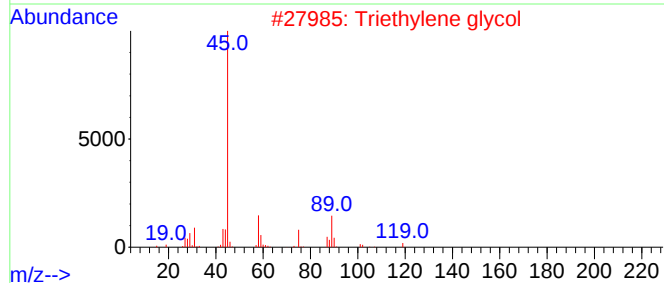
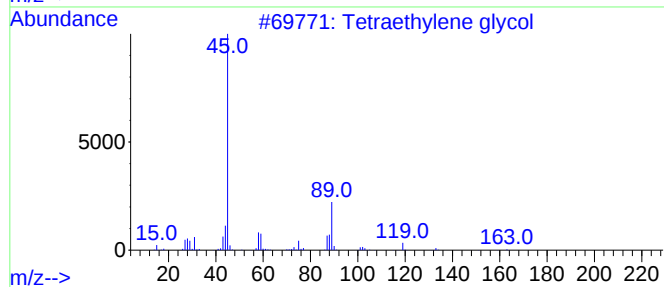
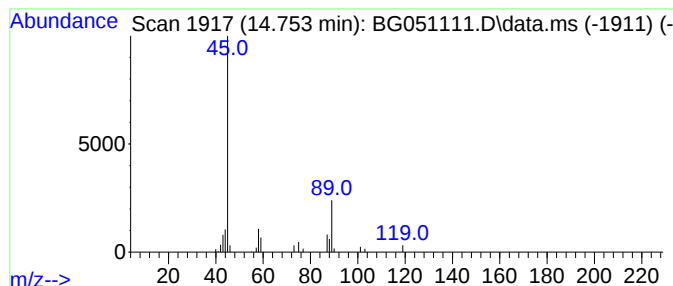
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Peak Number 4 Tetraethylene glycol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.753	2.29 ng	51590	Acenaphthene-d10	14.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetraethylene glycol	194	C8H18O5	000112-60-7	83
2			Triethylene glycol	150	C6H14O4	000112-27-6	83
3			Pentaethylene glycol	238	C10H22O6	004792-15-8	83
4			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	72
5			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	56



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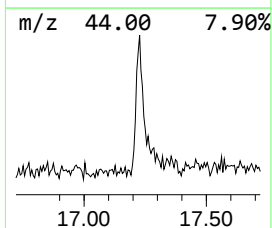
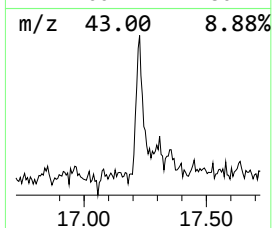
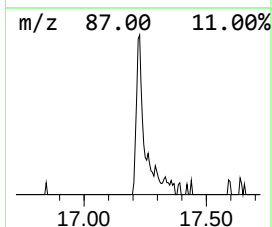
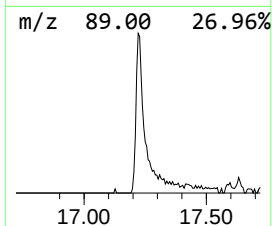
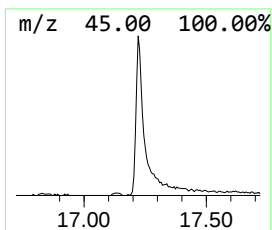
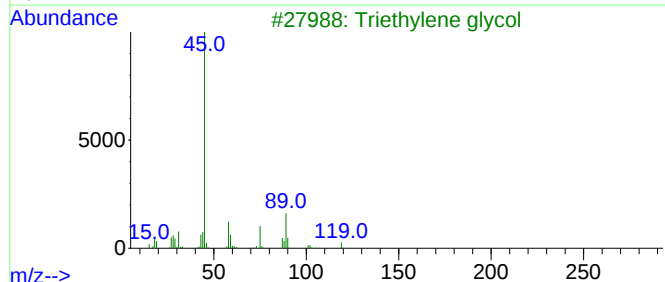
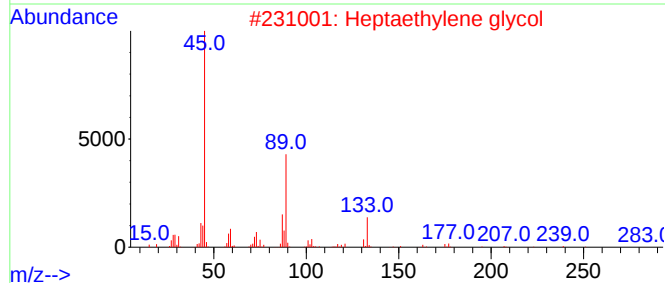
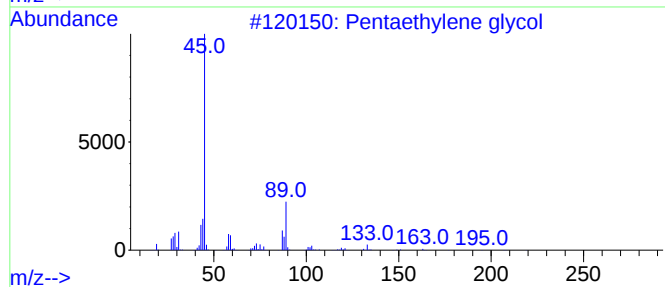
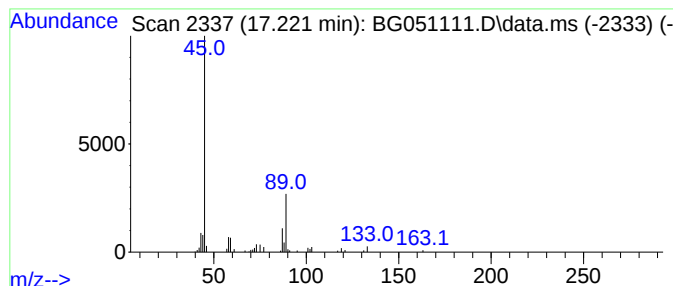
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Peak Number 5 Pentaethylene glycol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.221	3.83 ng	103056	Phenanthrene-d10	17.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentaethylene glycol	238	C10H22O6	004792-15-8	83
2			Heptaethylene glycol	326	C14H30O8	005617-32-3	83
3			Triethylene glycol	150	C6H14O4	000112-27-6	64
4			3,6,9,12-Tetraoxatetradecan-1-ol	222	C10H22O5	005650-20-4	56
5			Tetraethylene glycol	194	C8H18O5	000112-60-7	56



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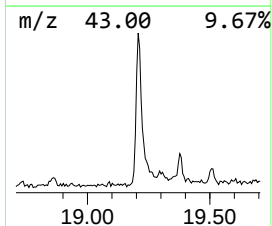
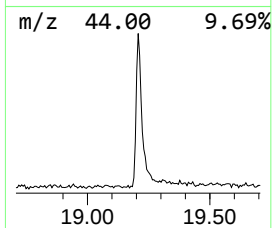
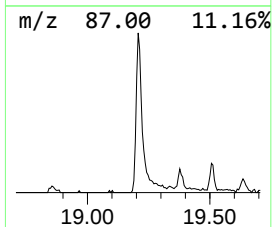
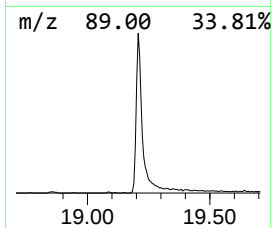
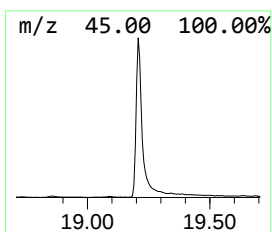
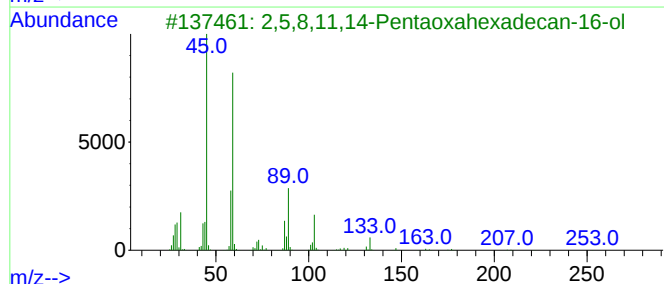
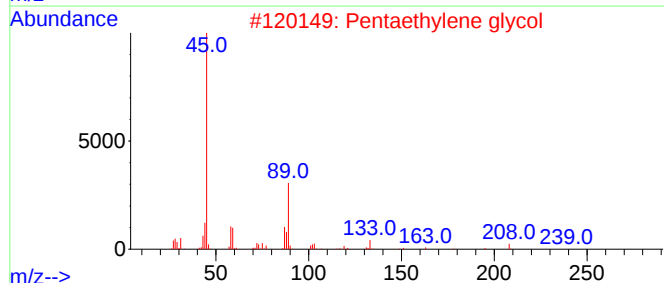
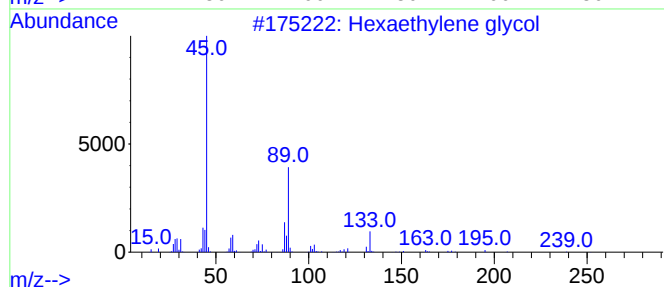
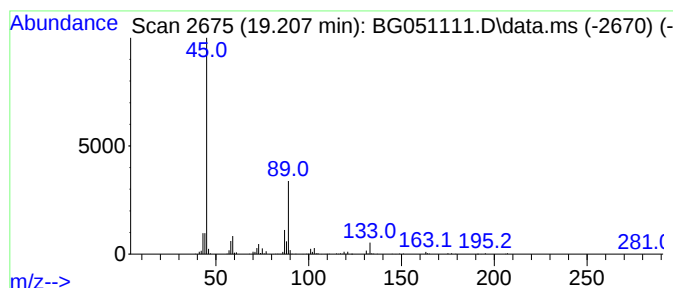
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexaethylene glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.207	18.04 ng	484869	Phenanthrene-d10	17.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexaethylene glycol	282	C12H26O7	002615-15-8	91
2			Pentaethylene glycol	238	C10H22O6	004792-15-8	90
3			2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	83
4			3,6,9,12-Tetraoxatetradecan-1-ol	222	C10H22O5	005650-20-4	78
5			Ethanol, 2-[2-(2-methoxyethoxy)e...	164	C7H16O4	000112-35-6	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111821\
Data File : BG051111.D
Acq On : 18 Nov 2021 18:51
Operator : CG/JU
Sample : M4695-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

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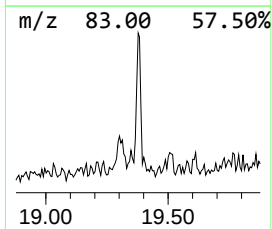
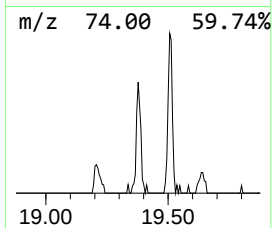
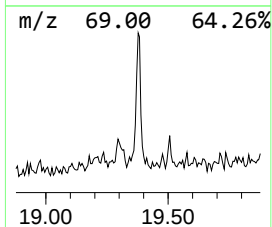
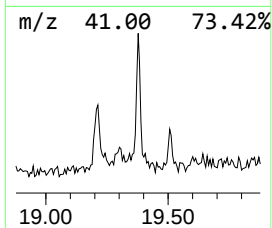
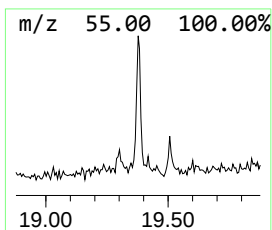
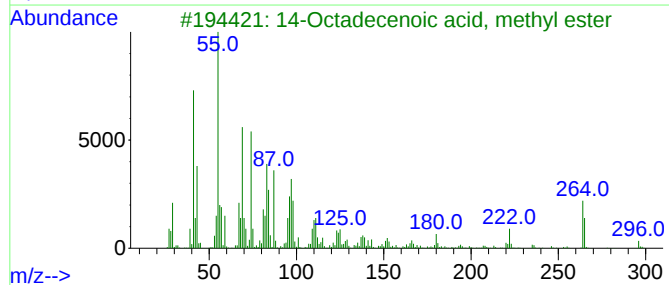
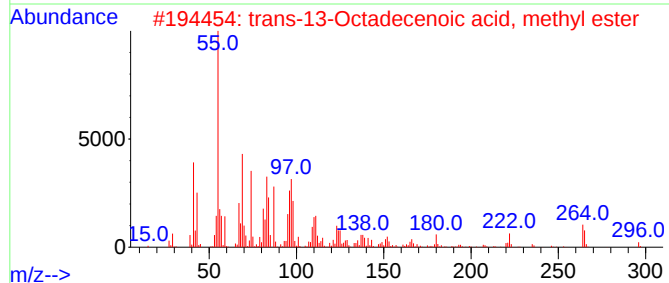
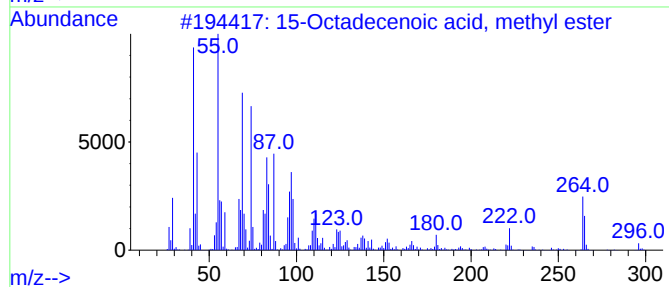
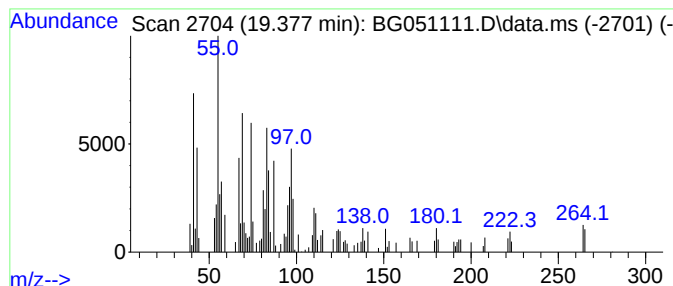
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 15-Octadecenoic acid, methyl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.377	2.14 ng	57622	Phenanthrene-d10	17.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91
2			trans-13-Octadecenoic acid, methyl ester	296	C19H36O2	1000333-61-3	91
3			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
4			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	90
5			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111821\
Data File : BG051111.D
Acq On : 18 Nov 2021 18:51
Operator : CG/JU
Sample : M4695-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

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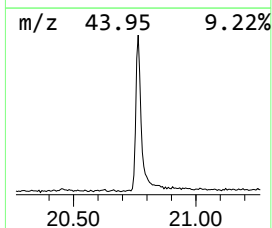
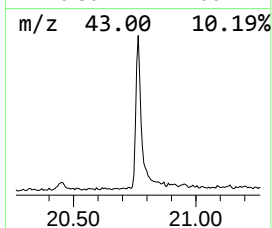
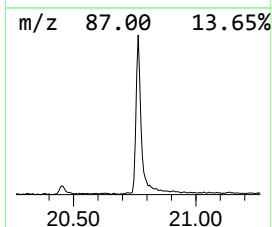
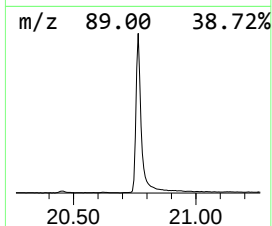
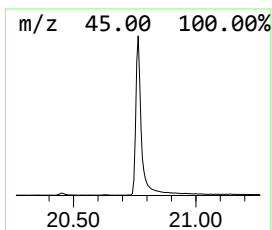
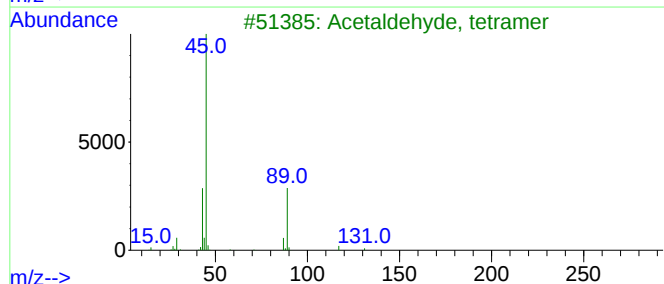
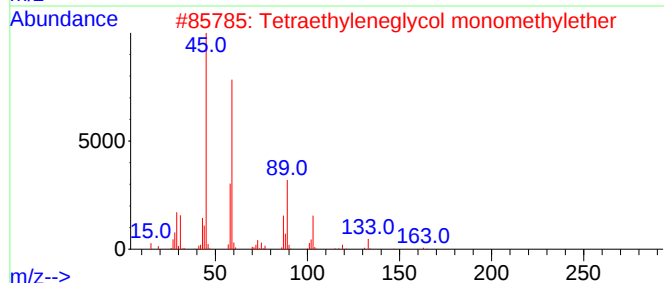
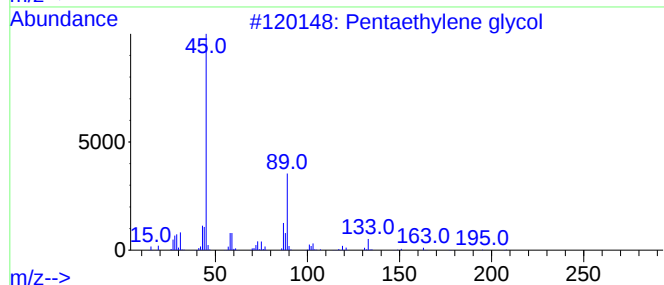
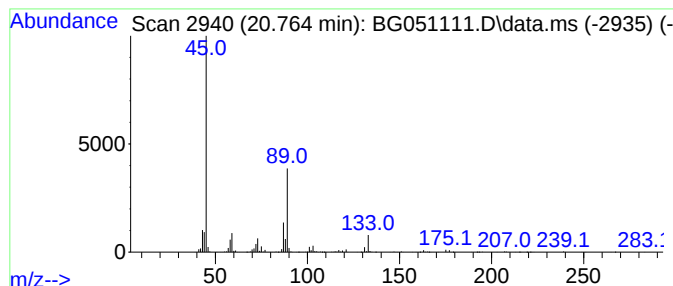
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetraethyleneglycol monomet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.764	41.67 ng	1117640	Chrysene-d12	21.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentaethylene glycol	238	C10H22O6	004792-15-8	83
2			Tetraethyleneglycol monomethylether	208	C9H20O5	023783-42-8	83
3			Acetaldehyde, tetramer	176	C8H16O4	000108-62-3	72
4			2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	72
5			2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111821\
Data File : BG051111.D
Acq On : 18 Nov 2021 18:51
Operator : CG/JU
Sample : M4695-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

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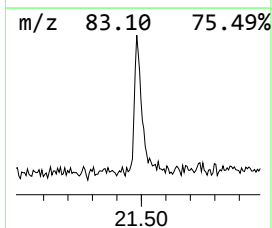
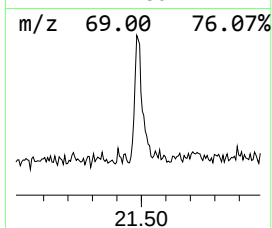
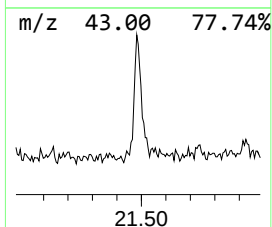
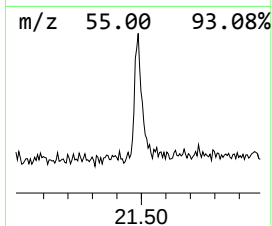
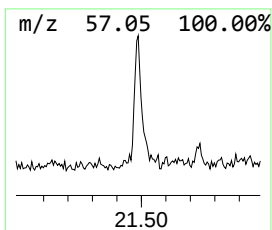
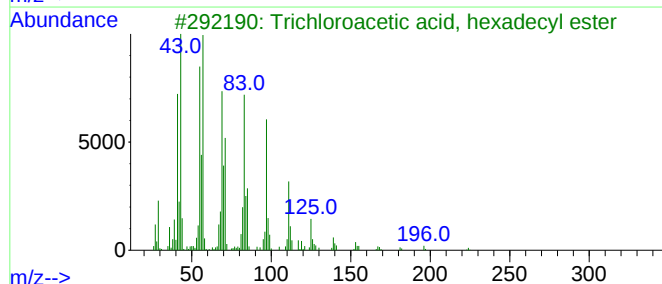
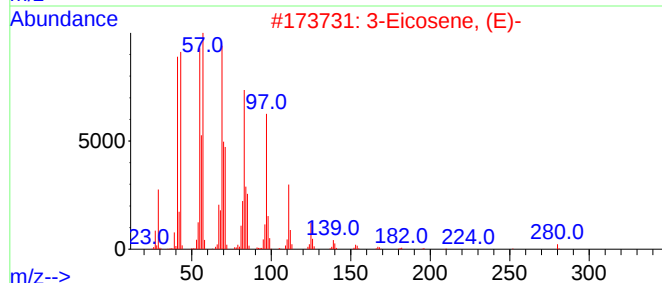
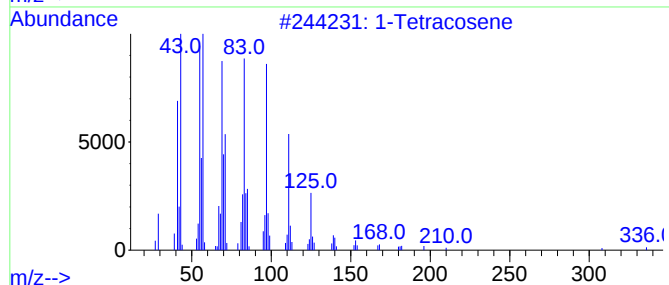
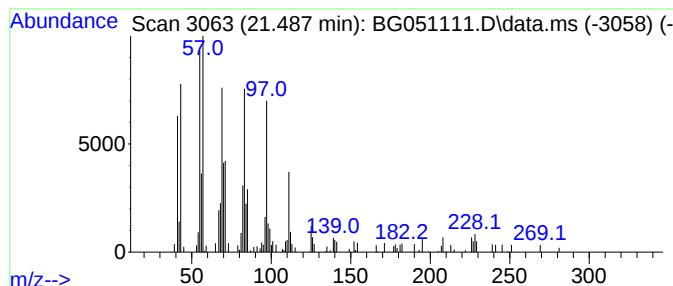
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Tetracosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.486	3.97 ng	106511	Chrysene-d12	21.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetracosene	336	C24H48	010192-32-2	94
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4			1-Tricosene	322	C23H46	018835-32-0	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111821\
Data File : BG051111.D
Acq On : 18 Nov 2021 18:51
Operator : CG/JU
Sample : M4695-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

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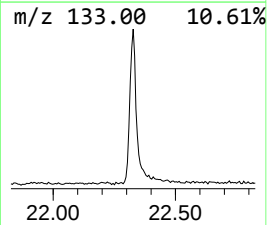
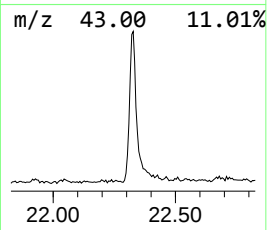
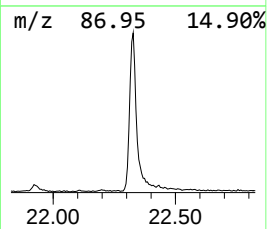
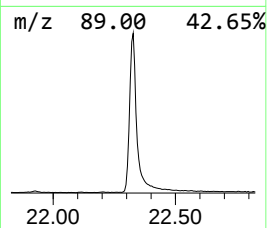
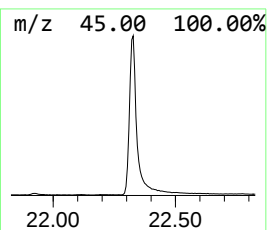
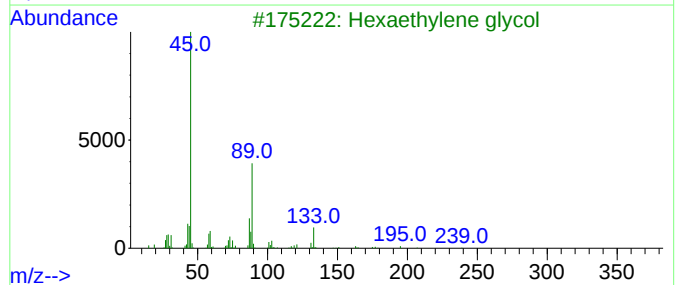
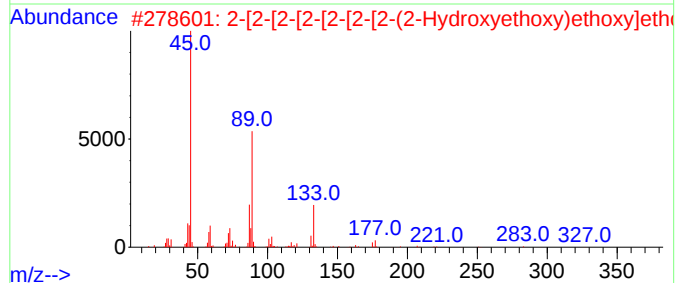
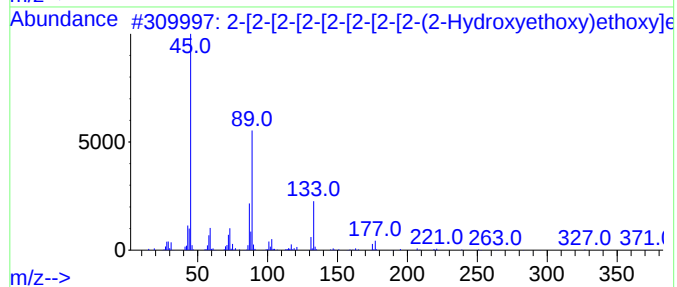
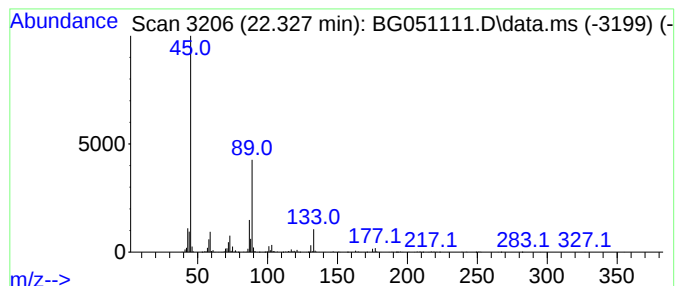
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-[2-[2-[2-[2-[2-[2-(2-H... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.327	49.14 ng	1318010	Chrysene-d12	21.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2	-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38010	003386-18-3	91	
2	2	-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H3409	005117-19-1	91	
3	Hexaethylene glycol	282	C12H2607	002615-15-8	91		
4	Heptaethylene glycol	326	C14H3008	005617-32-3	72		
5	Acetaldehyde, tetramer	176	C8H1604	000108-62-3	64		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111821\
Data File : BG051111.D
Acq On : 18 Nov 2021 18:51
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Sample : M4695-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

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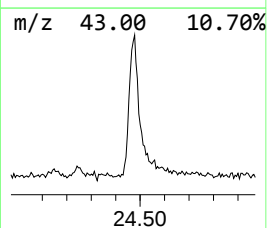
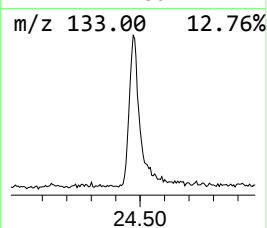
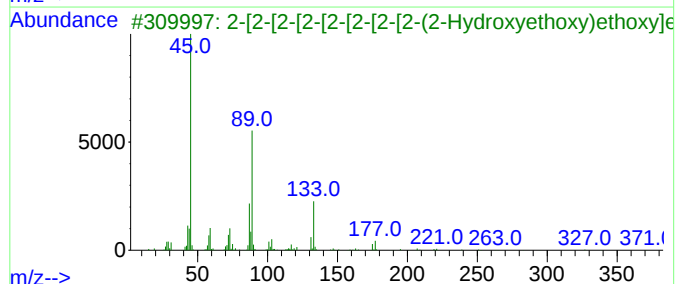
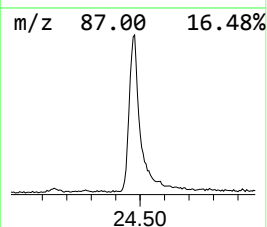
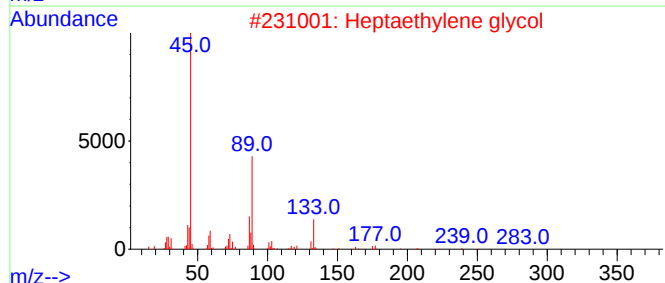
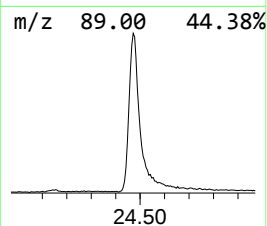
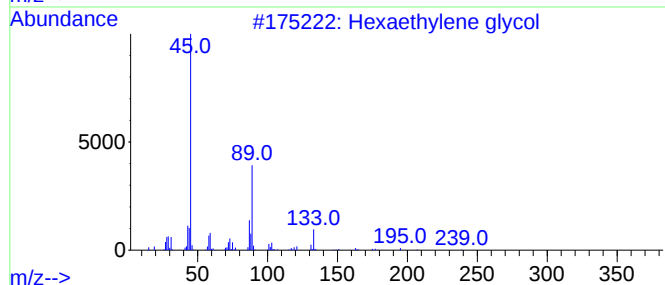
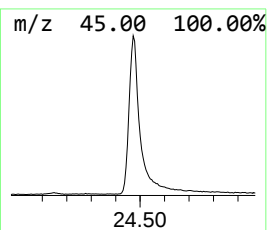
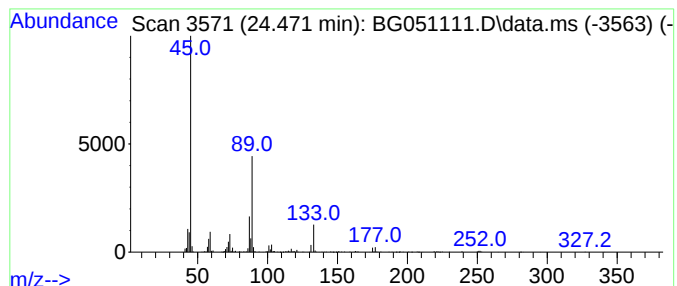
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heptaethylene glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.471	40.19 ng	984920	Perylene-d12	25.300

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexaethylene glycol	282	C12H26O7	002615-15-8	91
2			Heptaethylene glycol	326	C14H30O8	005617-32-3	91
3			2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	91
4			2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	91
5			2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	006809-70-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111821\
Data File : BG051111.D
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Sample : M4695-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

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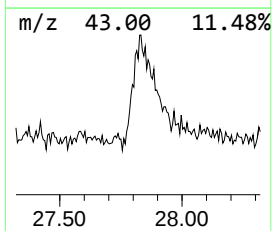
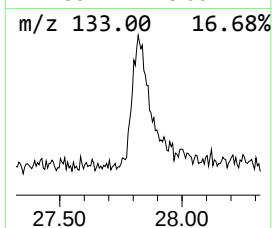
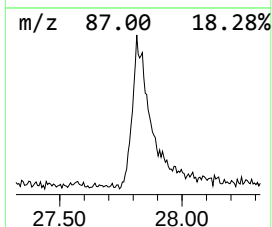
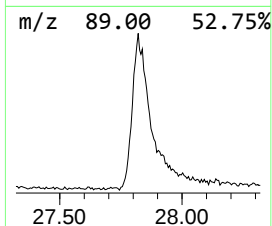
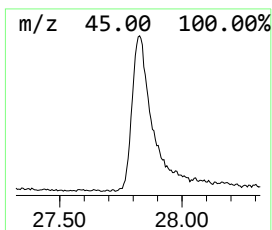
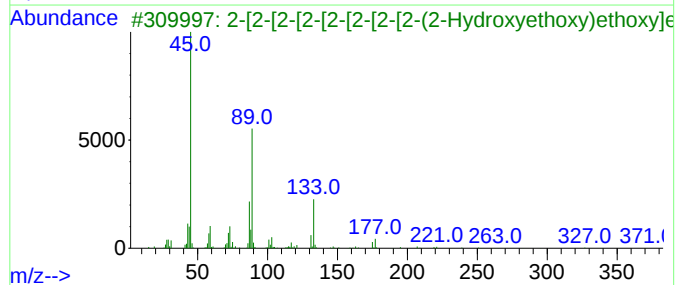
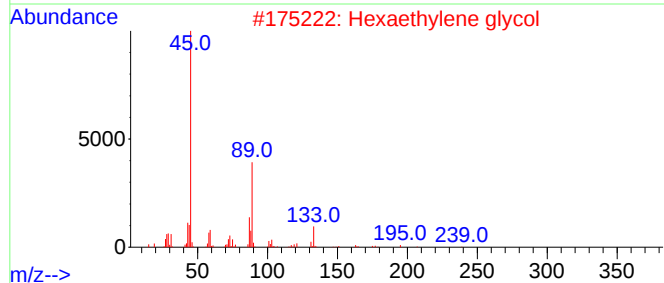
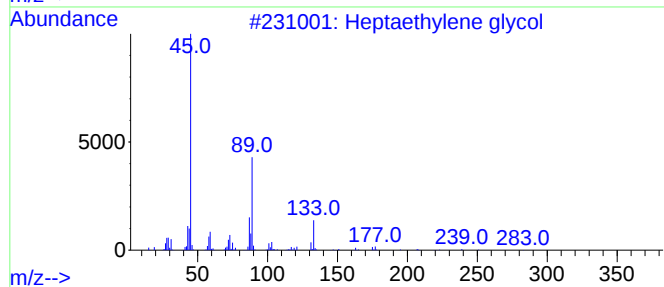
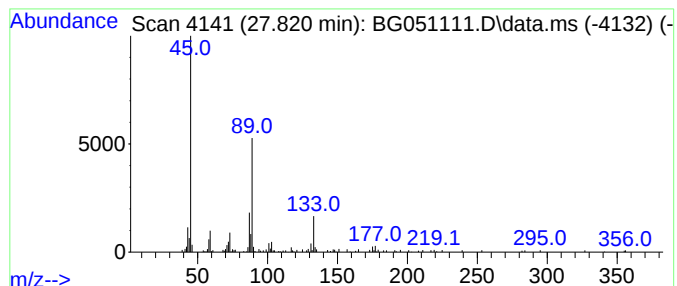
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown27.820 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.820	13.42 ng	328732	Perylene-d12	25.300

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptaethylene glycol	326	C14H30O8	005617-32-3	91
2		Hexaethylene glycol	282	C12H26O7	002615-15-8	90
3		2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	76
4		2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	72
5		Tetraethylene glycol	194	C8H18O5	000112-60-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111821\
 Data File : BG051111.D
 Acq On : 18 Nov 2021 18:51
 Operator : CG/JU
 Sample : M4695-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 218

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111321.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
unknown3.854	3.854	4.6	ng	48086	1	8.220	207903	20.0
Ethanol, 1-(2-b...	10.793	6.5	ng	102969	2	11.046	314612	20.0
3-(2-Hydroxyeth...	13.766	3.4	ng	77289	3	14.847	450901	20.0
Tetraethylene g...	14.753	2.3	ng	51590	3	14.847	450901	20.0
Pentaethylene g...	17.221	3.8	ng	103056	4	17.597	537666	20.0
Hexaethylene gl...	19.207	18.0	ng	484869	4	17.597	537666	20.0
15-Octadecenoic...	19.377	2.1	ng	57622	4	17.597	537666	20.0
Tetraethylenegl...	20.764	41.7	ng	1117640	5	21.892	536436	20.0
1-Tetracosene	21.486	4.0	ng	106511	5	21.892	536436	20.0
2-[2-[2-[2-[2-[...	22.327	49.1	ng	1318010	5	21.892	536436	20.0
Heptaethylene g...	24.471	40.2	ng	984920	6	25.300	490090	20.0
unknown27.820	27.820	13.4	ng	328732	6	25.300	490090	20.0