

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051424\
 Data File : BG061191.D
 Acq On : 14 May 2024 15:53
 Operator : MA/JU
 Sample : P2330-22
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 H-3(5.0-6.0)

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-BG043024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061191.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.071	9	14	21	rVB4	10725	22963	1.73%	0.320%
2	3.147	21	27	42	rVB	240208	377112	28.41%	5.247%
3	3.670	111	116	126	rBV	18571	29287	2.21%	0.407%
4	5.521	425	431	441	rBV	319569	489503	36.88%	6.811%
5	7.107	692	701	711	rBV	312646	538856	40.59%	7.497%
6	7.924	834	840	847	rVB	95287	154750	11.66%	2.153%
7	9.081	1030	1037	1046	rVB	180381	323209	24.35%	4.497%
8	10.497	1271	1278	1287	rBV3	11291	23924	1.80%	0.333%
9	10.721	1308	1316	1325	rVB	106665	187450	14.12%	2.608%
10	13.176	1727	1734	1744	rBV	449352	683685	51.50%	9.513%
11	14.557	1962	1969	1976	rBV	181867	277635	20.92%	3.863%
12	14.775	1998	2006	2012	rBV6	9172	21024	1.58%	0.293%
13	16.050	2216	2223	2234	rBV	476394	745342	56.15%	10.370%
14	17.307	2430	2437	2442	rBV	264132	412321	31.06%	5.737%
15	17.348	2442	2444	2450	rVB	14994	16754	1.26%	0.233%
16	18.206	2585	2590	2598	rBV2	17811	29143	2.20%	0.405%
17	19.128	2743	2747	2752	rBV	53456	62799	4.73%	0.874%
18	19.363	2781	2787	2791	rBV	20876	31787	2.39%	0.442%
19	19.722	2846	2848	2856	rVB	17701	23761	1.79%	0.331%
20	19.922	2875	2882	2892	rBV	1024990	1327423	100.00%	18.469%
21	20.239	2929	2936	2940	rBV	45354	62109	4.68%	0.864%
22	20.732	3015	3020	3024	rBV4	9566	16294	1.23%	0.227%
23	21.232	3100	3105	3116	rBV2	42285	87342	6.58%	1.215%
24	21.561	3154	3161	3168	rBV2	311827	519838	39.16%	7.233%
25	22.354	3290	3296	3300	rBV2	18771	33910	2.55%	0.472%
26	23.206	3436	3441	3449	rVB3	39937	81651	6.15%	1.136%
27	23.805	3538	3543	3551	rVB5	15237	30420	2.29%	0.423%
28	23.987	3572	3574	3584	rVB9	7200	15629	1.18%	0.217%
29	24.687	3681	3693	3703	rBV	187631	561239	42.28%	7.809%

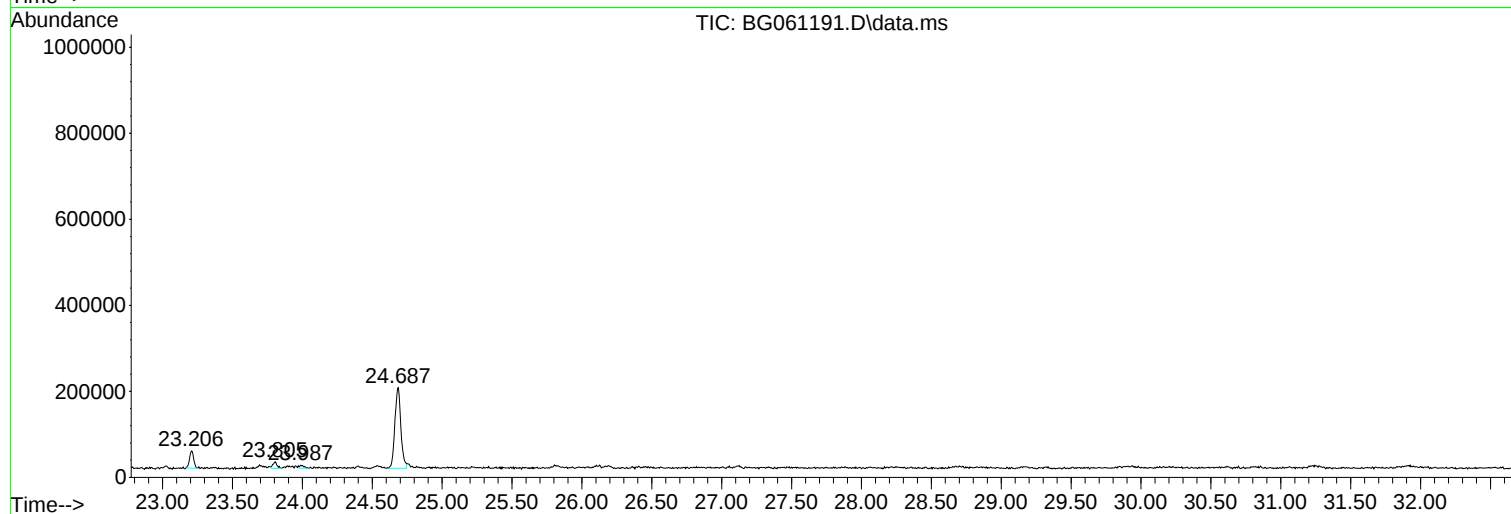
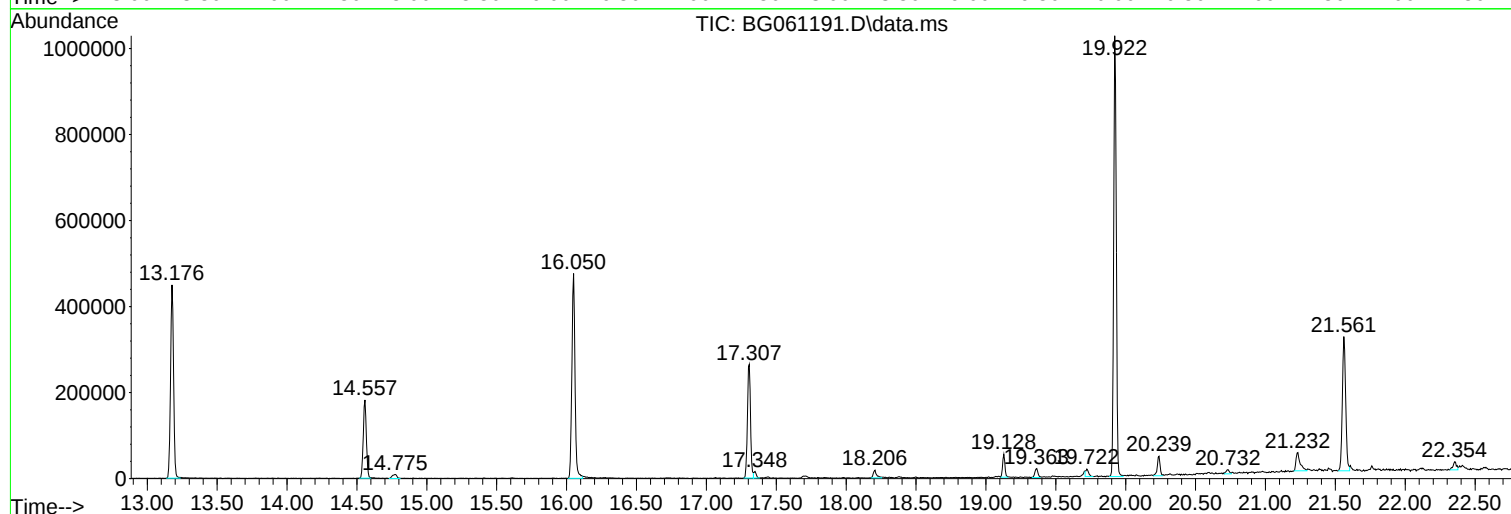
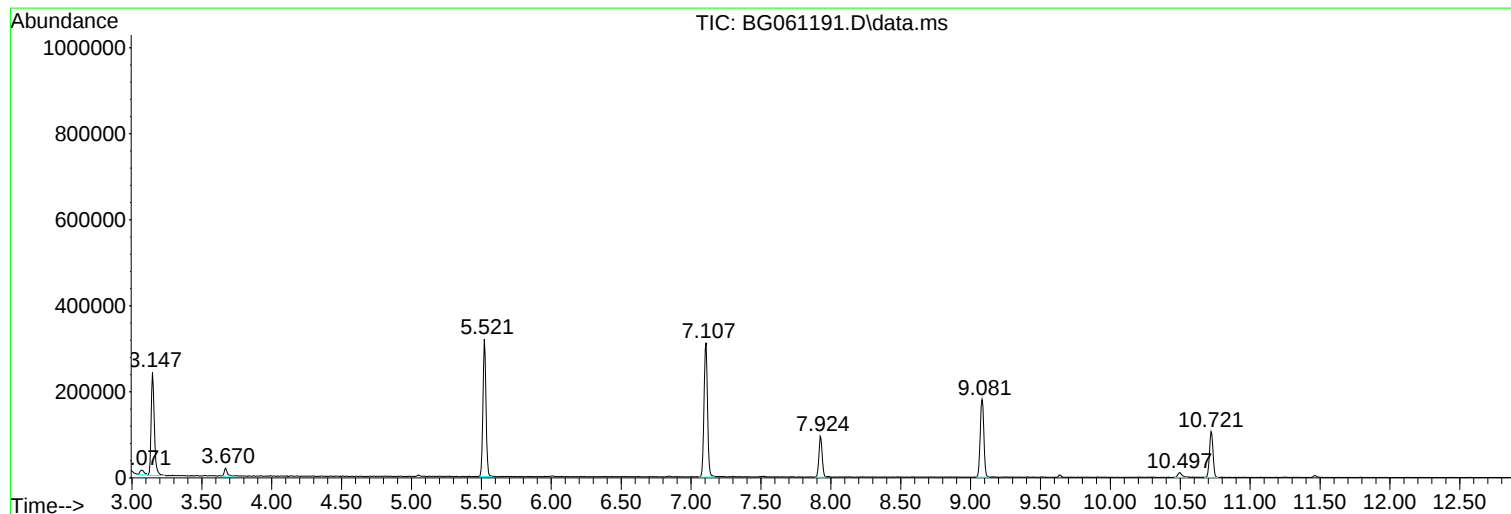
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Instrument :
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ClientSampleId :
H-3(5.0-6.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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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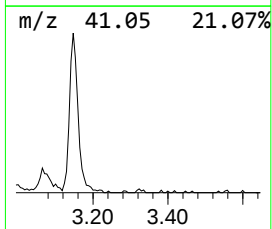
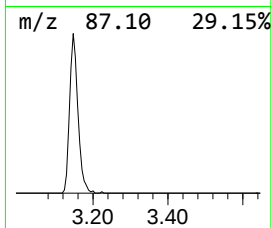
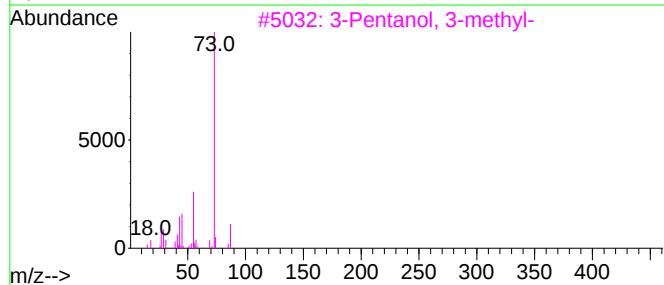
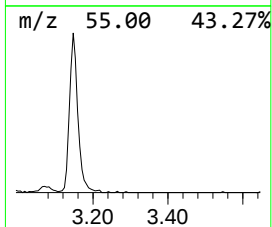
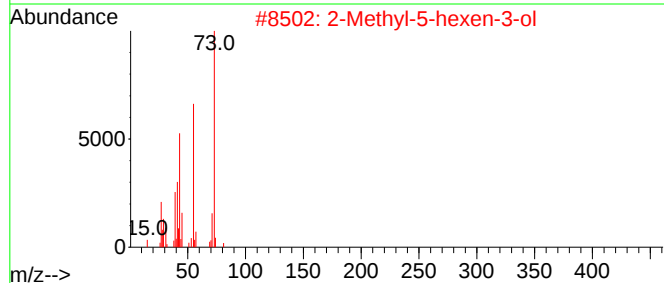
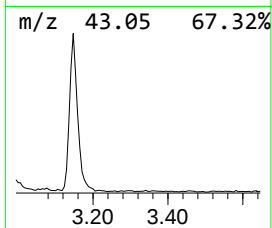
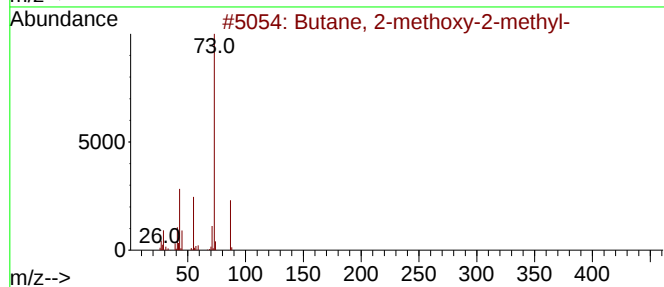
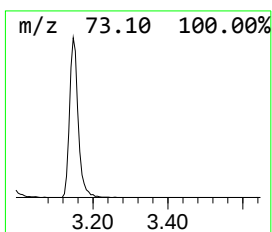
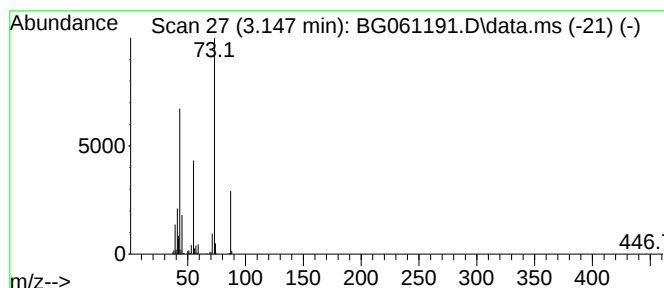
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.147	48.74 ng	377112	1,4-Dichlorobenzene-d4	7.924

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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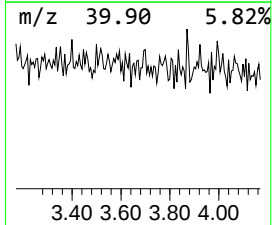
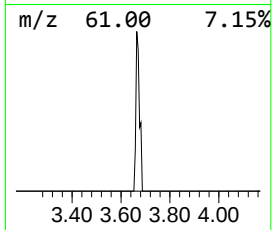
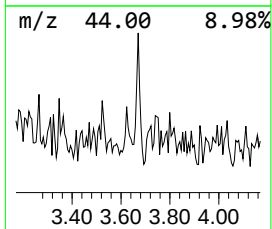
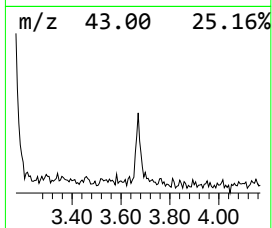
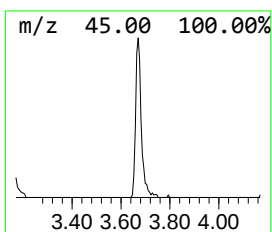
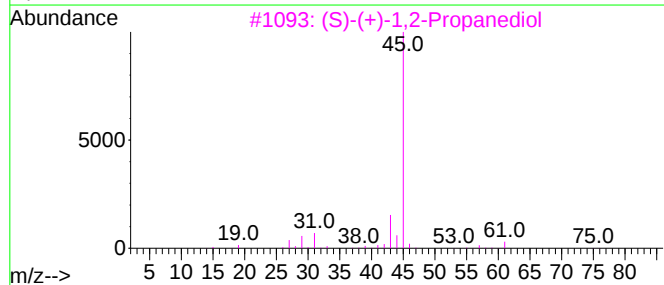
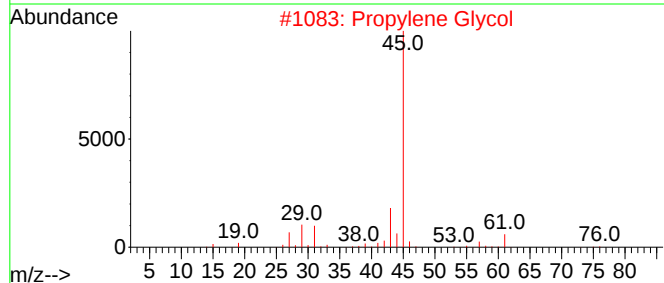
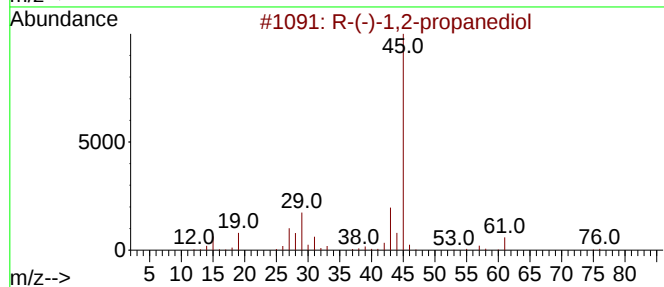
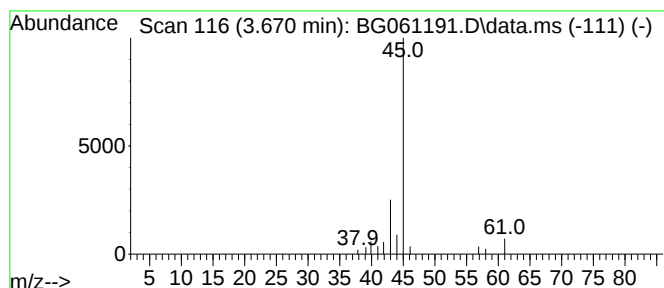
Instrument :
BNA_G
ClientSampleId :
H-3(5.0-6.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 R-(-)-1,2-propanediol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.670	3.79 ng	29287	1,4-Dichlorobenzene-d4	7.924	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2	Propylene Glycol	76	C3H8O2	000057-55-6	9
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Methane, nitroso-	45	CH3NO	000865-40-7	4



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Instrument :
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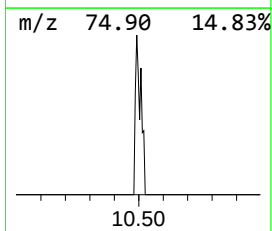
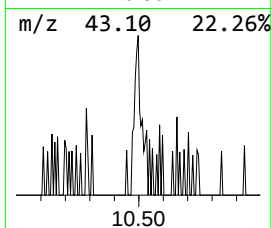
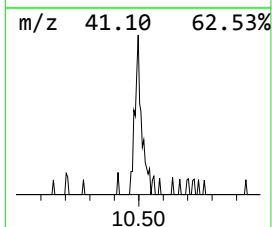
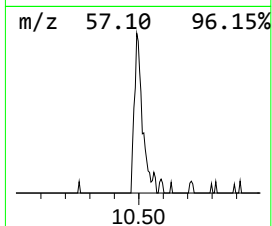
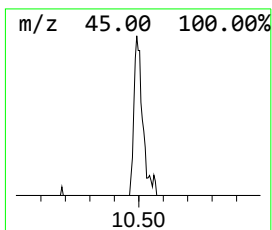
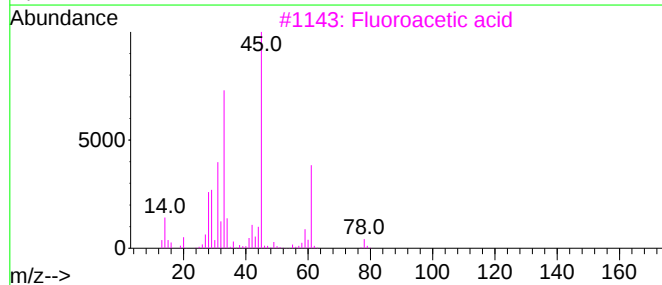
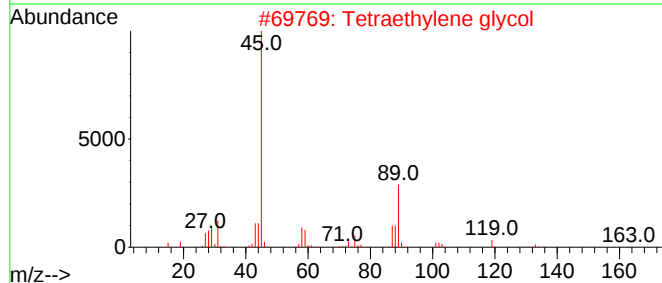
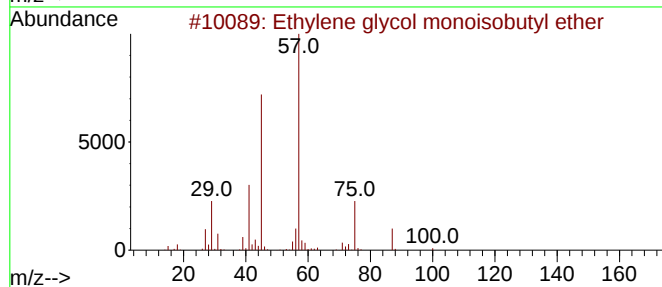
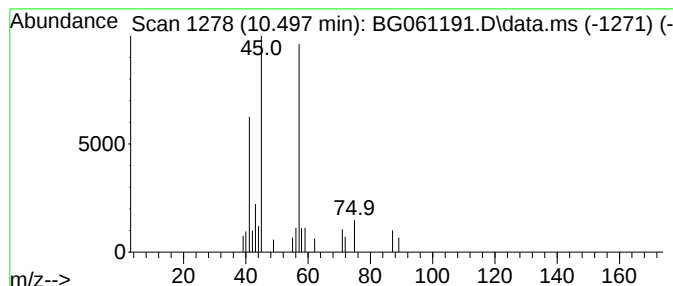
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown10.497 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.497	2.55 ng	23924	Naphthalene-d8	10.726

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
2			Tetraethylene glycol	194	C8H18O5	000112-60-7	28
3			Fluoroacetic acid	78	C2H3FO2	000144-49-0	28
4			2-Propanol, 1-(2-propenyloxy)-	116	C6H12O2	021460-36-6	23
5			2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	9



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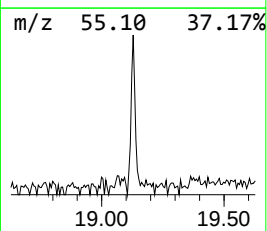
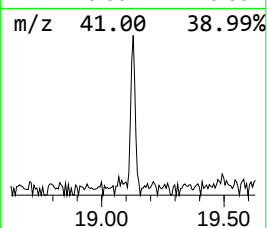
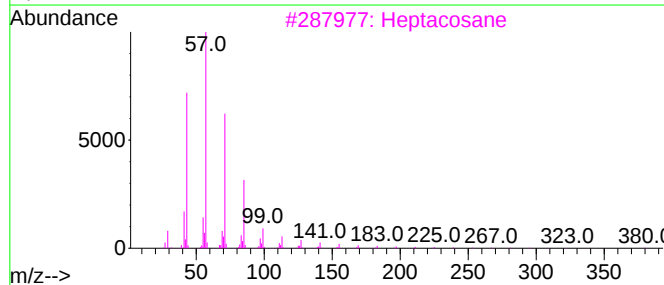
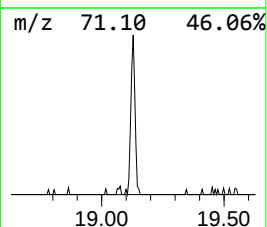
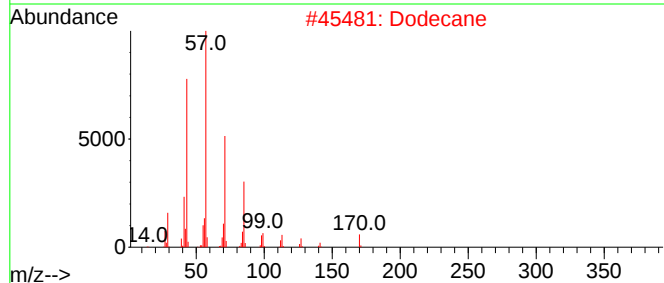
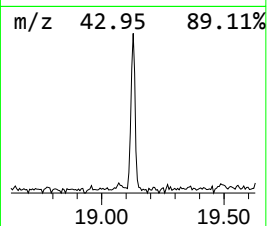
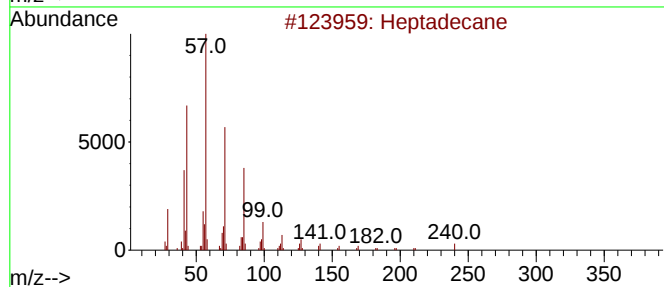
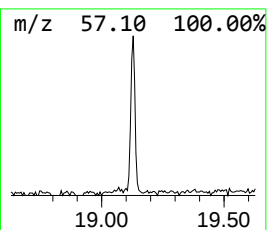
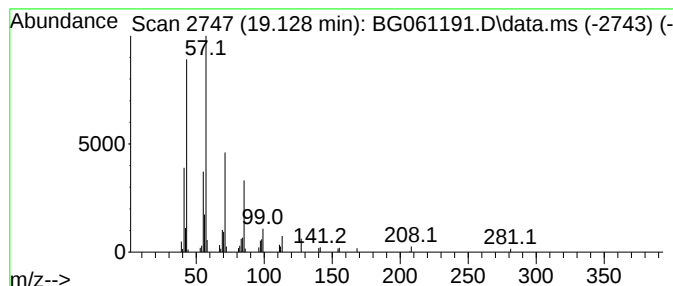
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.128	3.05 ng	62799	Phenanthrene-d10	17.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	87
2			Dodecane	170	C12H26	000112-40-3	86
3			Heptacosane	380	C27H56	000593-49-7	86
4			Pentadecane	212	C15H32	000629-62-9	86
5			Hexacosane	366	C26H54	000630-01-3	86



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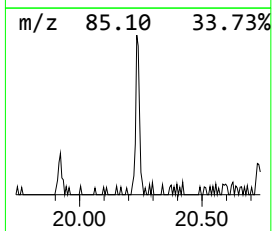
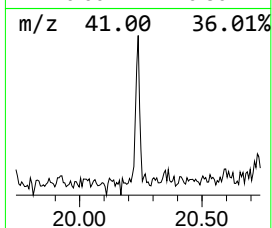
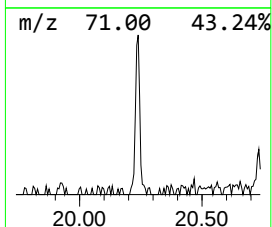
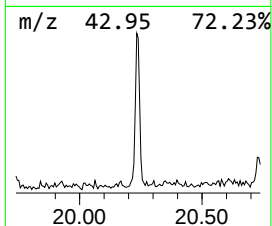
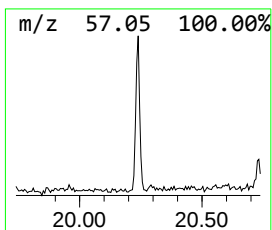
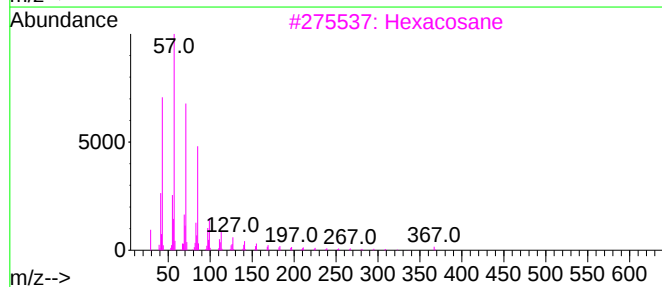
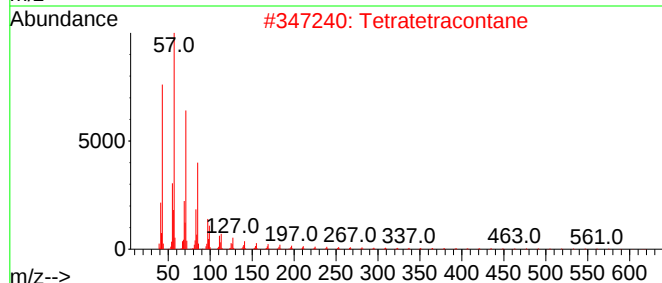
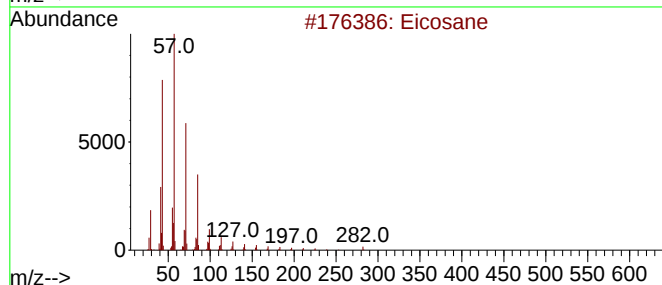
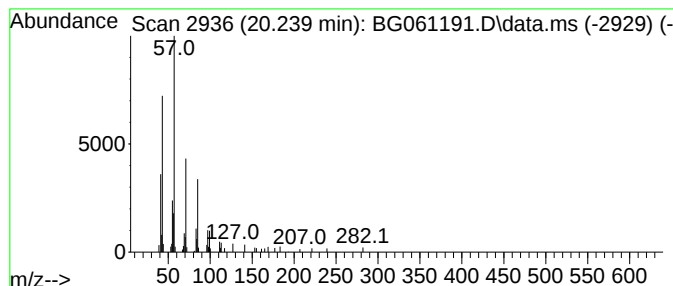
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.239	2.39 ng	62109	Chrysene-d12	21.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	93
2	Tetratetracontane			619	C44H90	007098-22-8	86
3	Hexacosane			366	C26H54	000630-01-3	86
4	Hexatriacontane			507	C36H74	000630-06-8	86
5	Sulfurous acid, butyl undecyl ester			292	C15H32O3S	1000309-17-8	86



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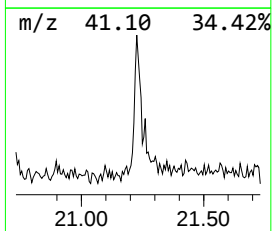
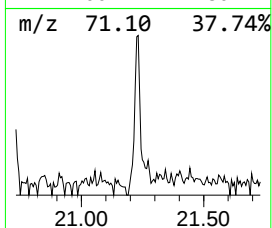
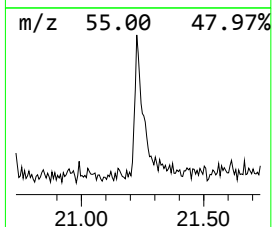
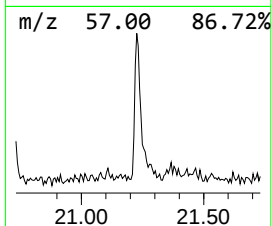
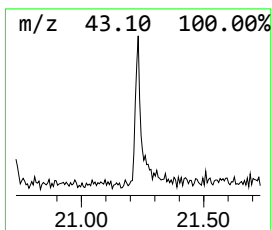
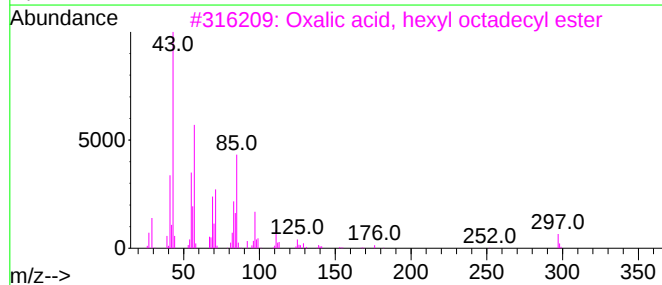
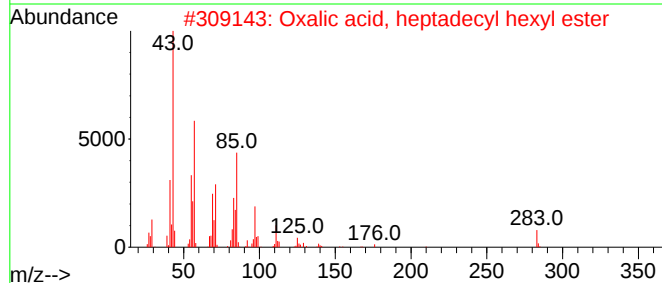
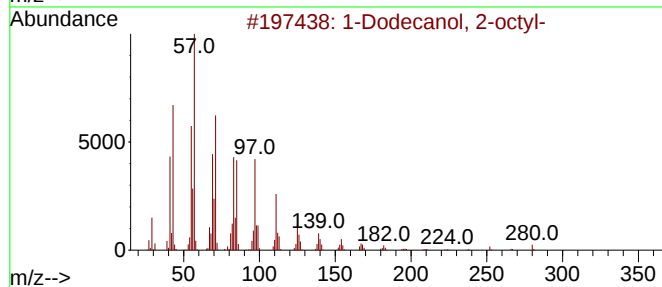
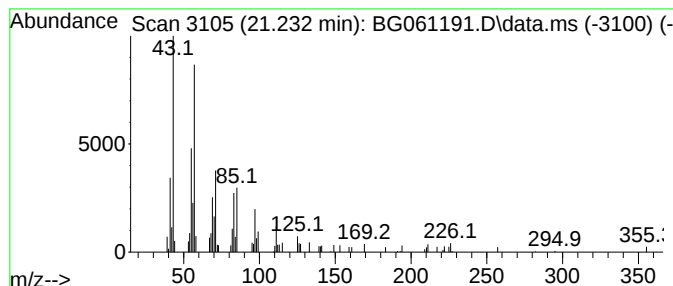
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Dodecanol, 2-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.232	3.36 ng	87342	Chrysene-d12	21.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-		298	C20H42O		005333-42-6	83
2	Oxalic acid, heptadecyl hexyl ester		412	C25H48O4		1000309-25-1	74
3	Oxalic acid, hexyl octadecyl ester		426	C26H50O4		1000309-25-2	72
4	Carbonic acid, octadecyl prop-1-...		354	C22H42O3		1000383-11-5	72
5	Carbonic acid, hexadecyl prop-1-...		326	C20H38O3		1000382-90-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051424\
Data File : BG061191.D
Acq On : 14 May 2024 15:53
Operator : MA/JU
Sample : P2330-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
H-3(5.0-6.0)

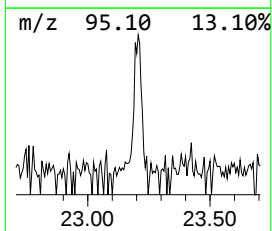
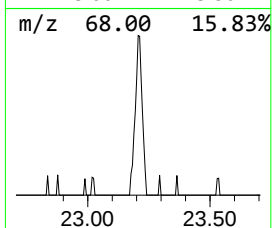
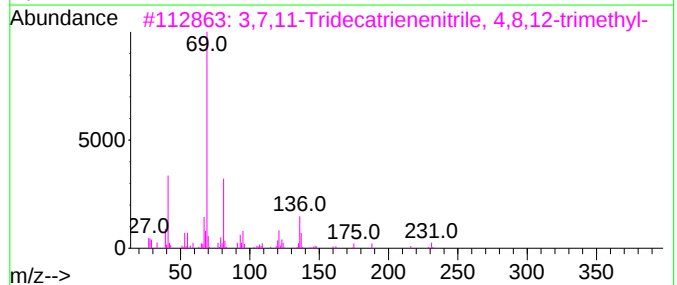
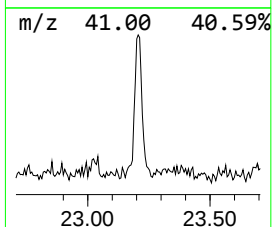
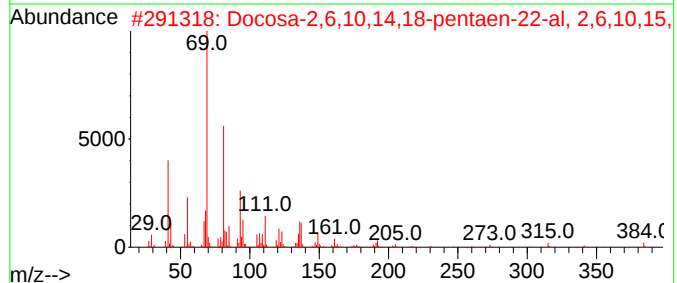
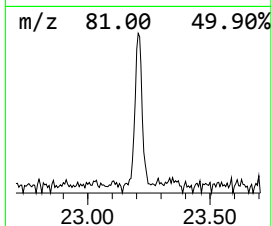
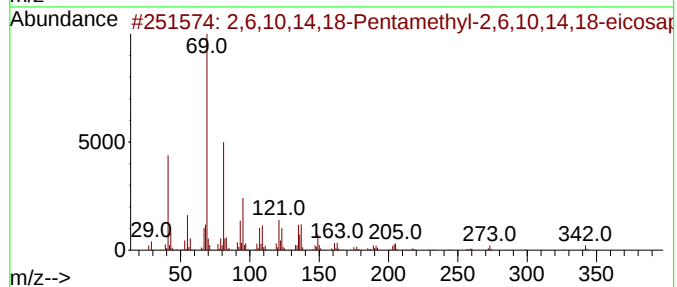
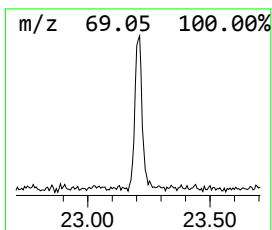
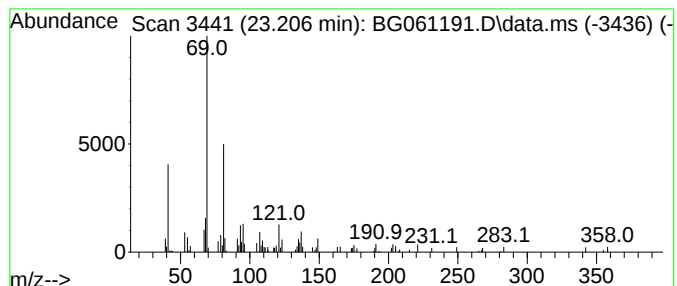
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2,6,10,14,18-Pentamethyl-2,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.206	2.91 ng	81651	Perylene-d12	24.681

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	87		
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80		
3	3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	64		
4	Supraene	410	C30H50	007683-64-9	59		
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051424\
Data File : BG061191.D
Acq On : 14 May 2024 15:53
Operator : MA/JU
Sample : P2330-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
H-3(5.0-6.0)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.147	48.7	ng	377112	1	7.924	154750	20.0
R-(-)-1,2-propa...	3.670	3.8	ng	29287	1	7.924	154750	20.0
unknown10.497	10.497	2.5	ng	23924	2	10.726	187450	20.0
Heptadecane	19.128	3.0	ng	62799	4	17.307	412321	20.0
Eicosane	20.239	2.4	ng	62109	5	21.561	519838	20.0
1-Dodecanol, 2-...	21.232	3.4	ng	87342	5	21.561	519838	20.0
2,6,10,14,18-Pe...	23.206	2.9	ng	81651	6	24.681	561239	20.0