

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
 Data File : BG055555.D
 Acq On : 11 Nov 2022 1:47
 Operator : CG/JU
 Sample : N5360-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20221114-COMP-13

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-BG110922.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055555.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.328	3	7	13	rBV	247015	395793	12.91%	2.251%
2	5.326	340	347	355	rVB	170298	266893	8.70%	1.518%
3	5.796	419	427	439	rBV	1113442	1794784	58.54%	10.206%
4	7.400	692	700	711	rBV	1115025	1916611	62.51%	10.899%
5	8.269	841	848	855	rBV	192775	329609	10.75%	1.874%
6	9.439	1037	1047	1057	rBV	618690	1096162	35.75%	6.233%
7	10.843	1280	1286	1294	rBV	43642	68482	2.23%	0.389%
8	11.095	1321	1329	1338	rVB	263020	455097	14.84%	2.588%
9	13.516	1733	1741	1748	rVB	1366659	2153550	70.24%	12.246%
10	14.885	1967	1974	1982	rVB	415128	637010	20.78%	3.622%
11	16.366	2218	2226	2237	rBV	1362808	2075664	67.70%	11.804%
12	17.623	2433	2440	2451	rBV	565686	815730	26.60%	4.639%
13	17.735	2454	2459	2463	rBV3	24071	34572	1.13%	0.197%
14	18.487	2582	2587	2595	rBV2	78220	119094	3.88%	0.677%
15	19.744	2797	2801	2812	rBV3	38211	63427	2.07%	0.361%
16	20.214	2874	2881	2887	rBV	2256542	3066171	100.00%	17.436%
17	21.007	3012	3016	3020	rVB3	32511	41027	1.34%	0.233%
18	21.530	3100	3105	3115	rBV2	123184	191120	6.23%	1.087%
19	21.918	3165	3171	3182	rVB2	569864	972357	31.71%	5.529%
20	22.112	3201	3204	3209	rVB	33184	46875	1.53%	0.267%
21	22.758	3311	3314	3324	rVB3	28218	55756	1.82%	0.317%
22	25.338	3743	3753	3770	rVB	325812	989303	32.27%	5.626%

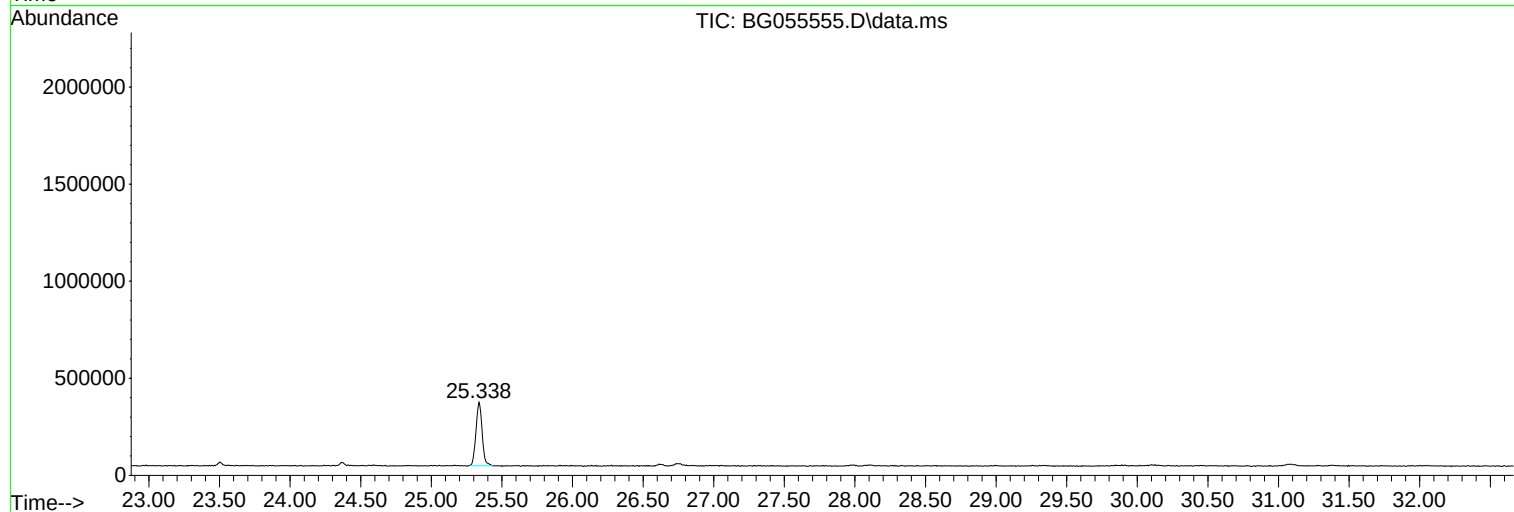
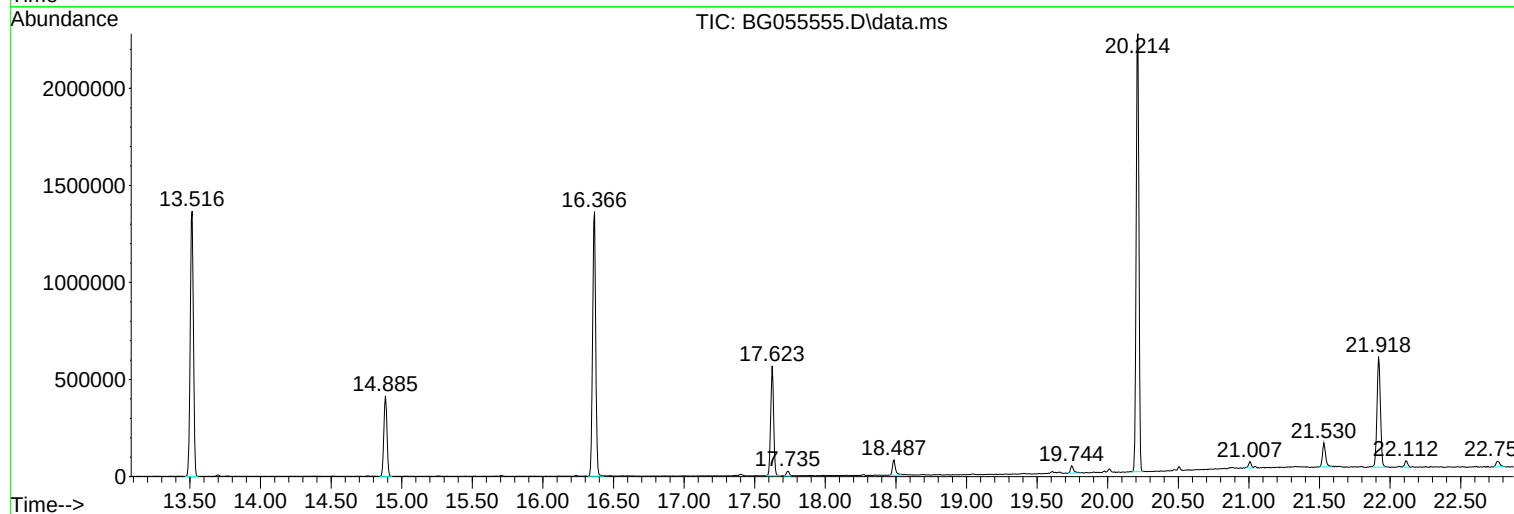
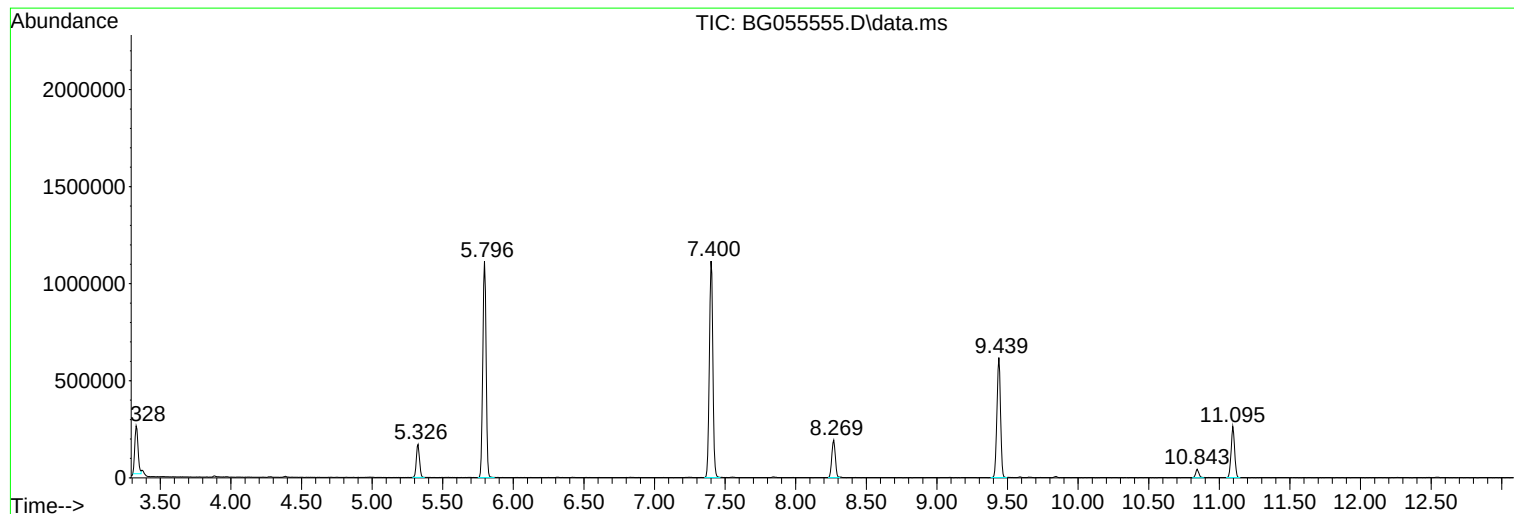
Sum of corrected areas: 17585087

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055555.D
Acq On : 11 Nov 2022 1:47
Operator : CG/JU
Sample : N5360-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221114-COMP-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055555.D
Acq On : 11 Nov 2022 1:47
Operator : CG/JU
Sample : N5360-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221114-COMP-13

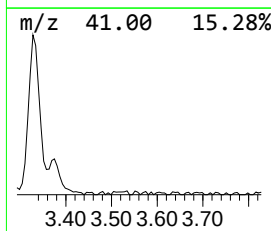
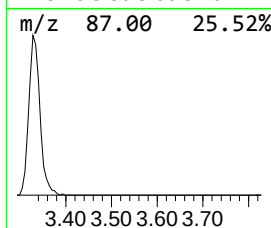
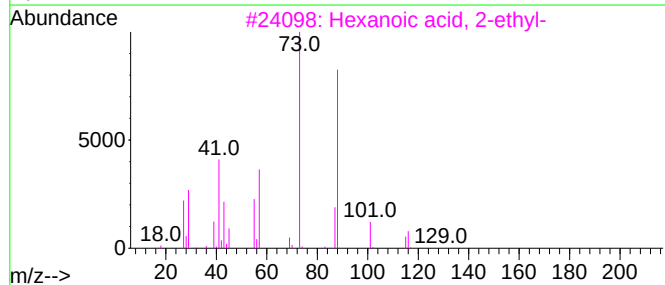
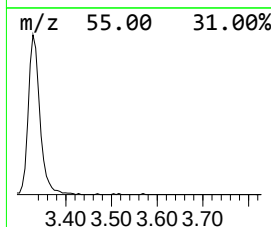
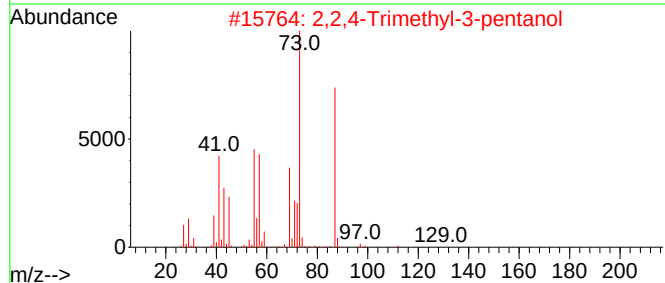
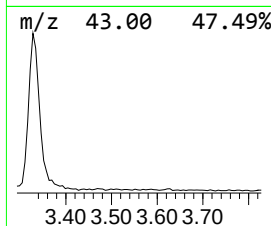
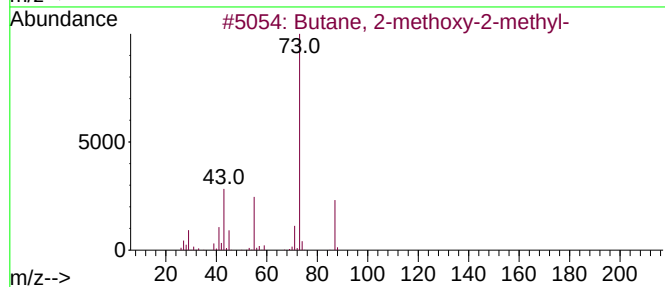
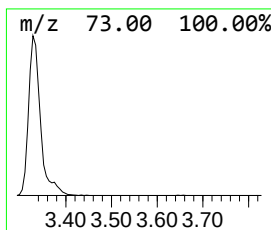
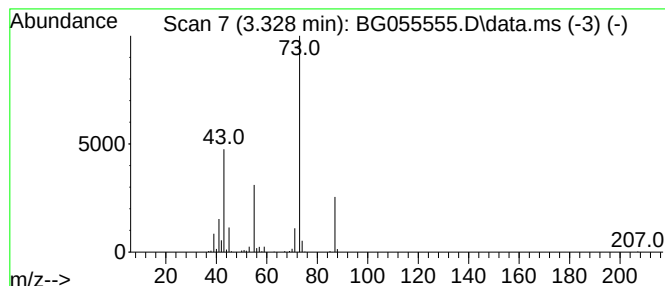
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.328	24.02 ng	395793	1,4-Dichlorobenzene-d4	8.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	28
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055555.D
Acq On : 11 Nov 2022 1:47
Operator : CG/JU
Sample : N5360-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221114-COMP-13

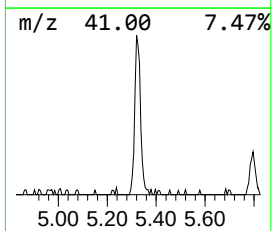
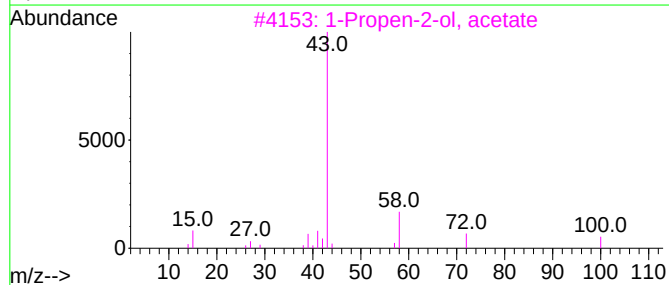
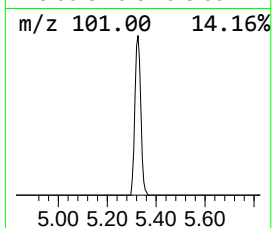
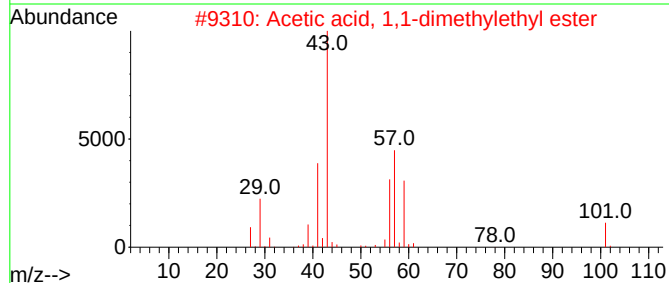
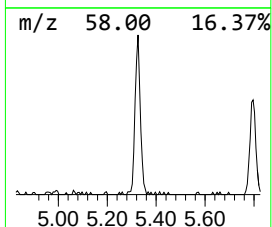
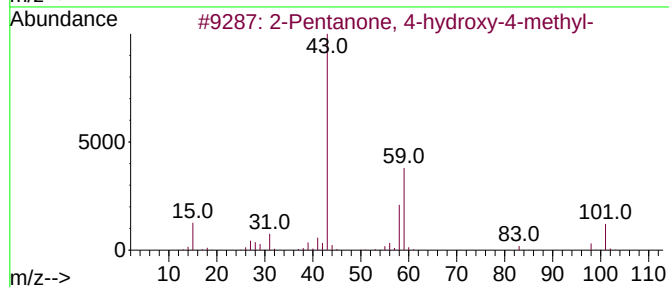
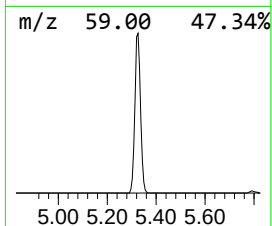
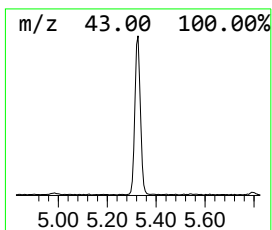
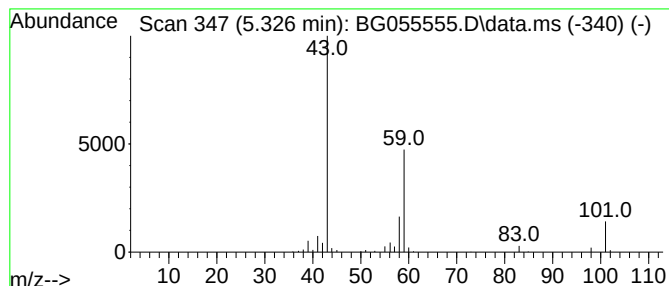
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.326	16.19 ng	266893	1,4-Dichlorobenzene-d4	8.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	8



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055555.D
Acq On : 11 Nov 2022 1:47
Operator : CG/JU
Sample : N5360-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221114-COMP-13

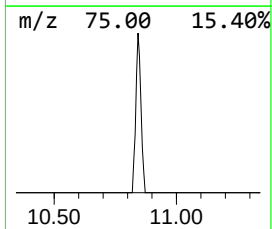
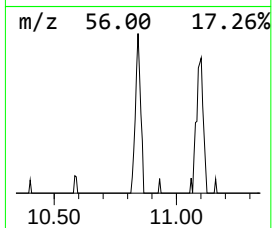
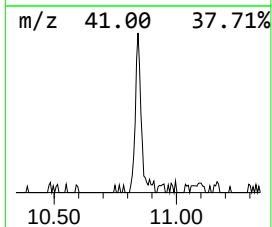
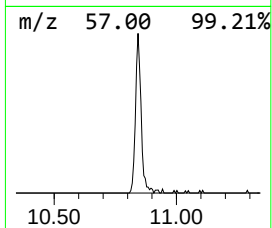
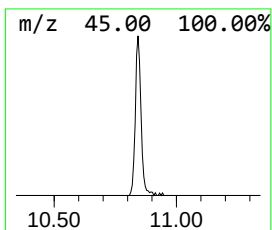
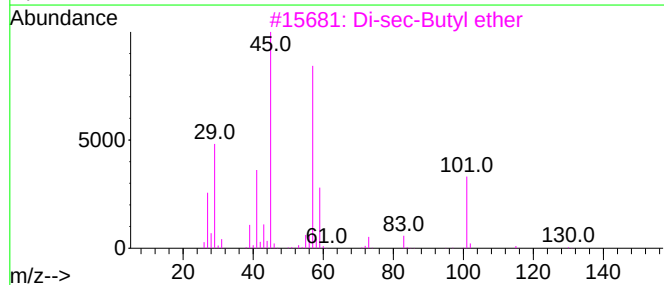
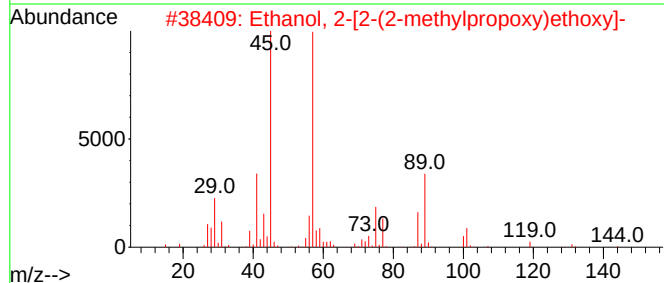
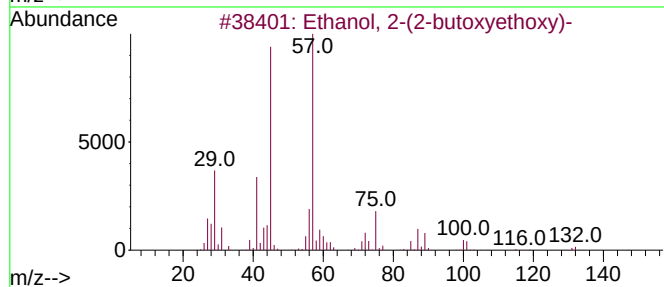
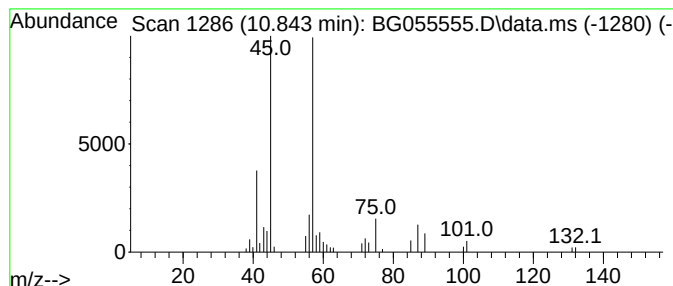
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.843	3.01 ng	68482	Naphthalene-d8	11.095

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	74
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	50
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055555.D
Acq On : 11 Nov 2022 1:47
Operator : CG/JU
Sample : N5360-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

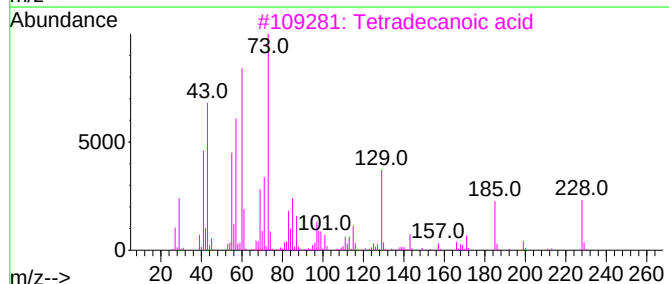
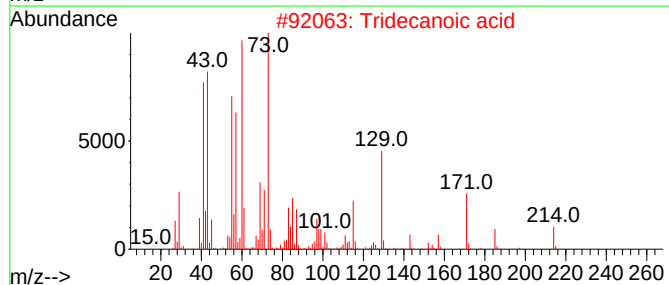
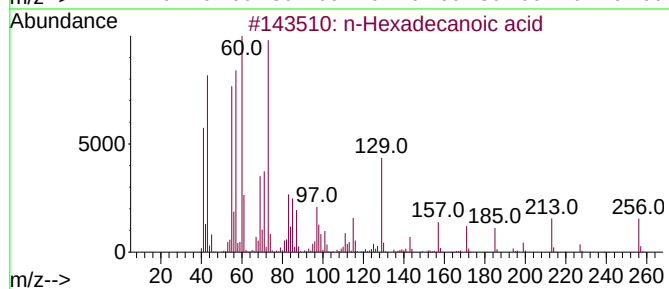
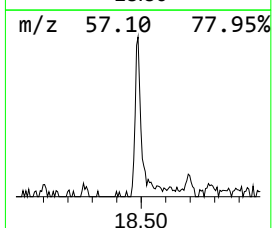
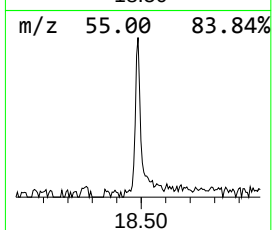
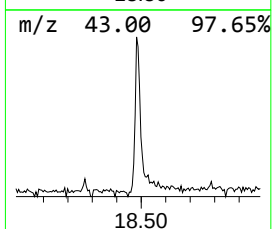
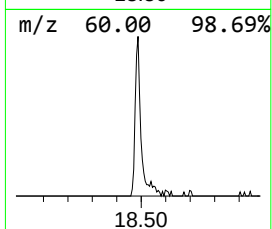
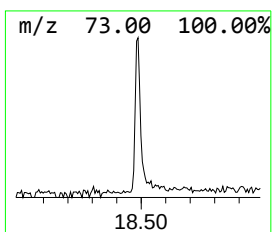
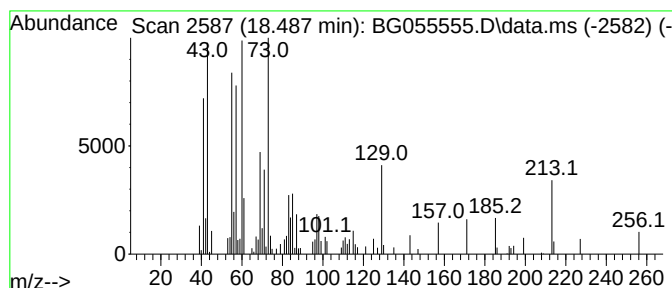
Instrument :
BNA_G
ClientSampleId :
20221114-COMP-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.487	2.92 ng	119094	Phenanthrene-d10		17.623	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	93
2	Tridecanoic acid		214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	83
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	83
5	n-Decanoic acid		172	C10H20O2	000334-48-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055555.D
Acq On : 11 Nov 2022 1:47
Operator : CG/JU
Sample : N5360-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221114-COMP-13

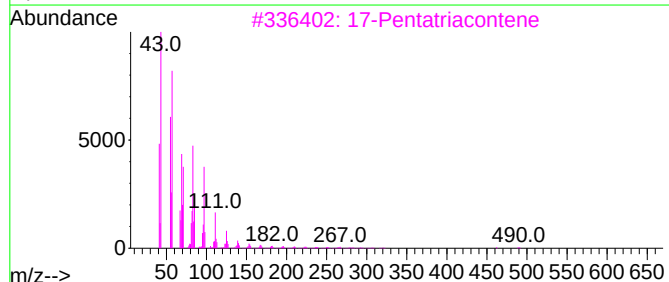
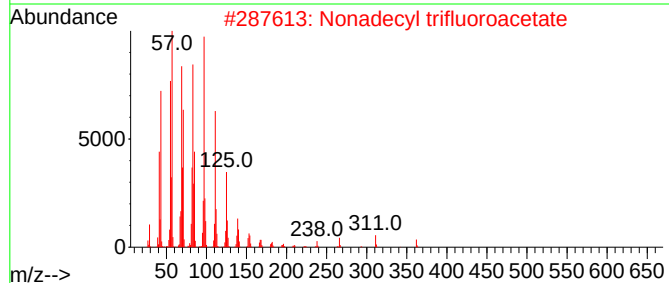
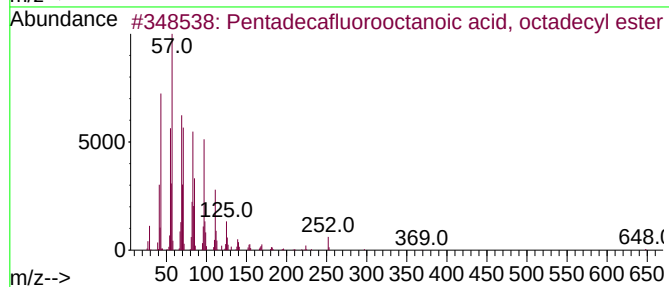
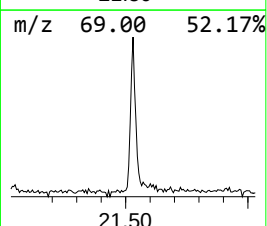
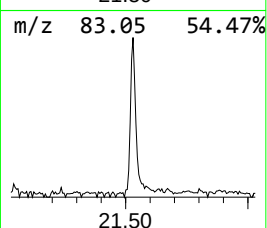
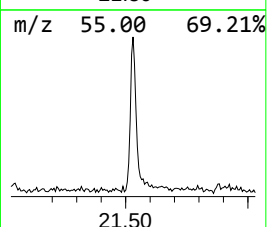
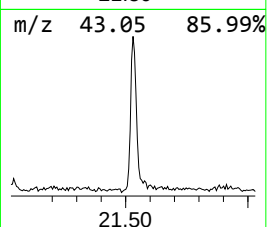
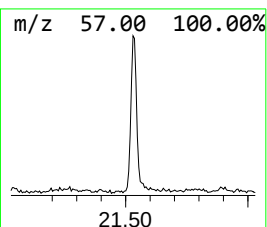
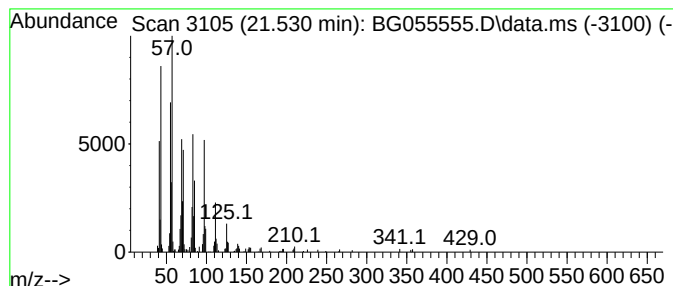
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.530	3.93 ng	191120	Chrysene-d12	21.918

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
3			17-Pentatriacontene	491	C35H70	006971-40-0	90
4			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	81
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
Data File : BG055555.D
Acq On : 11 Nov 2022 1:47
Operator : CG/JU
Sample : N5360-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221114-COMP-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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...	3.328	24.0	ng	395793	1	8.269	329609	20.0
2-Pentanone, 4-...	5.326	16.2	ng	266893	1	8.269	329609	20.0
Ethanol, 2-(2-b...	10.843	3.0	ng	68482	2	11.095	455097	20.0
n-Hexadecanoic ...	18.487	2.9	ng	119094	4	17.623	815730	20.0
Pentadecafluoro...	21.530	3.9	ng	191120	5	21.918	972357	20.0