

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101022\
 Data File : BG055115.D
 Acq On : 10 Oct 2022 16:40
 Operator : CG/JU
 Sample : N5052-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 551B-1

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-BG100322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055115.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.364	8	13	30	rVB	748408	1145949	16.51%	5.864%
2	5.373	348	355	363	rBV	63350	95263	1.37%	0.487%
3	5.849	429	436	445	rVB	303922	498350	7.18%	2.550%
4	7.453	700	709	720	rVB	204713	354636	5.11%	1.815%
5	8.329	850	858	865	rBV	103717	175447	2.53%	0.898%
6	9.498	1049	1057	1066	rVB	381569	671658	9.68%	3.437%
7	10.902	1290	1296	1308	rBV	80849	143556	2.07%	0.735%
8	11.161	1333	1340	1349	rBV	138636	247116	3.56%	1.264%
9	13.570	1742	1750	1757	rBV	1063244	1632115	23.51%	8.351%
10	14.939	1973	1983	1990	rBV	256785	391777	5.64%	2.005%
11	16.413	2227	2234	2244	rBV	1106758	1642965	23.67%	8.407%
12	17.459	2405	2412	2429	rVB	287887	473946	6.83%	2.425%
13	17.671	2442	2448	2455	rVB	379707	572740	8.25%	2.931%
14	18.523	2588	2593	2602	rBV	71883	111424	1.61%	0.570%
15	18.617	2602	2609	2614	rBV	4716612	6940915	100.00%	35.516%
16	20.250	2880	2887	2894	rBV	2359143	3125752	45.03%	15.994%
17	21.966	3172	3179	3186	rBV	379585	641660	9.24%	3.283%
18	25.415	3756	3766	3780	rVB3	217256	677989	9.77%	3.469%

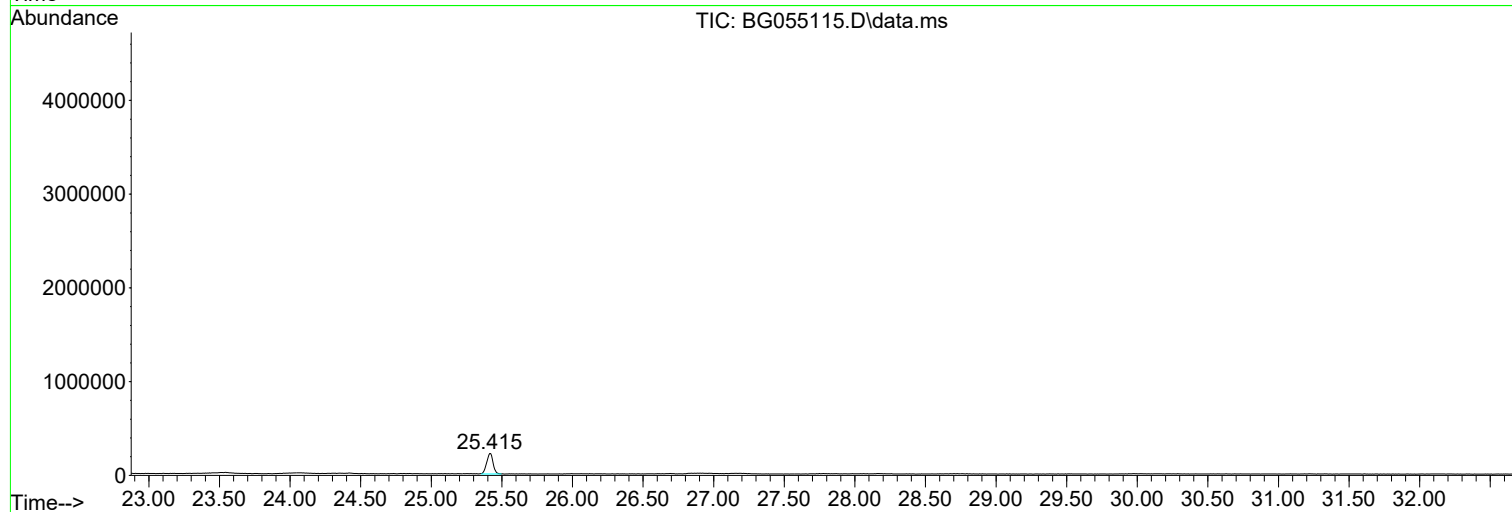
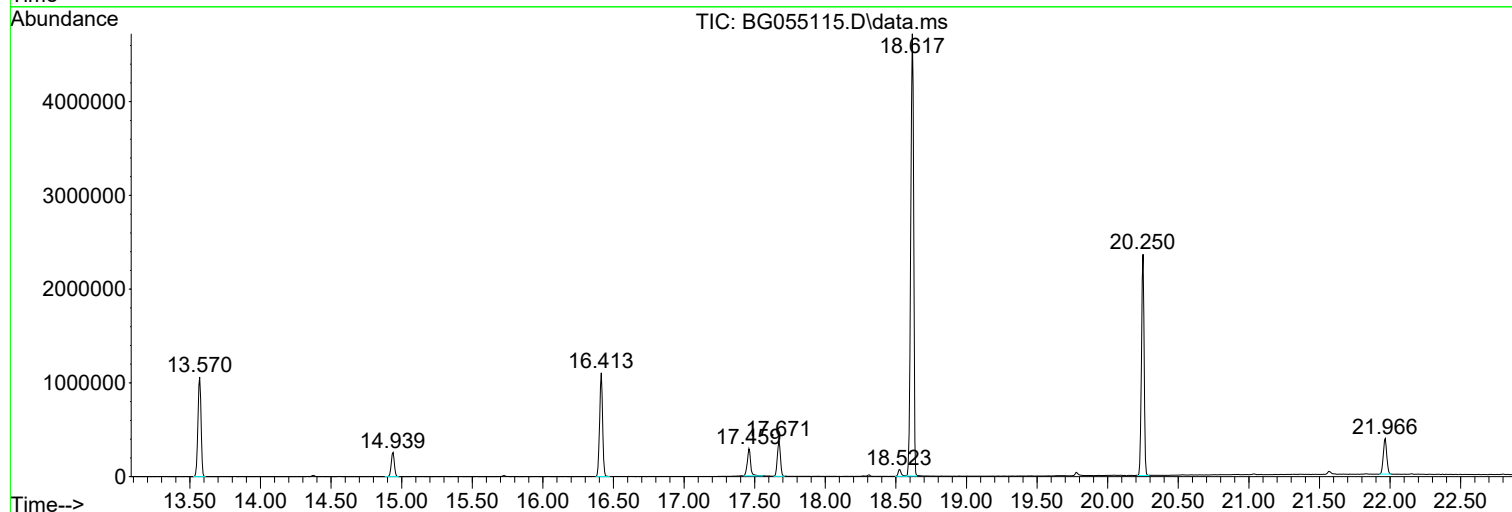
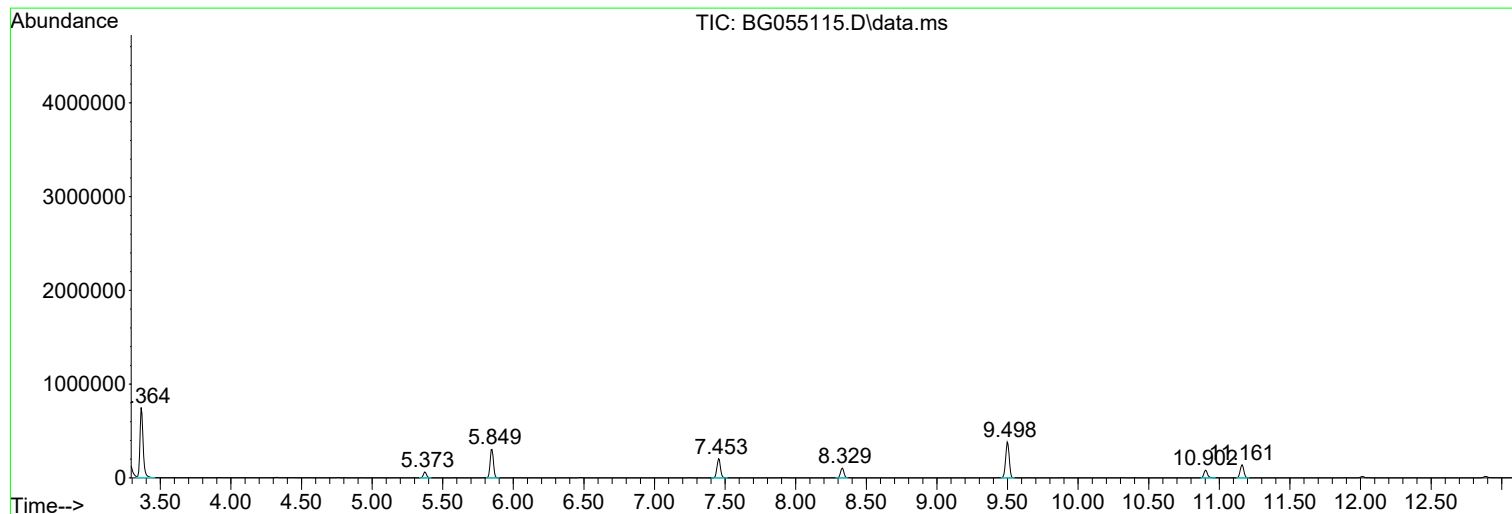
Sum of corrected areas: 19543258

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101022\
Data File : BG055115.D
Acq On : 10 Oct 2022 16:40
Operator : CG/JU
Sample : N5052-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
551B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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\BG101022\
Data File : BG055115.D
Acq On : 10 Oct 2022 16:40
Operator : CG/JU
Sample : N5052-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
551B-1

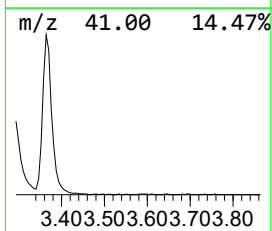
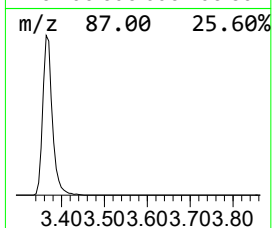
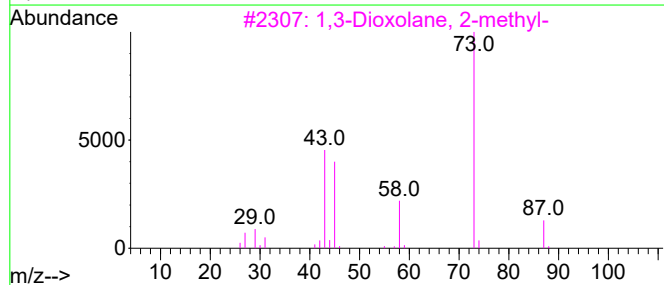
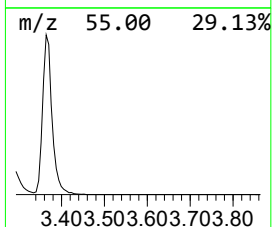
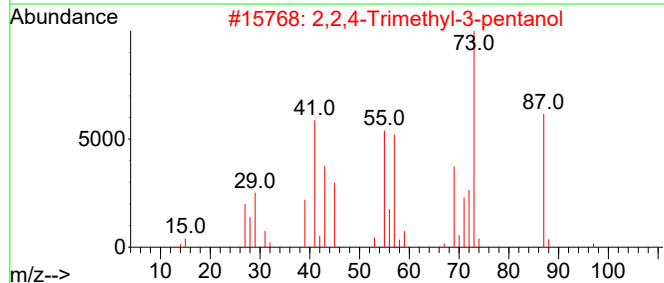
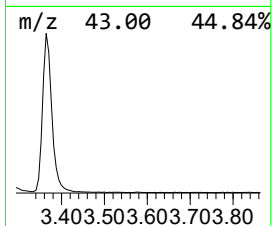
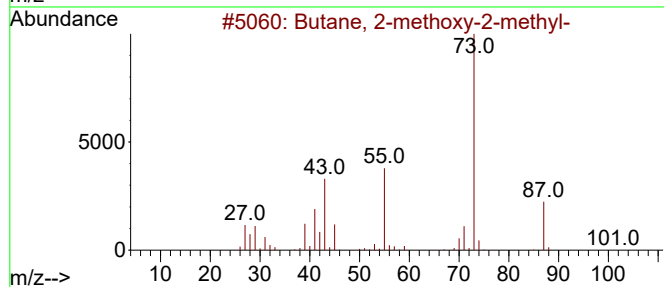
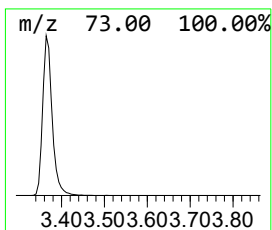
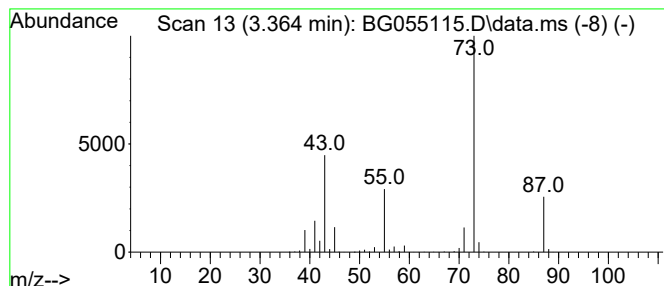
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.364	130.63 ng	1145950	1,4-Dichlorobenzene-d4	8.329

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101022\
Data File : BG055115.D
Acq On : 10 Oct 2022 16:40
Operator : CG/JU
Sample : N5052-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
551B-1

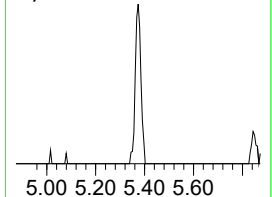
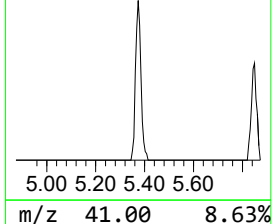
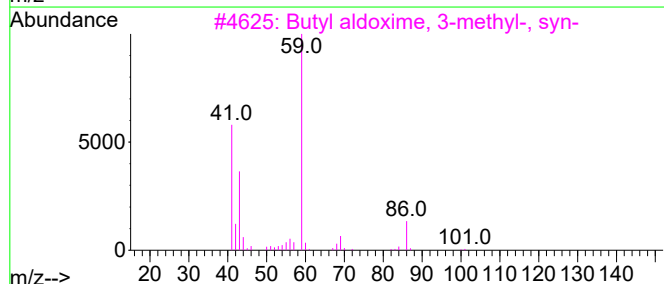
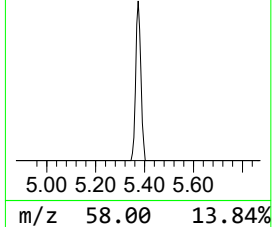
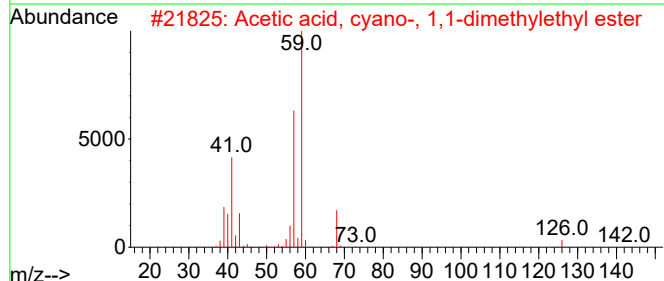
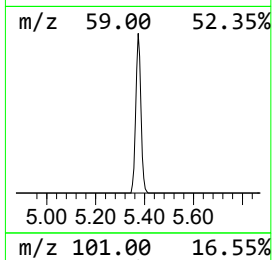
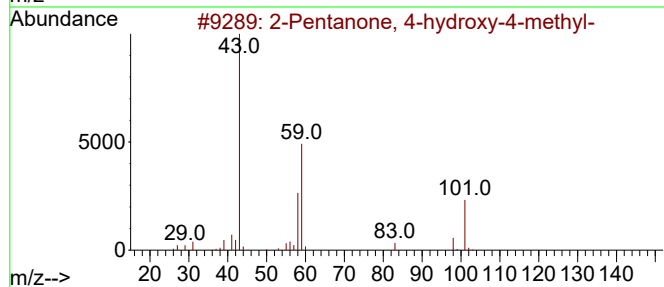
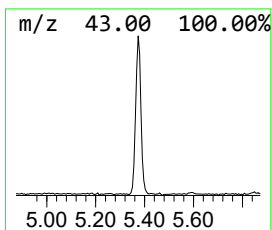
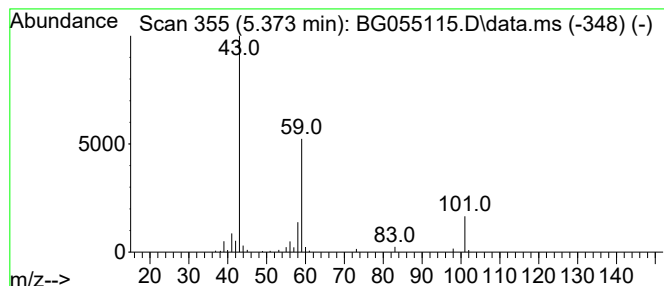
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.373	10.86 ng	95263	1,4-Dichlorobenzene-d4	8.329

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16	
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101022\
Data File : BG055115.D
Acq On : 10 Oct 2022 16:40
Operator : CG/JU
Sample : N5052-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
551B-1

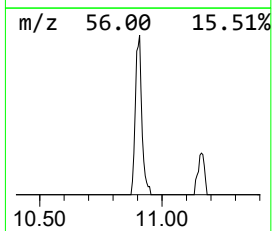
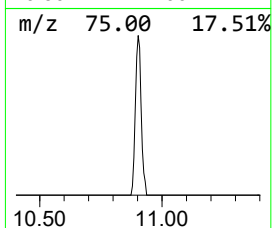
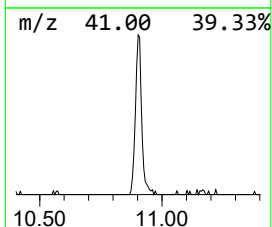
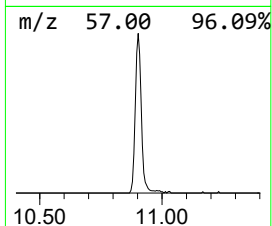
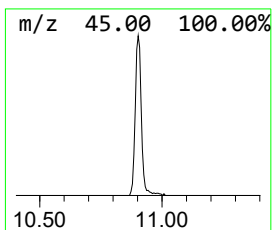
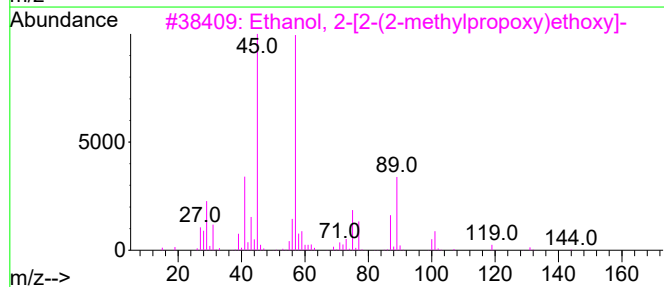
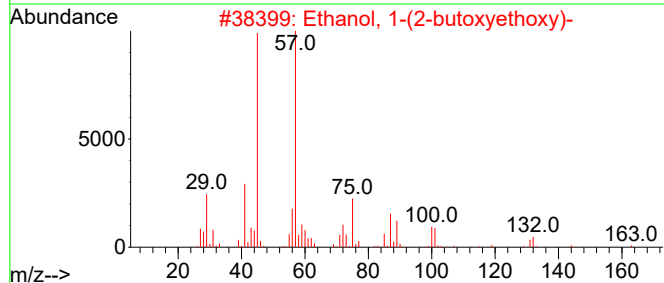
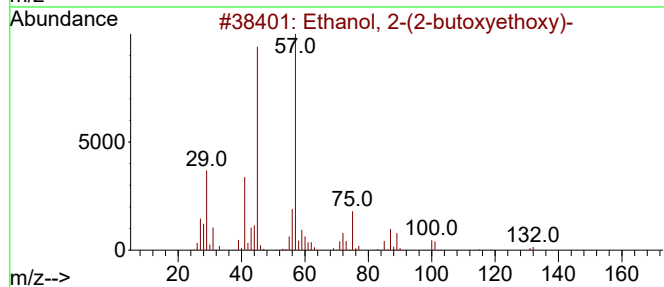
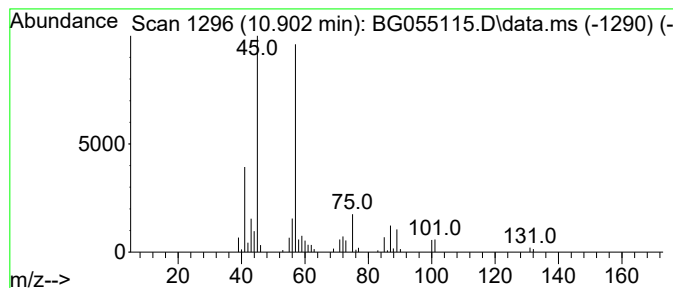
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.902	11.62 ng	143556	Naphthalene-d8	11.161

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5			Propanoic acid, 3-methoxy-2-meth...	132	C6H12O3	003852-11-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101022\
Data File : BG055115.D
Acq On : 10 Oct 2022 16:40
Operator : CG/JU
Sample : N5052-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

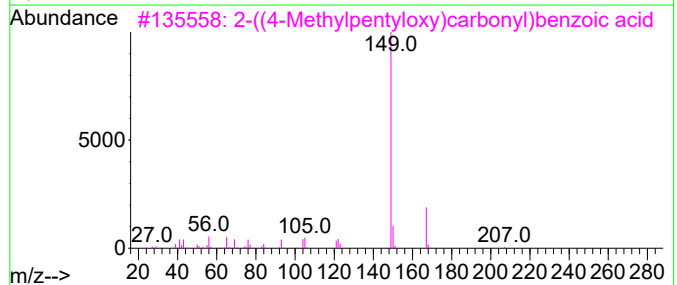
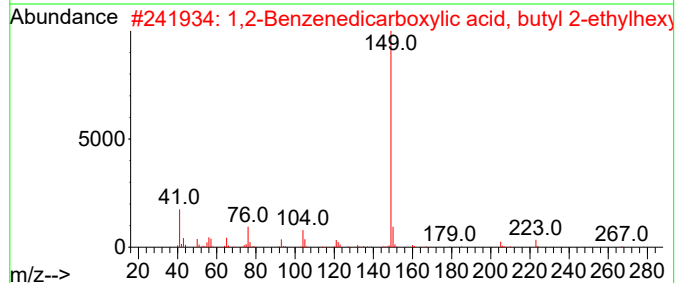
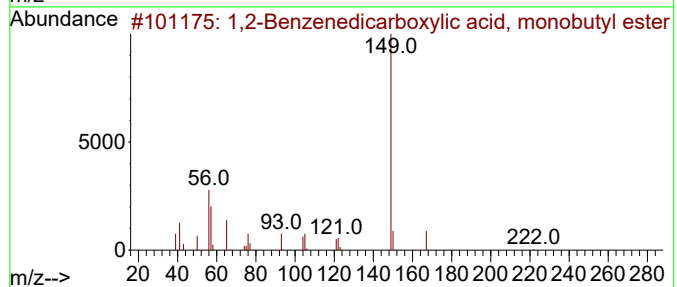
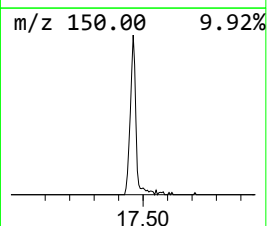
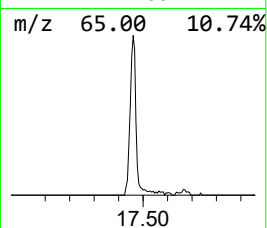
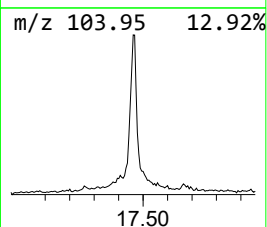
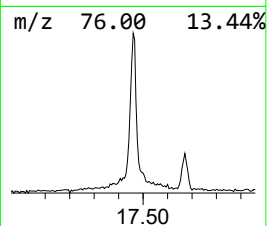
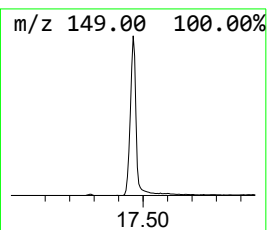
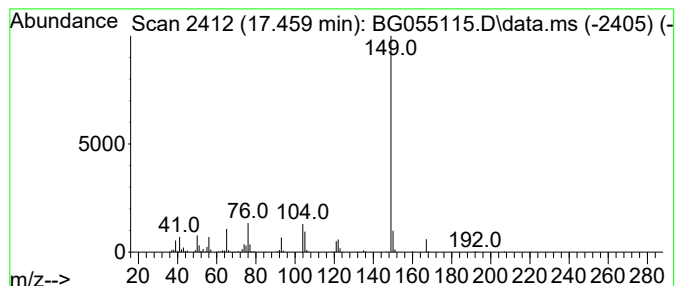
Instrument :
BNA_G
ClientSampleId :
551B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1,2-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.459	16.55 ng	473946	Phenanthrene-d10	17.671	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, mo...	222	C12H14O4	000131-70-4	83
2	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	83
3	2-((4-Methylpentyloxy)carbonyl)b...	250	C14H18O4	848131-14-6	83
4	1,2-Benzenedicarboxylic acid, bi...	250	C14H18O4	000605-45-8	78
5	Phthalic acid, monoethyl ester	278	C16H22O4	005393-19-1	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101022\
Data File : BG055115.D
Acq On : 10 Oct 2022 16:40
Operator : CG/JU
Sample : N5052-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
551B-1

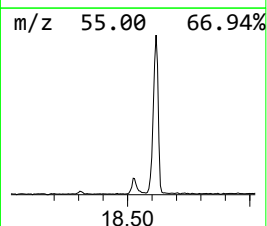
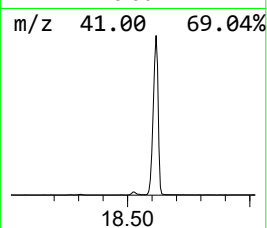
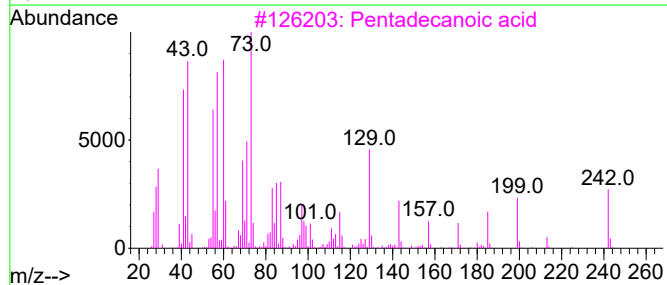
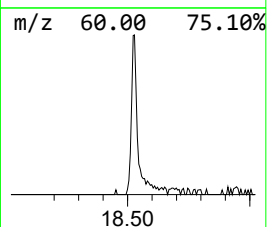
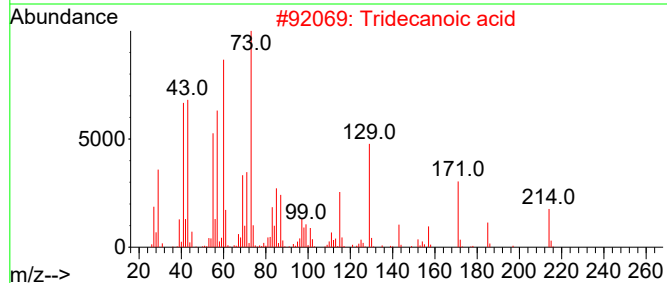
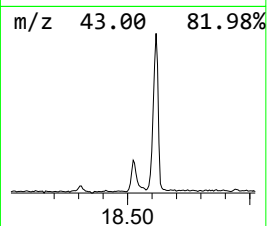
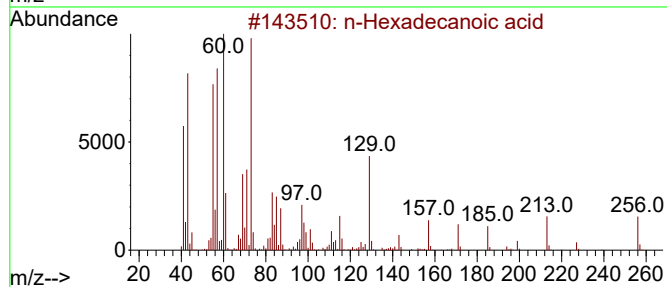
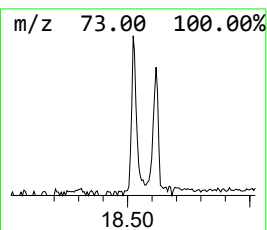
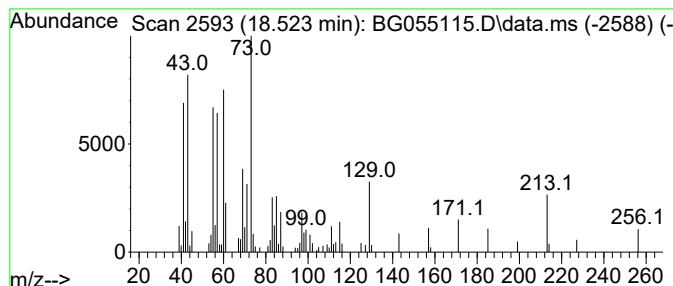
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.523	3.89 ng	111424	Phenanthrene-d10	17.671

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			1-(p-Toluidino)-1-deoxy-.beta.-d...	269	C13H19NO5	1000226-06-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101022\
Data File : BG055115.D
Acq On : 10 Oct 2022 16:40
Operator : CG/JU
Sample : N5052-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
551B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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...	3.364	130.6	ng	1145950	1	8.329	175447	20.0
2-Pentanone, 4-...	5.373	10.9	ng	95263	1	8.329	175447	20.0
Ethanol, 2-(2-b...	10.902	11.6	ng	143556	2	11.161	247116	20.0
1,2-Benzenedica...	17.459	16.6	ng	473946	4	17.671	572740	20.0
n-Hexadecanoic ...	18.523	3.9	ng	111424	4	17.671	572740	20.0