

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
 Data File : BG055609.D
 Acq On : 14 Nov 2022 18:04
 Operator : CG/JU
 Sample : N5561-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-25

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: BG055609.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.321	3	5	21	rVB	232069	396455	13.20%	2.375%
2	5.318	339	345	354	rVB	169572	273134	9.09%	1.636%
3	5.794	419	426	439	rBV	884736	1447129	48.17%	8.668%
4	7.404	690	700	710	rBV	902256	1556702	51.82%	9.325%
5	8.262	837	846	853	rBV	190730	331414	11.03%	1.985%
6	9.437	1037	1046	1056	rBV	539634	952748	31.71%	5.707%
7	10.835	1277	1284	1297	rBV	148444	271161	9.03%	1.624%
8	11.094	1320	1328	1337	rVB	288120	497418	16.56%	2.980%
9	13.515	1732	1740	1747	rVB	1388213	2188557	72.85%	13.110%
10	14.883	1966	1973	1980	rVB	450589	715928	23.83%	4.288%
11	16.370	2219	2226	2236	rVB	1173033	1859972	61.91%	11.141%
12	17.627	2433	2440	2446	rBV	578460	866659	28.85%	5.191%
13	18.268	2545	2549	2553	rVB	26720	35649	1.19%	0.214%
14	18.485	2581	2586	2593	rBV	157967	237475	7.90%	1.422%
15	19.660	2783	2786	2792	rVB	33060	50945	1.70%	0.305%
16	19.748	2797	2801	2810	rBV	73478	121364	4.04%	0.727%
17	20.213	2875	2880	2886	rBV	2251410	3004181	100.00%	17.995%
18	21.535	3101	3105	3115	rVB	88408	153047	5.09%	0.917%
19	21.928	3166	3172	3178	rBV	513966	851235	28.34%	5.099%
20	25.354	3748	3755	3770	rVB2	275068	883170	29.40%	5.290%

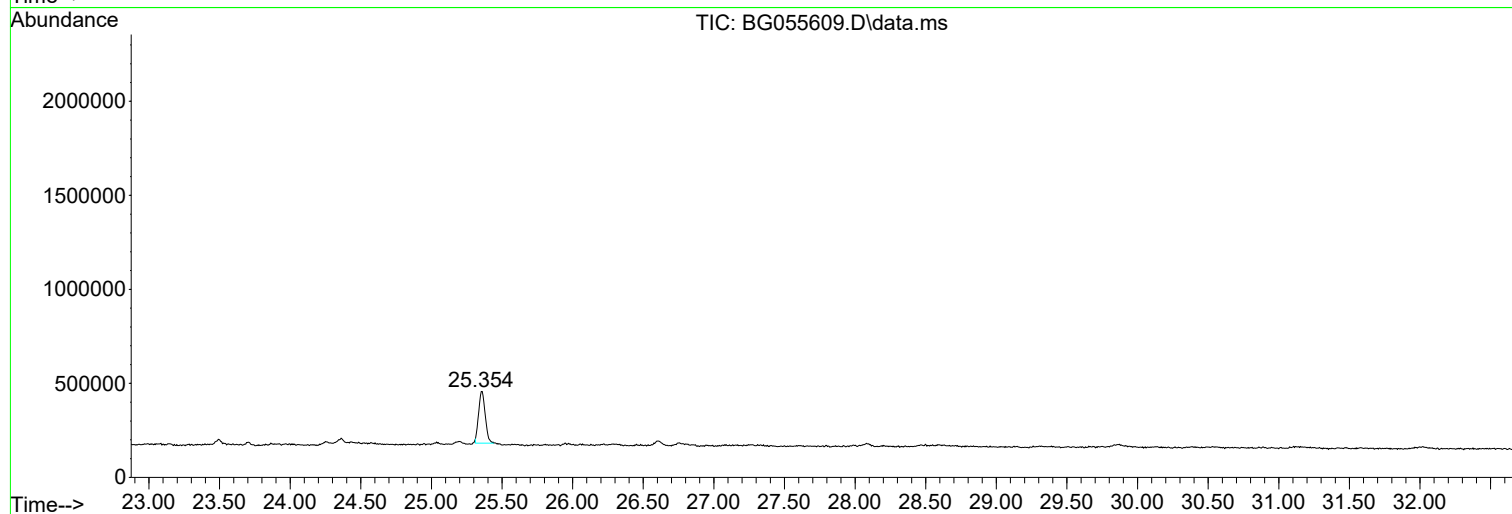
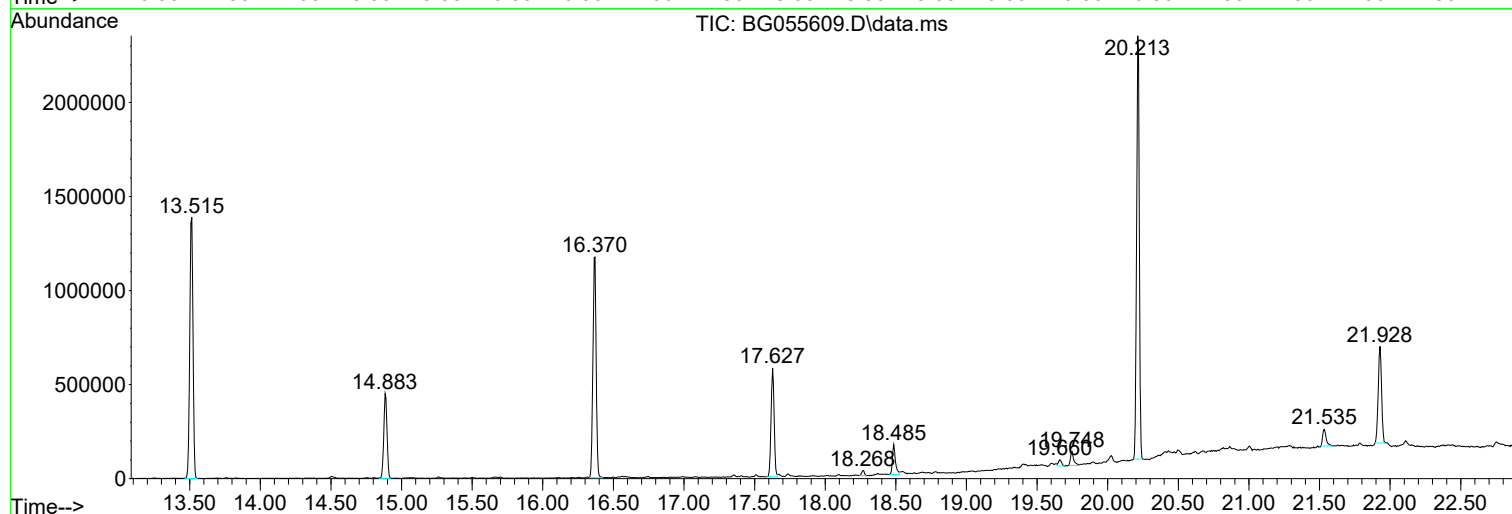
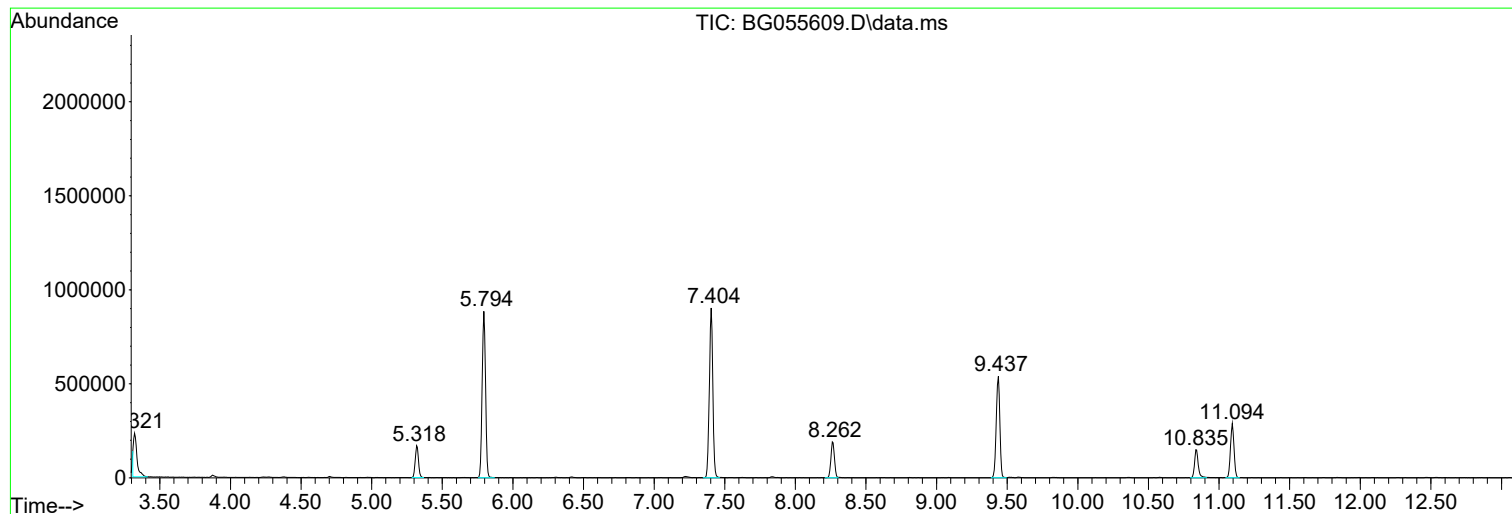
Sum of corrected areas: 16694343

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055609.D
Acq On : 14 Nov 2022 18:04
Operator : CG/JU
Sample : N5561-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-25

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\BG111422\
Data File : BG055609.D
Acq On : 14 Nov 2022 18:04
Operator : CG/JU
Sample : N5561-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-25

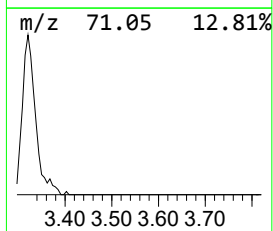
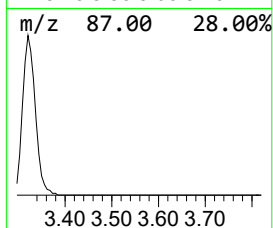
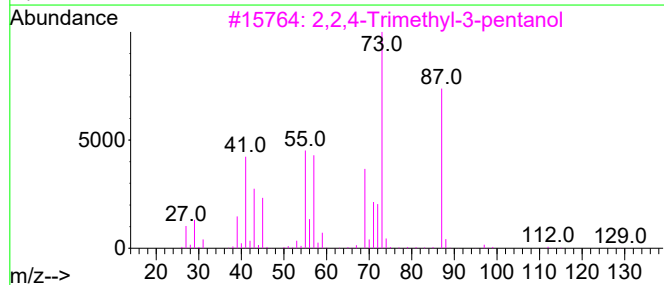
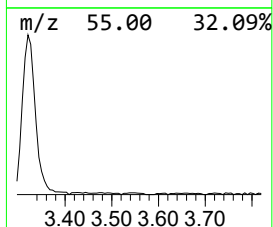
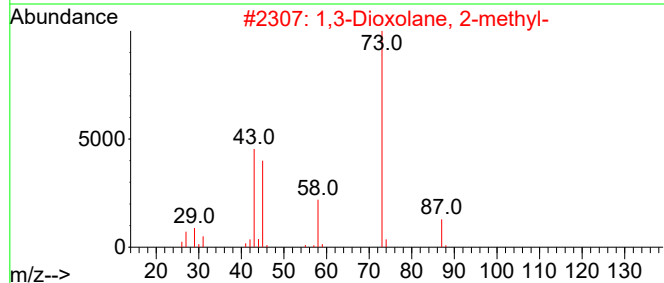
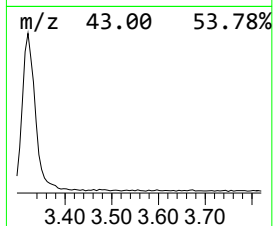
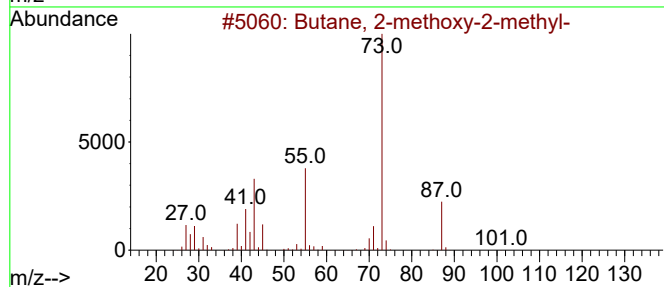
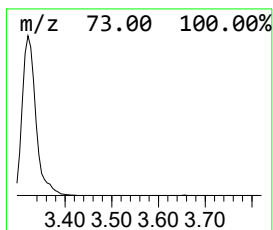
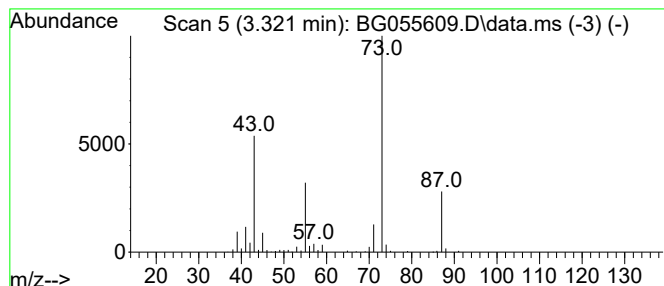
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.321	23.93 ng	396455	1,4-Dichlorobenzene-d4	8.262

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	47
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	42
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055609.D
Acq On : 14 Nov 2022 18:04
Operator : CG/JU
Sample : N5561-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

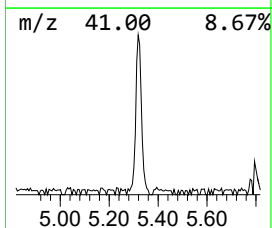
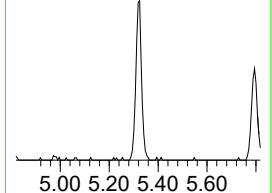
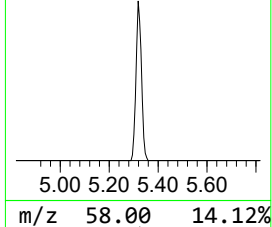
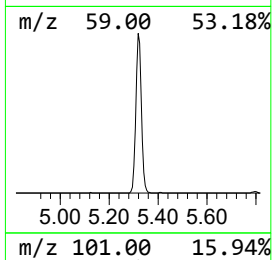
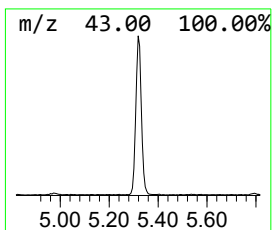
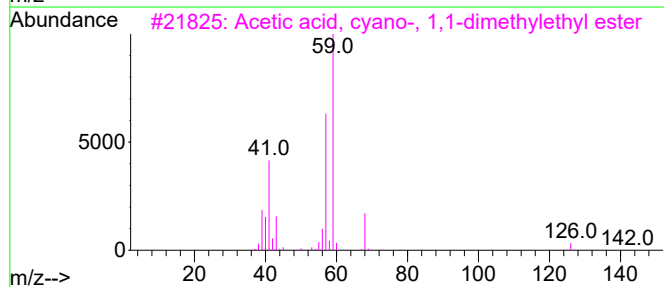
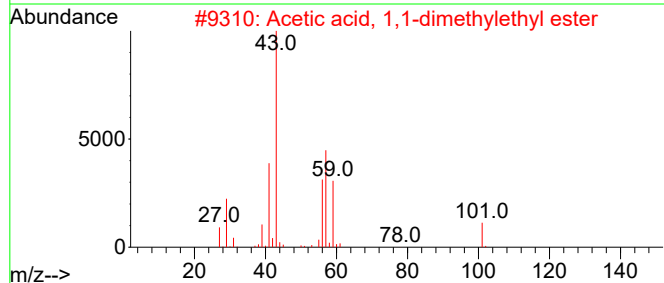
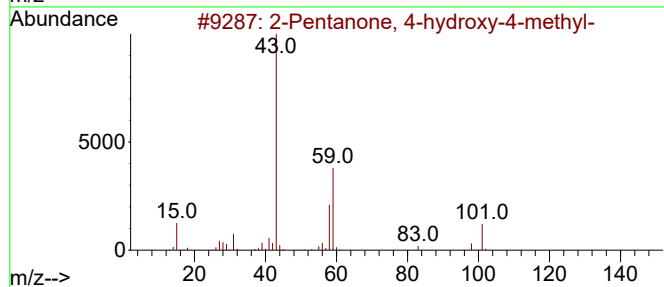
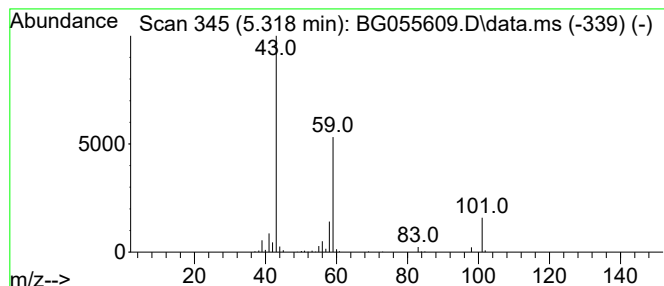
Instrument :
BNA_G
ClientSampleId :
SB-25

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.	
5.318	16.48 ng	273134	1,4-Dichlorobenzene-d4	8.262	
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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055609.D
Acq On : 14 Nov 2022 18:04
Operator : CG/JU
Sample : N5561-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-25

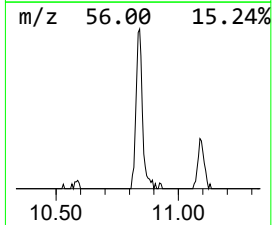
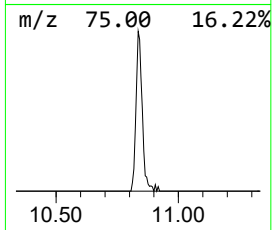
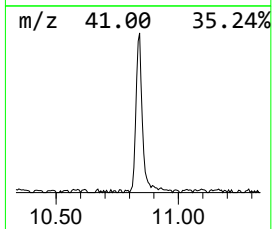
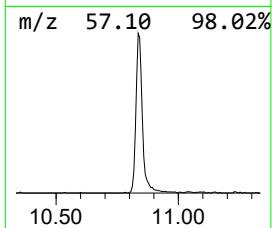
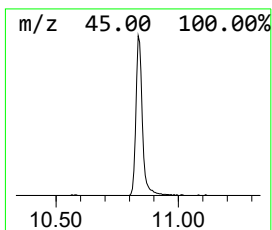
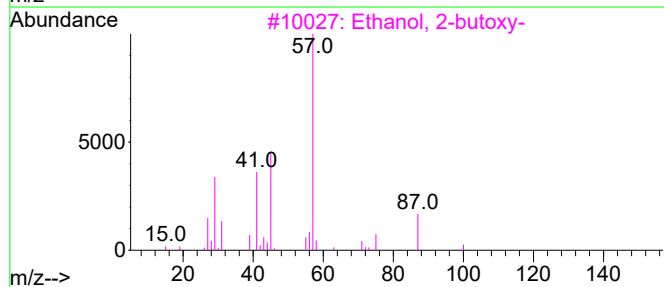
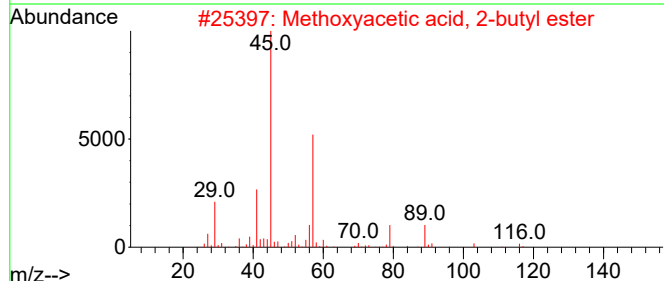
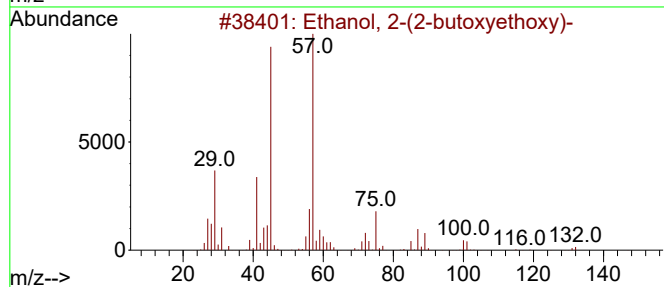
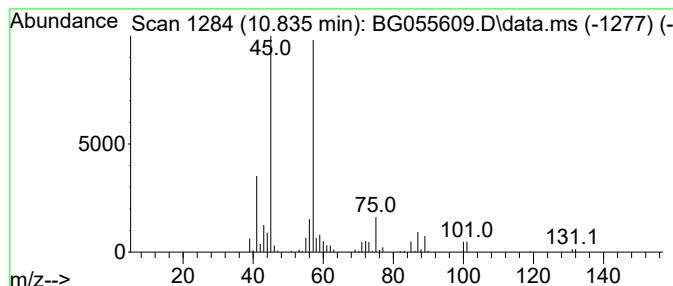
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.835	10.90 ng	271161	Naphthalene-d8	11.094

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	53
3			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	53
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055609.D
Acq On : 14 Nov 2022 18:04
Operator : CG/JU
Sample : N5561-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-25

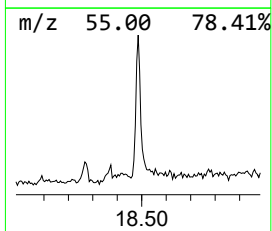
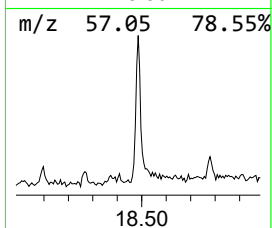
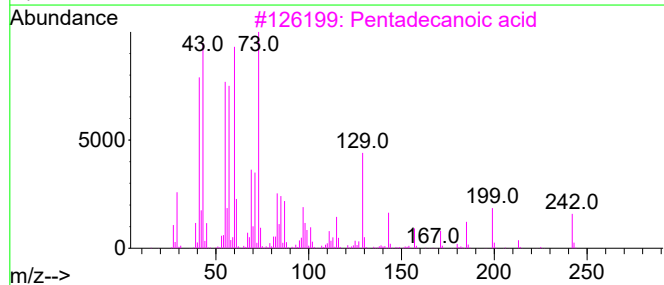
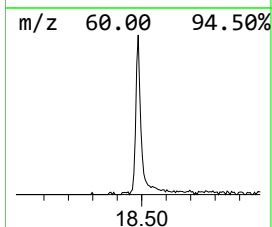
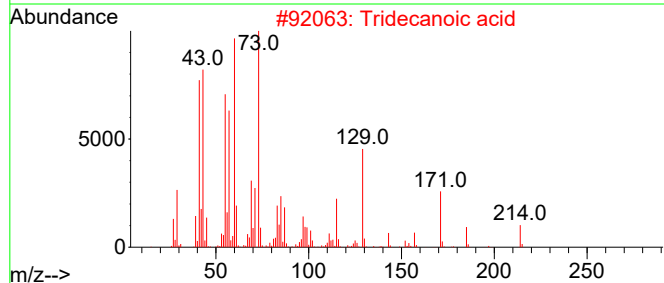
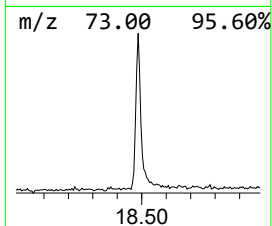
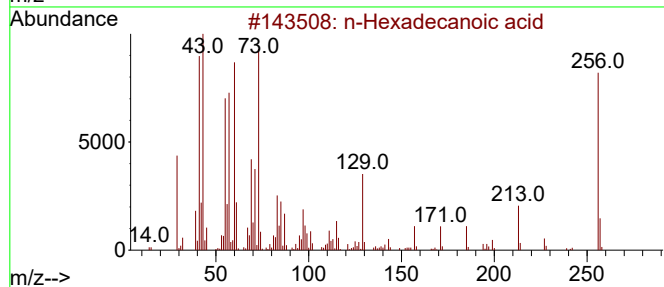
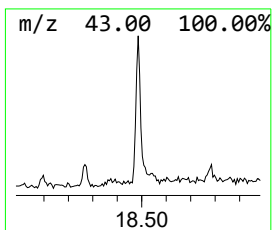
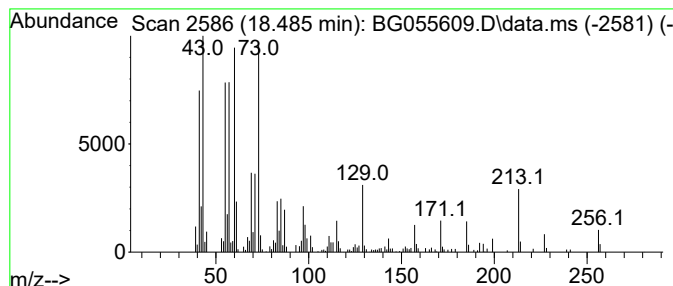
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.485	5.48 ng	237475	Phenanthrene-d10	17.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055609.D
Acq On : 14 Nov 2022 18:04
Operator : CG/JU
Sample : N5561-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-25

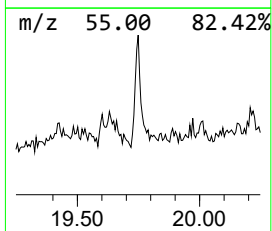
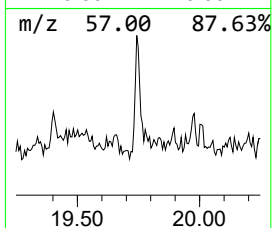
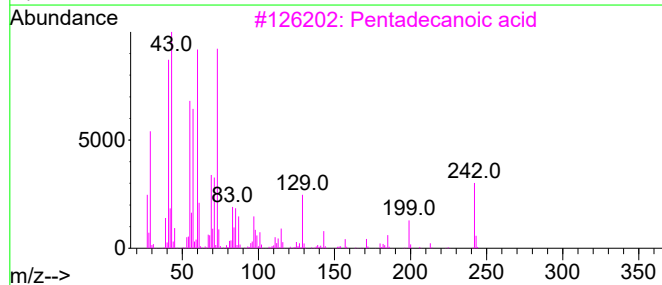
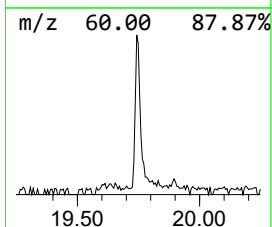
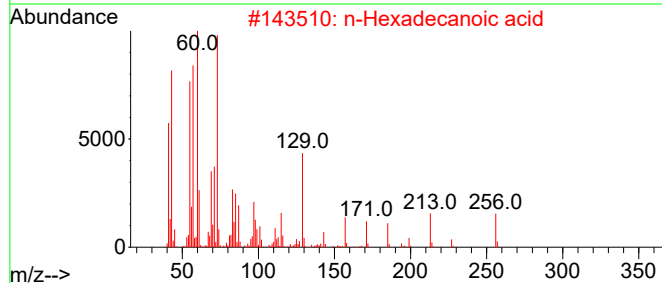
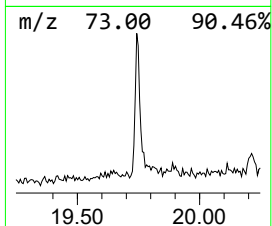
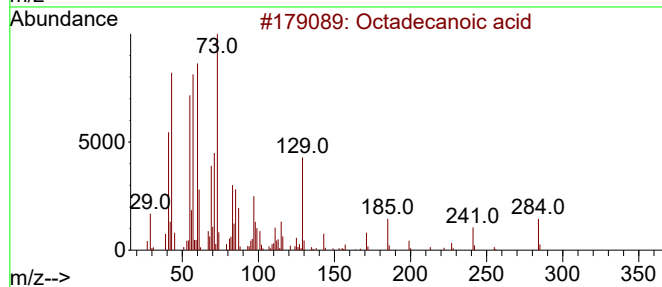
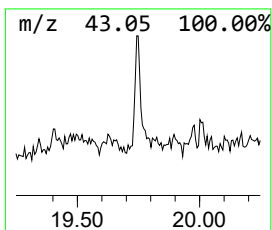
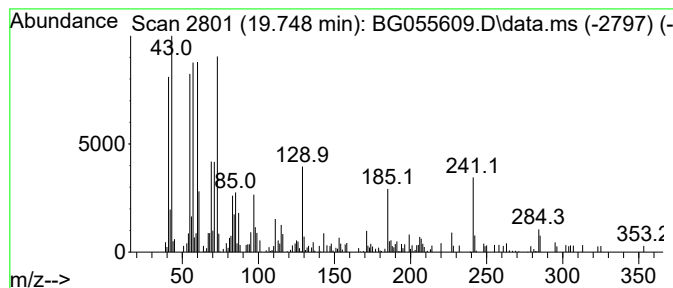
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.748	2.80 ng	121364	Phenanthrene-d10	17.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055609.D
Acq On : 14 Nov 2022 18:04
Operator : CG/JU
Sample : N5561-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-25

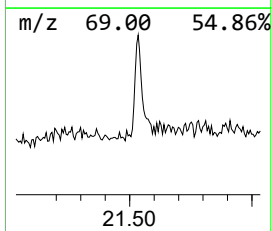
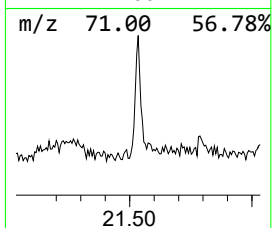
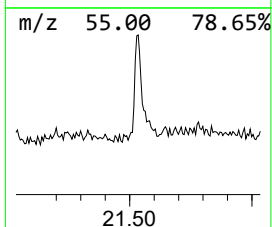
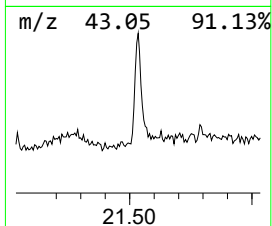
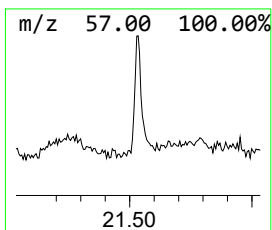
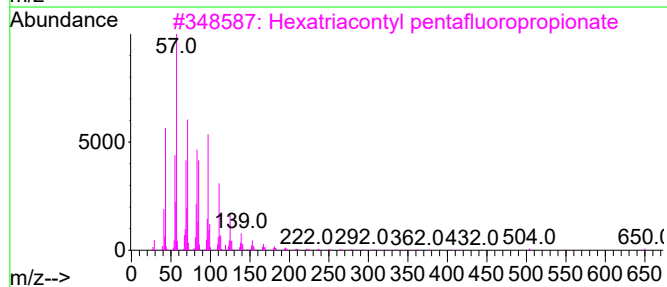
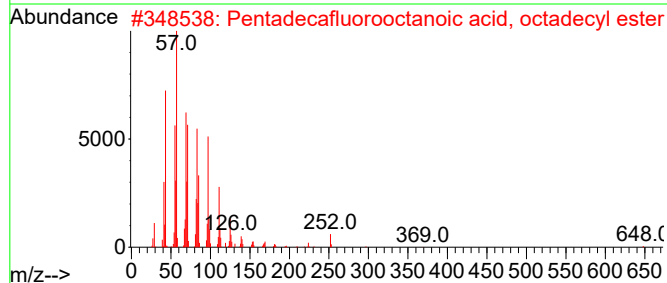
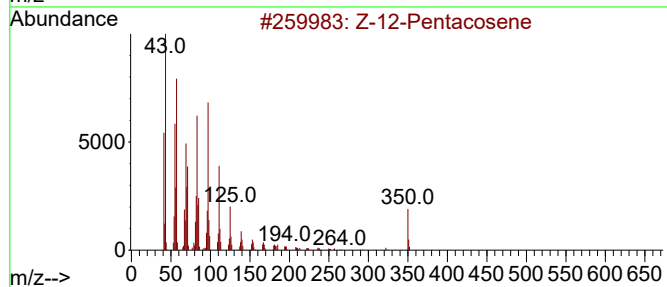
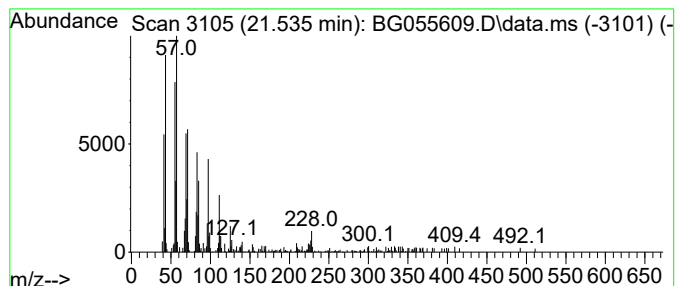
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Z-12-Pentacosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.535	3.60 ng	153047	Chrysene-d12	21.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Z-12-Pentacosene	350	C25H50	1000131-09-4	93
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
3			Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	90
4			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
5			Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055609.D
Acq On : 14 Nov 2022 18:04
Operator : CG/JU
Sample : N5561-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-25

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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
Butane, 2-metho...	3.321	23.9	ng	396455	1	8.262	331414	20.0
2-Pentanone, 4-...	5.318	16.5	ng	273134	1	8.262	331414	20.0
Ethanol, 2-(2-b...	10.835	10.9	ng	271161	2	11.094	497418	20.0
n-Hexadecanoic ...	18.485	5.5	ng	237475	4	17.627	866659	20.0
Octadecanoic acid	19.748	2.8	ng	121364	4	17.627	866659	20.0
Z-12-Pentacosene	21.535	3.6	ng	153047	5	21.928	851235	20.0