

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
 Data File : BG055565.D
 Acq On : 11 Nov 2022 13:39
 Operator : CG/JU
 Sample : N5531-13
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-28B

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: BG055565.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.326	3	6	11	rVB	118716	149003	3.17%	0.774%
2	4.707	235	241	248	rVB	55145	83640	1.78%	0.434%
3	5.324	339	346	355	rBV	394418	622045	13.23%	3.229%
4	5.794	419	426	440	rVB	1153049	1848480	39.32%	9.596%
5	7.404	692	700	716	rBV	1106299	1906485	40.55%	9.897%
6	8.268	838	847	854	rBV	168758	281137	5.98%	1.459%
7	9.437	1038	1046	1056	rBV	638901	1126021	23.95%	5.846%
8	10.841	1279	1285	1299	rBV	37119	67026	1.43%	0.348%
9	11.099	1321	1329	1340	rBV	205443	374951	7.98%	1.947%
10	13.514	1732	1740	1747	rBV	1683762	2588830	55.07%	13.440%
11	14.883	1966	1973	1981	rVB	326731	517028	11.00%	2.684%
12	16.364	2218	2225	2240	rBV	1494497	2260104	48.08%	11.733%
13	17.621	2434	2439	2446	rBV	451152	690143	14.68%	3.583%
14	18.268	2545	2549	2554	rBV	39196	49344	1.05%	0.256%
15	19.554	2764	2768	2772	rBV	40194	47682	1.01%	0.248%
16	20.212	2874	2880	2889	rBV	3572409	4701182	100.00%	24.406%
17	21.528	3099	3104	3114	rBV2	69519	119924	2.55%	0.623%
18	21.922	3164	3171	3181	rBV2	495460	881289	18.75%	4.575%
19	23.708	3471	3475	3482	rVB3	33243	58032	1.23%	0.301%
20	25.336	3743	3752	3768	rVB2	293643	890368	18.94%	4.622%

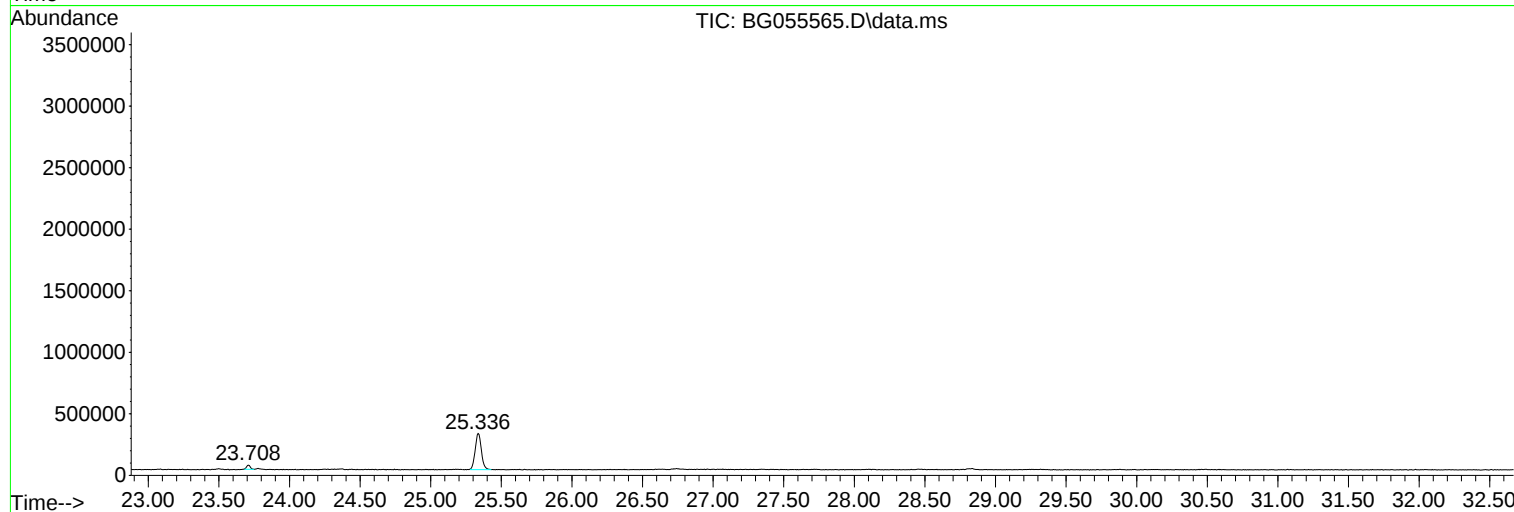
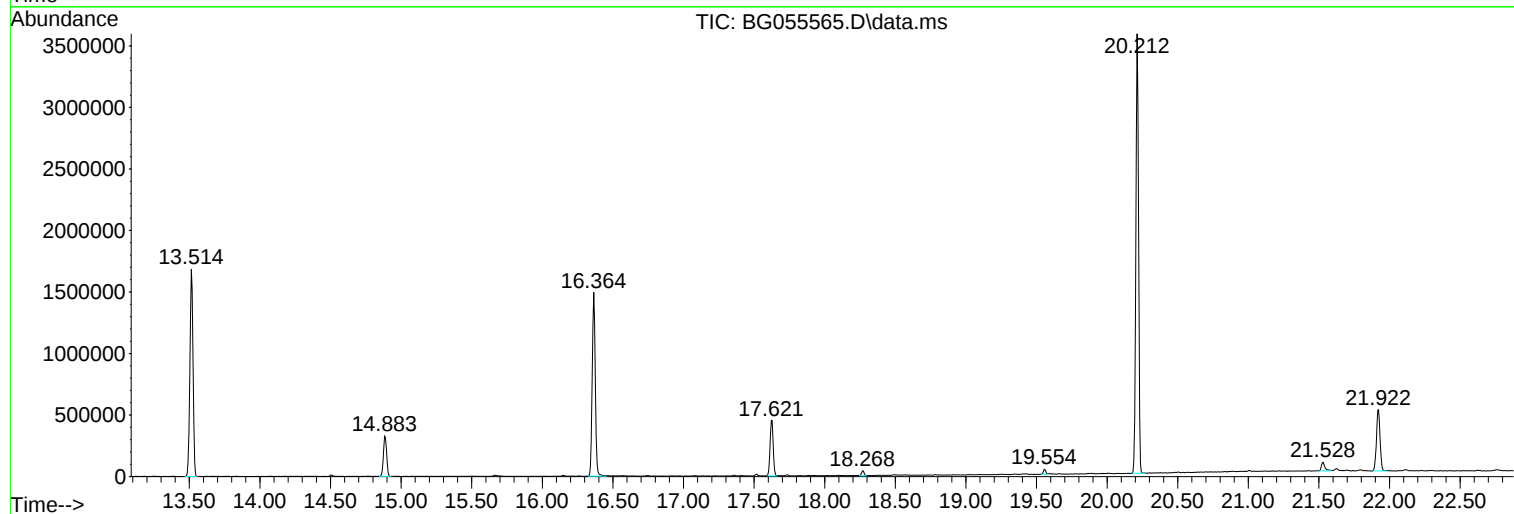
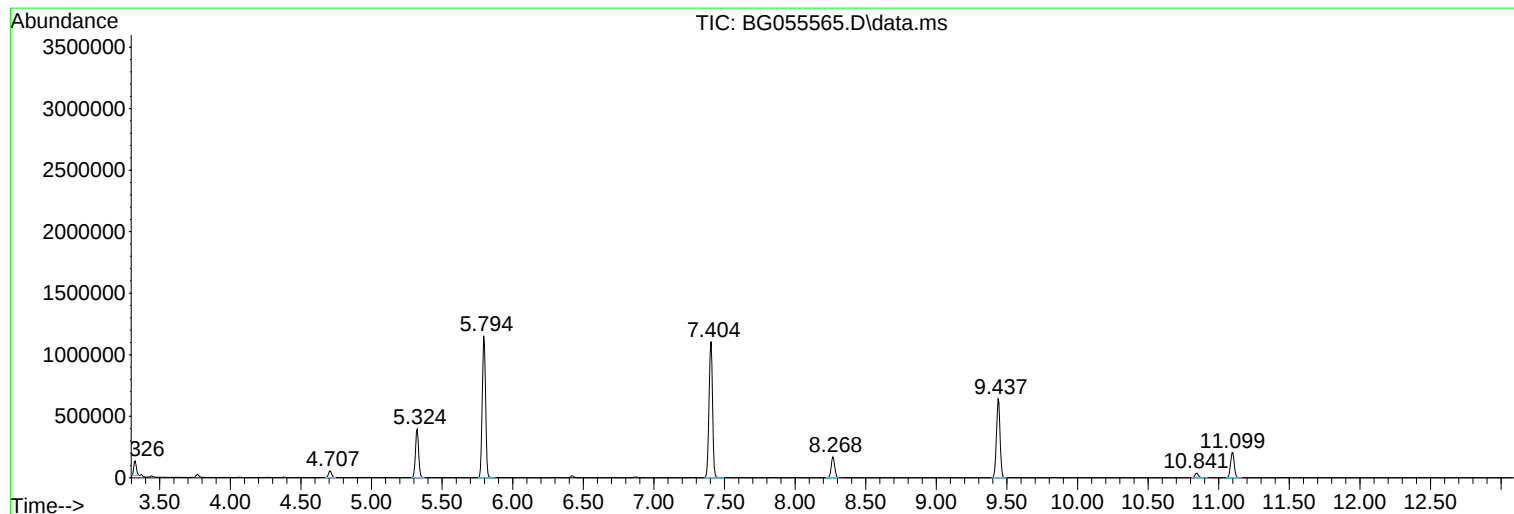
Sum of corrected areas: 19262714

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055565.D
Acq On : 11 Nov 2022 13:39
Operator : CG/JU
Sample : N5531-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-28B

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\BG111122\
Data File : BG055565.D
Acq On : 11 Nov 2022 13:39
Operator : CG/JU
Sample : N5531-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-28B

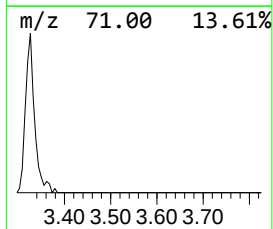
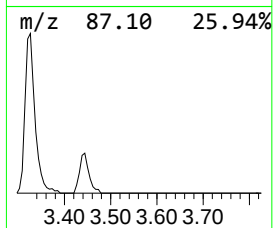
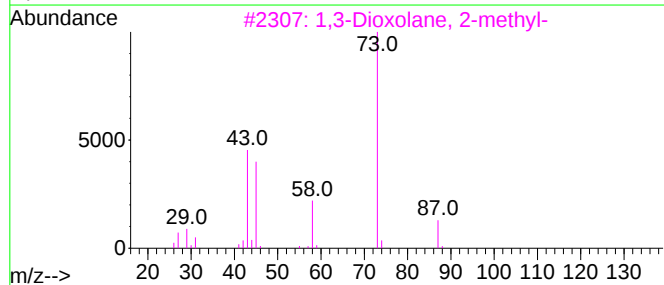
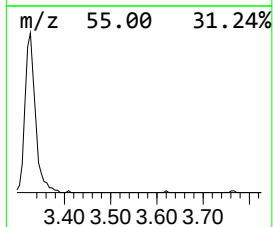
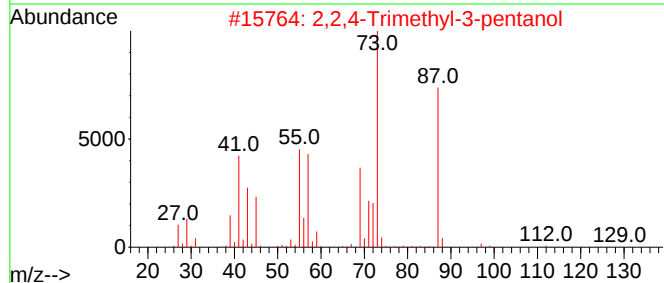
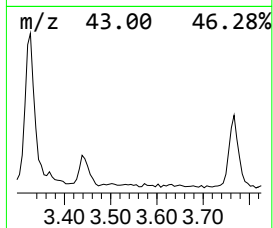
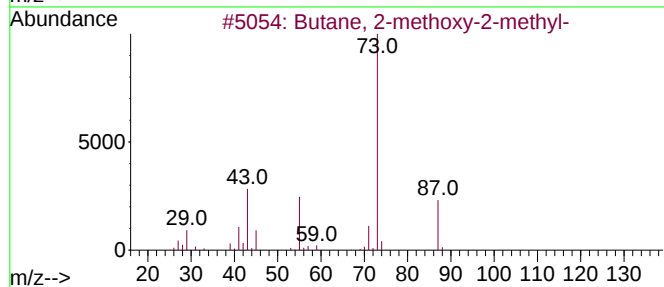
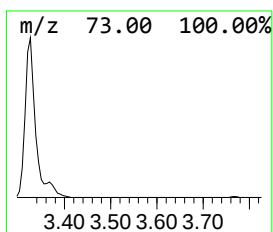
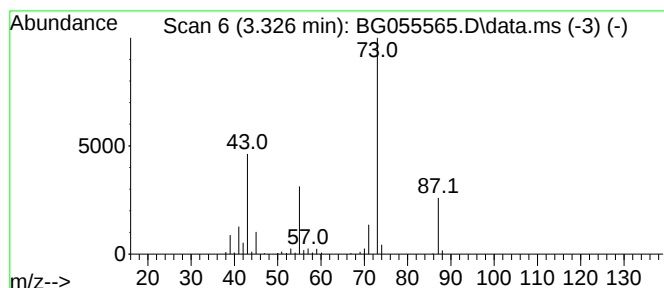
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.326	10.60 ng	149003	1,4-Dichlorobenzene-d4	8.268

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055565.D
Acq On : 11 Nov 2022 13:39
Operator : CG/JU
Sample : N5531-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-28B

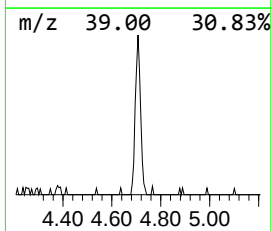
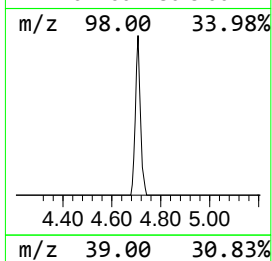
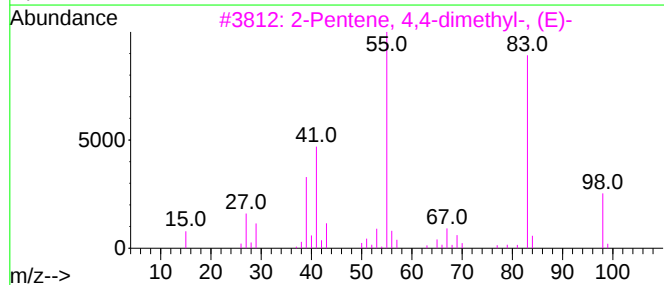
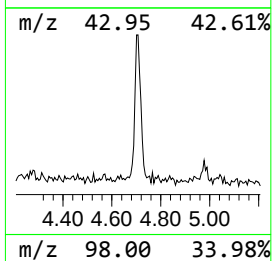
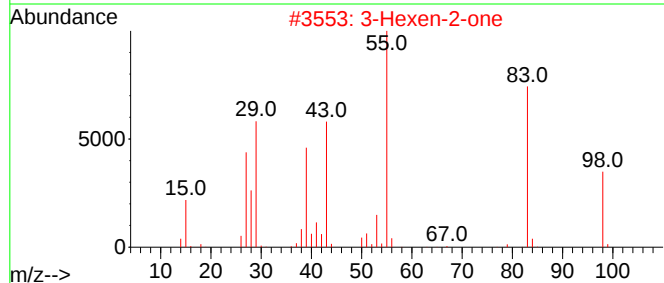
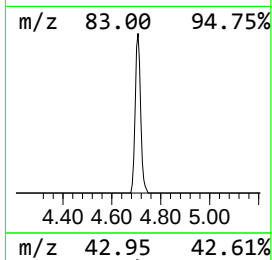
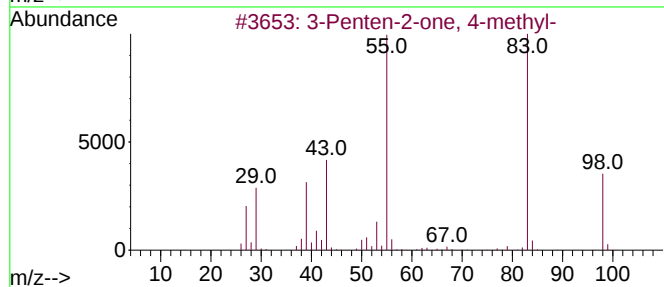
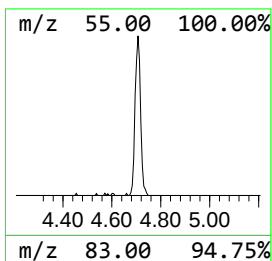
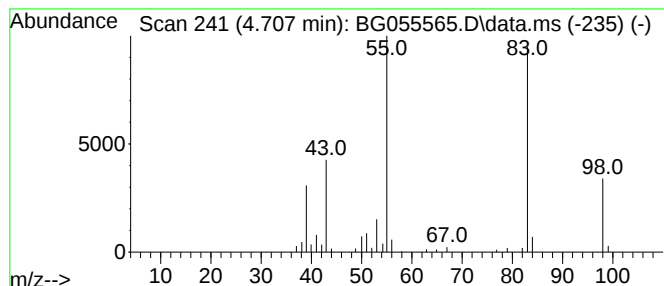
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.707	5.95 ng	83640	1,4-Dichlorobenzene-d4	8.268

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055565.D
Acq On : 11 Nov 2022 13:39
Operator : CG/JU
Sample : N5531-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-28B

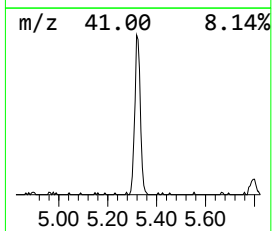
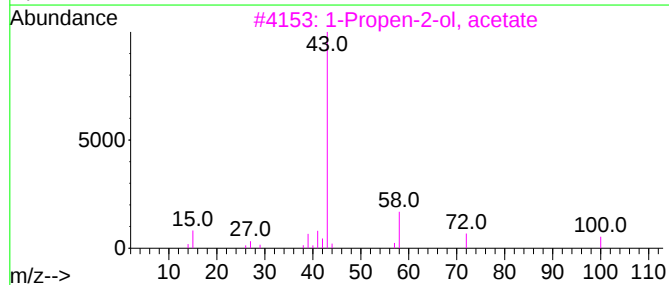
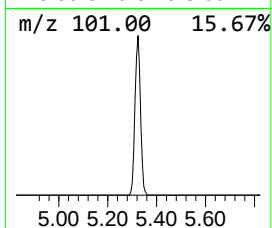
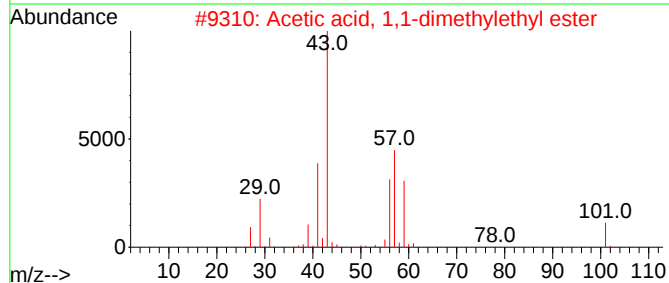
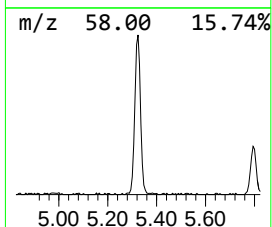
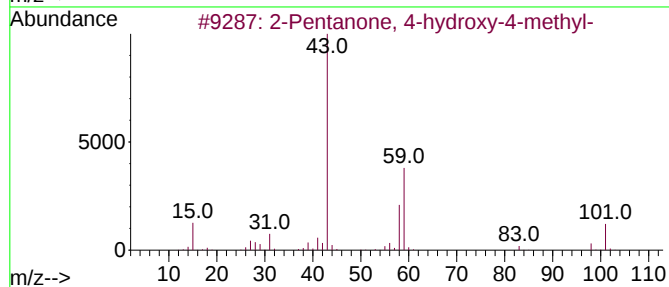
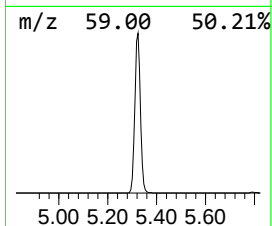
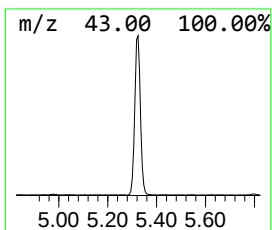
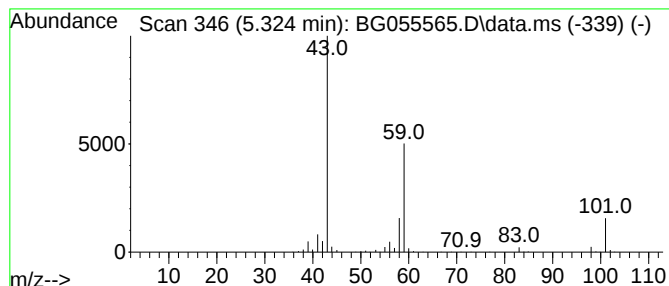
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.324	44.25 ng	622045	1,4-Dichlorobenzene-d4	8.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
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			Acetone	58	C3H6O	000067-64-1	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055565.D
Acq On : 11 Nov 2022 13:39
Operator : CG/JU
Sample : N5531-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

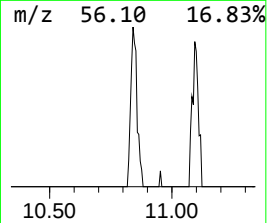
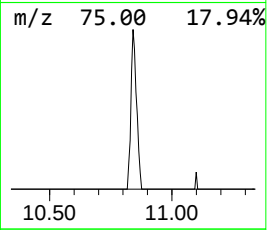
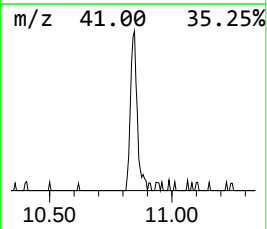
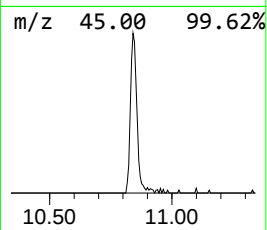
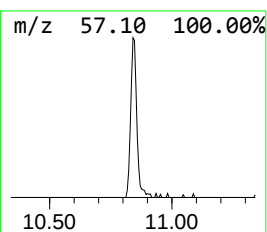
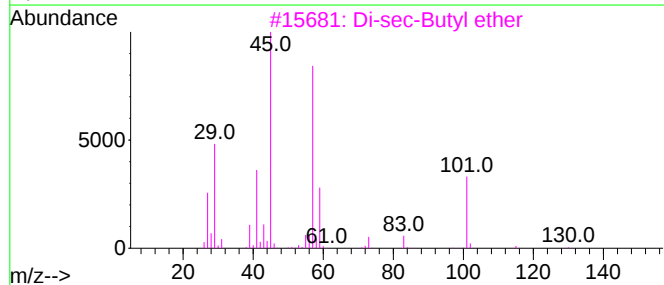
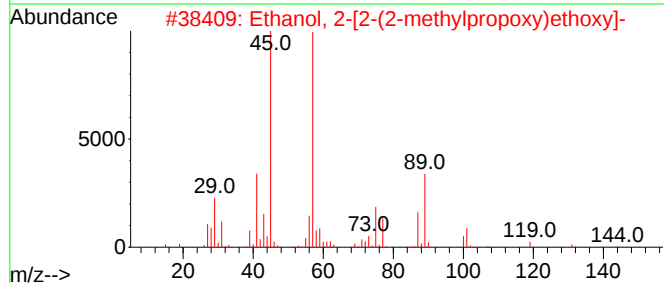
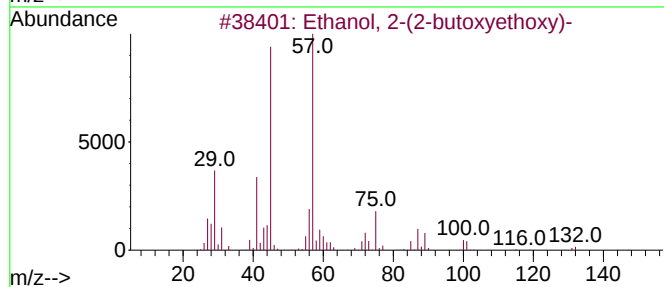
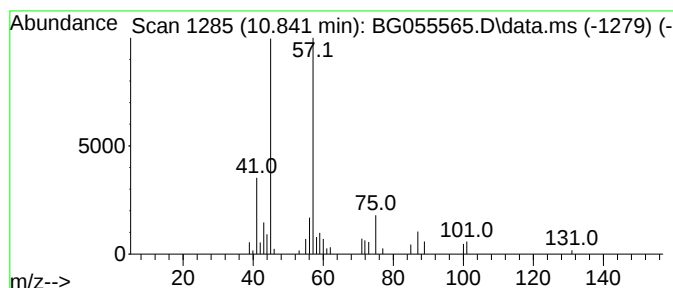
Instrument :
BNA_G
ClientSampleId :
SB-28B

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 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.841	3.58 ng	67026	Naphthalene-d8	11.100	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
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	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055565.D
Acq On : 11 Nov 2022 13:39
Operator : CG/JU
Sample : N5531-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-28B

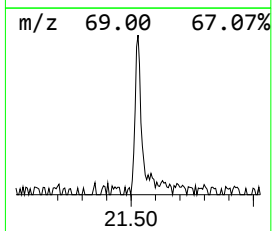
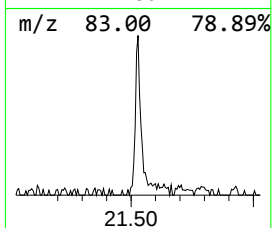
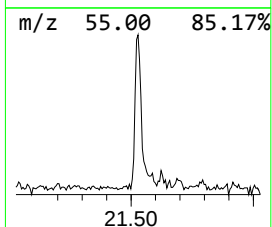
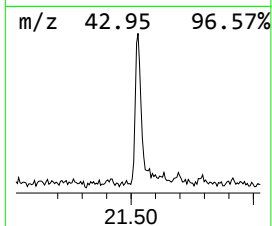
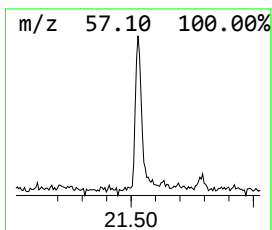
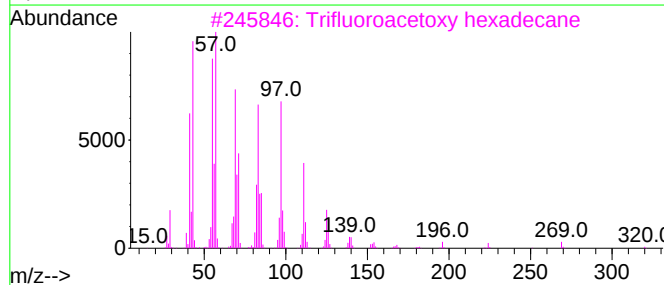
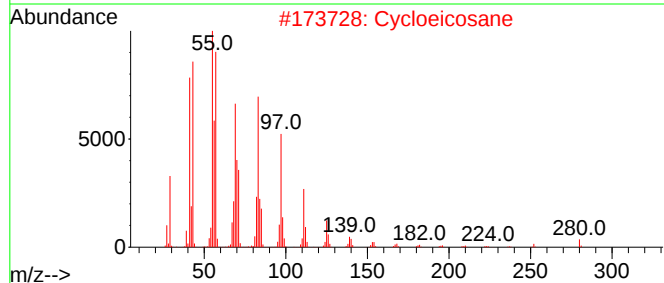
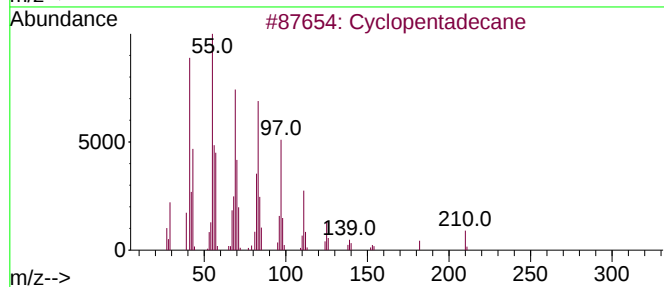
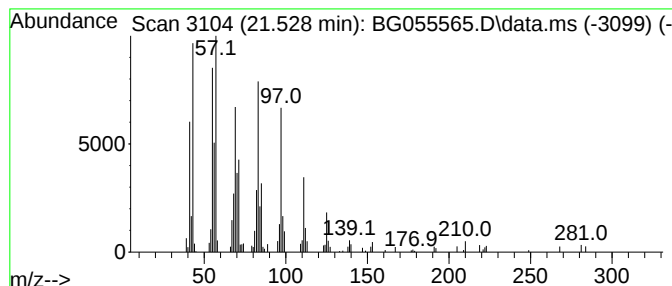
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.528	2.72 ng	119924	Chrysene-d12	21.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	93
2			Cycloeicosane	280	C20H40	000296-56-0	91
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
5			1-Hexacosene	364	C26H52	018835-33-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055565.D
Acq On : 11 Nov 2022 13:39
Operator : CG/JU
Sample : N5531-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-28B

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...	3.326	10.6	ng	149003	1	8.268	281137	20.0
3-Penten-2-one,...	4.707	6.0	ng	83640	1	8.268	281137	20.0
2-Pentanone, 4-...	5.324	44.3	ng	622045	1	8.268	281137	20.0
Ethanol, 2-(2-b...	10.841	3.6	ng	67026	2	11.100	374951	20.0
Cyclopentadecane	21.528	2.7	ng	119924	5	21.916	881289	20.0