

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122922\
 Data File : BG056163.D
 Acq On : 29 Dec 2022 20:59
 Operator : CG/JU
 Sample : N6226-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TWP01

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056163.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	7	13	27	rVB	430696	747363	21.87%	5.708%
2	5.379	350	356	363	rVB	79828	121300	3.55%	0.926%
3	5.855	430	437	445	rBV	290950	465081	13.61%	3.552%
4	7.465	704	711	721	rVB	181098	314102	9.19%	2.399%
5	8.335	850	859	871	rBB	138668	234152	6.85%	1.788%
6	9.510	1049	1059	1068	rBV	349495	637153	18.64%	4.866%
7	11.167	1332	1341	1352	rBV	182217	319406	9.35%	2.439%
8	11.425	1378	1385	1392	rBB	60088	95048	2.78%	0.726%
9	12.935	1632	1642	1646	rBV4	18890	34974	1.02%	0.267%
10	13.570	1743	1750	1761	rVB	1346493	2147047	62.82%	16.397%
11	14.945	1974	1984	1992	rBV	335182	520602	15.23%	3.976%
12	15.656	2099	2105	2113	rBV	28688	40395	1.18%	0.309%
13	16.419	2229	2235	2250	rBV	767326	1201935	35.17%	9.179%
14	17.677	2442	2449	2457	rBV	496789	762434	22.31%	5.823%
15	18.599	2601	2606	2615	rVB2	25042	39409	1.15%	0.301%
16	20.250	2881	2887	2893	rBV	2690043	3417886	100.00%	26.103%
17	21.560	3105	3110	3121	rVB3	78351	140864	4.12%	1.076%
18	21.972	3173	3180	3188	rVB2	521413	912813	26.71%	6.971%
19	25.426	3757	3768	3779	rVB2	307846	941929	27.56%	7.194%

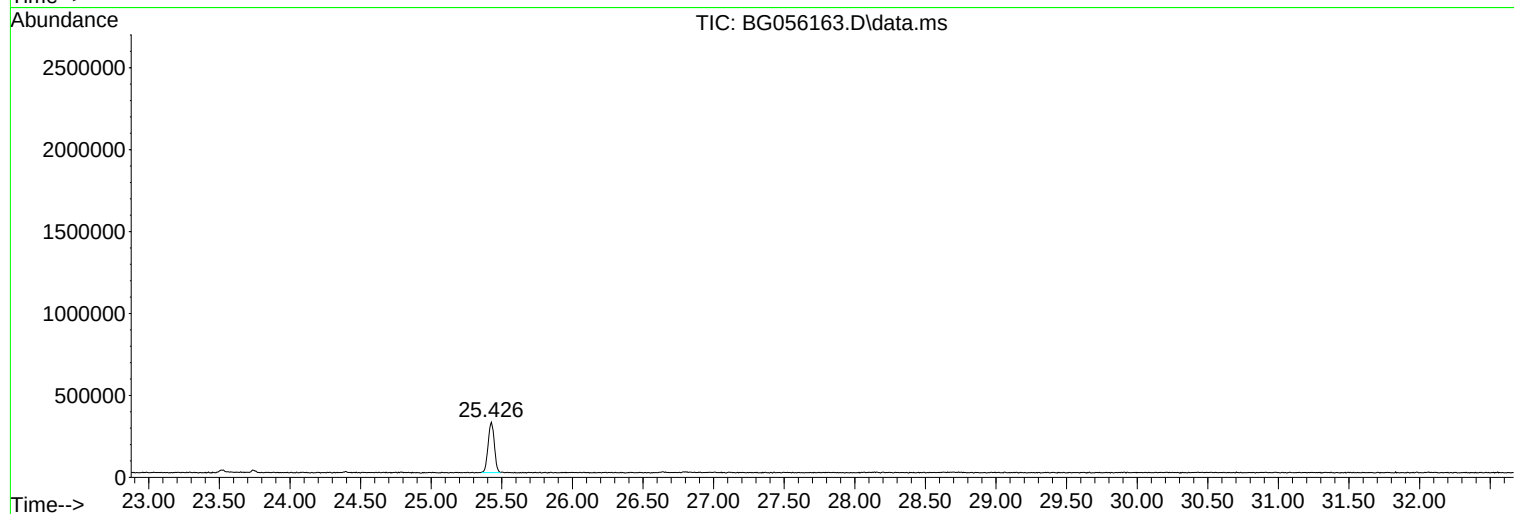
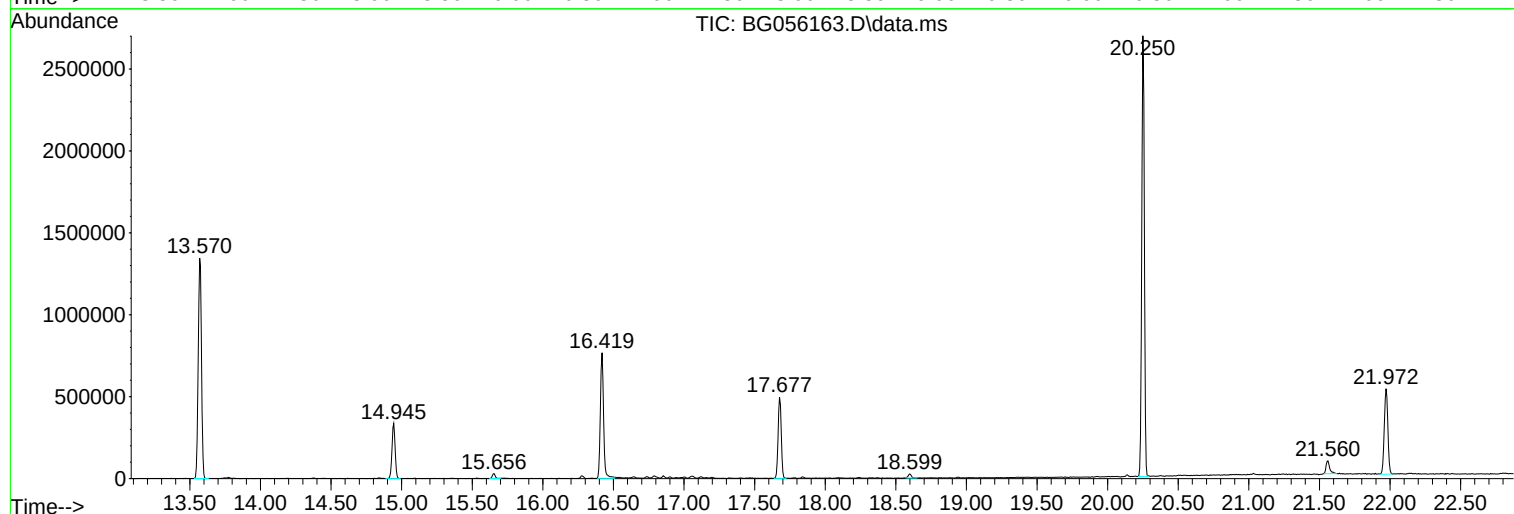
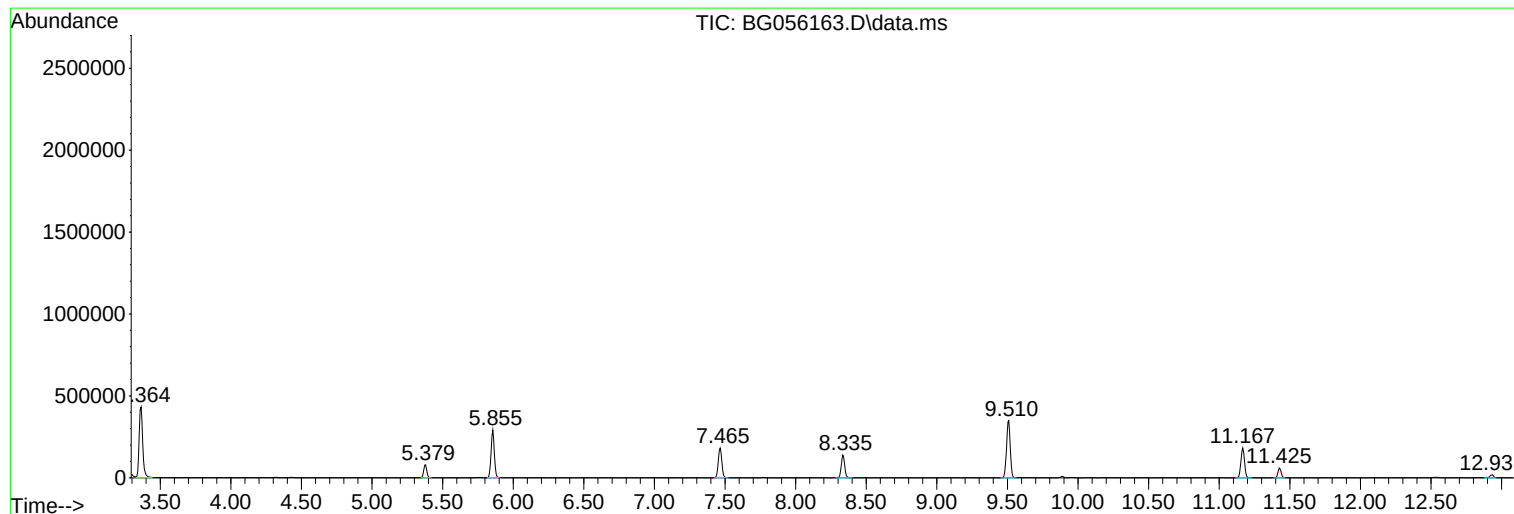
Sum of corrected areas: 13093893

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122922\
Data File : BG056163.D
Acq On : 29 Dec 2022 20:59
Operator : CG/JU
Sample : N6226-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TWP01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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\BG122922\
Data File : BG056163.D
Acq On : 29 Dec 2022 20:59
Operator : CG/JU
Sample : N6226-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TWP01

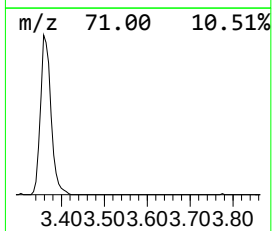
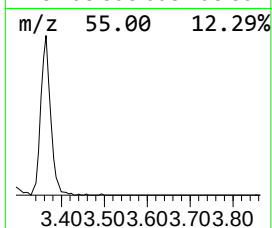
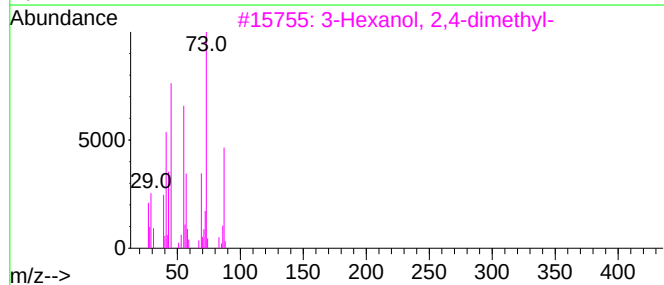
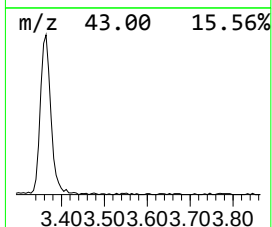
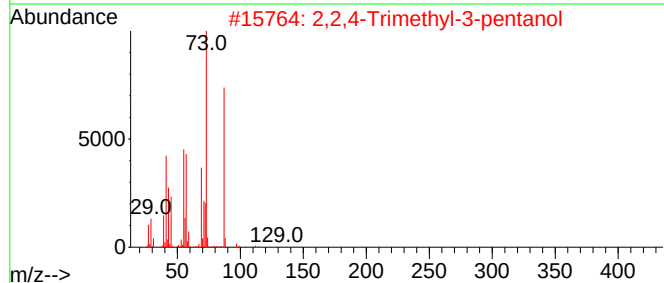
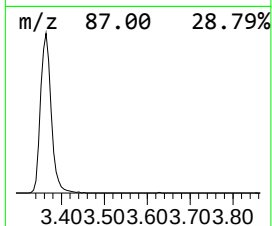
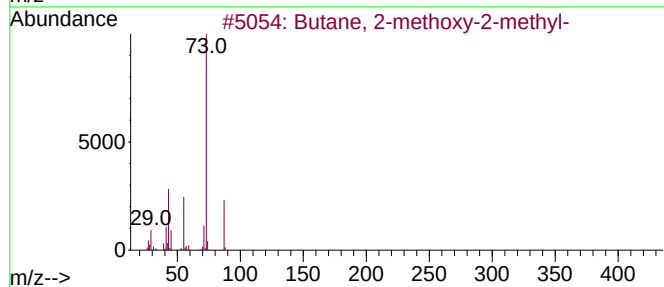
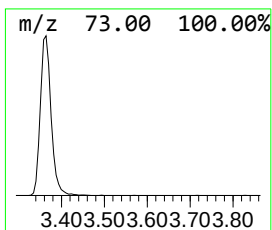
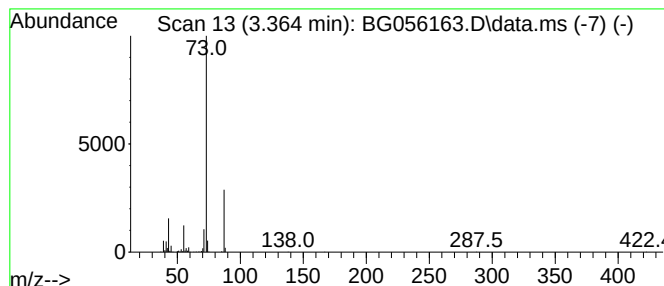
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	63.84 ng	747363	1,4-Dichlorobenzene-d4	8.335

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	9
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122922\
Data File : BG056163.D
Acq On : 29 Dec 2022 20:59
Operator : CG/JU
Sample : N6226-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TWP01

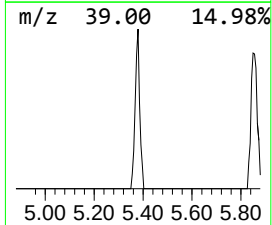
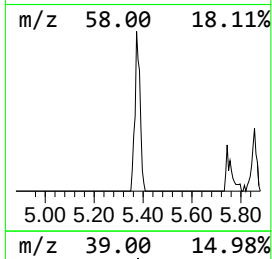
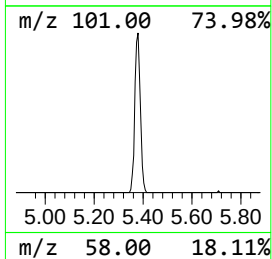
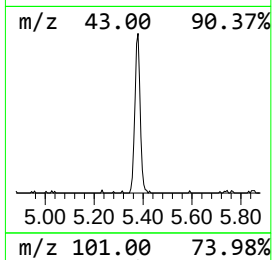
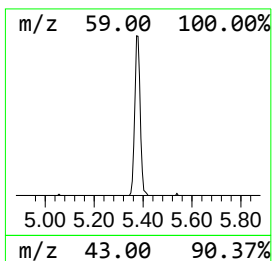
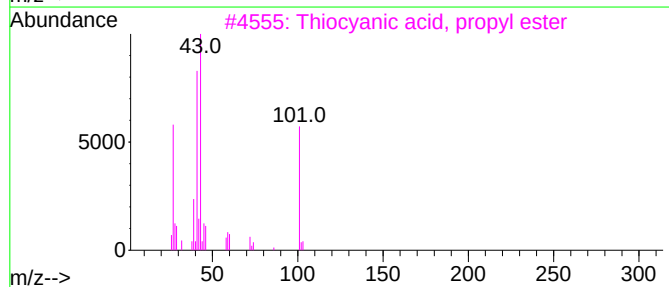
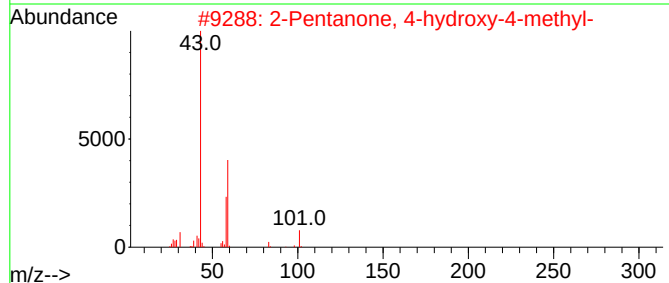
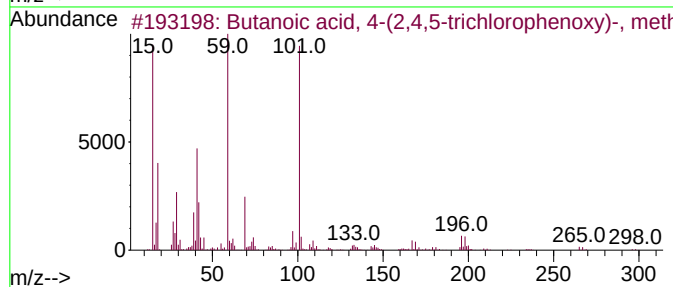
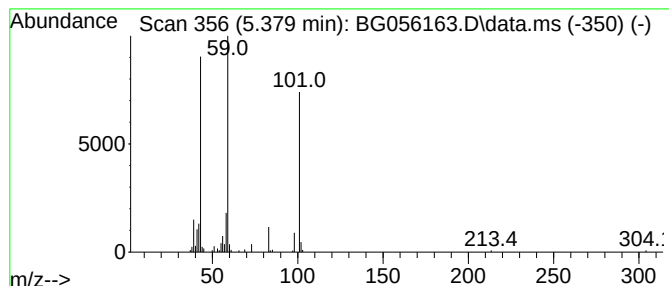
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butanoic acid, 4-(2,4,5-tri... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.379	10.36 ng	121300	1,4-Dichlorobenzene-d4	8.335

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 4-(2,4,5-trichlor...	296	C11H11Cl3O3	025333-21-5	64
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
3			Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	43
4			Butanoic acid, 4-iodo-, methyl e...	228	C5H9IO2	014273-85-9	40
5			Isopropyl methyl carbonate	118	C5H10O3	051729-83-0	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122922\
Data File : BG056163.D
Acq On : 29 Dec 2022 20:59
Operator : CG/JU
Sample : N6226-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

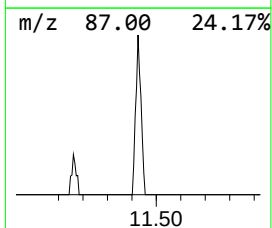
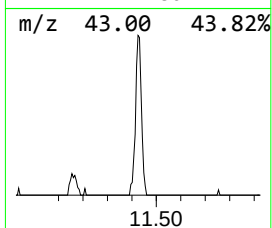
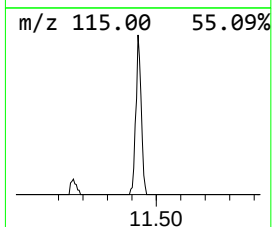
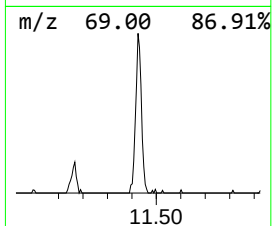
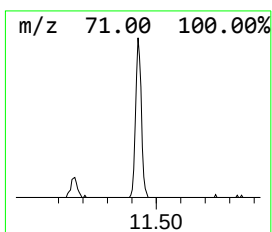
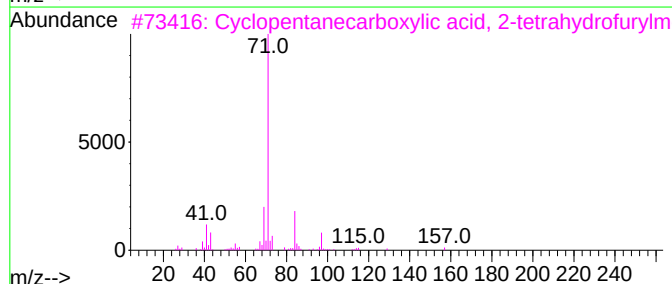
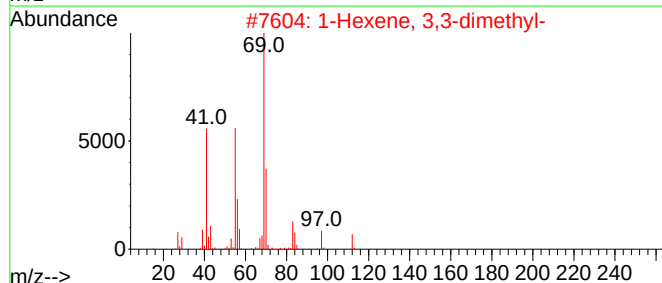
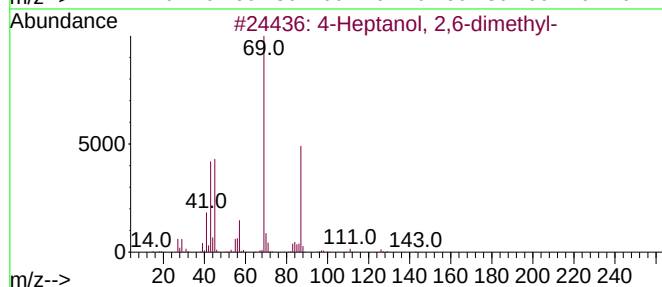
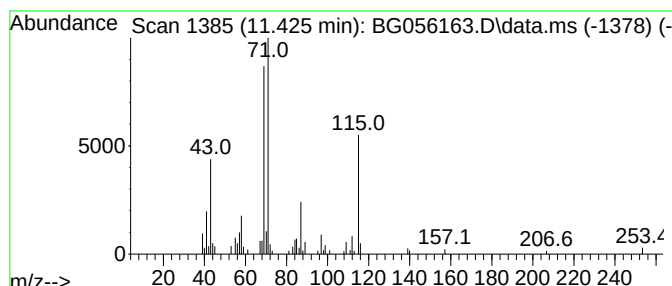
Instrument :
BNA_G
ClientSampleId :
TWP01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown11.425 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.425	5.95 ng	95048	Naphthalene-d8		11.167	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-		144	C9H20O	000108-82-7	27
2	1-Hexene, 3,3-dimethyl-		112	C8H16	003404-77-1	25
3	Cyclopentanecarboxylic acid, 2-t...		198	C11H18O3	1000282-42-9	22
4	Morpholine, 2,6-dimethyl-		115	C6H13NO	000141-91-3	22
5	Butyric acid, 1-propylpentyl ester		200	C12H24O2	020286-46-8	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122922\
Data File : BG056163.D
Acq On : 29 Dec 2022 20:59
Operator : CG/JU
Sample : N6226-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TWP01

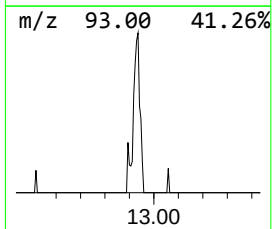
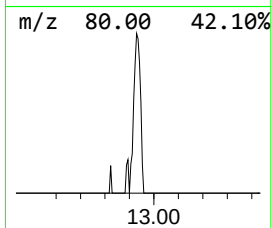
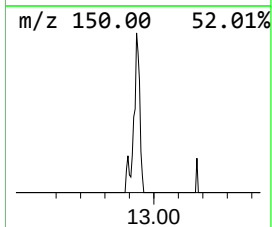
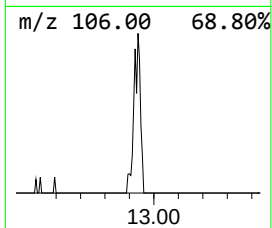
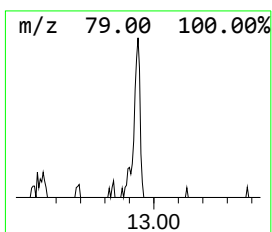
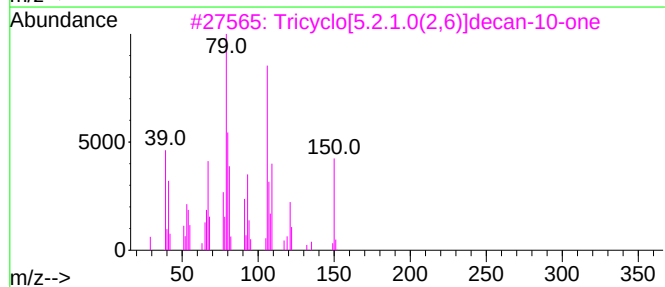
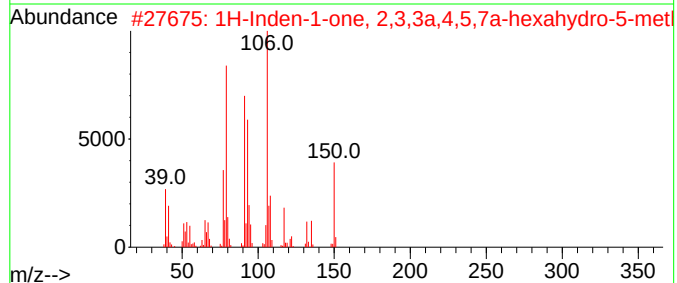
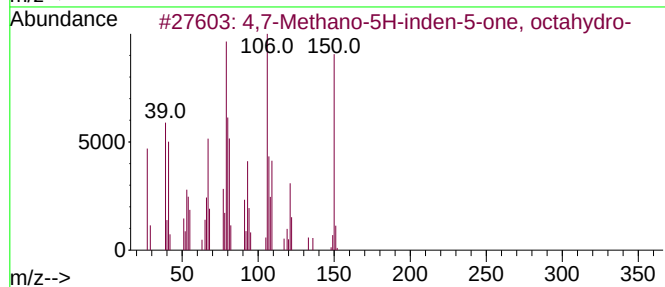
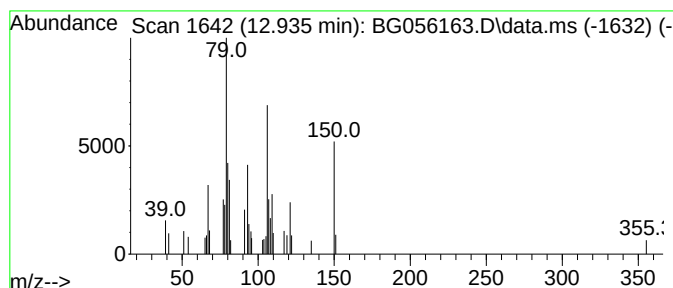
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 4,7-Methano-5H-inden-5-one,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.935	2.19 ng	34974	Naphthalene-d8	11.167

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,7-Methano-5H-inden-5-one, octa...	150	C10H14O	013380-94-4	92
2			1H-Inden-1-one, 2,3,3a,4,5,7a-he...	150	C10H14O	1000221-37-4	64
3			Tricyclo[5.2.1.0(2,6)]decan-10-one	150	C10H14O	103385-97-3	64
4			3a,6-Methano-3aH-inden-5(4H)-one...	150	C10H14O	016489-26-2	50
5			1(2H)-Pentalenone, hexahydro-5-m...	150	C10H14O	120587-85-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122922\
Data File : BG056163.D
Acq On : 29 Dec 2022 20:59
Operator : CG/JU
Sample : N6226-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

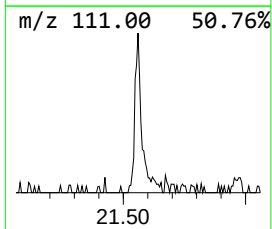
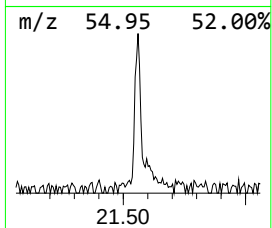
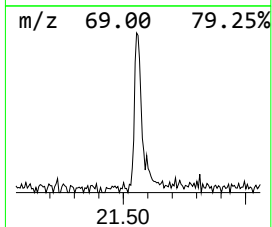
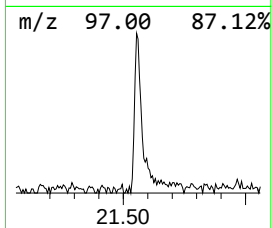
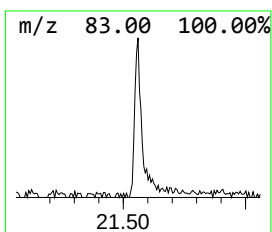
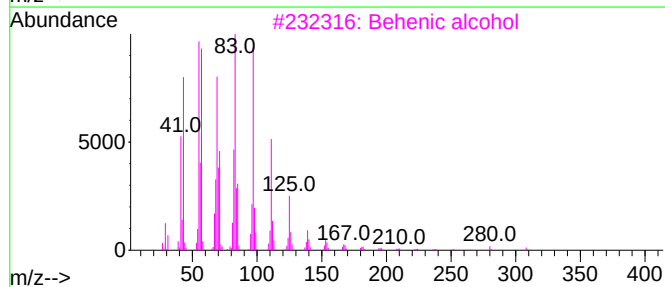
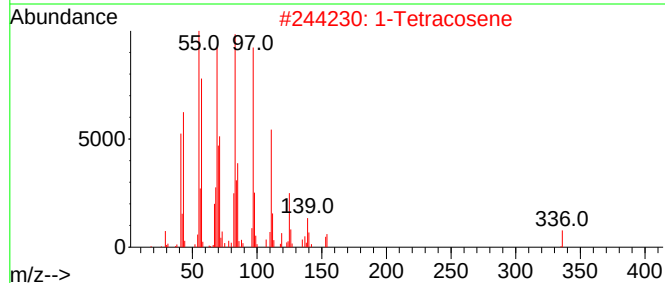
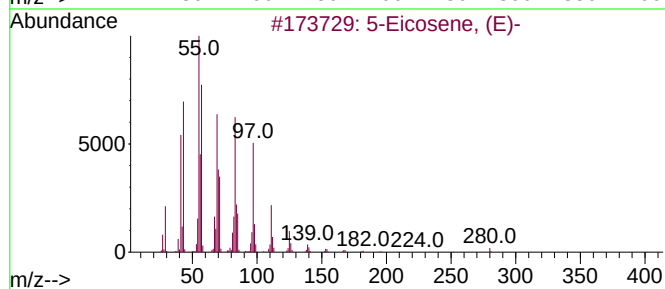
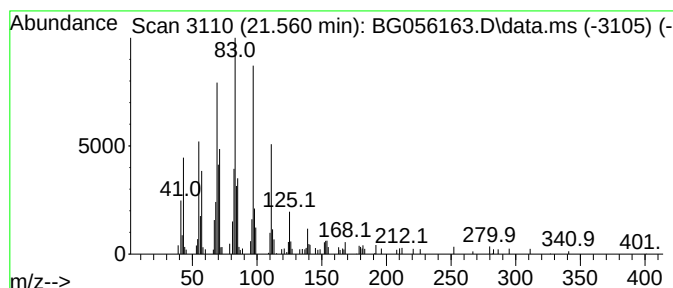
Instrument :
BNA_G
ClientSampleId :
TWP01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.560	3.09 ng	140864	Chrysene-d12	21.972	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
2	1-Tetracosene	336	C24H48	010192-32-2	90
3	Behenic alcohol	326	C22H46O	000661-19-8	90
4	1-Octadecanol	270	C18H38O	000112-92-5	90
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122922\
Data File : BG056163.D
Acq On : 29 Dec 2022 20:59
Operator : CG/JU
Sample : N6226-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TWP01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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	63.8	ng	747363	1	8.335	234152	20.0
Butanoic acid, ...	5.379	10.4	ng	121300	1	8.335	234152	20.0
unknown11.425	11.425	6.0	ng	95048	2	11.167	319406	20.0
4,7-Methano-5H-...	12.935	2.2	ng	34974	2	11.167	319406	20.0
5-Eicosene, (E)-	21.560	3.1	ng	140864	5	21.972	912813	20.0