

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
 Data File : BG055967.D
 Acq On : 14 Dec 2022 20:09
 Operator : CG/JU
 Sample : N6024-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-Q

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-BG121322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055967.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.403	15	19	24	rBV	9359	12170	1.15%	0.331%
2	5.412	356	361	367	rBB	19670	29547	2.79%	0.804%
3	5.888	435	442	449	rBB	153484	237543	22.44%	6.465%
4	7.498	708	716	723	rBB	159214	275308	26.00%	7.493%
5	8.368	859	864	870	rBB	19539	31920	3.01%	0.869%
6	9.543	1057	1064	1071	rBB	94529	162591	15.36%	4.425%
7	11.205	1340	1347	1353	rBB	29161	48760	4.61%	1.327%
8	13.608	1749	1756	1763	rBB	363402	543970	51.38%	14.806%
9	14.977	1983	1989	1995	rBB	55146	84068	7.94%	2.288%
10	16.317	2211	2217	2222	rBB	44181	62719	5.92%	1.707%
11	16.452	2233	2240	2249	rBV	422907	632344	59.72%	17.211%
12	17.710	2447	2454	2461	rBV	75412	116610	11.01%	3.174%
13	18.562	2594	2599	2605	rBV3	21847	29174	2.76%	0.794%
14	20.289	2887	2893	2899	rBV	811324	1058786	100.00%	28.818%
15	21.611	3113	3118	3123	rBV3	19222	28721	2.71%	0.782%
16	22.016	3178	3187	3195	rBV2	84185	154534	14.60%	4.206%
17	25.512	3771	3782	3793	rBV3	52410	165306	15.61%	4.499%

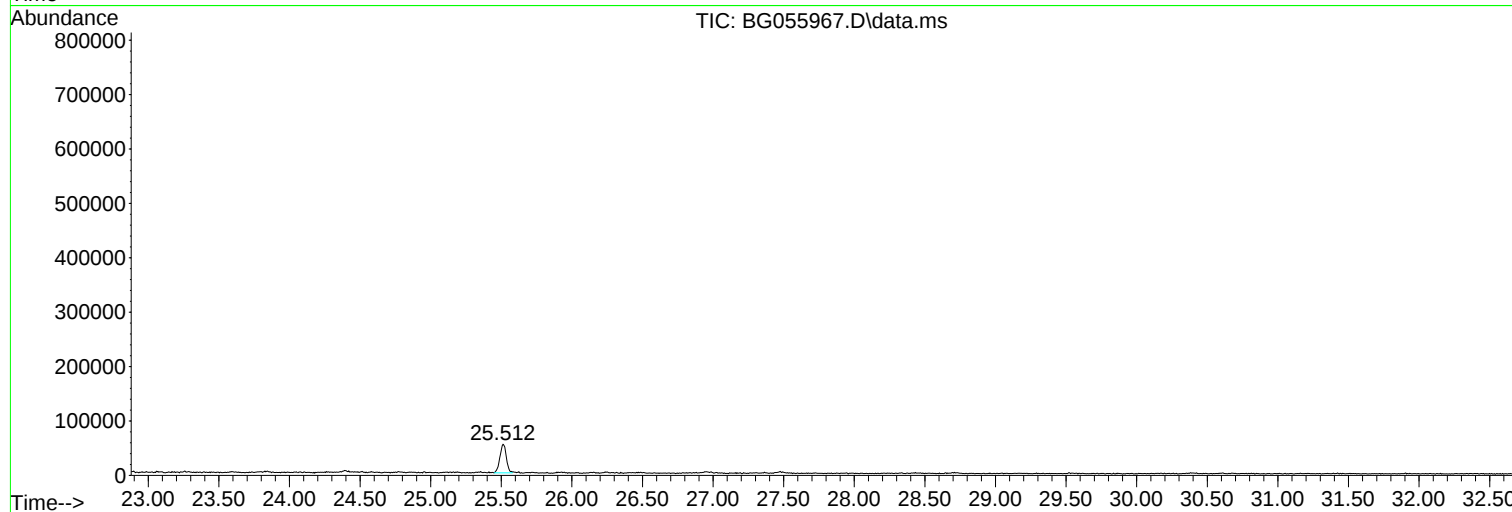
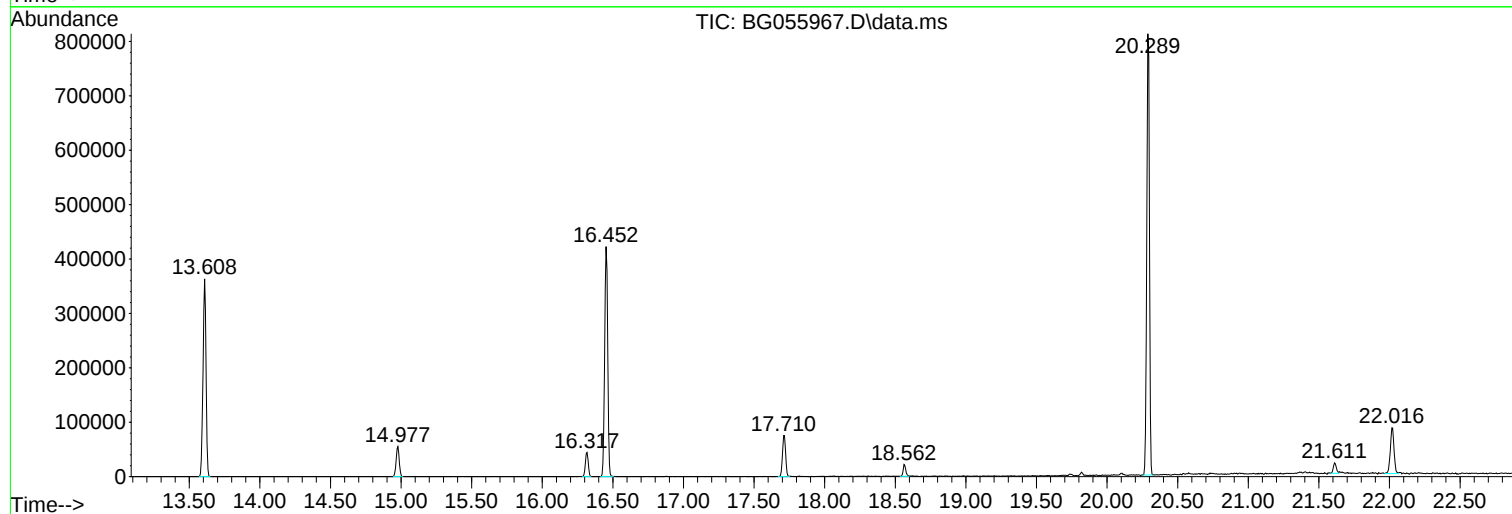
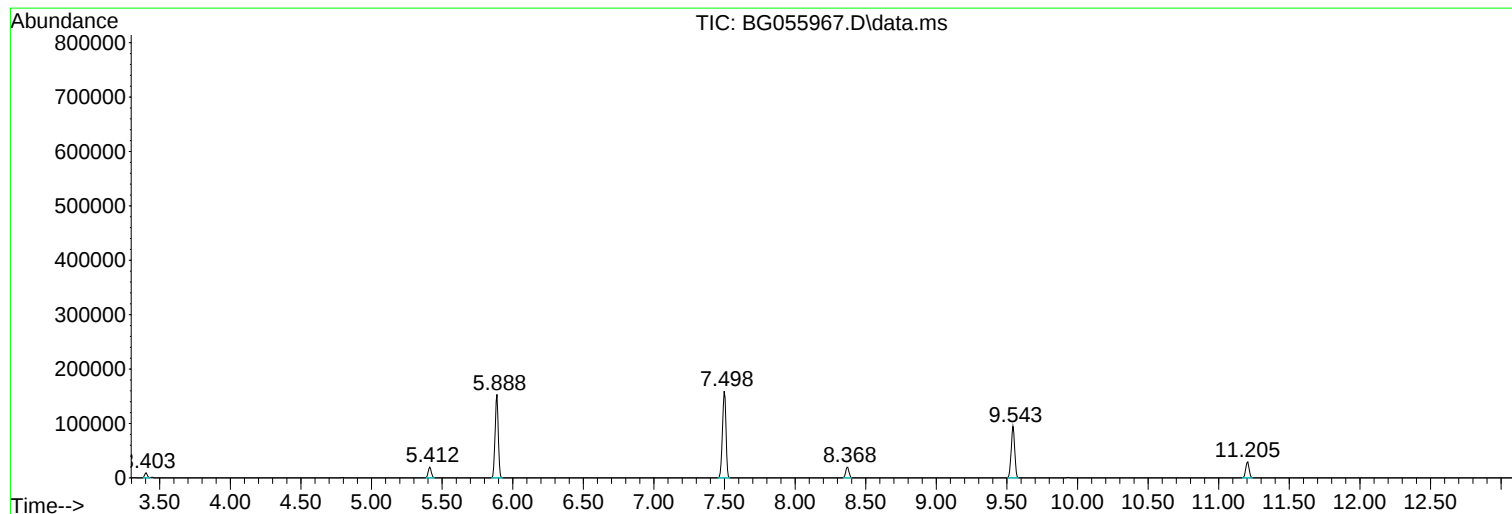
Sum of corrected areas: 3674071

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
Data File : BG055967.D
Acq On : 14 Dec 2022 20:09
Operator : CG/JU
Sample : N6024-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-Q

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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\BG121422\
Data File : BG055967.D
Acq On : 14 Dec 2022 20:09
Operator : CG/JU
Sample : N6024-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-Q

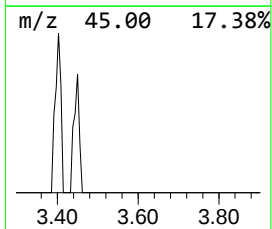
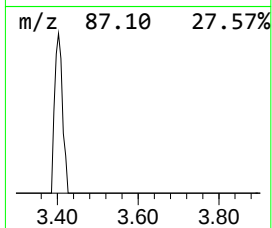
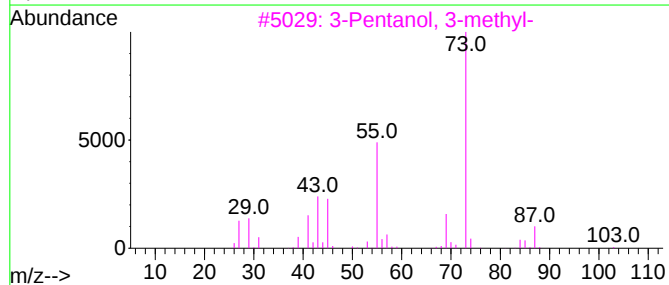
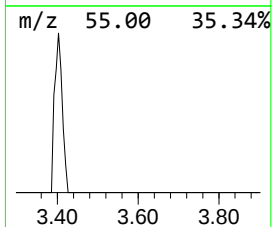
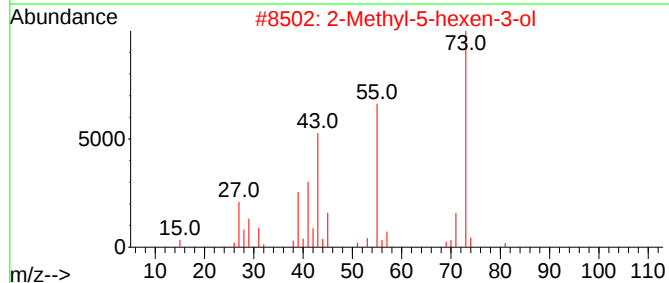
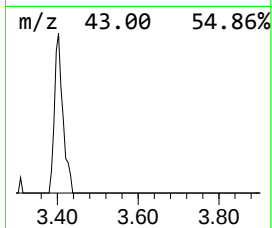
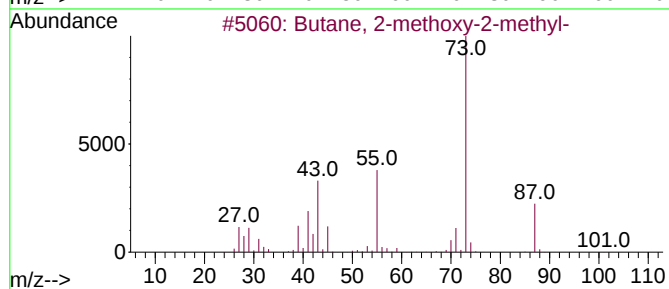
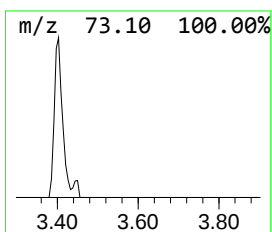
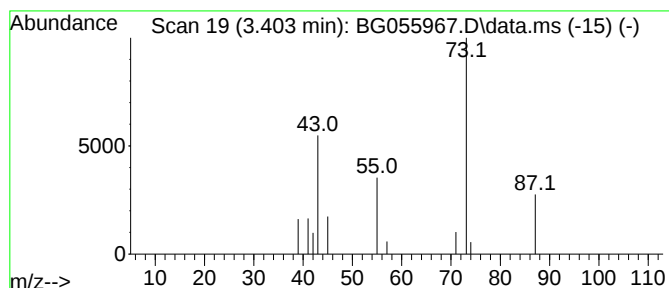
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.403	7.63 ng	12170	1,4-Dichlorobenzene-d4	8.368

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
3		3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	9
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
5		1-Pentanamine	87	C5H13N	000110-58-7	7



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
Data File : BG055967.D
Acq On : 14 Dec 2022 20:09
Operator : CG/JU
Sample : N6024-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-Q

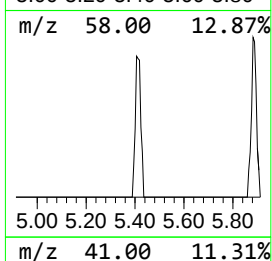
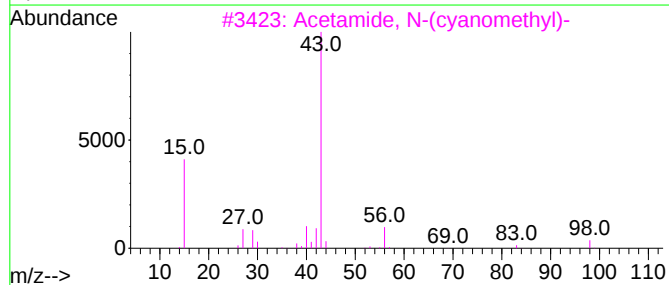
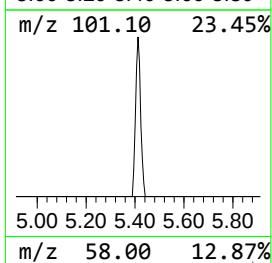
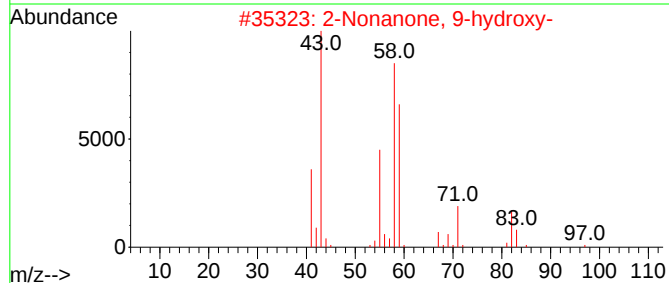
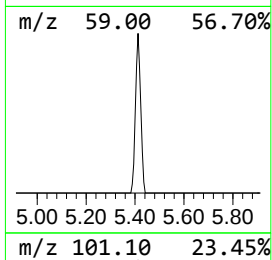
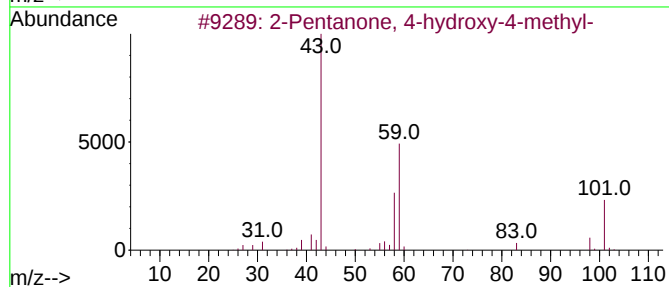
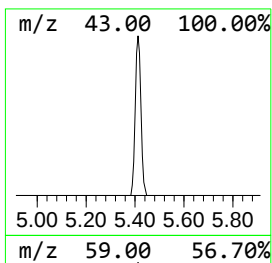
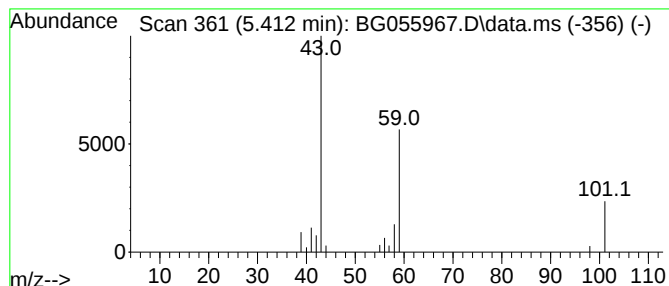
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.412	18.51 ng	29547	1,4-Dichlorobenzene-d4	8.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36
3			Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9
4			Butane	58	C4H10	000106-97-8	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
Data File : BG055967.D
Acq On : 14 Dec 2022 20:09
Operator : CG/JU
Sample : N6024-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-Q

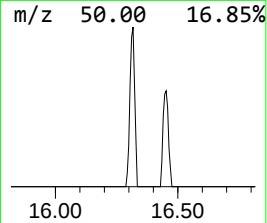
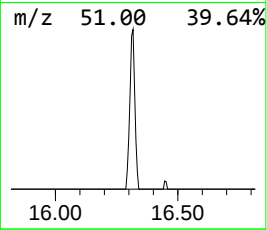
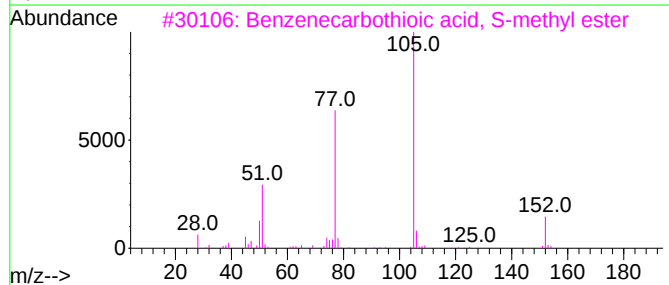
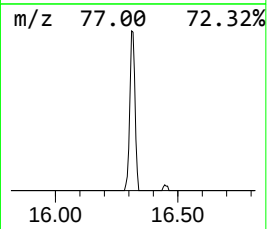
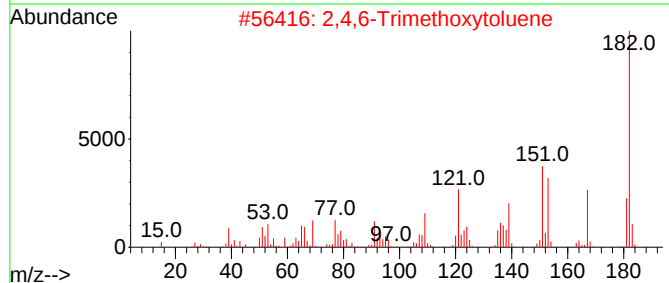
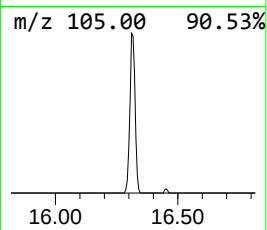
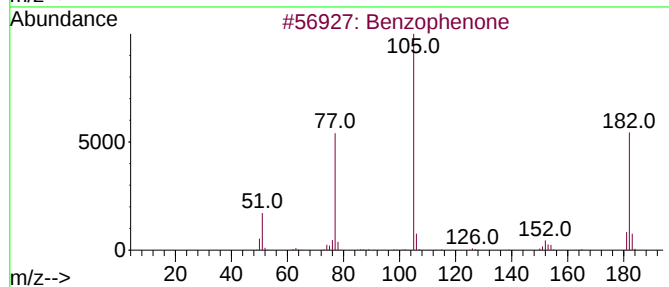
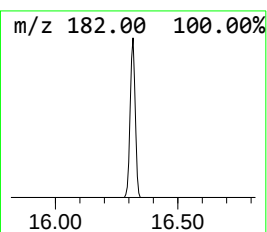
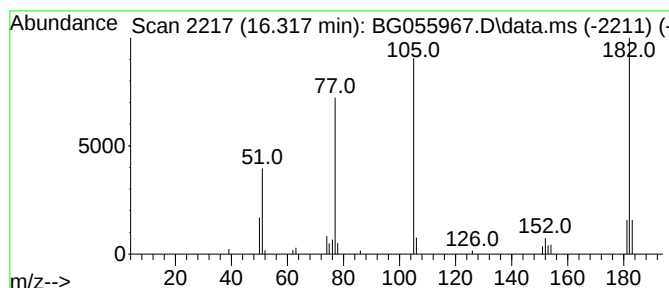
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.317	14.92 ng	62719	Acenaphthene-d10	14.977

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	43
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	41
4			1-Methyl-1,6-diazaplenalene	182	C12H10N2	079691-99-9	38
5			2-Methyl-1H-perimidine	182	C12H10N2	005157-10-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
Data File : BG055967.D
Acq On : 14 Dec 2022 20:09
Operator : CG/JU
Sample : N6024-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-Q

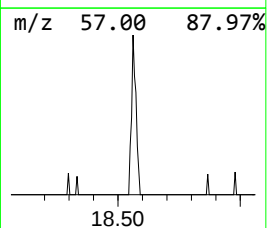
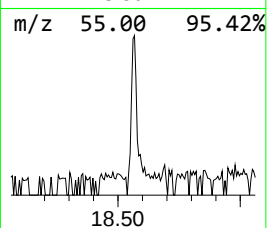
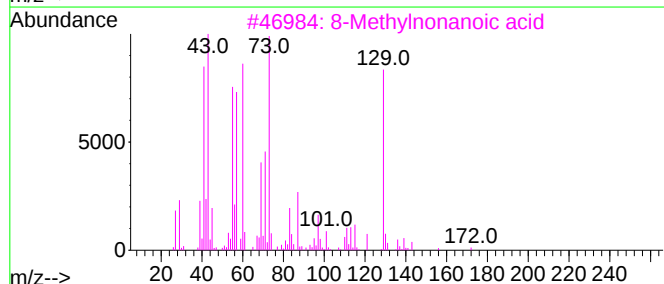
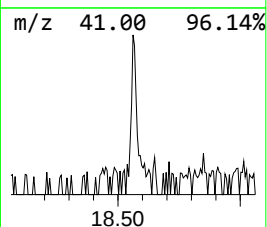
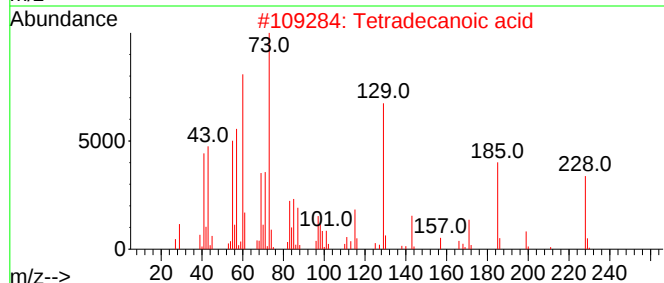
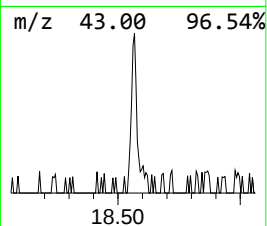
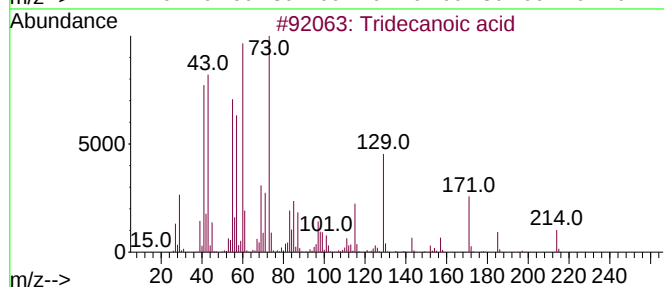
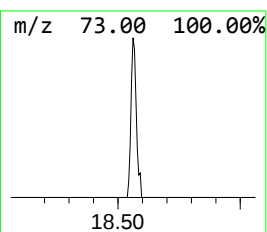
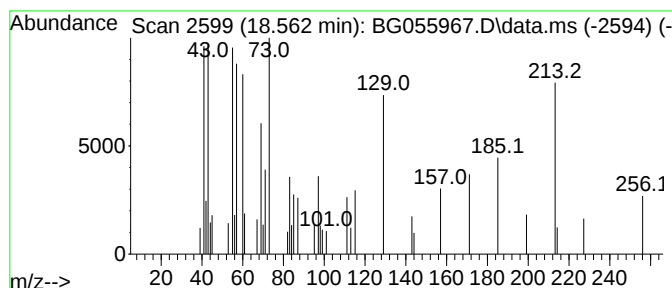
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.561	5.00 ng	29174	Phenanthrene-d10	17.715

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	90
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	49
3			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	41
4			Adipic acid, hexyl isobutyl ester	286	C16H30O4	1000324-09-6	38
5			Adipic acid, hexyl 3-pentyl ester	300	C17H32O4	1000324-60-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
Data File : BG055967.D
Acq On : 14 Dec 2022 20:09
Operator : CG/JU
Sample : N6024-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

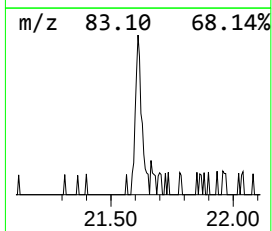
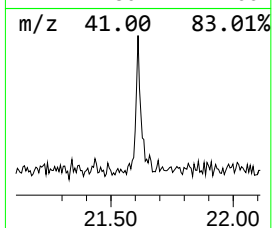
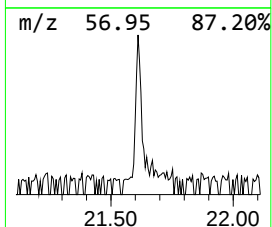
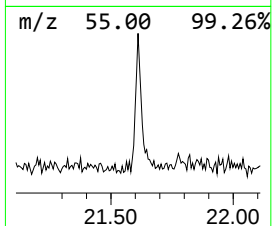
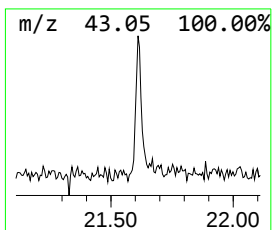
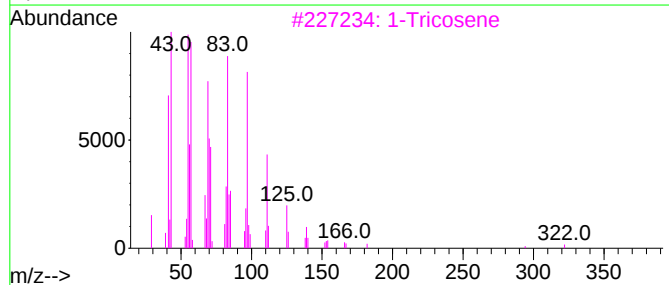
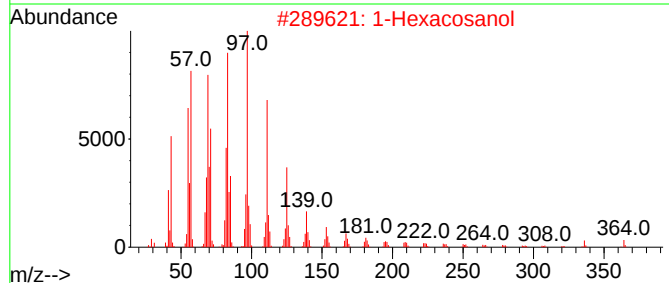
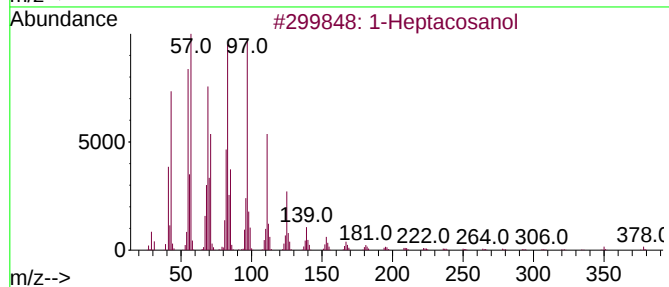
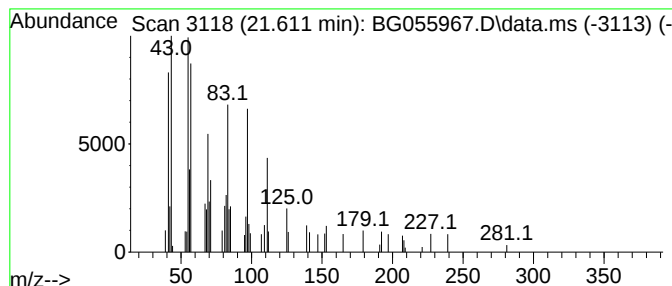
Instrument :
BNA_G
ClientSampleId :
TP-Q

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.611	3.72 ng	28721	Chrysene-d12	22.016	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	1-Hexacosanol	382	C26H54O	000506-52-5	93
3	1-Tricosene	322	C23H46	018835-32-0	93
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	90
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
Data File : BG055967.D
Acq On : 14 Dec 2022 20:09
Operator : CG/JU
Sample : N6024-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-Q

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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...	3.403	7.6	ng	12170	1	8.368	31920	20.0
2-Pentanone, 4-...	5.412	18.5	ng	29547	1	8.368	31920	20.0
Benzophenone	16.317	14.9	ng	62719	3	14.977	84068	20.0
Tridecanoic acid	18.561	5.0	ng	29174	4	17.715	116610	20.0
1-Heptacosanol	21.611	3.7	ng	28721	5	22.016	154534	20.0