

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041223\
 Data File : BG057072.D
 Acq On : 12 Apr 2023 20:50
 Operator : CG/JU
 Sample : 02283-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20230327-COMP-5

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-BG033023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057072.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.435	317	323	330	rVB	37312	59465	4.54%	1.070%
2	5.917	396	405	415	rBV	345500	546911	41.75%	9.842%
3	7.538	674	681	692	rBV	336109	585287	44.68%	10.532%
4	8.402	821	828	835	rBV	52926	87679	6.69%	1.578%
5	9.582	1021	1029	1037	rBV	197288	344920	26.33%	6.207%
6	11.245	1303	1312	1319	rBV	65587	116472	8.89%	2.096%
7	13.642	1713	1720	1728	rBV	515870	786086	60.00%	14.146%
8	15.016	1944	1954	1961	rBV2	112504	173056	13.21%	3.114%
9	16.355	2176	2182	2188	rBV	30926	42809	3.27%	0.770%
10	16.497	2200	2206	2214	rBV	446820	676269	51.62%	12.169%
11	17.754	2414	2420	2427	rVB	148064	226295	17.27%	4.072%
12	18.594	2556	2563	2573	rBV2	29734	44692	3.41%	0.804%
13	20.327	2852	2858	2863	rBV	1031510	1310094	100.00%	23.575%
14	21.631	3075	3080	3093	rBV2	35993	69737	5.32%	1.255%
15	22.071	3149	3155	3163	rBV2	142824	246292	18.80%	4.432%
16	25.608	3745	3757	3766	rVB	77323	241064	18.40%	4.338%

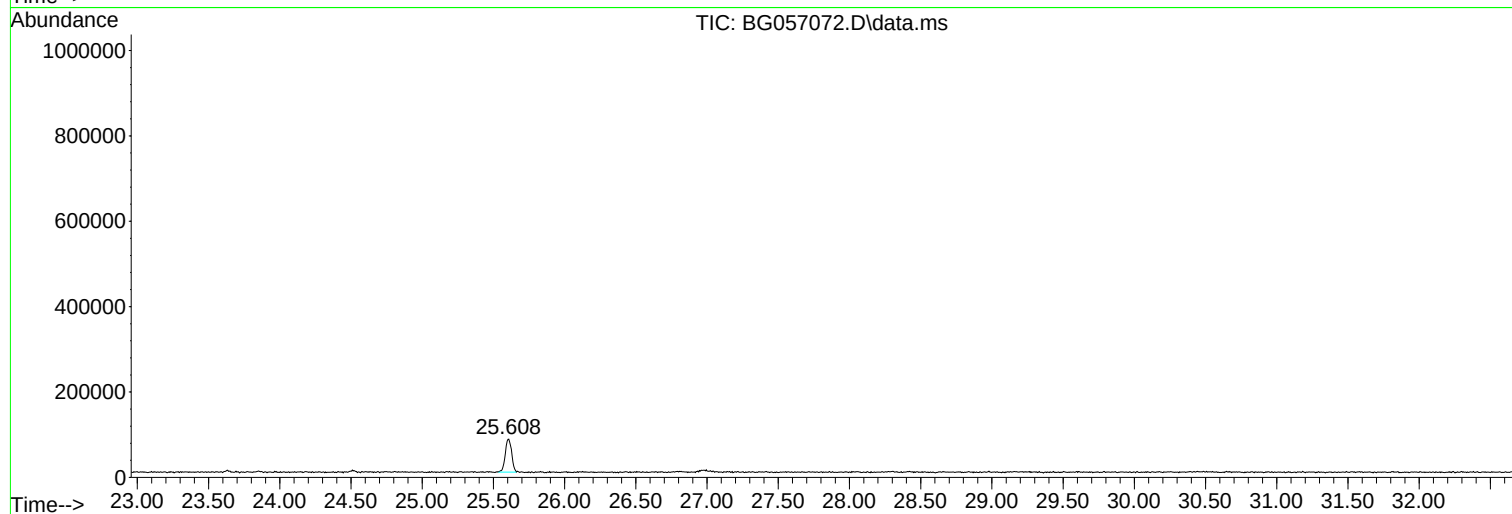
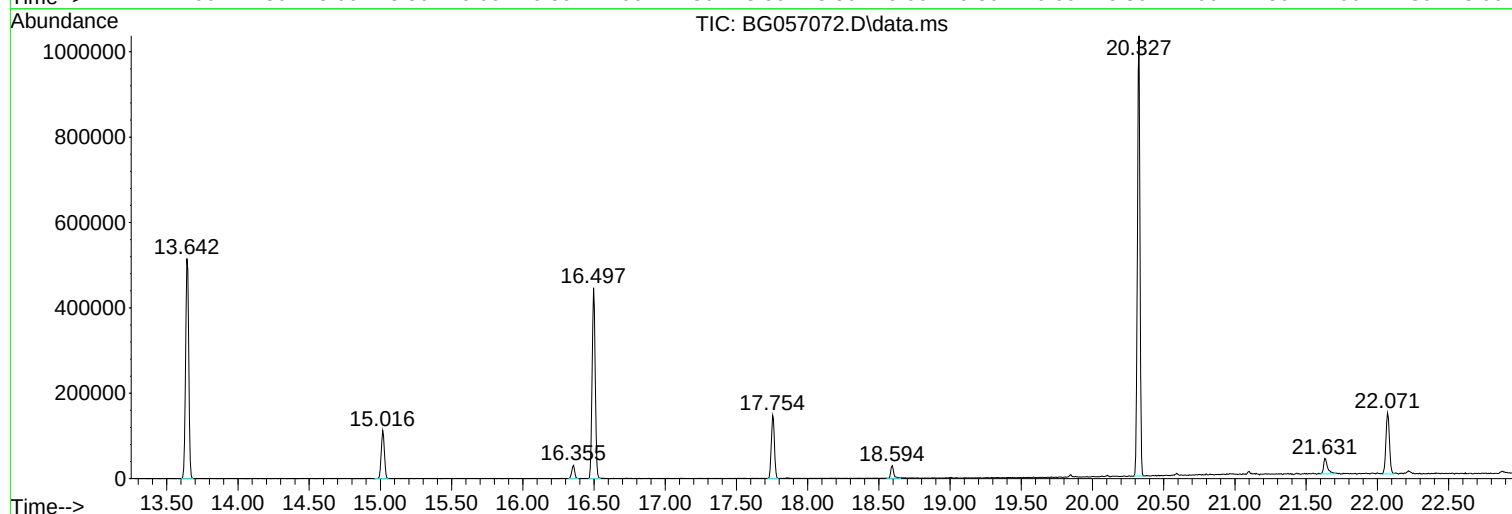
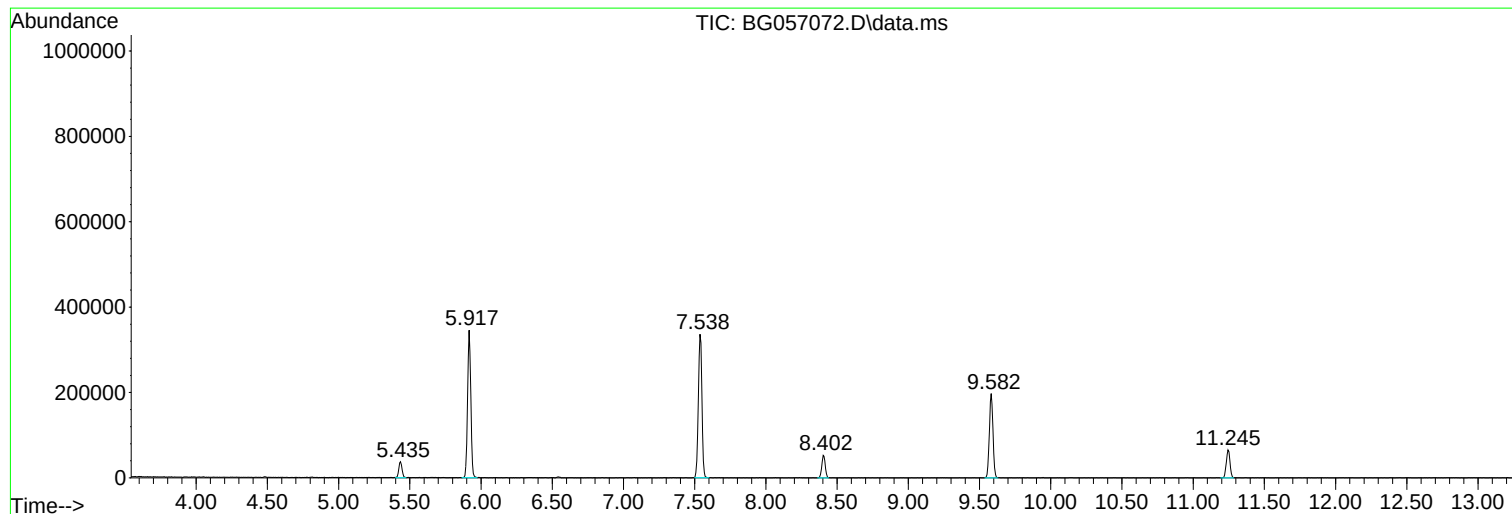
Sum of corrected areas: 5557128

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041223\
Data File : BG057072.D
Acq On : 12 Apr 2023 20:50
Operator : CG/JU
Sample : 02283-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20230327-COMP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.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\BG041223\
Data File : BG057072.D
Acq On : 12 Apr 2023 20:50
Operator : CG/JU
Sample : 02283-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20230327-COMP-5

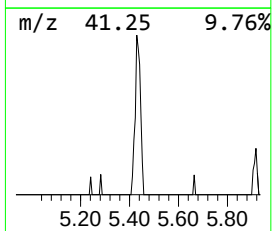
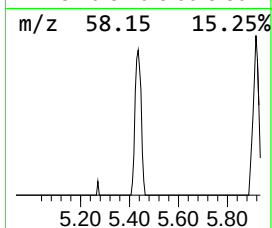
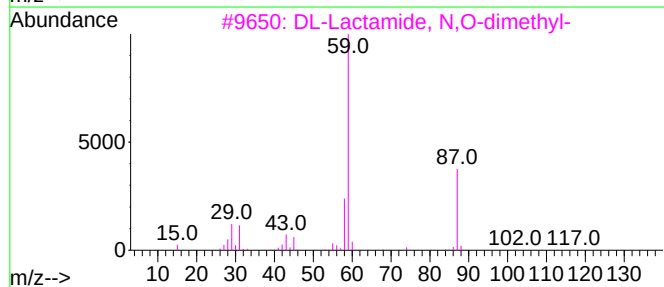
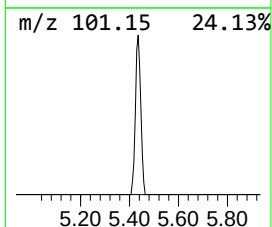
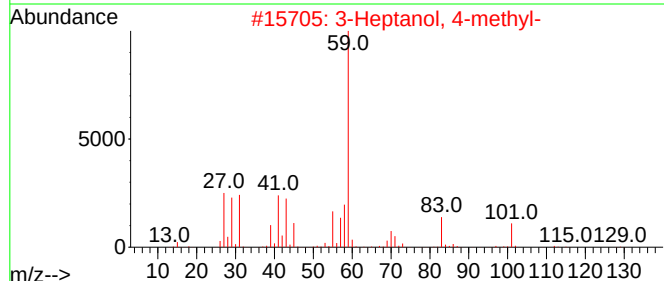
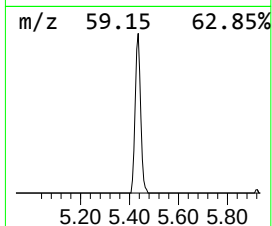
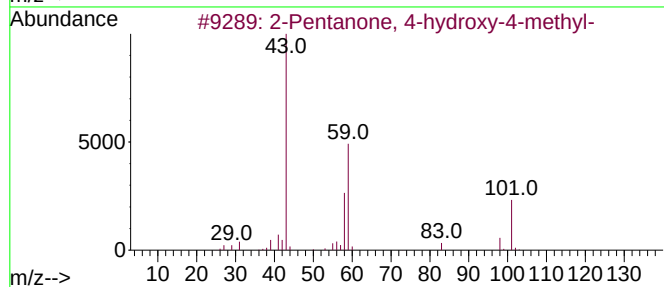
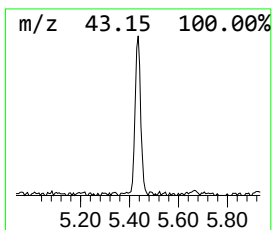
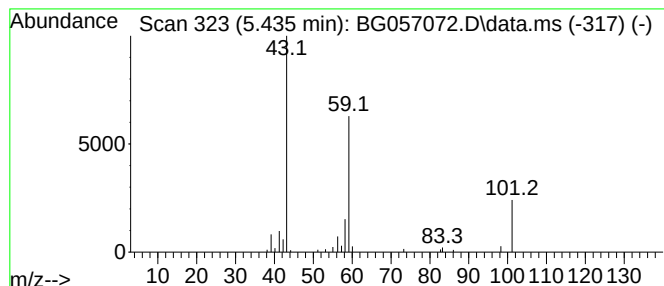
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.435	13.56 ng	59465	1,4-Dichlorobenzene-d4	8.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	25		
3	DL-Lactamide, N,O-dimethyl-	117	C5H11NO2	1000452-56-3	23		
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041223\
Data File : BG057072.D
Acq On : 12 Apr 2023 20:50
Operator : CG/JU
Sample : 02283-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20230327-COMP-5

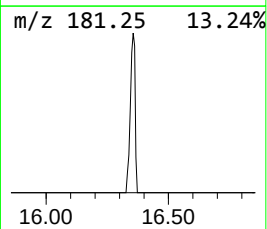
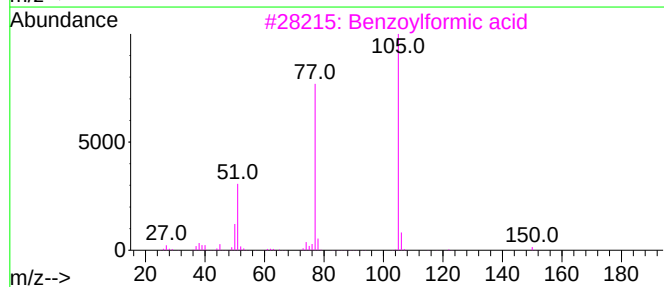
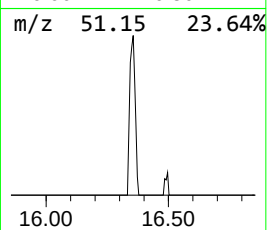
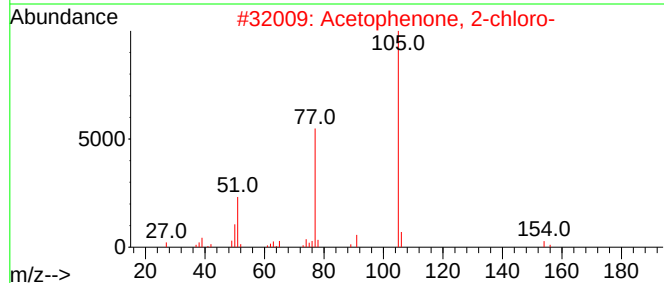
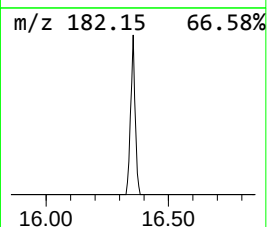
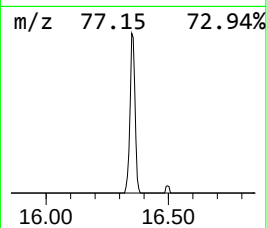
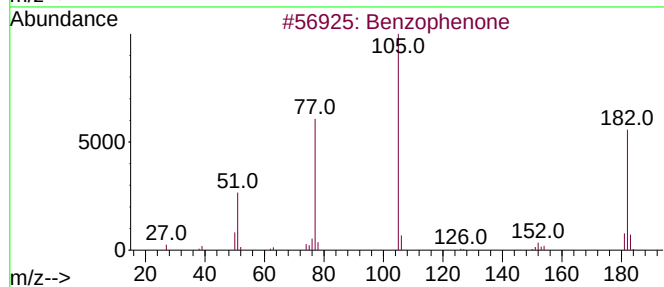
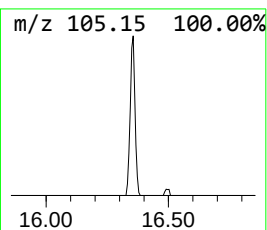
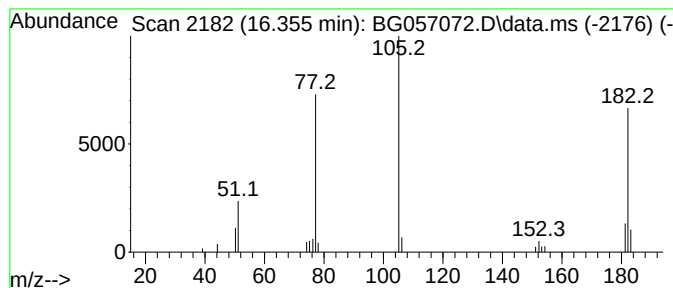
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.355	4.95 ng	42809	Acenaphthene-d10	15.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			Benzoylformic acid	150	C8H6O3	000611-73-4	47
4			Benzoic acid, (4-nitrophenyl)-me...	269	C14H11N3O3	028123-77-5	47
5			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041223\
Data File : BG057072.D
Acq On : 12 Apr 2023 20:50
Operator : CG/JU
Sample : 02283-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20230327-COMP-5

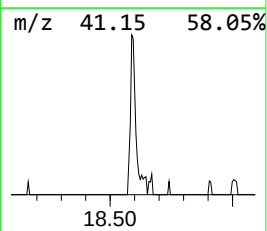
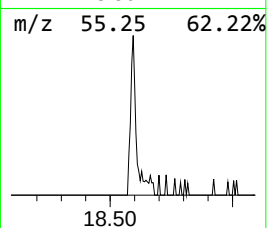
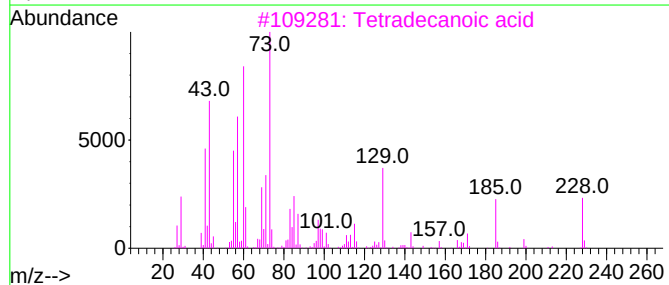
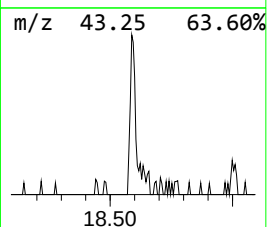
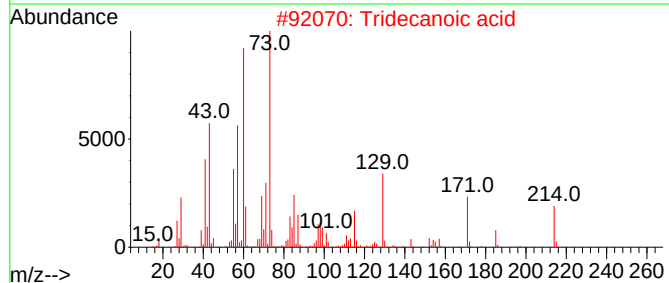
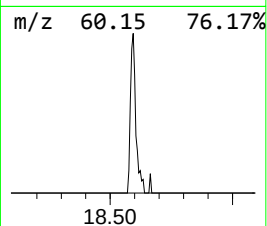
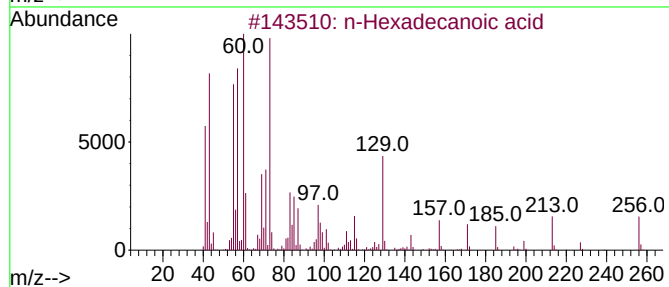
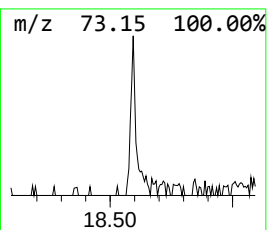
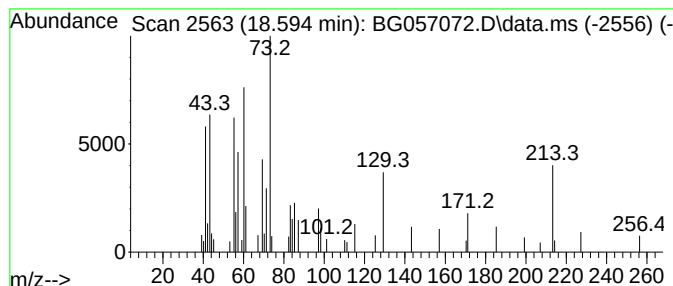
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.594	3.95 ng	44692	Phenanthrene-d10	17.754

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
2			Tridecanoic acid	214	C13H26O2	000638-53-9	70
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041223\
Data File : BG057072.D
Acq On : 12 Apr 2023 20:50
Operator : CG/JU
Sample : 02283-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20230327-COMP-5

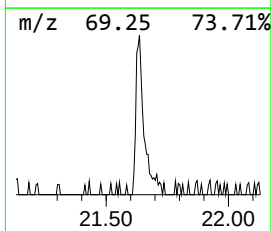
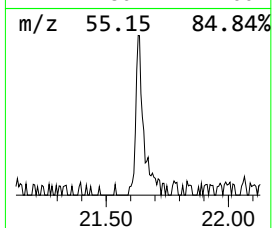
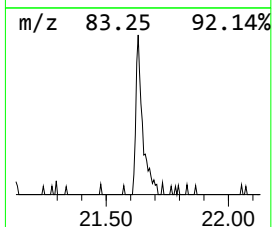
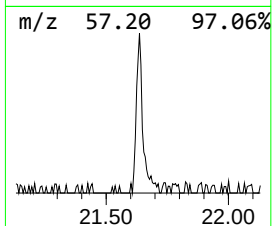
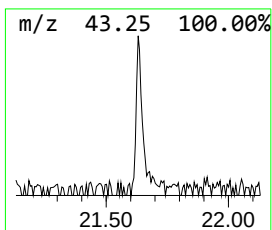
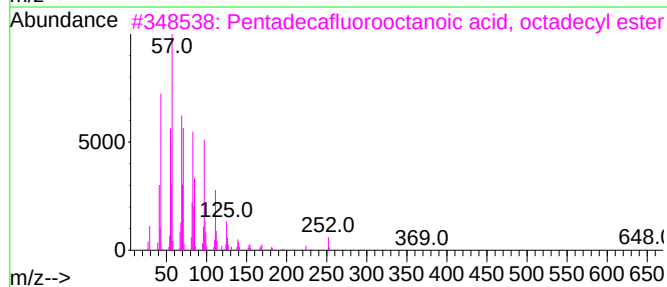
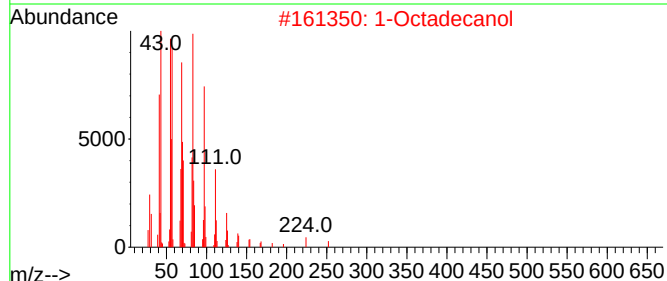
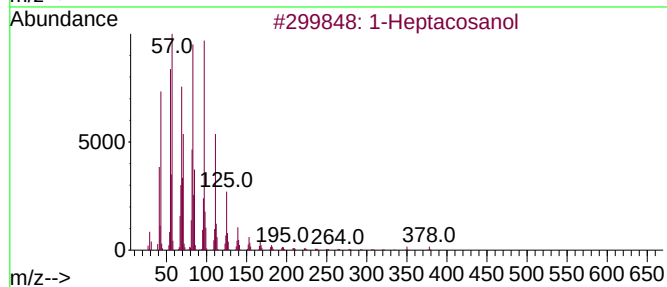
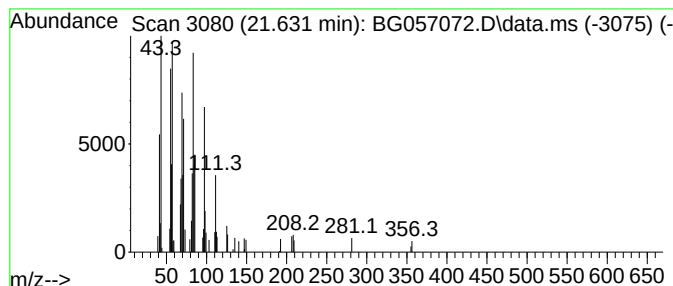
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Heptacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.631	5.66 ng	69737	Chrysene-d12	22.071

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	83
2			1-Octadecanol	270	C18H38O	000112-92-5	81
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	81
4			Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	81
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041223\
Data File : BG057072.D
Acq On : 12 Apr 2023 20:50
Operator : CG/JU
Sample : 02283-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20230327-COMP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.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
2-Pentanone, 4-...	5.435	13.6	ng	59465	1	8.407	87679	20.0
Benzophenone	16.355	5.0	ng	42809	3	15.016	173056	20.0
n-Hexadecanoic ...	18.594	4.0	ng	44692	4	17.754	226295	20.0
1-Heptacosanol	21.631	5.7	ng	69737	5	22.071	246292	20.0