

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
 Data File : BG049860.D
 Acq On : 16 Aug 2021 21:50
 Operator : CG/JU
 Sample : M3407-11
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 26S

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-BG080321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049860.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.138	11	17	24	rBV	87335	159553	1.70%	0.936%
2	5.588	427	434	444	rBV	413940	702767	7.51%	4.124%
3	7.192	699	707	721	rBV	439580	793955	8.48%	4.659%
4	8.026	840	849	857	rBV	117377	202823	2.17%	1.190%
5	9.201	1041	1049	1060	rBV	289253	522845	5.58%	3.068%
6	10.851	1321	1330	1337	rBV	155083	281446	3.01%	1.652%
7	13.301	1739	1747	1754	rBV	647451	1018558	10.88%	5.977%
8	14.681	1973	1982	1988	rBV	245312	392812	4.20%	2.305%
9	16.174	2223	2236	2243	rBV	588054	947903	10.12%	5.562%
10	17.437	2444	2451	2455	rBV	271012	417185	4.46%	2.448%
11	20.045	2889	2895	2901	rBV	815205	1074475	11.48%	6.305%
12	21.343	3111	3116	3122	rBV2	110360	203483	2.17%	1.194%
13	21.719	3172	3180	3185	rBV	243119	427965	4.57%	2.511%
14	22.630	3291	3335	3350	rVB5	1083868	9363204	100.00%	54.944%
15	24.991	3729	3737	3747	rVB3	148068	412675	4.41%	2.422%
16	31.794	4885	4895	4896	rBV8	57124	119780	1.28%	0.703%

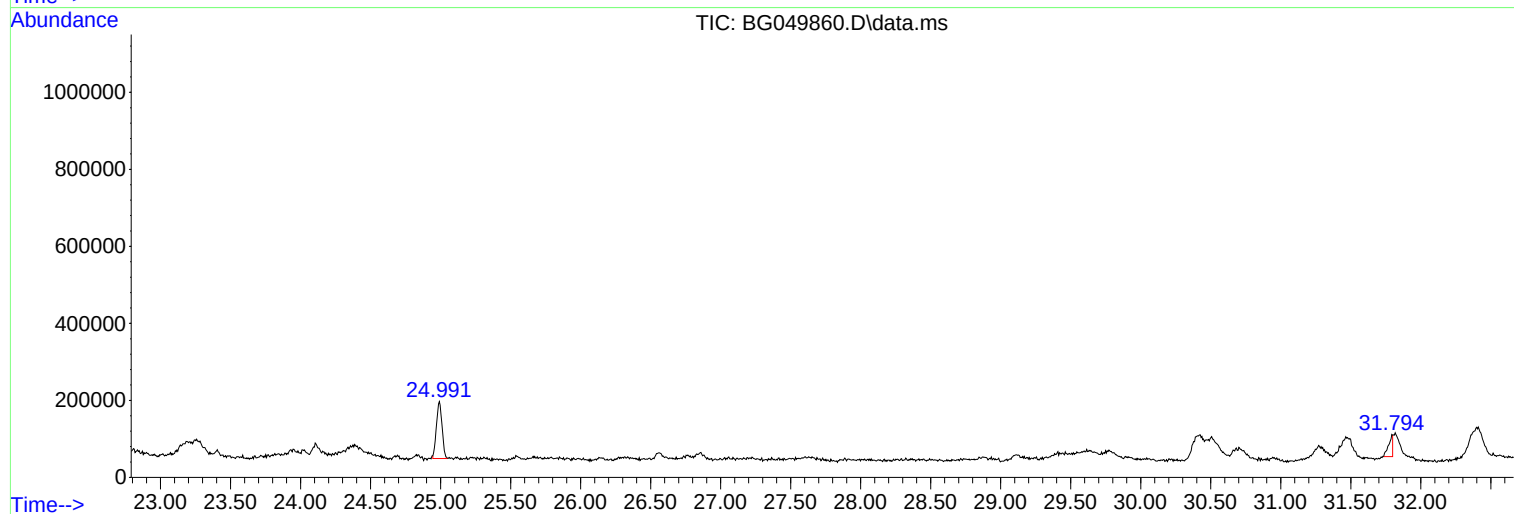
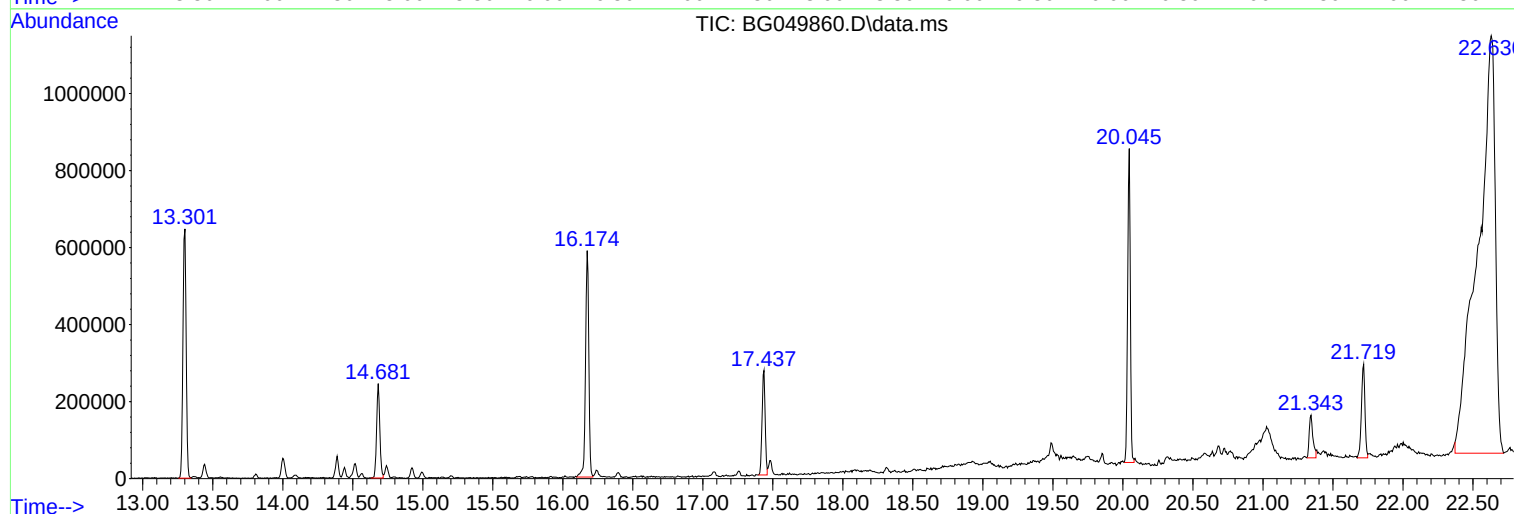
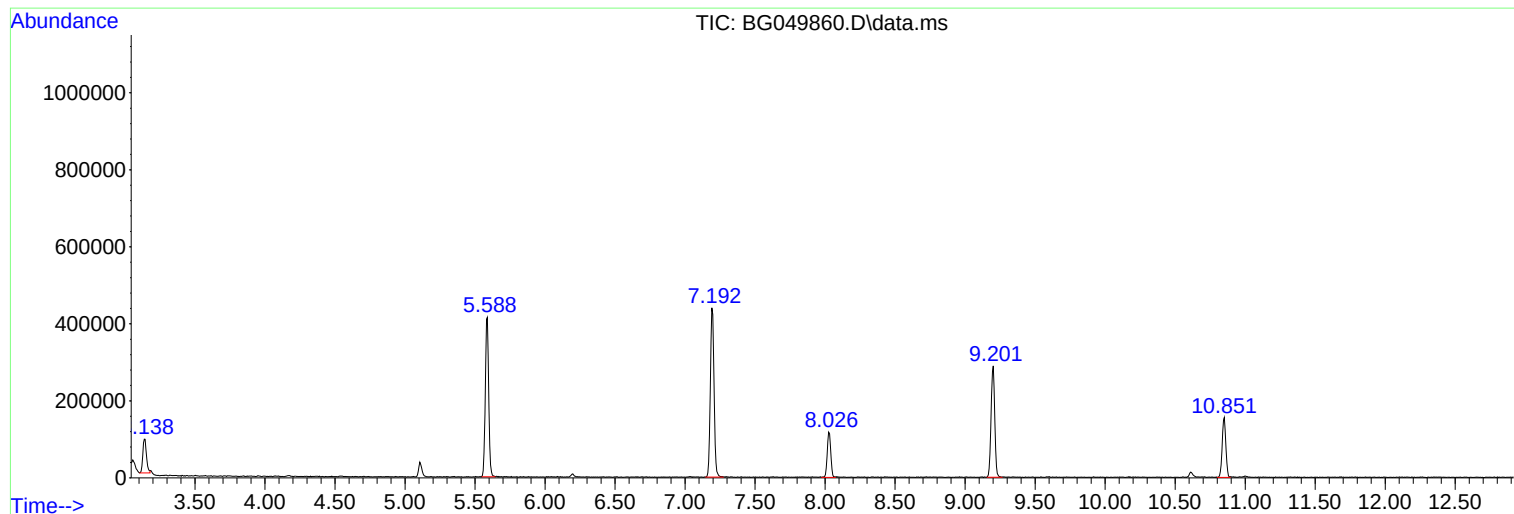
Sum of corrected areas: 17041429

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049860.D
Acq On : 16 Aug 2021 21:50
Operator : CG/JU
Sample : M3407-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
26S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.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\BG081621\
Data File : BG049860.D
Acq On : 16 Aug 2021 21:50
Operator : CG/JU
Sample : M3407-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
26S

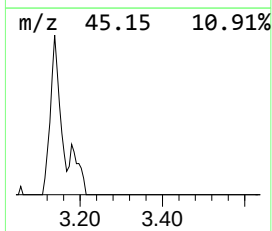
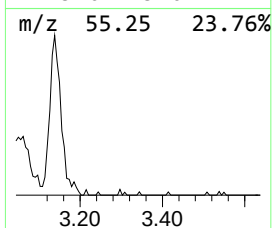
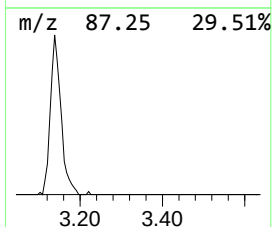
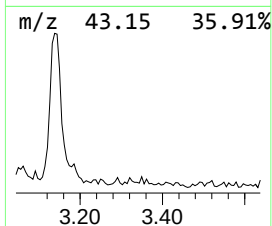
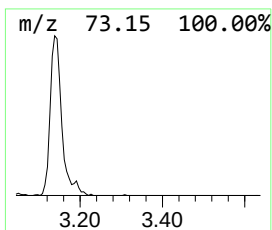
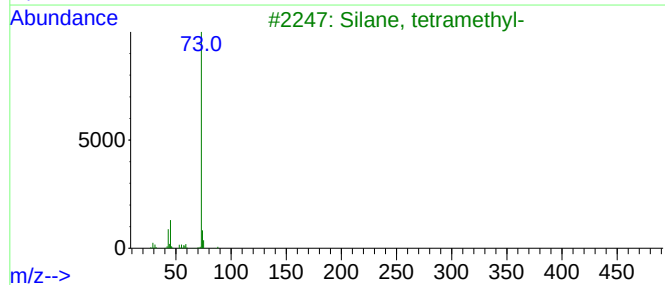
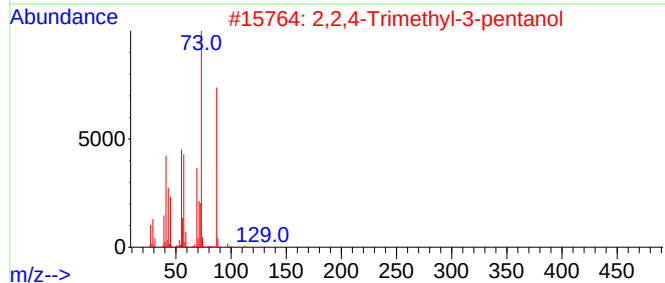
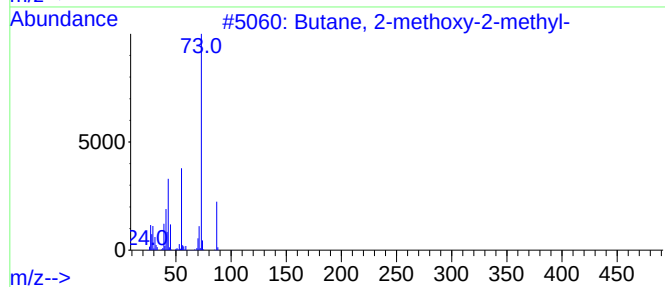
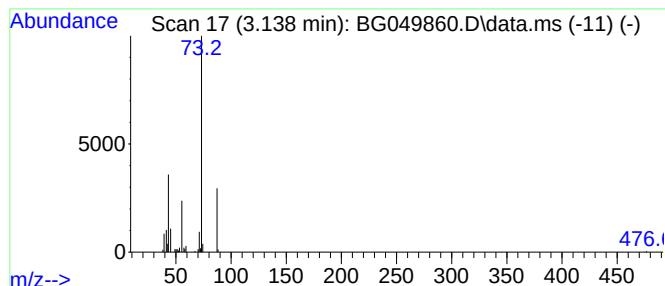
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.138	15.73 ng	159553	1,4-Dichlorobenzene-d4	8.032

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049860.D
Acq On : 16 Aug 2021 21:50
Operator : CG/JU
Sample : M3407-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
26S

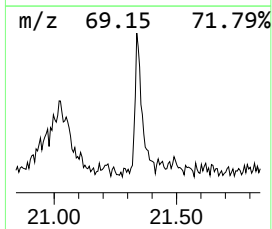
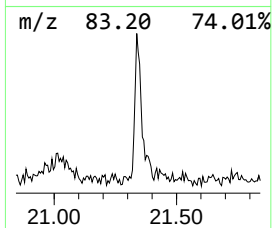
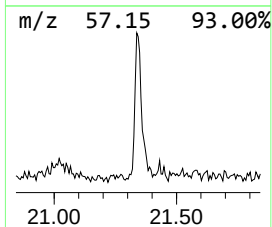
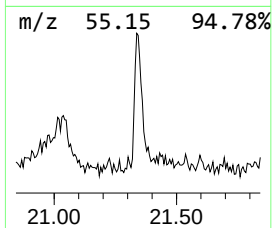
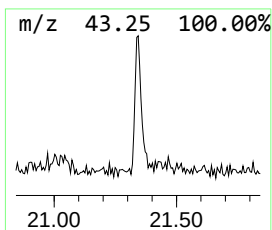
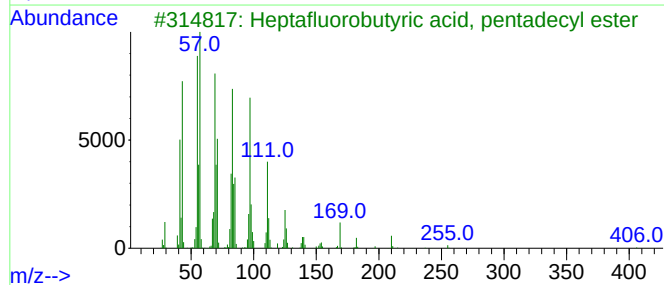
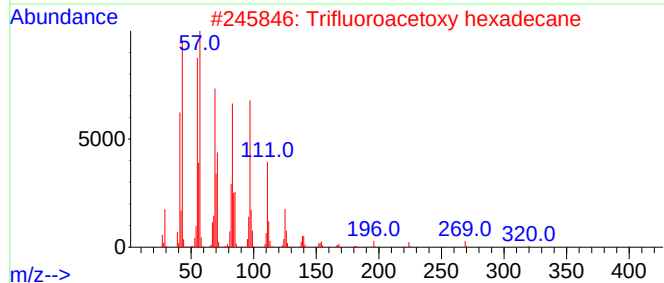
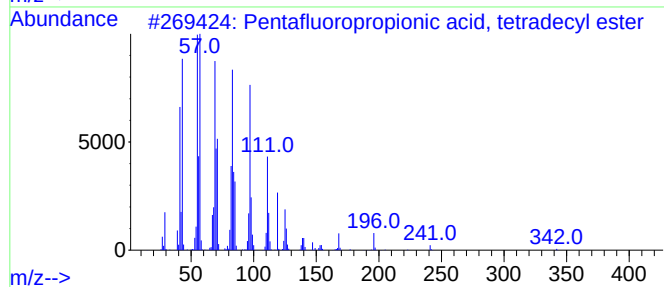
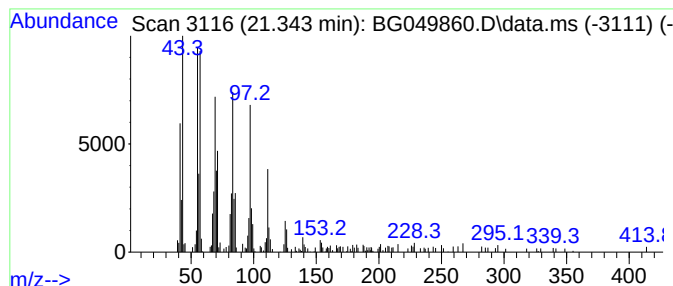
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.343	9.51 ng	203483	Chrysene-d12	21.719

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049860.D
Acq On : 16 Aug 2021 21:50
Operator : CG/JU
Sample : M3407-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
26S

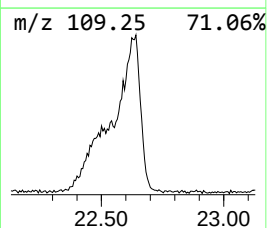
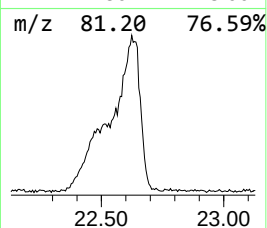
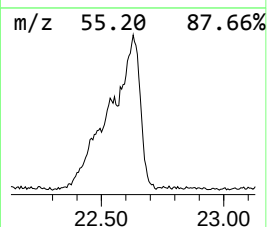
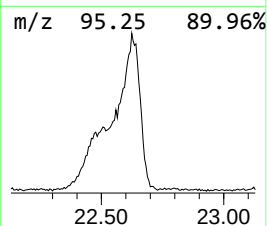
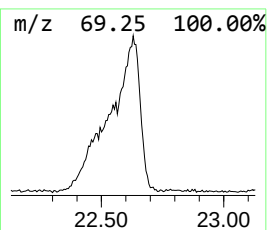
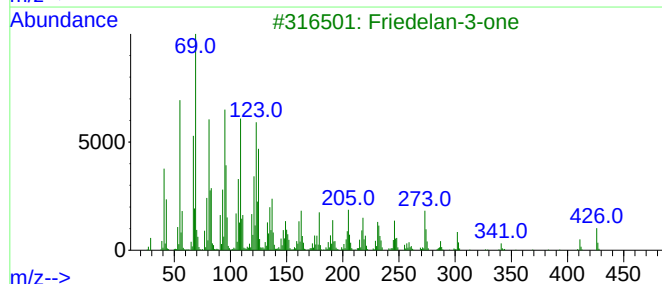
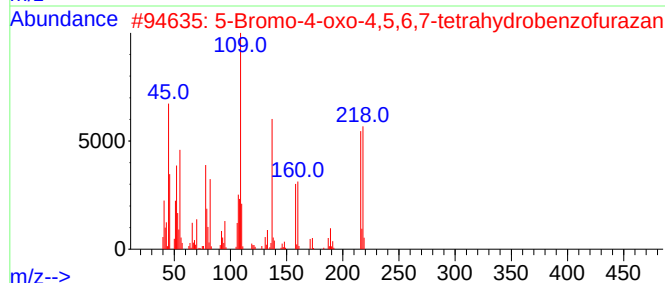
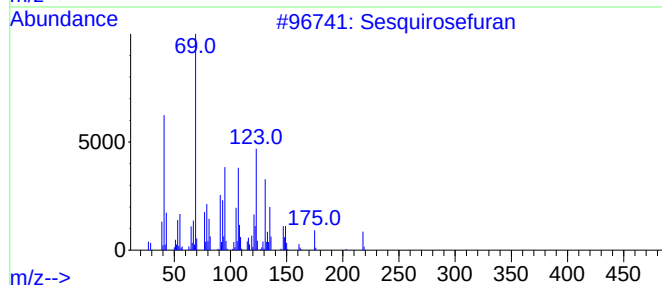
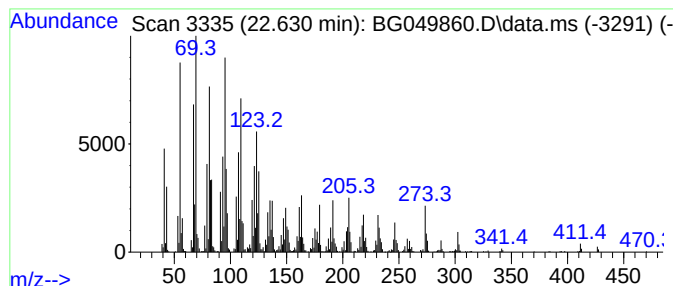
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Sesquirosefuran Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.630	437.57 ng	9363200	Chrysene-d12	21.719

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sesquirosefuran	218	C15H22O	039007-93-7	80
2			5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	59
3			Friedelan-3-one	426	C30H50O	000559-74-0	58
4			2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	52
5			2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049860.D
Acq On : 16 Aug 2021 21:50
Operator : CG/JU
Sample : M3407-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
26S

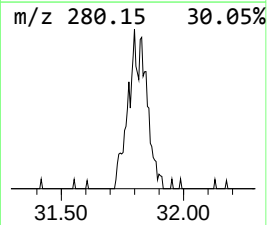
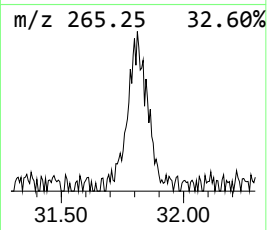
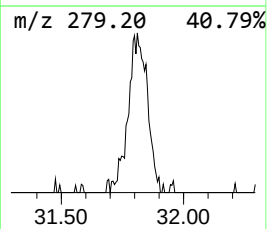
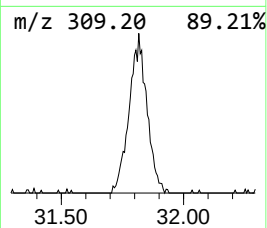
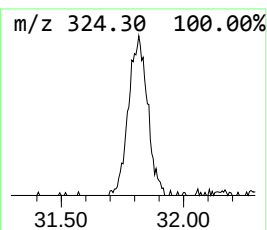
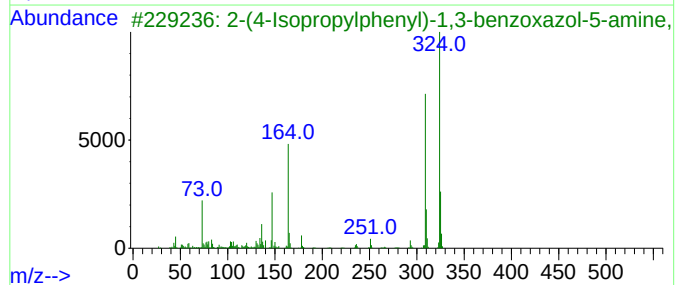
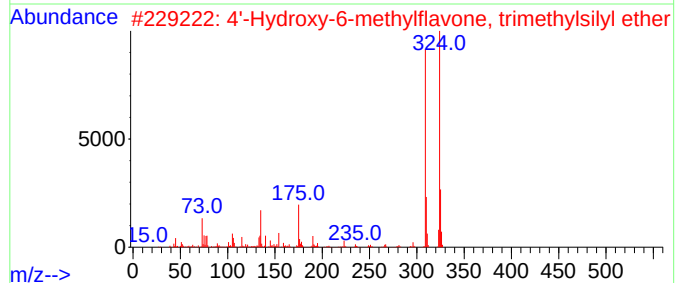
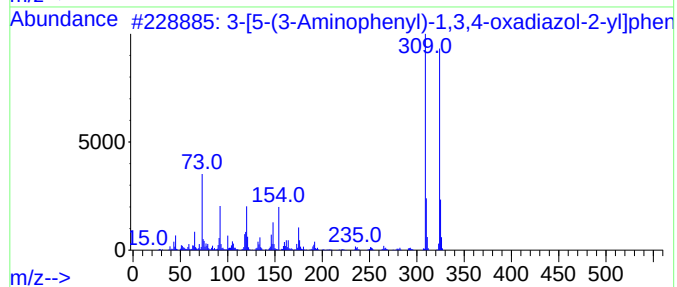
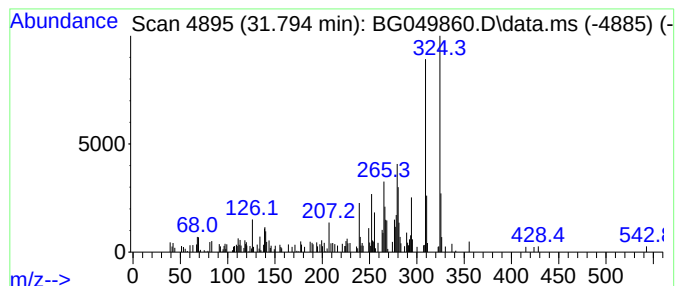
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 3-[5-(3-Aminophenyl)-1,3,4-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.794	5.81 ng	119780	Perylene-d12	24.991

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3	-[5-(3-Aminophenyl)-1,3,4-oxadi...	324	C17H20N4OSi	1000474-54-9	60	
2	4	'-Hydroxy-6-methylflavone, trim...	324	C19H20O3Si	1010454-24-9	53	
3	2	-(4-Isopropylphenyl)-1,3-benzox...	324	C19H24N2OSi	1000471-61-2	49	
4	[2](9,10)(1,2,3,4-Tetrahydroanth...	309	C23H19N	1000156-07-2	46		
5	3-Amino-7-dimethylamino-2-methyl...	324	C18H24N4Si	1000472-49-8	43		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049860.D
Acq On : 16 Aug 2021 21:50
Operator : CG/JU
Sample : M3407-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
26S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.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...	3.138	15.7	ng	159553	1	8.032	202823	20.0
Pentafluoroprop...	21.343	9.5	ng	203483	5	21.719	427965	20.0
Sesquirosefuran	22.630	437.6	ng	9363200	5	21.719	427965	20.0
3-[5-(3-Aminoph...	31.794	5.8	ng	119780	6	24.991	412675	20.0