

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
 Data File : BG057482.D
 Acq On : 20 May 2023 1:05
 Operator : CG/JU
 Sample : 02849-21
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP9

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-BG042723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057482.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.382	308	314	321	rBV	19308	29212	3.11%	0.658%
2	5.876	391	398	410	rBV	183019	301934	32.17%	6.801%
3	7.497	667	674	686	rBV	192963	335311	35.72%	7.553%
4	8.355	814	820	828	rBB	56303	92894	9.90%	2.092%
5	9.530	1013	1020	1030	rBV	118850	210492	22.42%	4.741%
6	11.192	1295	1303	1310	rBV	71872	126051	13.43%	2.839%
7	12.608	1538	1544	1554	rVB	113715	171023	18.22%	3.852%
8	13.589	1705	1711	1721	rVB	342972	523808	55.80%	11.798%
9	14.970	1940	1946	1952	rBV	126554	199081	21.21%	4.484%
10	16.303	2168	2173	2179	rBV	21808	29648	3.16%	0.668%
11	16.450	2192	2198	2209	rBV	282872	437167	46.57%	9.847%
12	17.707	2406	2412	2419	rBV	192694	277139	29.53%	6.242%
13	20.274	2843	2849	2856	rBV	755354	938658	100.00%	21.142%
14	21.408	3038	3042	3046	rVB	26319	33334	3.55%	0.751%
15	21.572	3066	3070	3086	rVB5	19225	44398	4.73%	1.000%
16	22.013	3138	3145	3151	rBV2	180364	305729	32.57%	6.886%
17	22.788	3271	3277	3282	rBV4	7824	15049	1.60%	0.339%
18	23.529	3399	3403	3411	rVB6	8310	15122	1.61%	0.341%
19	24.398	3545	3551	3558	rVB4	11012	25679	2.74%	0.578%
20	25.420	3719	3725	3730	rBV5	8101	18610	1.98%	0.419%
21	25.508	3730	3740	3750	rVB	95571	286242	30.49%	6.447%
22	26.642	3927	3933	3940	rVB7	9425	23103	2.46%	0.520%

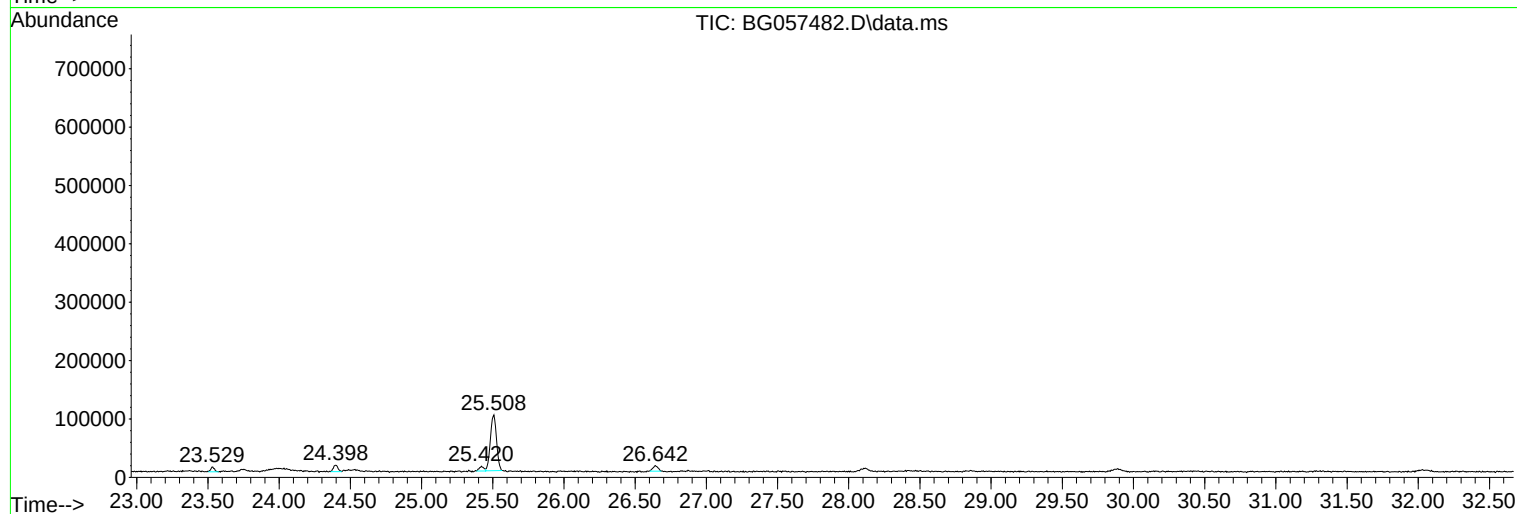
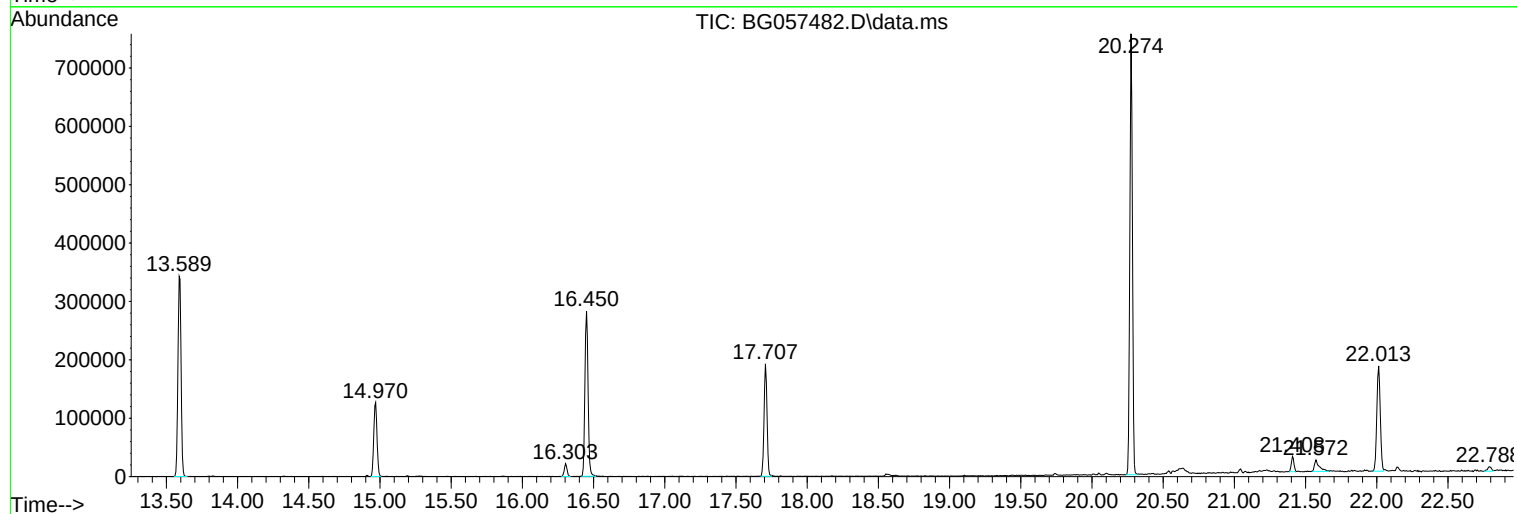
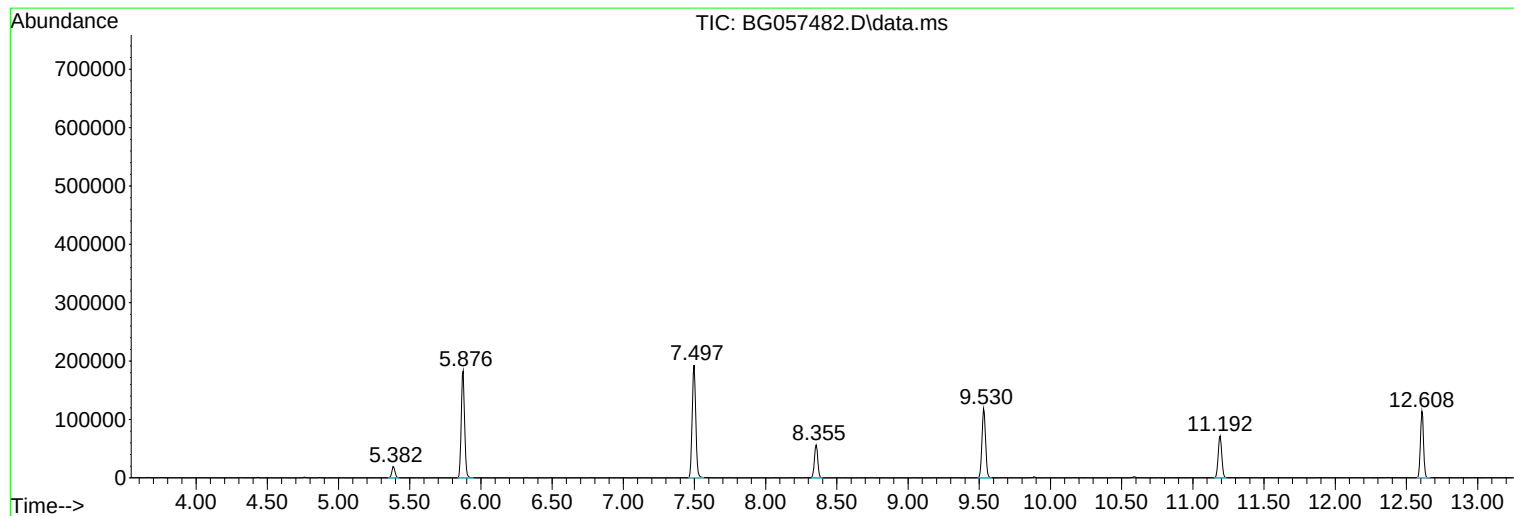
Sum of corrected areas: 4439684

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057482.D
Acq On : 20 May 2023 1:05
Operator : CG/JU
Sample : 02849-21
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.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\BG051923\
Data File : BG057482.D
Acq On : 20 May 2023 1:05
Operator : CG/JU
Sample : 02849-21
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP9

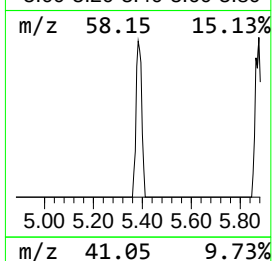
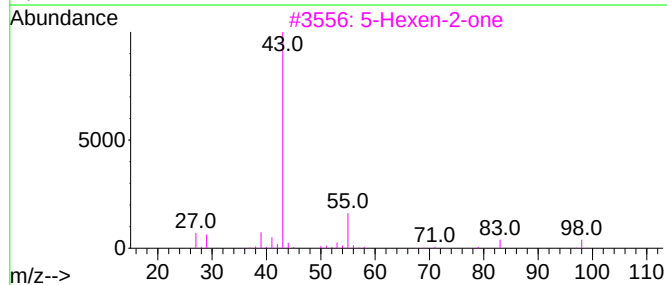
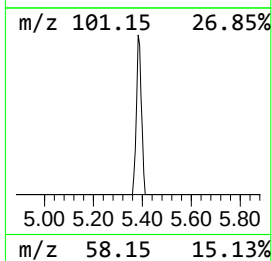
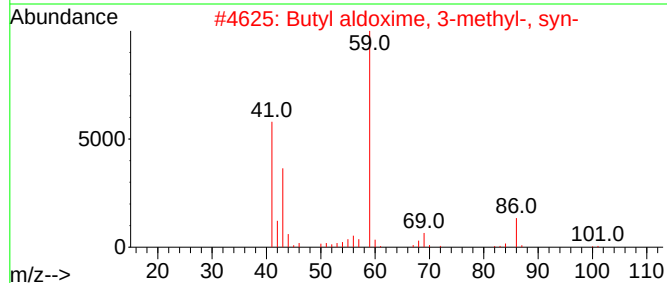
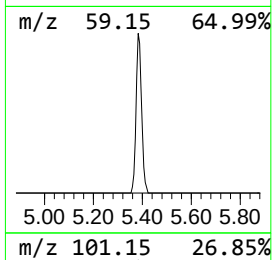
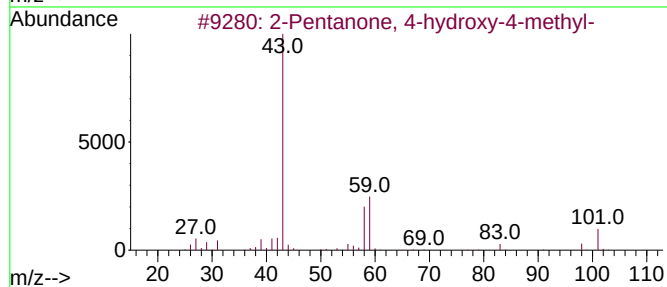
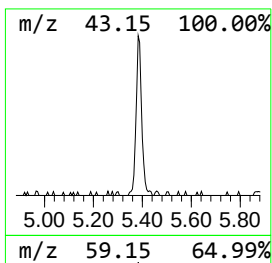
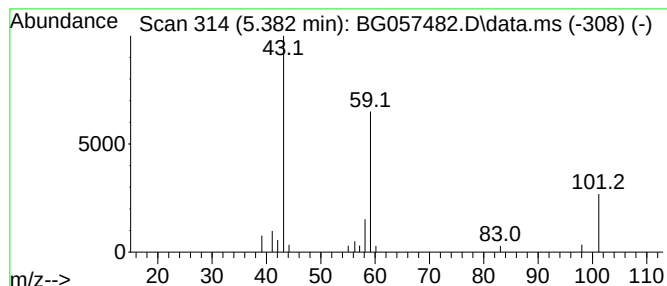
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.382	6.29 ng	29212	1,4-Dichlorobenzene-d4	8.355

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17	
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057482.D
Acq On : 20 May 2023 1:05
Operator : CG/JU
Sample : 02849-21
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP9

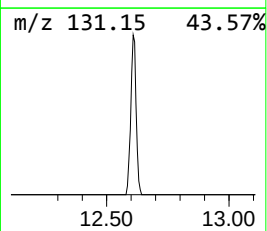
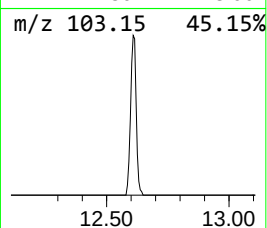
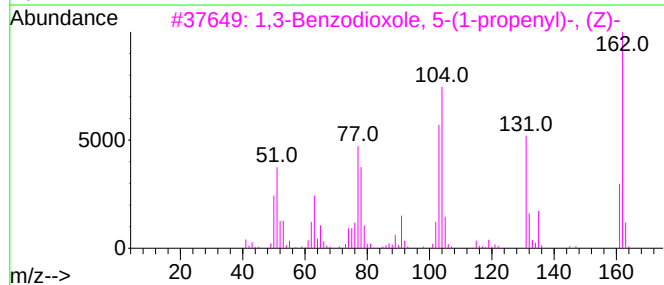
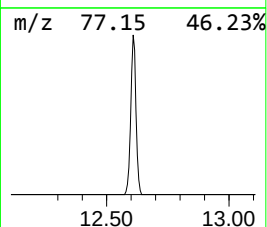
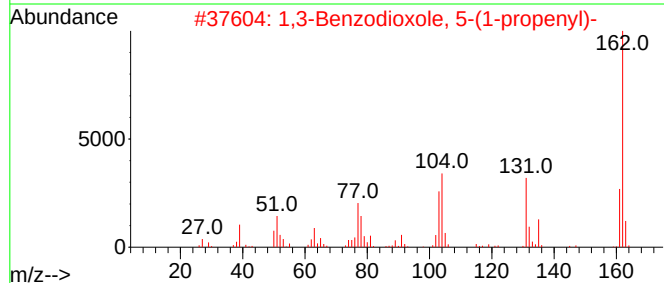
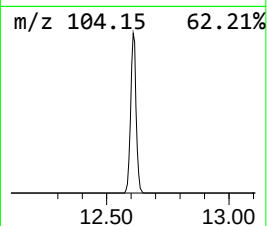
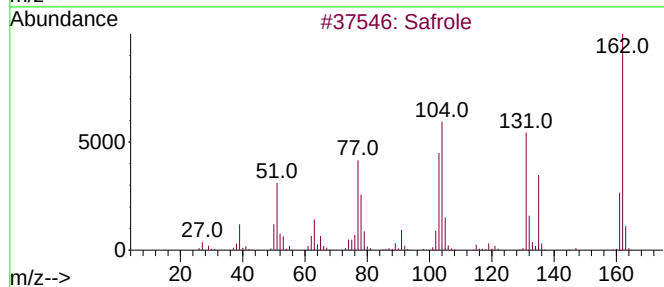
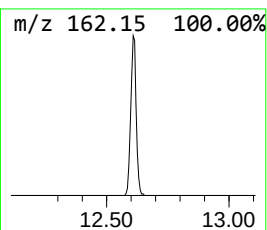
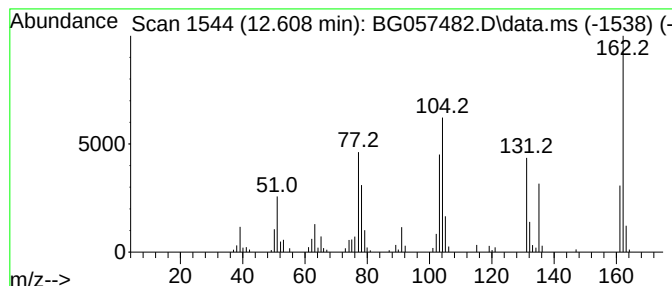
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Safole Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.608	27.14 ng	171023	Naphthalene-d8	11.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Safole	162	C10H10O2	000094-59-7	98
2			1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	97
3			1,3-Benzodioxole, 5-(1-propenyl)-...	162	C10H10O2	017627-76-8	93
4			Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	90
5			1H-Isoindole-1,3(2H)-dione, 2-am...	162	C8H6N2O2	001875-48-5	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057482.D
Acq On : 20 May 2023 1:05
Operator : CG/JU
Sample : 02849-21
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP9

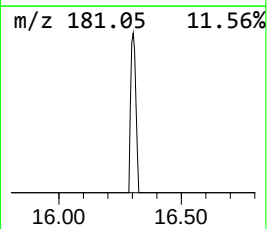
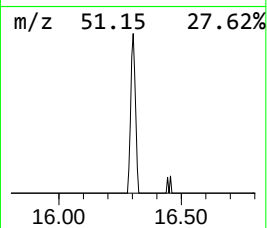
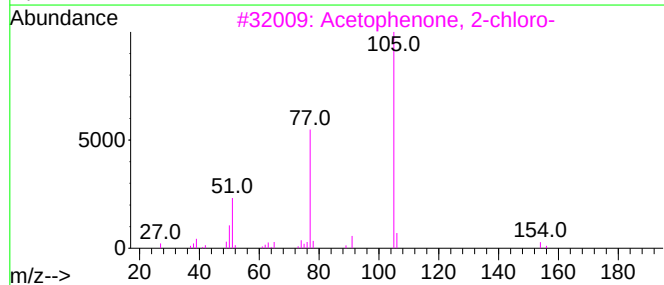
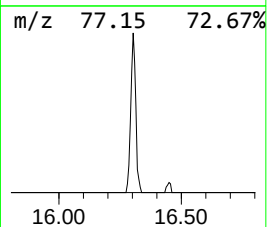
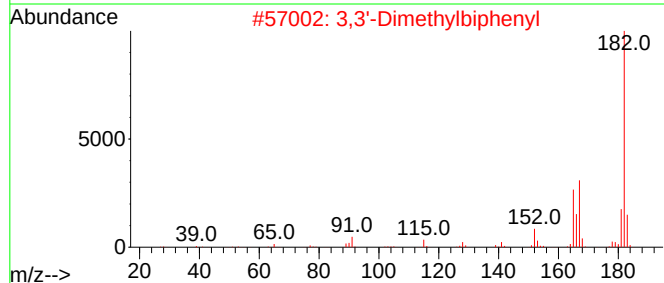
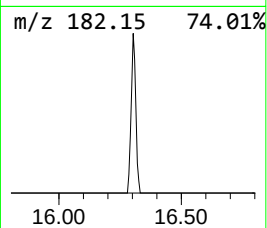
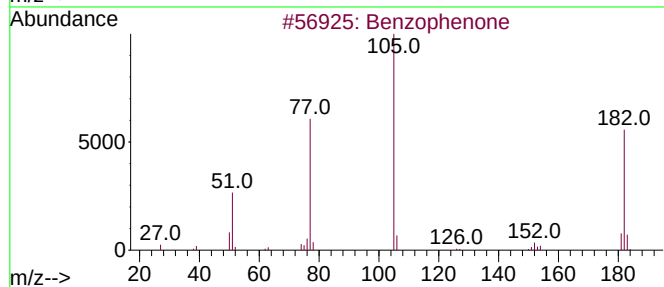
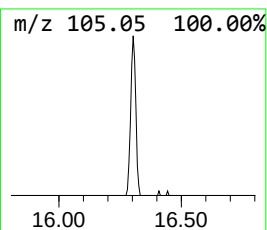
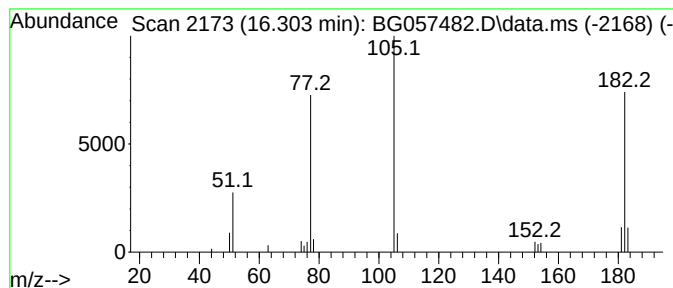
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.303	2.98 ng	29648	Acenaphthene-d10	14.970

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	94
2			3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	43
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	38
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	35
5			S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057482.D
Acq On : 20 May 2023 1:05
Operator : CG/JU
Sample : 02849-21
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP9

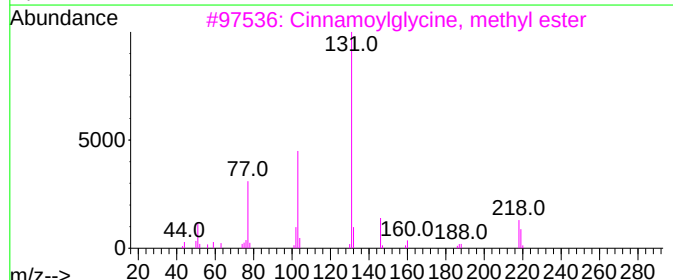
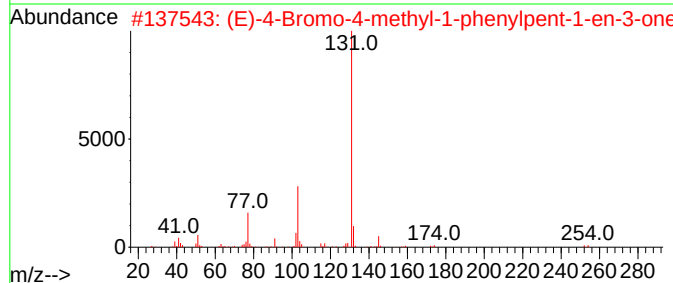
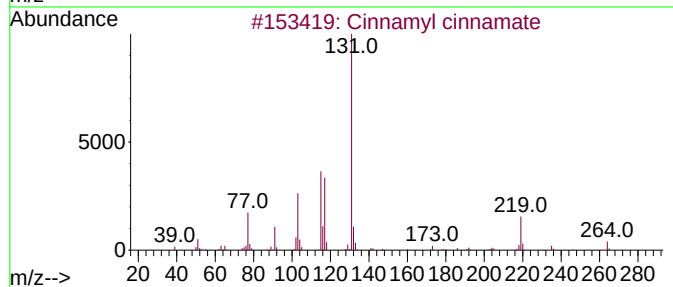
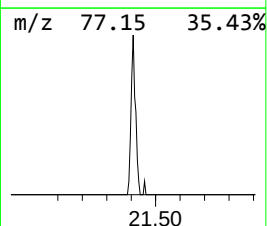
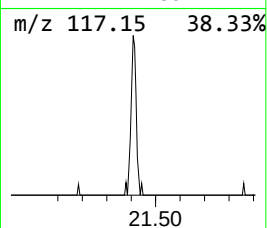
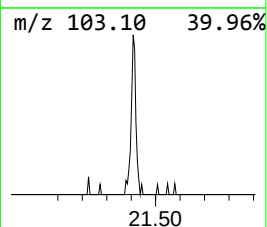
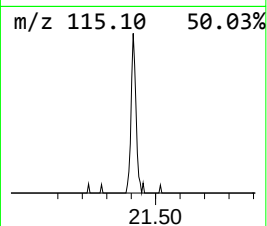
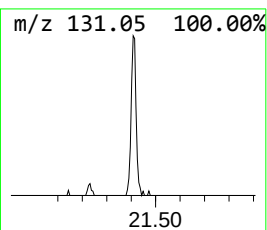
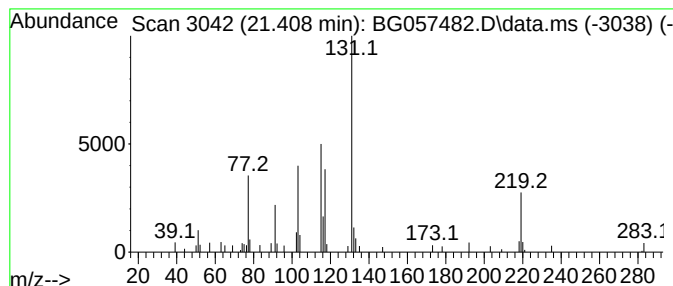
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Cinnamyl cinnamate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.408	2.18 ng	33334	Chrysene-d12	22.013

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	80
2			(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	43
3			Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	43
4			2-Propenoic acid, 3-phenyl-, met...	162	C10H10O2	001754-62-7	43
5			2-Propenoyl chloride, 3-phenyl-,...	166	C9H7ClO	017082-09-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057482.D
Acq On : 20 May 2023 1:05
Operator : CG/JU
Sample : 02849-21
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP9

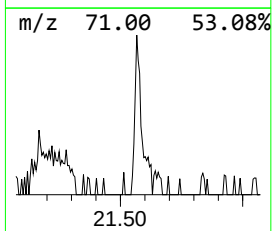
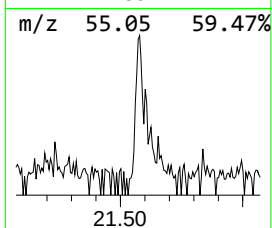
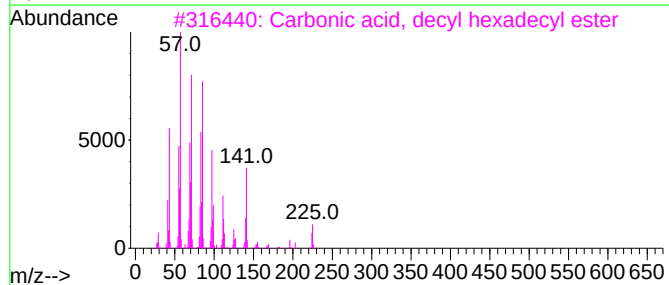
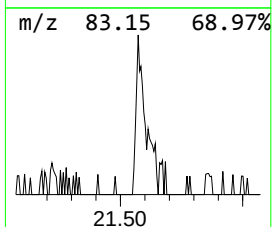
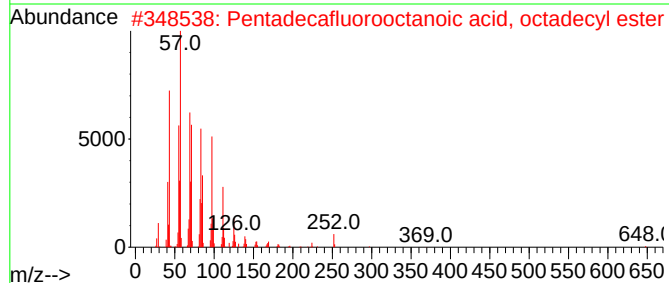
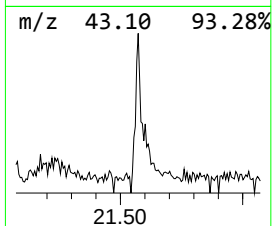
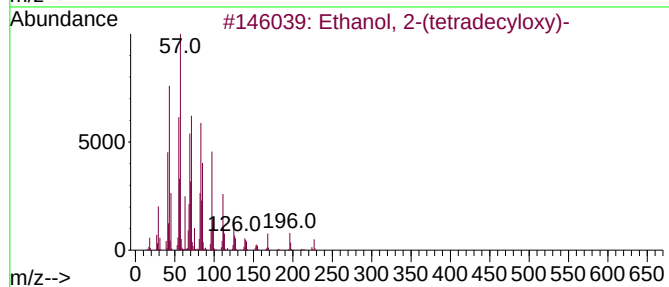
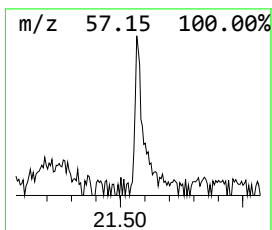
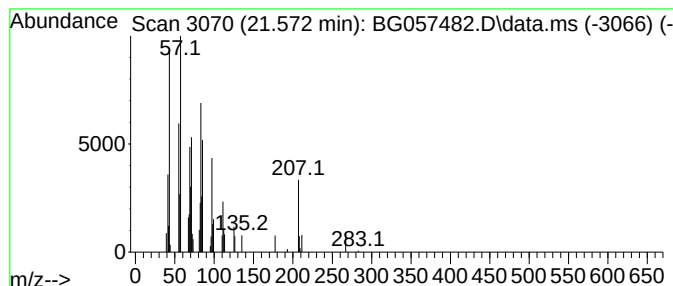
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.572	2.90 ng	44398	Chrysene-d12	22.013

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	81
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	68
3			Carbonic acid, decyl hexadecyl e...	426	C27H54O3	1000383-16-5	68
4			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	68
5			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051923\
Data File : BG057482.D
Acq On : 20 May 2023 1:05
Operator : CG/JU
Sample : 02849-21
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.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-...	5.382	6.3	ng	29212	1	8.355	92894	20.0
Safrole	12.608	27.1	ng	171023	2	11.192	126051	20.0
Benzophenone	16.303	3.0	ng	29648	3	14.970	199081	20.0
Cinnamyl cinnamate	21.408	2.2	ng	33334	5	22.013	305729	20.0
Ethanol, 2-(tet...	21.572	2.9	ng	44398	5	22.013	305729	20.0