

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
 Data File : BG057517.D
 Acq On : 23 May 2023 13:14
 Operator : CG/JU
 Sample : 02869-21
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP22

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: BG057517.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.389	308	315	320	rBV	19837	30812	2.13%	0.499%
2	5.876	389	398	411	rBV	296618	486101	33.59%	7.867%
3	7.498	665	674	685	rBV	316712	559193	38.64%	9.050%
4	8.355	814	820	828	rBB	68749	113334	7.83%	1.834%
5	9.536	1013	1021	1031	rVB	187447	329740	22.79%	5.337%
6	11.193	1296	1303	1310	rBV	86520	152669	10.55%	2.471%
7	13.595	1705	1712	1720	rBV	555577	825389	57.04%	13.358%
8	14.911	1929	1936	1940	rBV3	18597	25798	1.78%	0.418%
9	14.970	1940	1946	1956	rVB	139885	225037	15.55%	3.642%
10	16.309	2165	2174	2181	rBV	62911	91114	6.30%	1.475%
11	16.456	2189	2199	2213	rBV	452184	712209	49.22%	11.527%
12	17.713	2407	2413	2420	rBV	205698	308673	21.33%	4.996%
13	20.280	2843	2850	2857	rBV	1149910	1447003	100.00%	23.419%
14	21.414	3038	3043	3048	rVB	88838	119956	8.29%	1.941%
15	21.578	3066	3071	3079	rBV3	25422	56168	3.88%	0.909%
16	22.019	3140	3146	3157	rVB	218618	355986	24.60%	5.761%
17	25.526	3733	3743	3753	rVB2	110327	339592	23.47%	5.496%

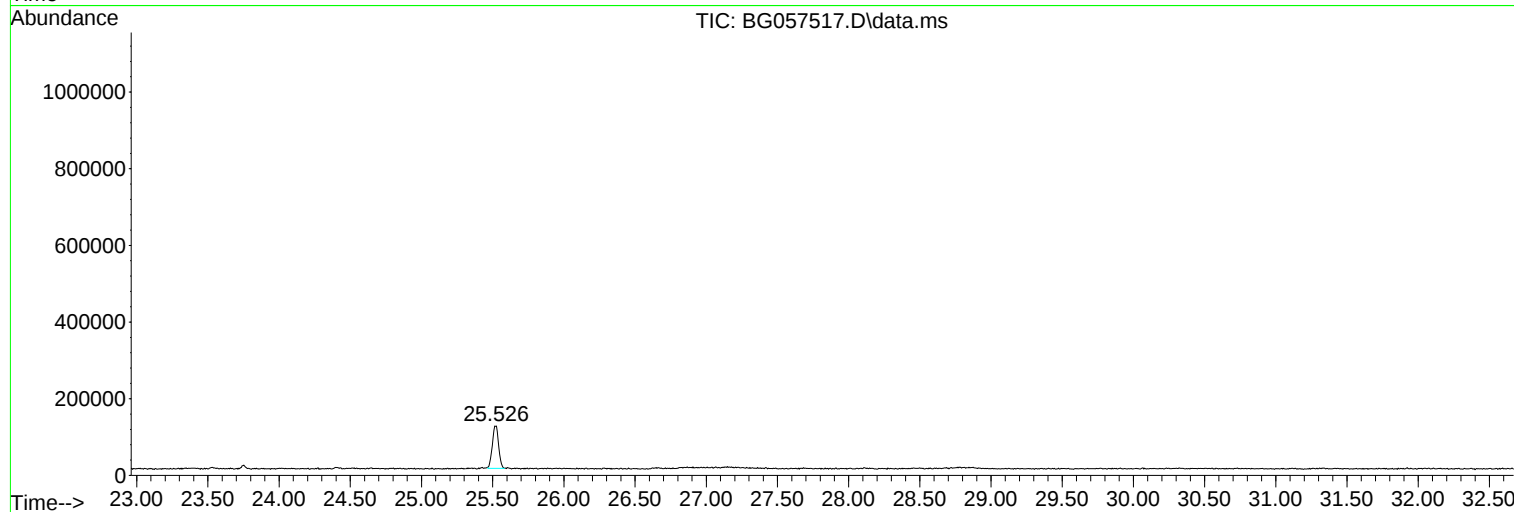
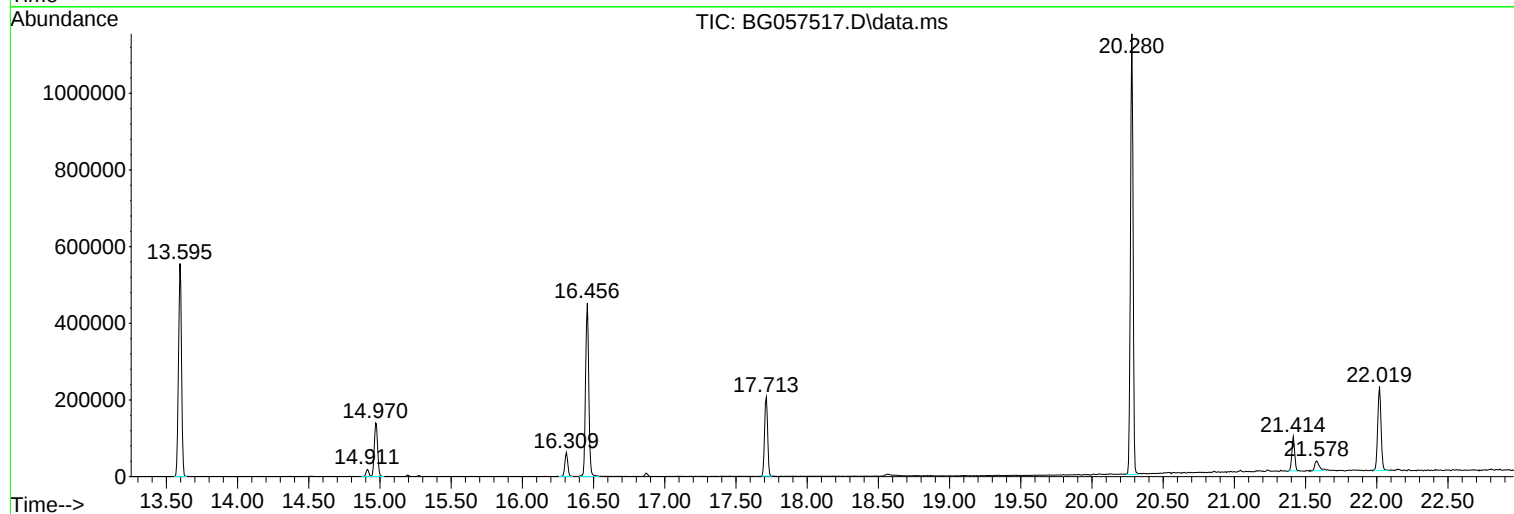
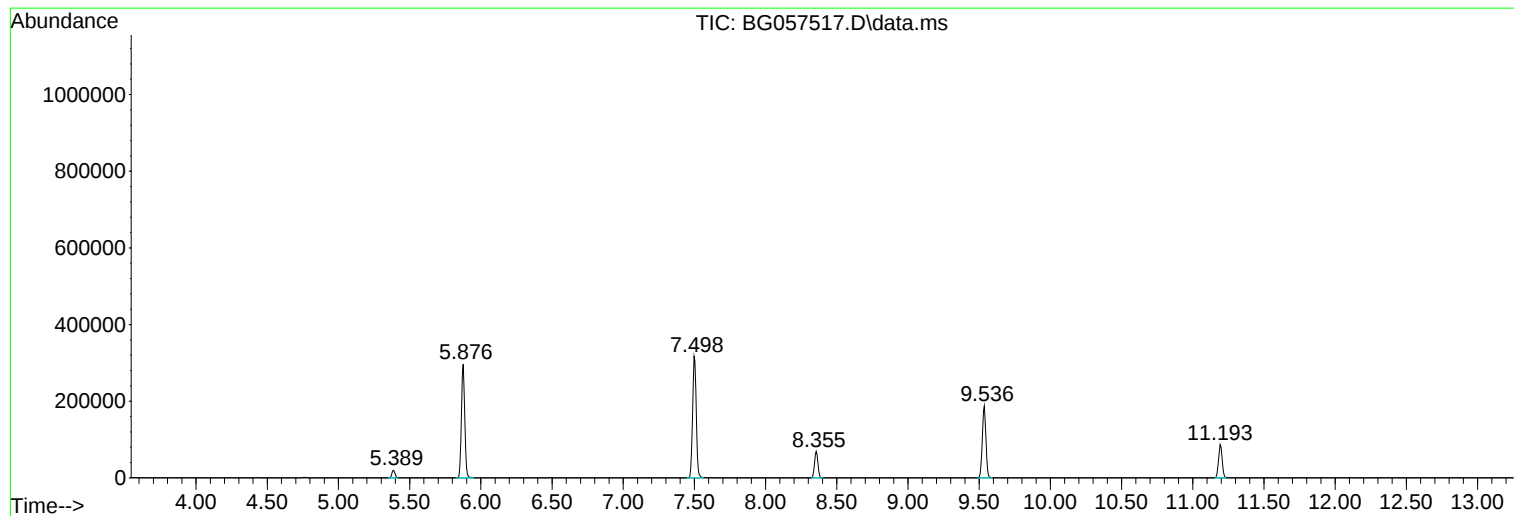
Sum of corrected areas: 6178774

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057517.D
Acq On : 23 May 2023 13:14
Operator : CG/JU
Sample : 02869-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP22

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\BG052323\
Data File : BG057517.D
Acq On : 23 May 2023 13:14
Operator : CG/JU
Sample : 02869-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP22

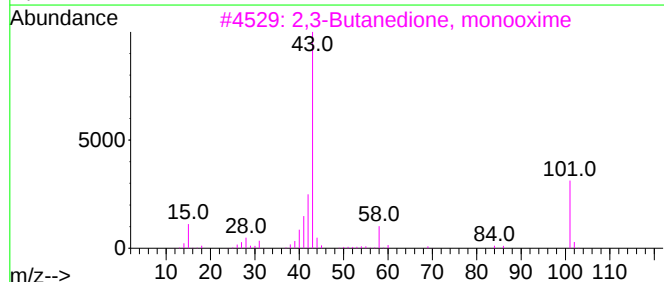
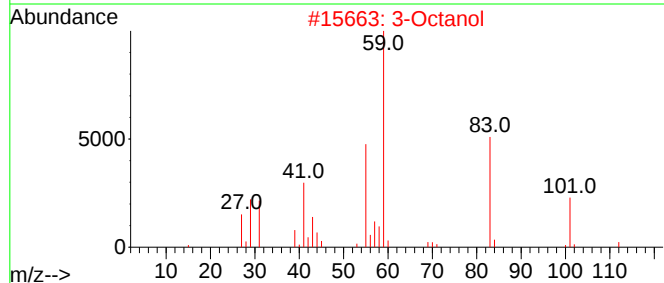
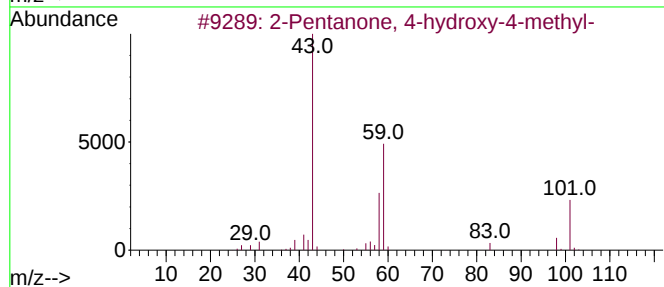
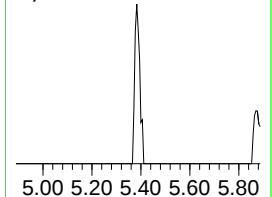
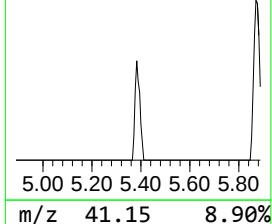
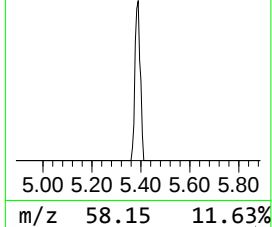
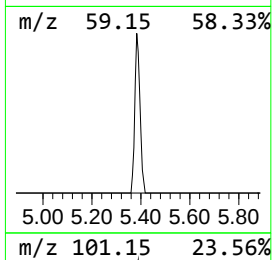
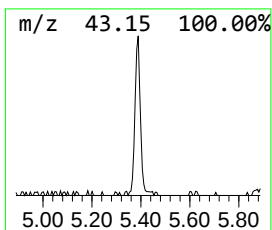
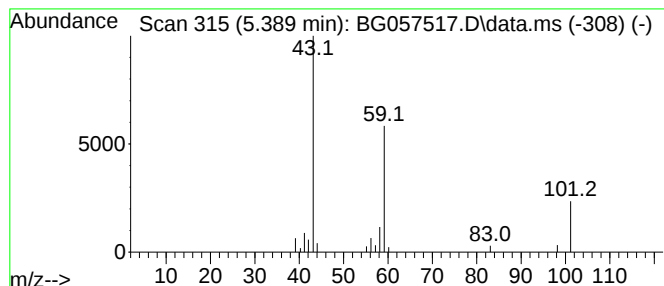
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.389	5.44 ng	30812	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	72
2		3-Octanol	130	C8H18O	000589-98-0	33
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
4		3-Heptanol	116	C7H16O	000589-82-2	25
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057517.D
Acq On : 23 May 2023 13:14
Operator : CG/JU
Sample : 02869-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP22

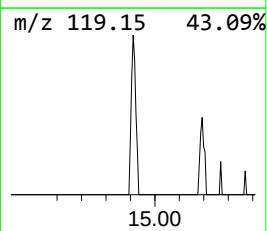
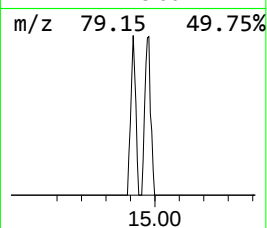
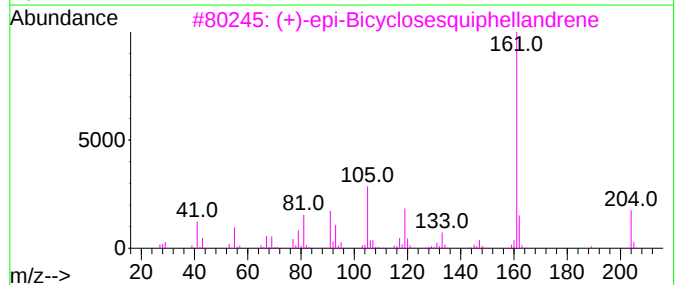
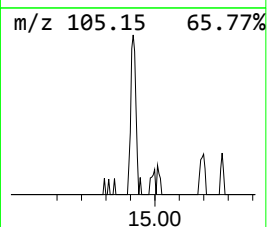
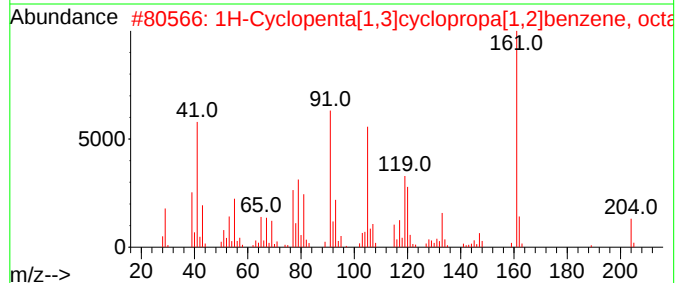
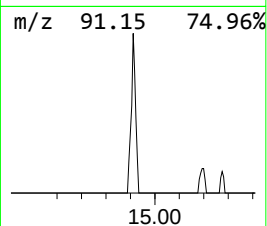
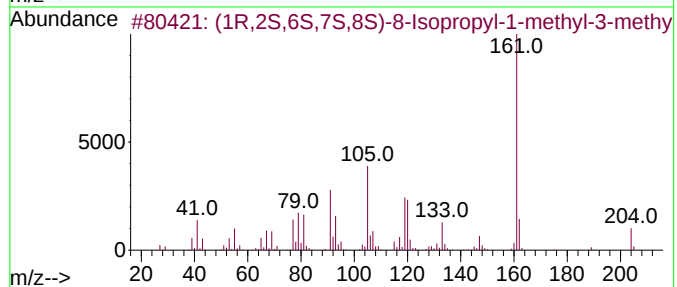
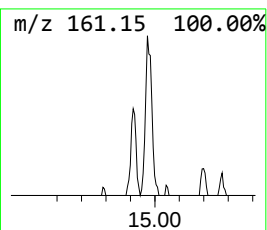
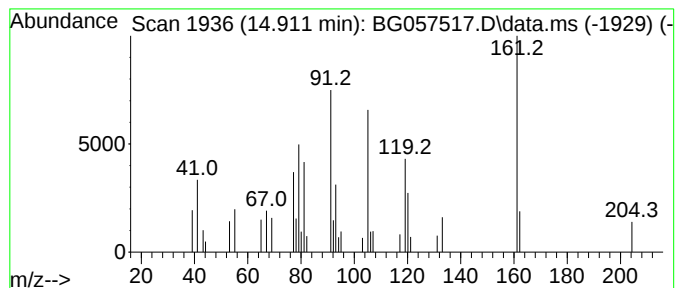
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 (1R,2S,6S,7S,8S)-8-Isopropy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.911	2.29 ng	25798	Acenaphthene-d10	14.970

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	91		
2	1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	90		
3	(+)-epi-Bicyclosquiphellandrene	204	C15H24	054274-73-6	70		
4	cis-Muurolo-4(15),5-diene	204	C15H24	157477-72-0	70		
5	Germacrene D	204	C15H24	023986-74-5	70		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057517.D
Acq On : 23 May 2023 13:14
Operator : CG/JU
Sample : 02869-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP22

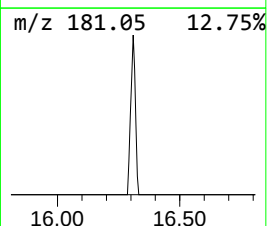
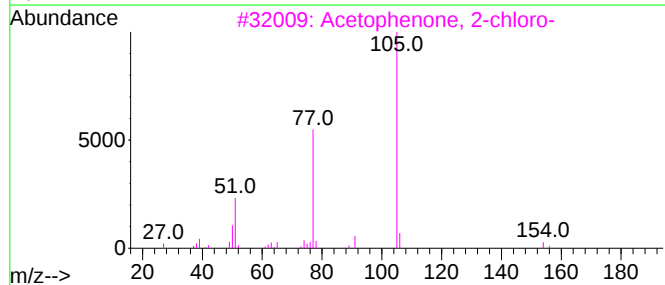
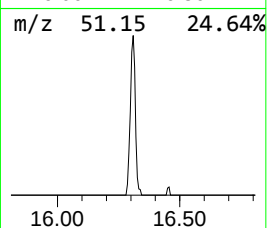
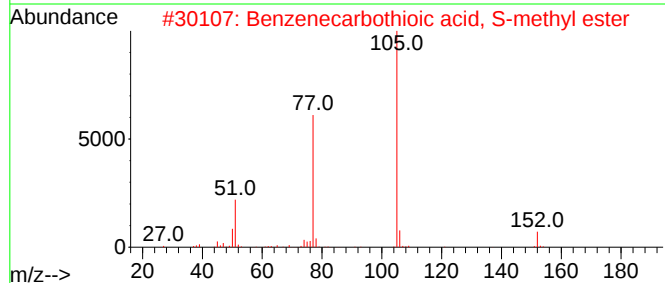
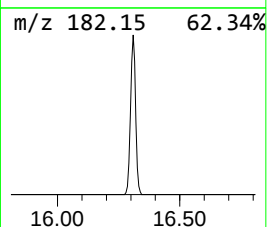
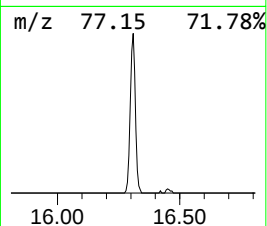
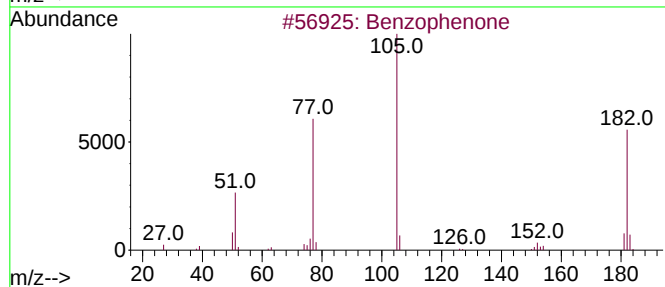
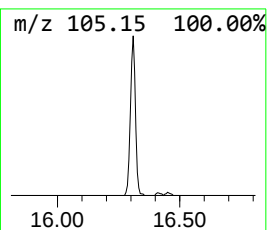
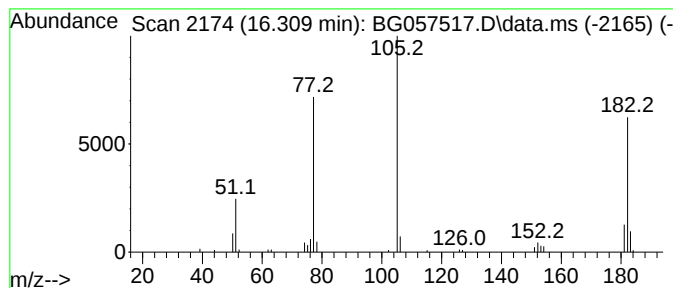
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.309	8.10 ng	91114	Acenaphthene-d10	14.970

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4			Phenacyl thiocyanate	177	C9H7NOS	005399-30-4	43
5			S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057517.D
Acq On : 23 May 2023 13:14
Operator : CG/JU
Sample : 02869-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP22

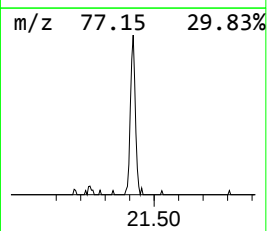
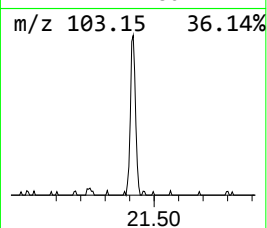
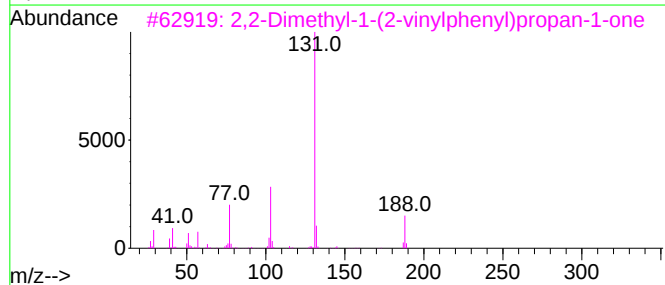
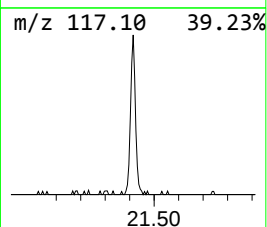
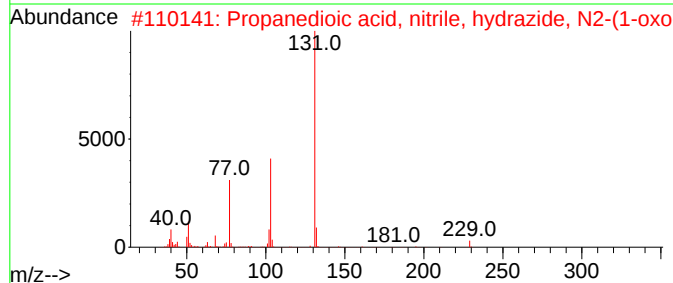
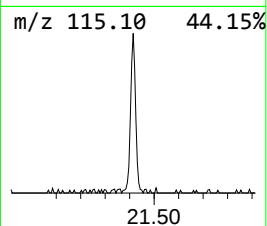
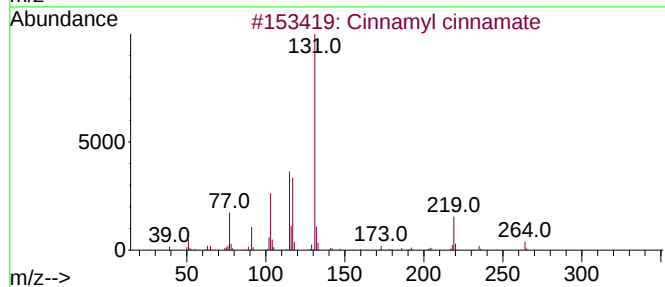
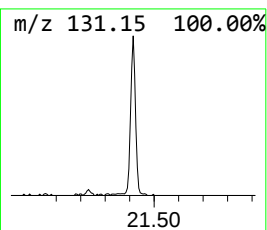
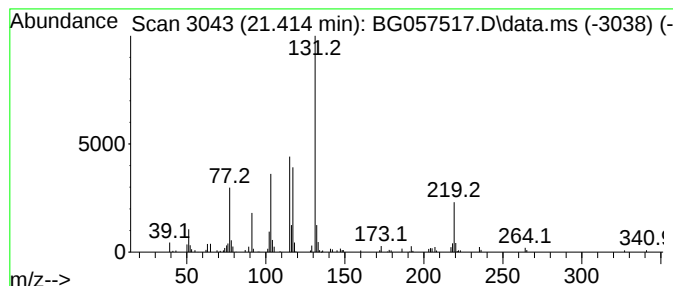
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Cinnamyl cinnamate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.414	6.74 ng	119956	Chrysene-d12	22.019

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			Propanedioic acid, nitrile, hydr...	229	C12H11N3O2	294878-35-6	46
3			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	43
4			trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	43
5			N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057517.D
Acq On : 23 May 2023 13:14
Operator : CG/JU
Sample : 02869-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP22

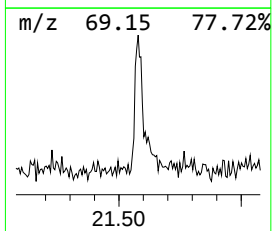
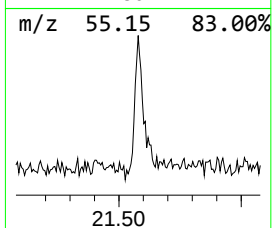
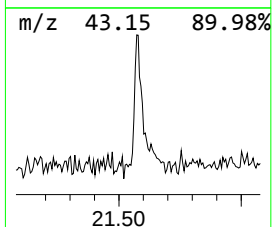
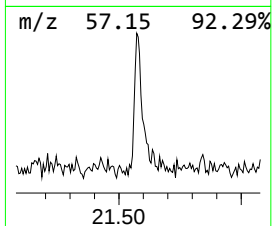
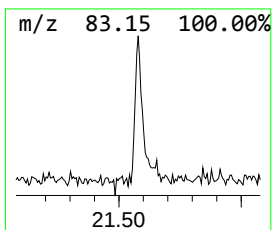
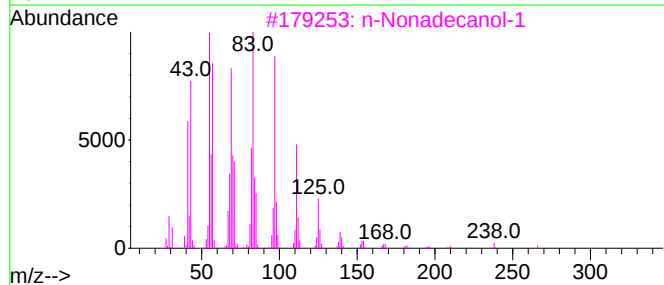
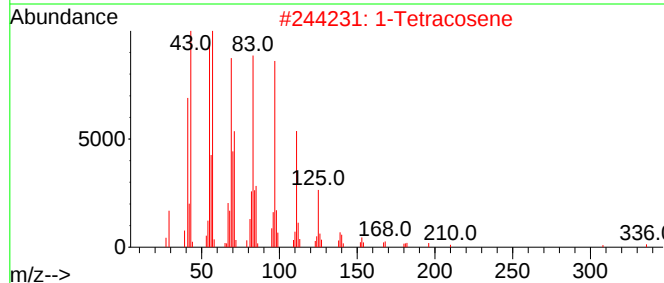
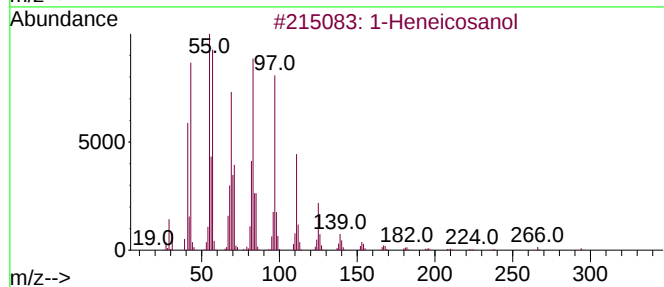
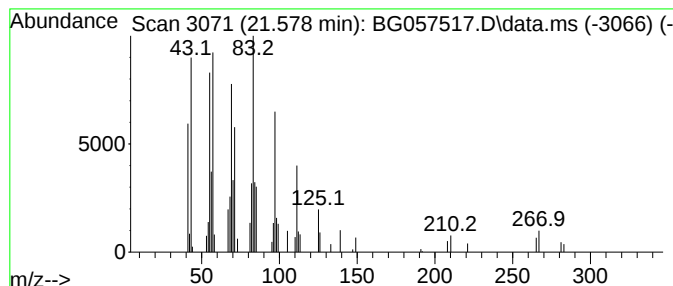
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.578	3.16 ng	56168	Chrysene-d12	22.019

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol			312	C21H44O	015594-90-8	90
2	1-Tetracosene			336	C24H48	010192-32-2	87
3	n-Nonadecanol-1			284	C19H40O	001454-84-8	87
4	1-Hexacosene			364	C26H52	018835-33-1	87
5	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057517.D
Acq On : 23 May 2023 13:14
Operator : CG/JU
Sample : 02869-21
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP22

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-...	5.389	5.4	ng	30812	1	8.355	113334	20.0
(1R,2S,6S,7S,8S...	14.911	2.3	ng	25798	3	14.970	225037	20.0
Benzophenone	16.309	8.1	ng	91114	3	14.970	225037	20.0
Cinnamyl cinnamate	21.414	6.7	ng	119956	5	22.019	355986	20.0
1-Heneicosanol	21.578	3.2	ng	56168	5	22.019	355986	20.0