

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
 Data File : BG055447.D
 Acq On : 3 Nov 2022 21:32
 Operator : CG/JU
 Sample : N5306-06
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DISSOLVED-20221166-COMP-01-MODIFIED-ELUTRIATE

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-BG110122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055447.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.273	333	338	351	rVB	20494	36153	1.67%	0.401%
2	5.761	415	421	438	rBV	211867	383251	17.76%	4.250%
3	7.382	690	697	714	rBV	167785	318142	14.74%	3.528%
4	8.234	833	842	855	rBB	98787	170947	7.92%	1.896%
5	9.409	1034	1042	1057	rBV	302457	548091	25.39%	6.079%
6	10.808	1274	1280	1299	rBV	114297	206361	9.56%	2.289%
7	11.060	1316	1323	1335	rVB	134758	245841	11.39%	2.727%
8	13.481	1727	1735	1746	rBV	880980	1402153	64.96%	15.551%
9	13.722	1769	1776	1786	rBV	28461	44301	2.05%	0.491%
10	14.850	1961	1968	1977	rVB	245302	369641	17.12%	4.100%
11	16.331	2214	2220	2235	rBV	697968	1055261	48.89%	11.703%
12	17.582	2427	2433	2444	rVB	313920	478294	22.16%	5.305%
13	18.211	2533	2540	2548	rBV3	59539	86334	4.00%	0.957%
14	18.434	2572	2578	2588	rBV2	27284	48342	2.24%	0.536%
15	19.362	2732	2736	2747	rVB2	119912	139638	6.47%	1.549%
16	20.161	2866	2872	2878	rBV	1664270	2158537	100.00%	23.939%
17	21.460	3087	3093	3107	rBV9	21150	78353	3.63%	0.869%
18	21.854	3154	3160	3173	rBV2	320416	539282	24.98%	5.981%
19	23.552	3442	3449	3456	rVB	67913	141014	6.53%	1.564%
20	25.226	3724	3734	3747	rVB3	194282	566703	26.25%	6.285%

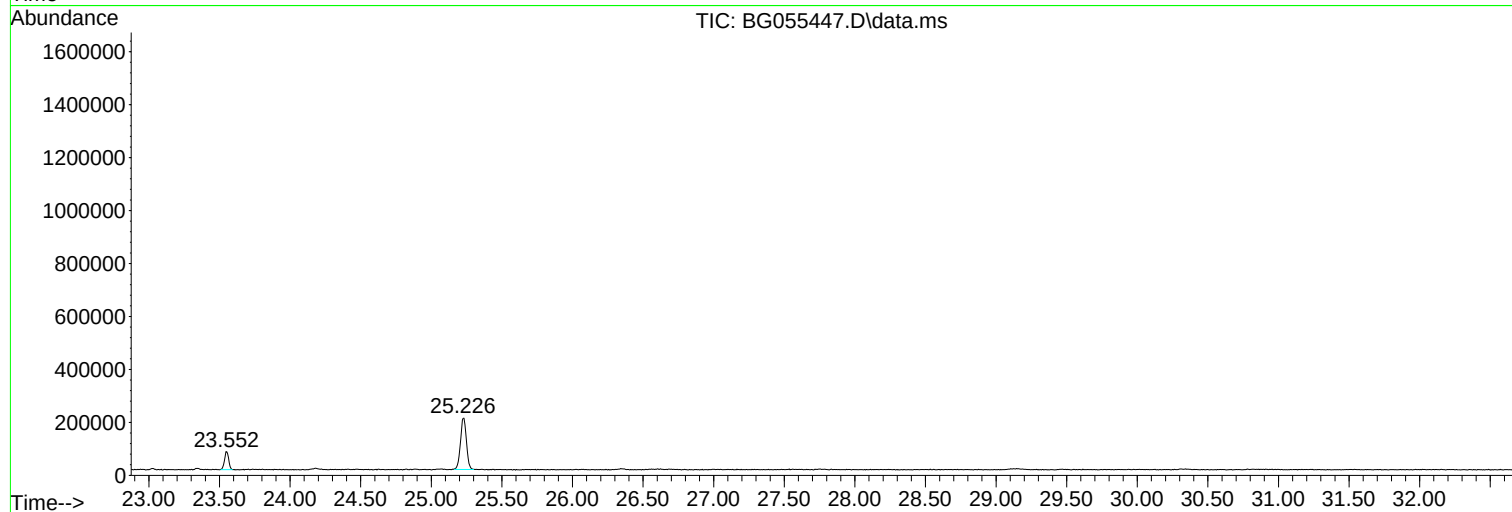
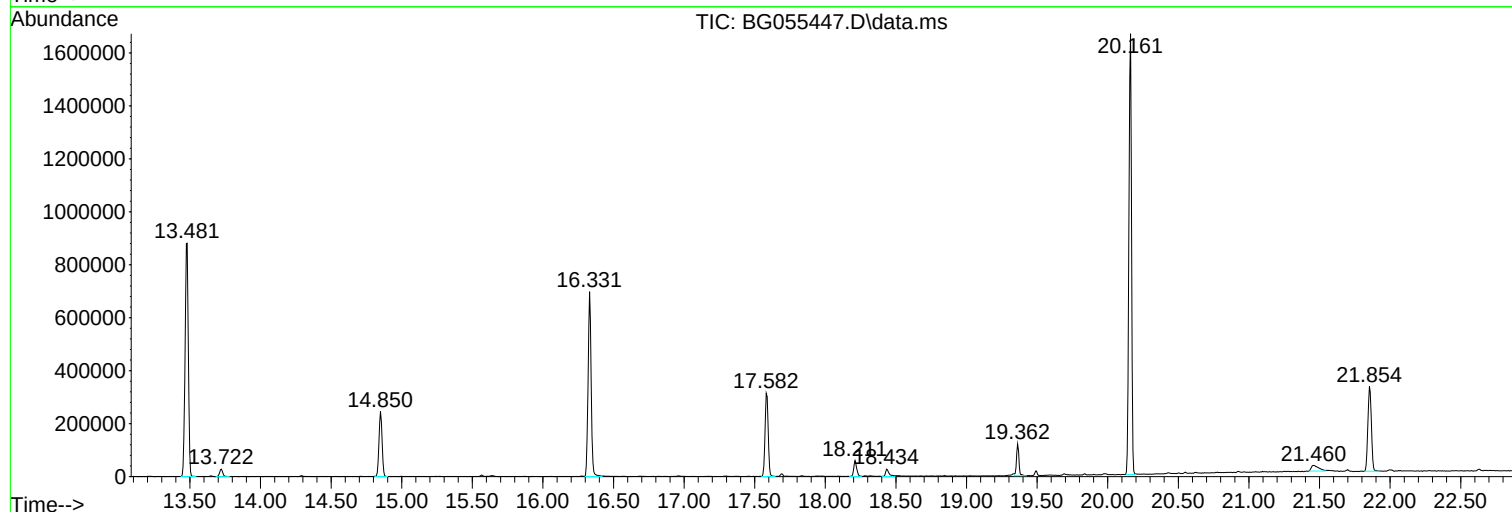
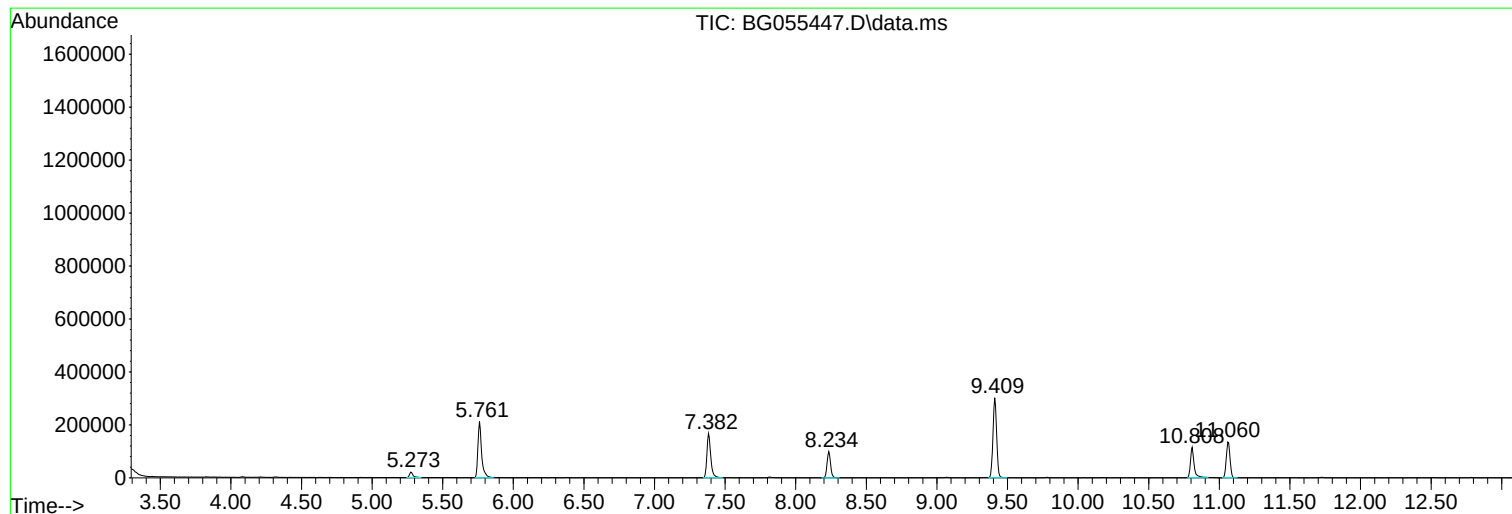
Sum of corrected areas: 9016639

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055447.D
Acq On : 3 Nov 2022 21:32
Operator : CG/JU
Sample : N5306-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221166-COMP-01-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.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\BG110322\
Data File : BG055447.D
Acq On : 3 Nov 2022 21:32
Operator : CG/JU
Sample : N5306-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221166-COMP-01-MODIFIED-ELUTRIATE

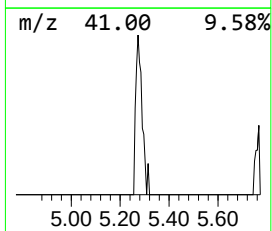
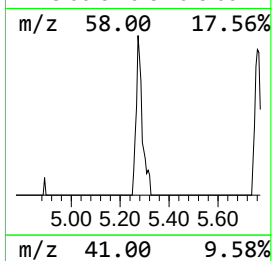
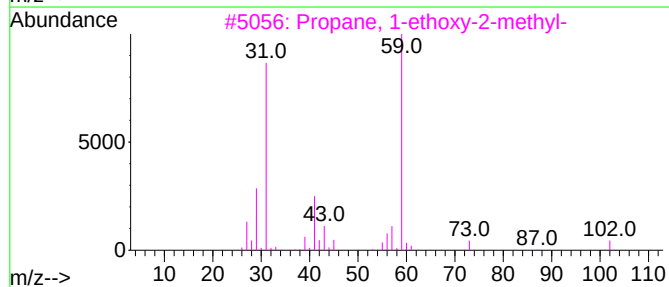
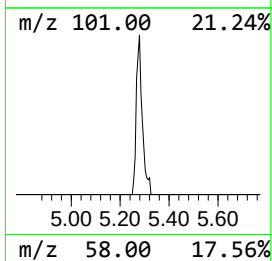
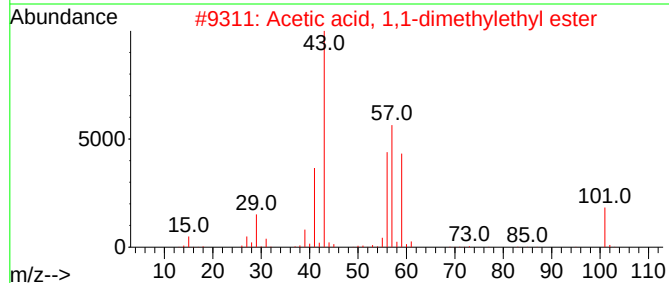
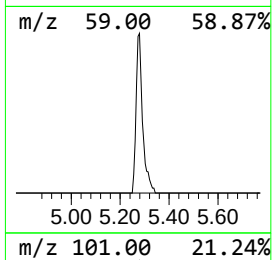
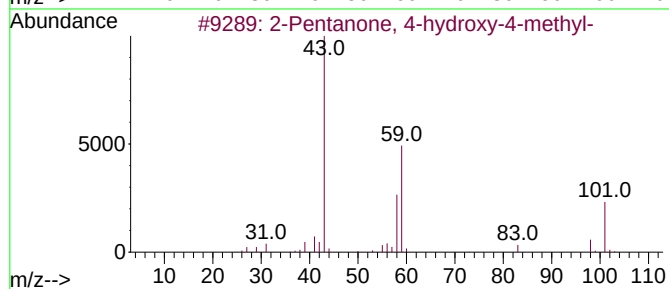
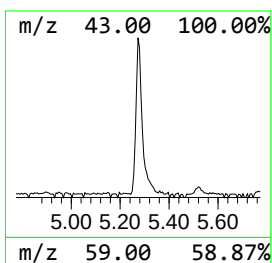
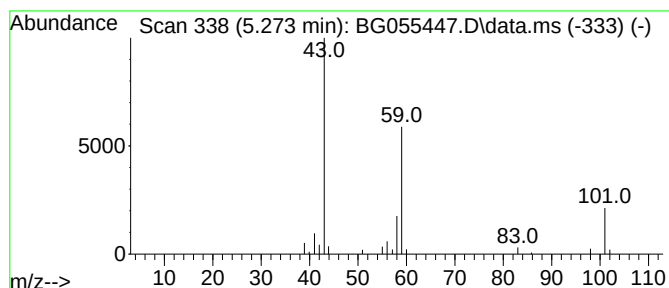
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.273	4.23 ng	36153	1,4-Dichlorobenzene-d4	8.234

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25		
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25		
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055447.D
Acq On : 3 Nov 2022 21:32
Operator : CG/JU
Sample : N5306-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

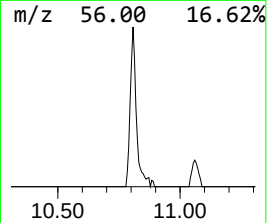
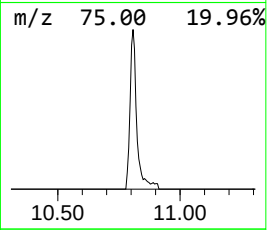
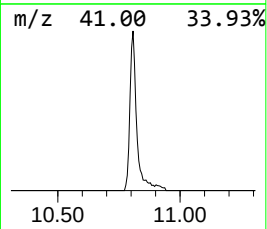
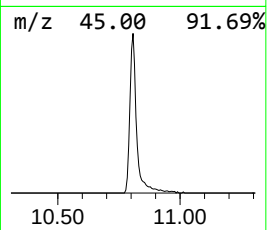
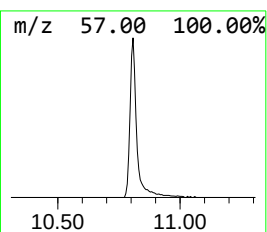
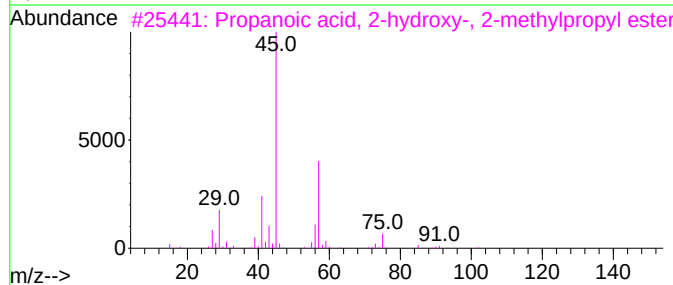
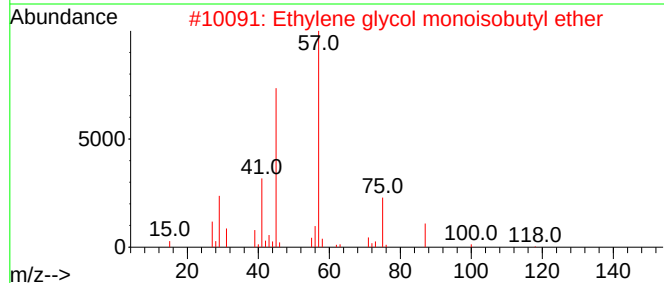
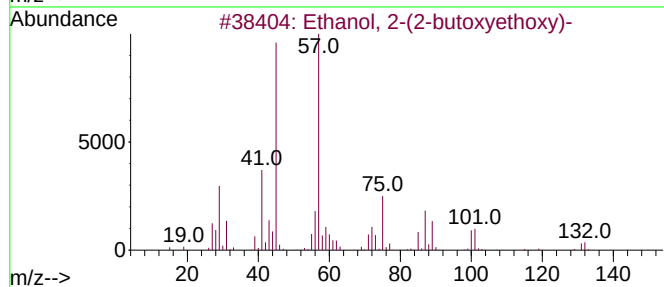
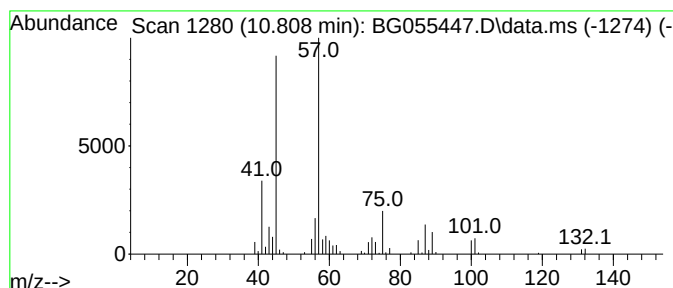
Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221166-COMP-01-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.808	16.79 ng	206361	Naphthalene-d8	11.066	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53
4	Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	53
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055447.D
Acq On : 3 Nov 2022 21:32
Operator : CG/JU
Sample : N5306-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221166-COMP-01-MODIFIED-ELUTRIATE

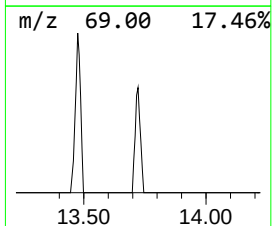
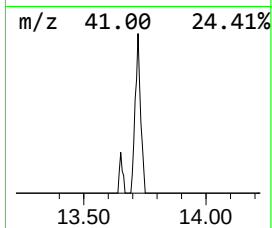
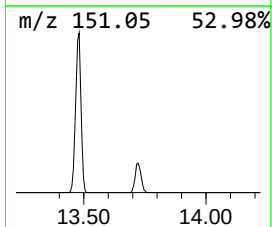
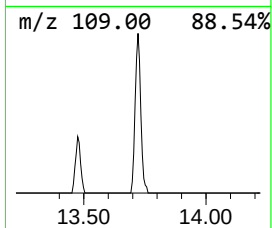
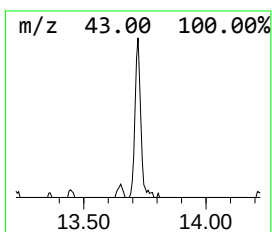
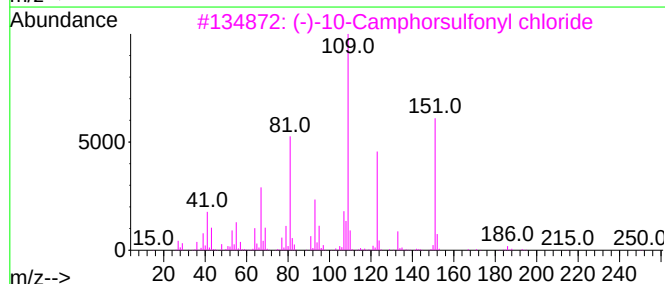
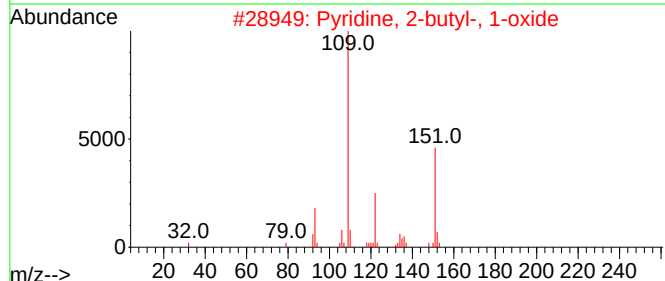
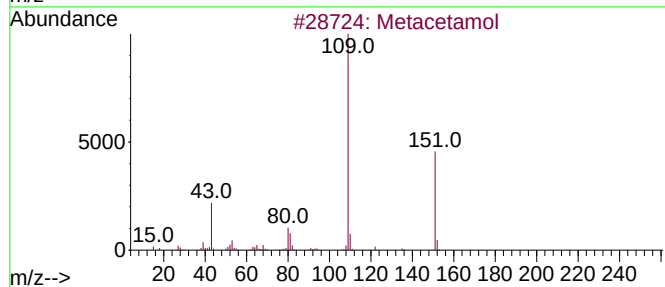
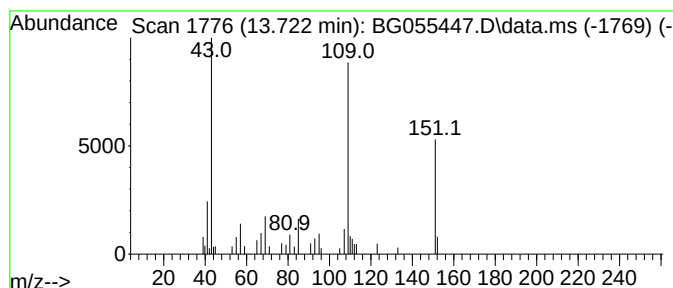
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Metacetamol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.722	2.40 ng	44301	Acenaphthene-d10	14.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Metacetamol	151	C8H9NO2	000621-42-1	58
2			Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
3			(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	50
4			Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	43
5			Acetaminophen	151	C8H9NO2	000103-90-2	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055447.D
Acq On : 3 Nov 2022 21:32
Operator : CG/JU
Sample : N5306-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221166-COMP-01-MODIFIED-ELUTRIATE

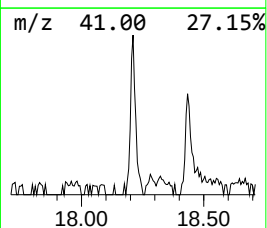
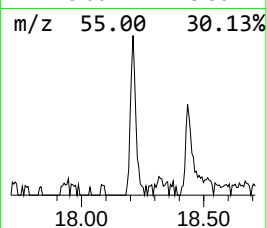
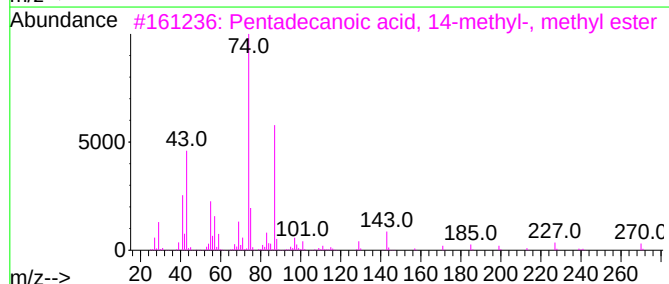
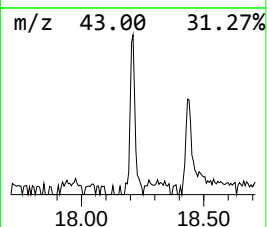
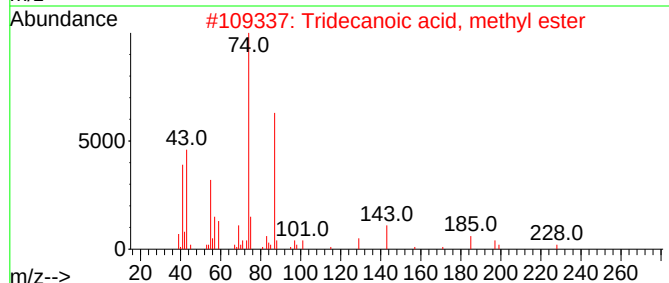
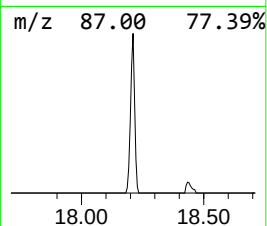
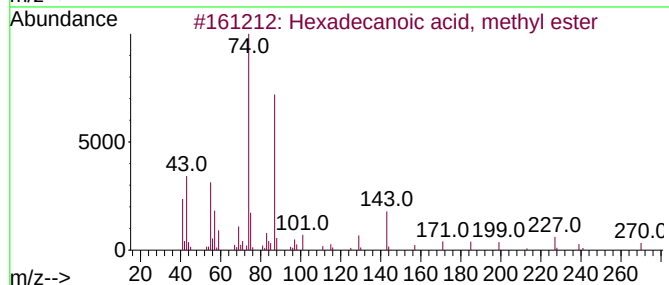
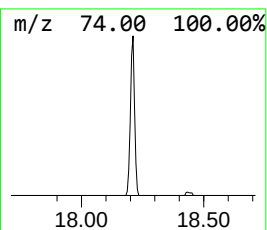
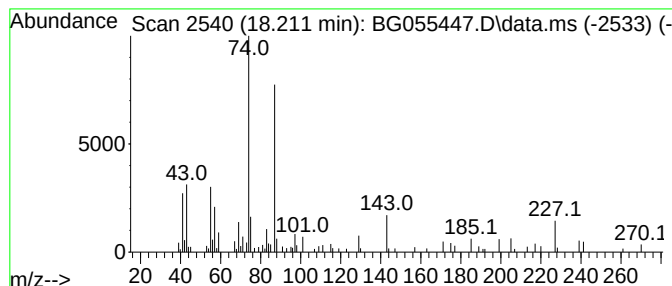
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.211	3.61 ng	86334	Phenanthrene-d10	17.582

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
4			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055447.D
Acq On : 3 Nov 2022 21:32
Operator : CG/JU
Sample : N5306-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221166-COMP-01-MODIFIED-ELUTRIATE

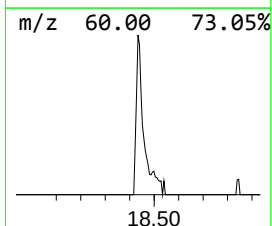
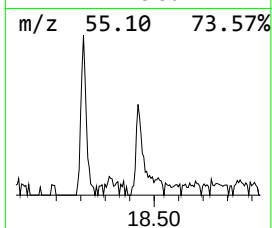
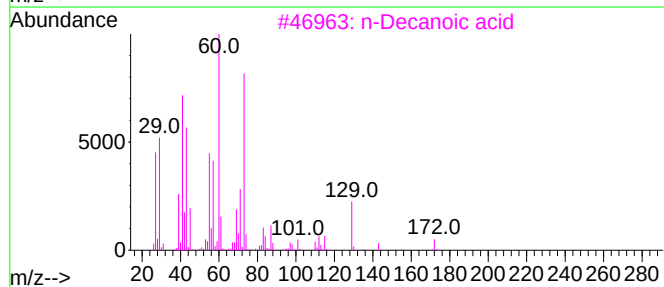
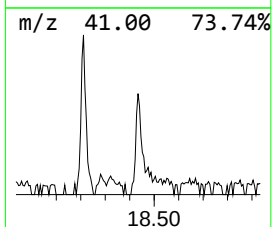
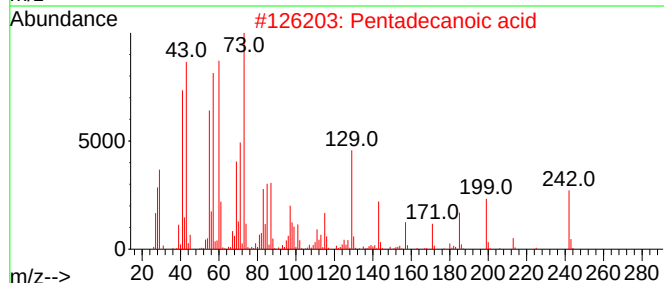
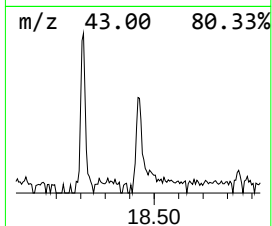
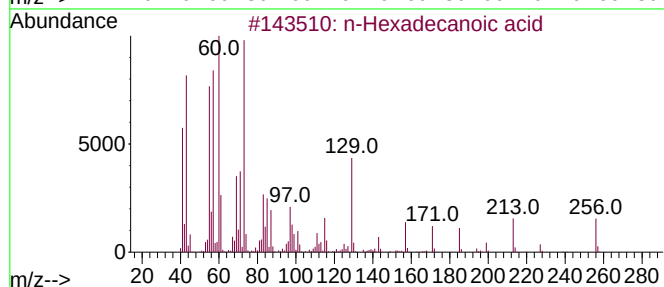
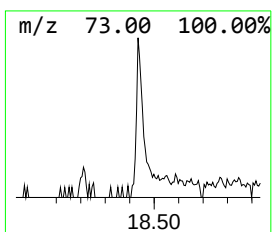
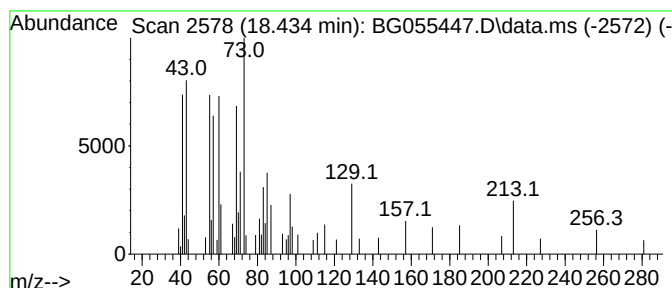
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.434	2.02 ng	48342	Phenanthrene-d10	17.582

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			n-Decanoic acid	172	C10H20O2	000334-48-5	50
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	50
5			D-Glucopyranoside, 4-O-decyl-	320	C16H32O6	1000158-00-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055447.D
Acq On : 3 Nov 2022 21:32
Operator : CG/JU
Sample : N5306-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221166-COMP-01-MODIFIED-ELUTRIATE

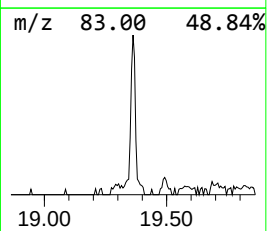
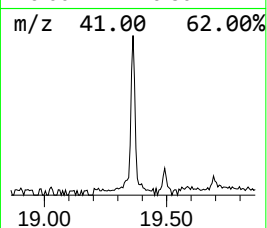
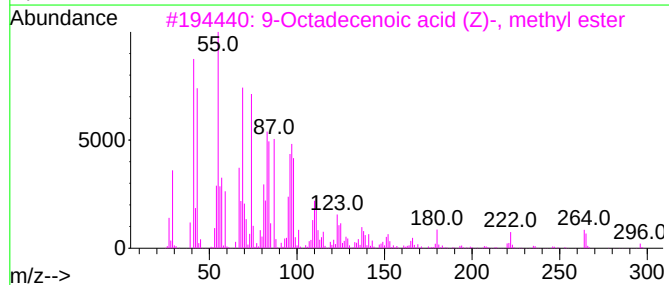
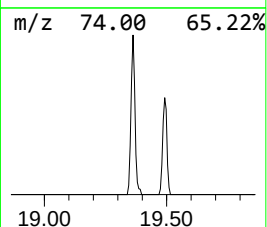
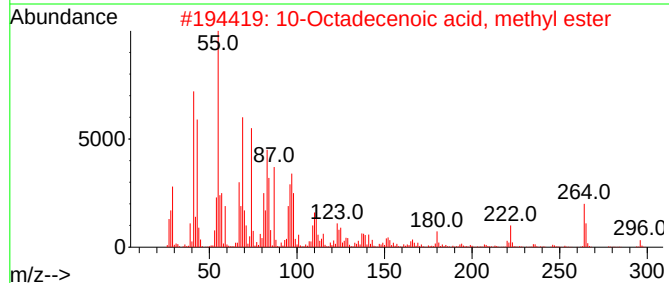
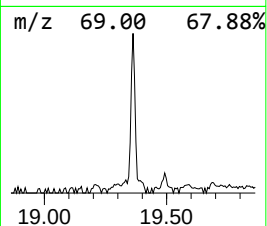
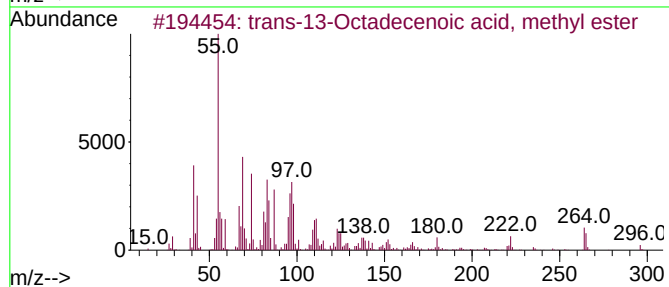
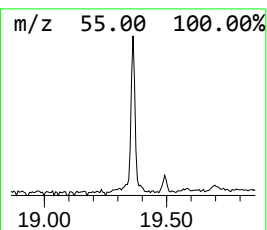
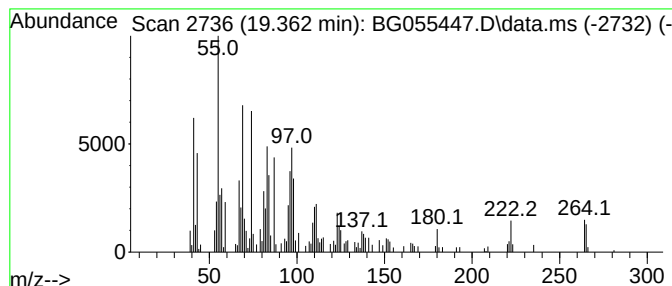
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 trans-13-Octadecenoic acid,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.362	5.84 ng	139638	Phenanthrene-d10	17.582

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	94
2			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
3			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
4			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
5			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055447.D
Acq On : 3 Nov 2022 21:32
Operator : CG/JU
Sample : N5306-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221166-COMP-01-MODIFIED-ELUTRIATE

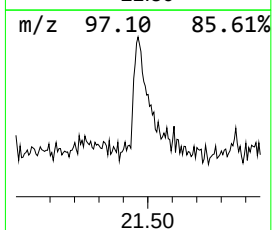
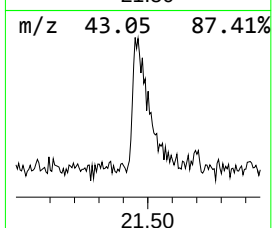
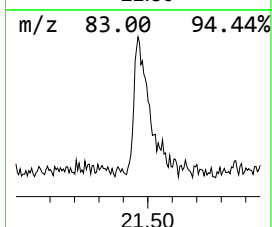
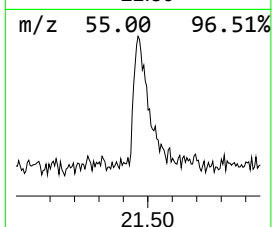
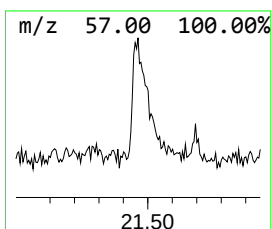
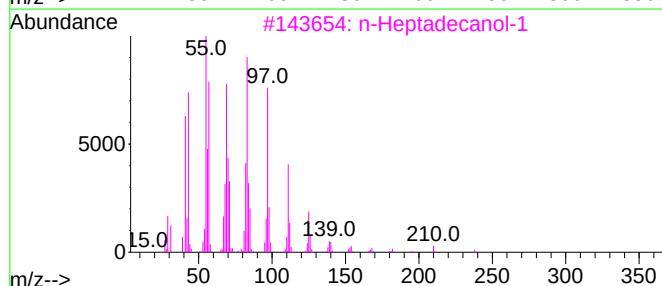
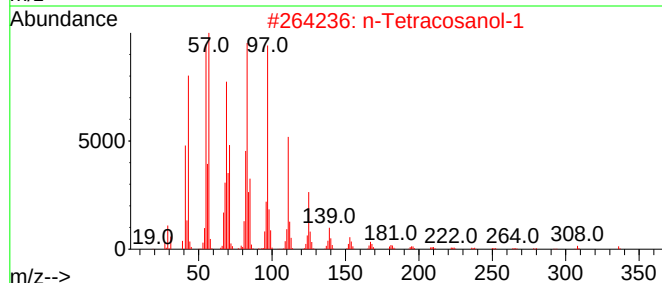
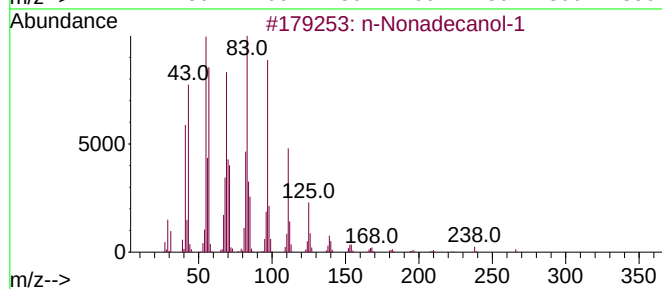
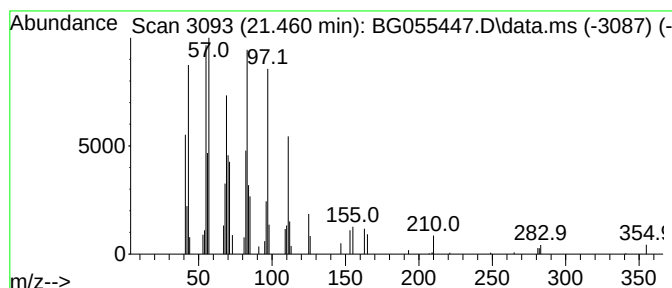
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Nonadecanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.460	2.91 ng	78353	Chrysene-d12	21.854

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3		n-Heptadecanol-1	256	C17H36O	001454-85-9	91
4		1-Octadecanol	270	C18H38O	000112-92-5	91
5		Behenic alcohol	326	C22H46O	000661-19-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055447.D
Acq On : 3 Nov 2022 21:32
Operator : CG/JU
Sample : N5306-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221166-COMP-01-MODIFIED-ELUTRIATE

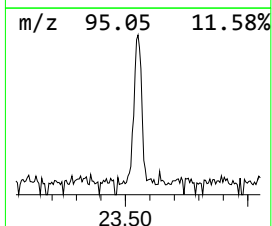
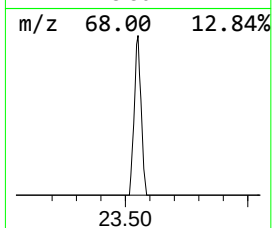
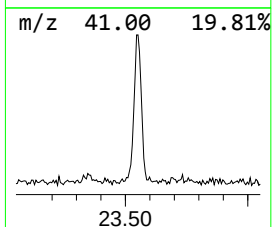
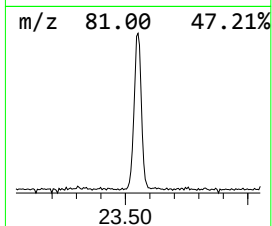
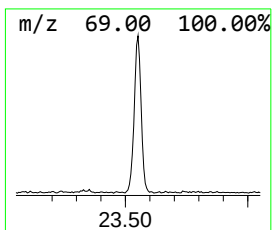
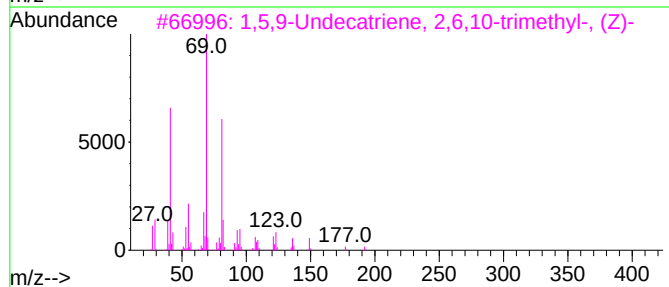
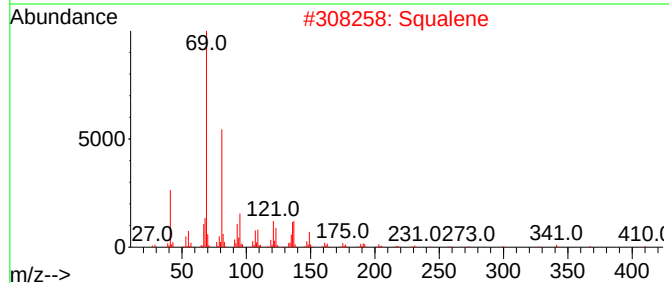
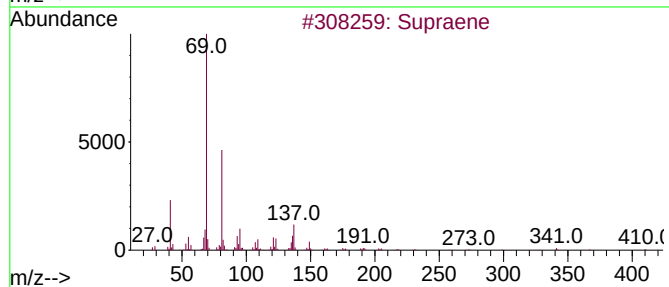
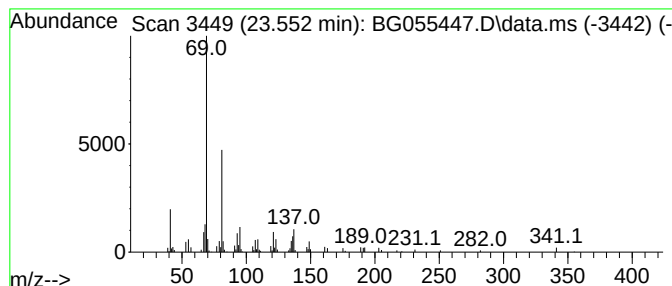
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.552	4.98 ng	141014	Perylene-d12	25.226

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	86
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055447.D
Acq On : 3 Nov 2022 21:32
Operator : CG/JU
Sample : N5306-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221166-COMP-01-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.273	4.2	ng	36153	1	8.234	170947	20.0
Ethanol, 2-(2-b...	10.808	16.8	ng	206361	2	11.066	245841	20.0
Metacetamol	13.722	2.4	ng	44301	3	14.850	369641	20.0
Hexadecanoic ac...	18.211	3.6	ng	86334	4	17.582	478294	20.0
n-Hexadecanoic ...	18.434	2.0	ng	48342	4	17.582	478294	20.0
trans-13-Octade...	19.362	5.8	ng	139638	4	17.582	478294	20.0
n-Nonadecanol-1	21.460	2.9	ng	78353	5	21.854	539282	20.0
Supraene	23.552	5.0	ng	141014	6	25.226	566703	20.0