

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120222\
 Data File : BG055876.D
 Acq On : 2 Dec 2022 16:25
 Operator : CG/JU
 Sample : N5830-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMP1-1201

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-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055876.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.247	326	333	347	rVB	86070	133815	5.61%	1.238%
2	5.729	409	415	425	rBV	275614	460087	19.28%	4.256%
3	7.350	683	691	708	rBV	189884	331603	13.89%	3.067%
4	8.196	829	835	842	rBV	111883	189000	7.92%	1.748%
5	9.371	1027	1035	1047	rBV	380465	683492	28.64%	6.323%
6	11.028	1308	1317	1325	rBV	165279	298548	12.51%	2.762%
7	13.449	1721	1729	1736	rBV	1097018	1726210	72.32%	15.968%
8	14.830	1958	1964	1976	rVB	300496	471147	19.74%	4.358%
9	16.310	2210	2216	2224	rBV	862223	1355408	56.79%	12.538%
10	17.444	2404	2409	2413	rBV	58821	76724	3.21%	0.710%
11	17.568	2424	2430	2440	rVB	371851	553082	23.17%	5.116%
12	18.431	2572	2577	2586	rBV	104292	183628	7.69%	1.699%
13	19.336	2724	2731	2732	rBV3	24579	47937	2.01%	0.443%
14	19.689	2788	2791	2800	rBV3	29768	44171	1.85%	0.409%
15	20.159	2864	2871	2876	rBV	1798154	2386763	100.00%	22.078%
16	21.451	3088	3091	3095	rBV3	23401	37780	1.58%	0.349%
17	21.504	3095	3100	3119	rVB4	45239	195533	8.19%	1.809%
18	21.857	3154	3160	3171	rVB	357309	596831	25.01%	5.521%
19	23.561	3443	3450	3458	rVB	201639	394090	16.51%	3.645%
20	25.235	3724	3735	3745	rVB2	212716	644551	27.01%	5.962%

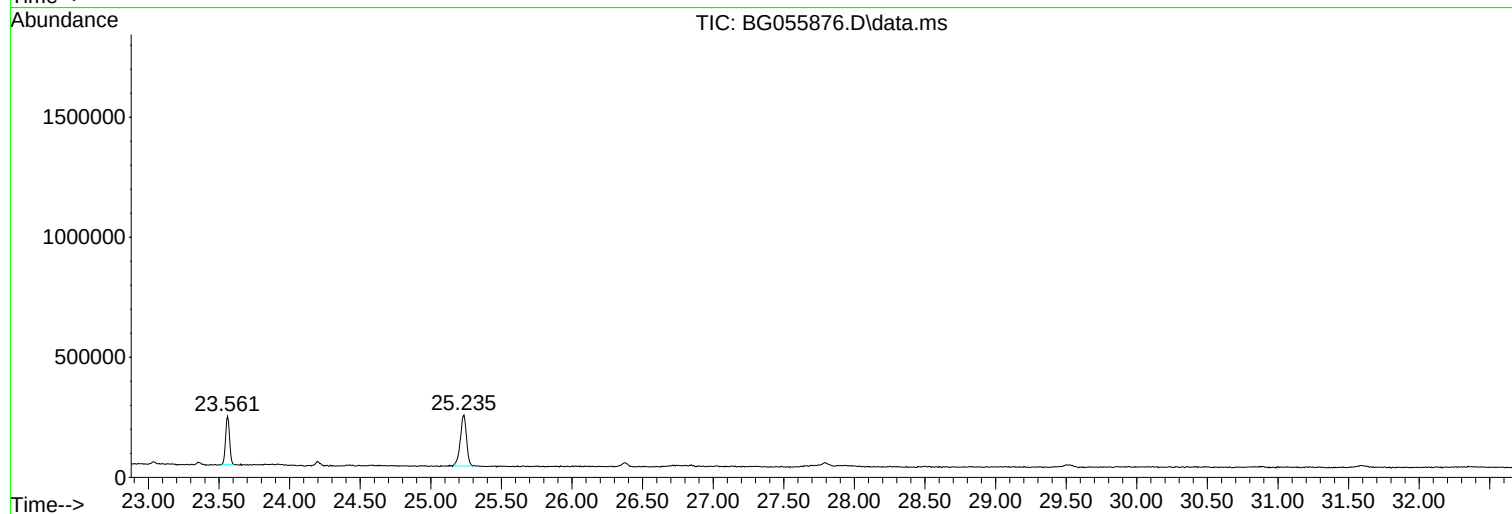
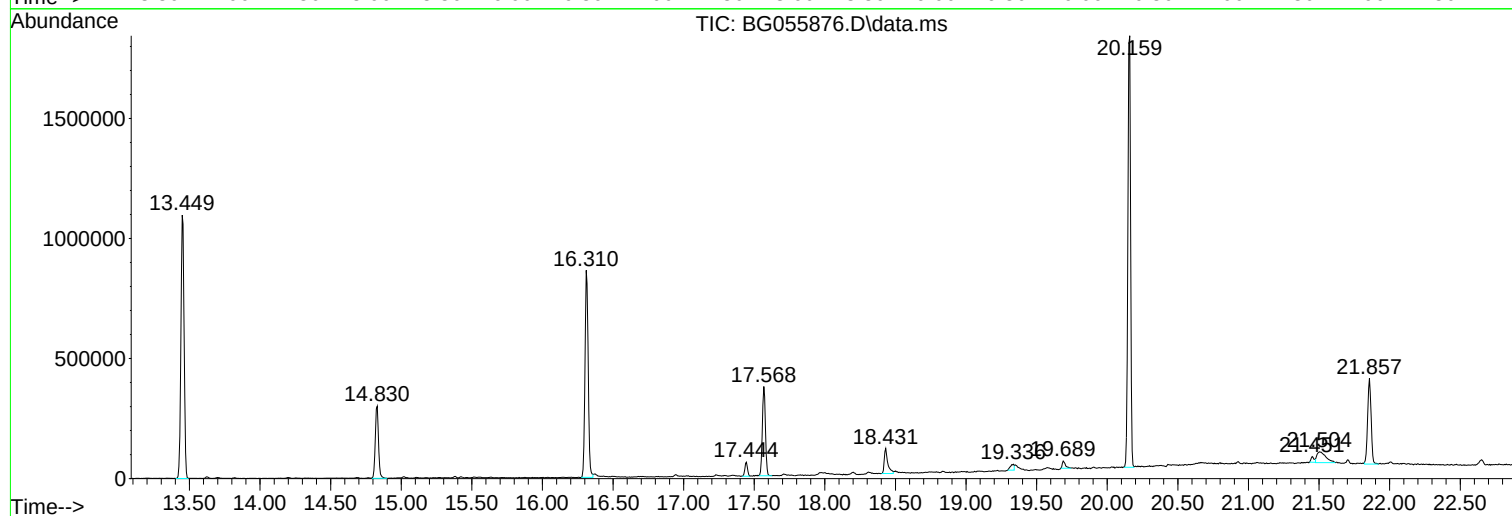
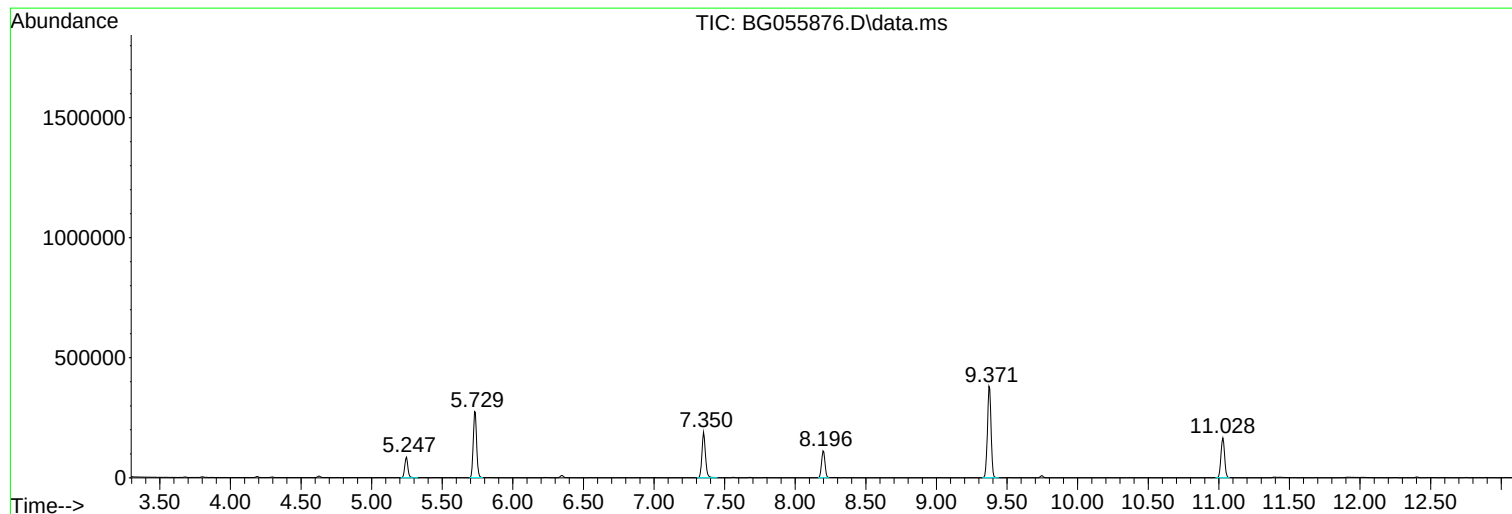
Sum of corrected areas: 10810400

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120222\
Data File : BG055876.D
Acq On : 2 Dec 2022 16:25
Operator : CG/JU
Sample : N5830-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP1-1201

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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\BG120222\
Data File : BG055876.D
Acq On : 2 Dec 2022 16:25
Operator : CG/JU
Sample : N5830-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP1-1201

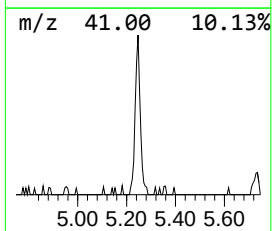
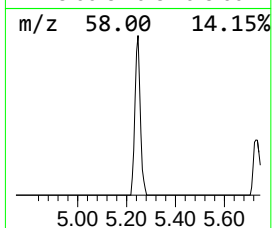
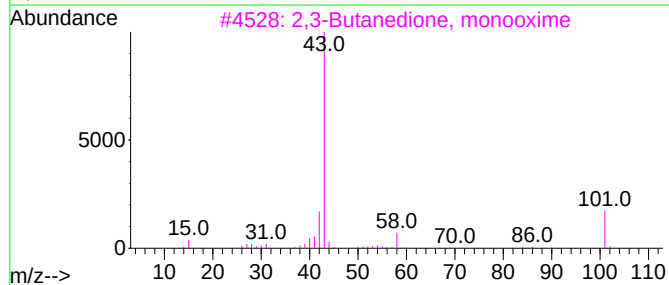
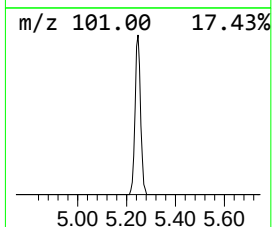
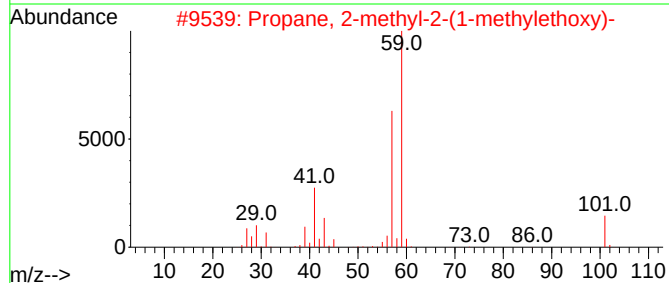
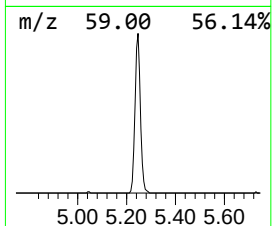
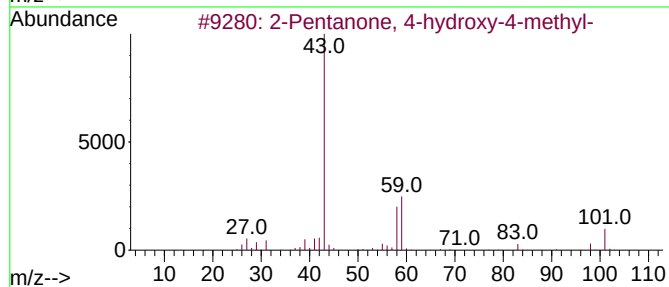
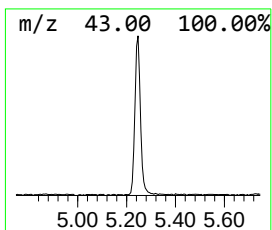
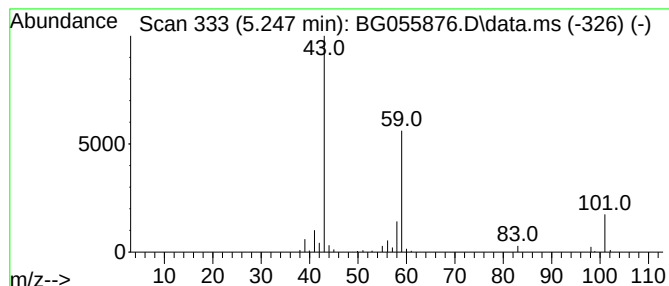
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.247	14.16 ng	133815	1,4-Dichlorobenzene-d4	8.202

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120222\
Data File : BG055876.D
Acq On : 2 Dec 2022 16:25
Operator : CG/JU
Sample : N5830-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP1-1201

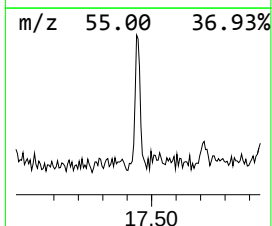
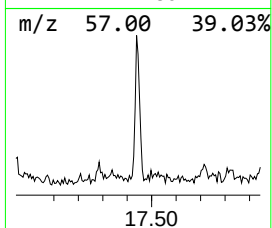
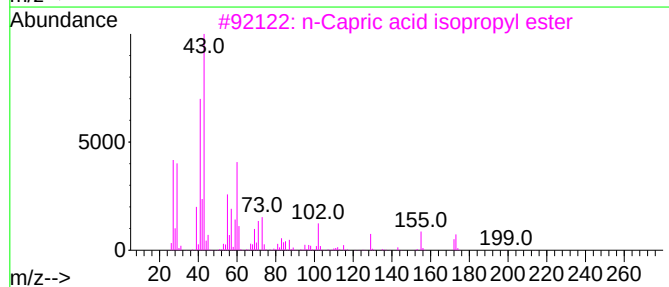
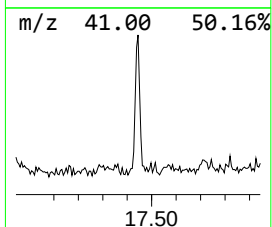
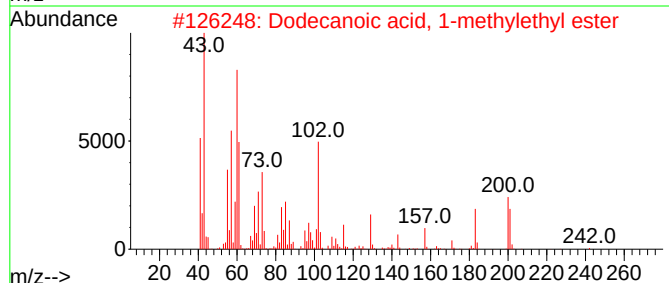
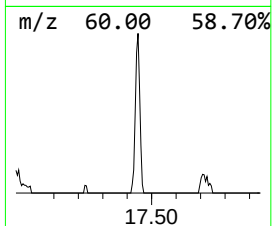
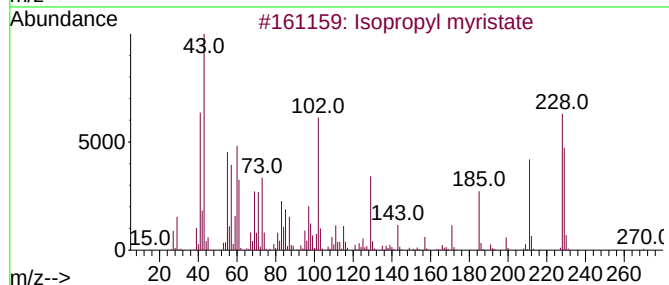
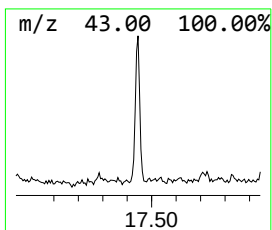
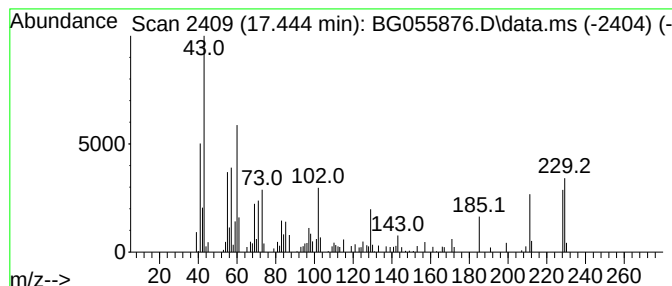
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Isopropyl myristate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.444	2.77 ng	76724	Phenanthrene-d10	17.568

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl myristate	270	C17H34O2	000110-27-0	74
2		Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	32
3		n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	22
4		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	14
5		n-Decanoic acid	172	C10H20O2	000334-48-5	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120222\
Data File : BG055876.D
Acq On : 2 Dec 2022 16:25
Operator : CG/JU
Sample : N5830-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP1-1201

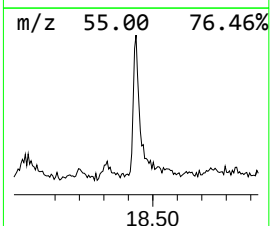
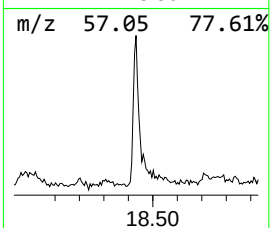
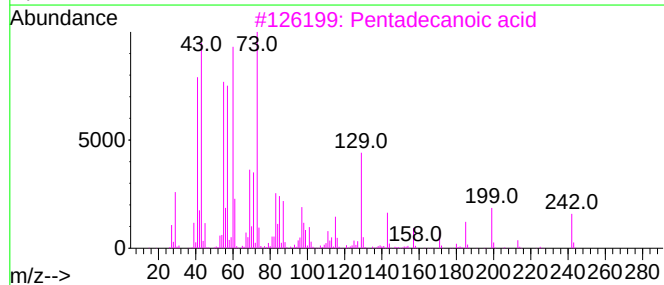
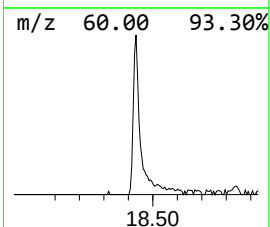
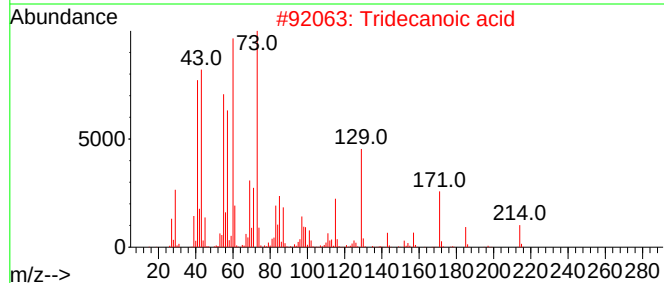
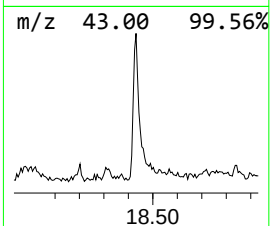
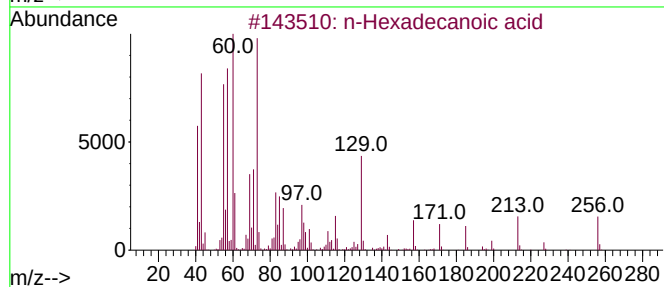
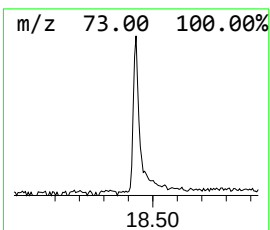
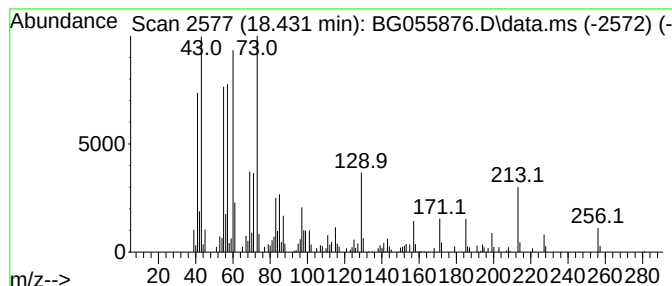
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.431	6.64 ng	183628	Phenanthrene-d10	17.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Dodecanoic acid	200	C12H24O2	000143-07-7	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120222\
Data File : BG055876.D
Acq On : 2 Dec 2022 16:25
Operator : CG/JU
Sample : N5830-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP1-1201

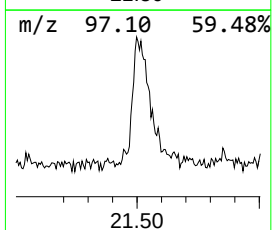
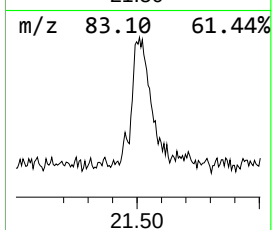
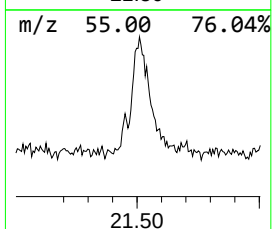
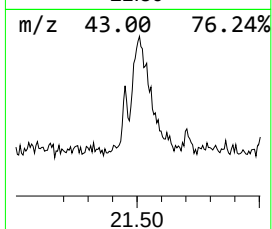
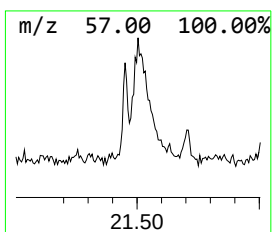
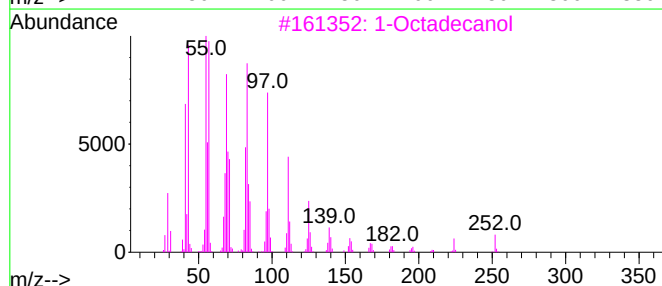
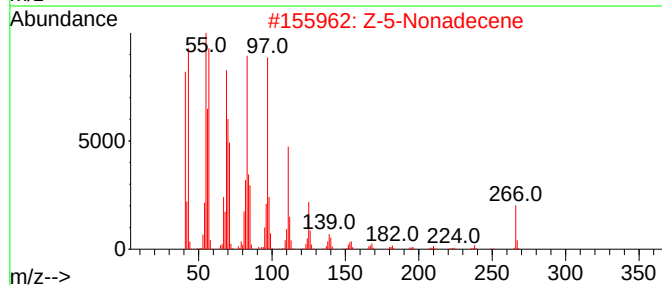
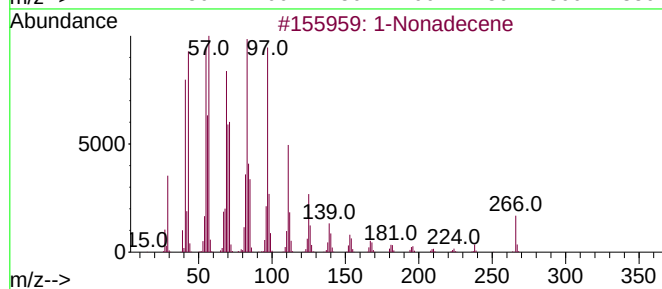
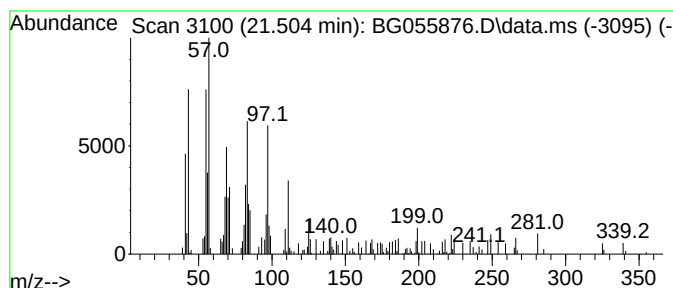
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.504	6.55 ng	195533	Chrysene-d12	21.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	93
2	Z-5-Nonadecene			266	C19H38	1000131-11-8	90
3	1-Octadecanol			270	C18H38O	000112-92-5	89
4	9-Nonadecene			266	C19H38	031035-07-1	89
5	1-Docosanol, methyl ether			340	C23H48O	1000333-91-9	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120222\
Data File : BG055876.D
Acq On : 2 Dec 2022 16:25
Operator : CG/JU
Sample : N5830-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP1-1201

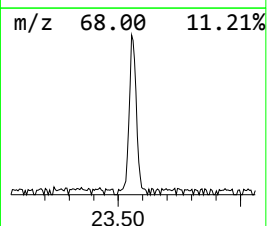
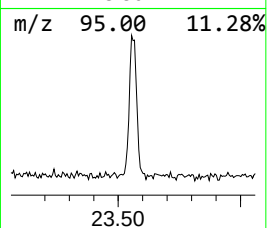
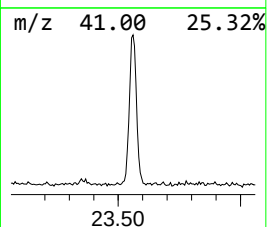
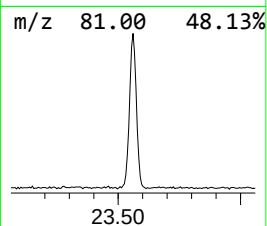
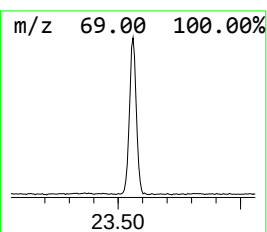
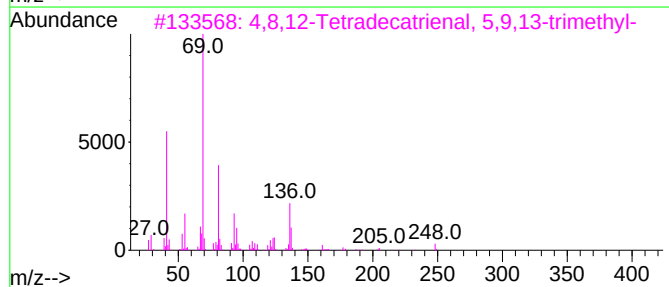
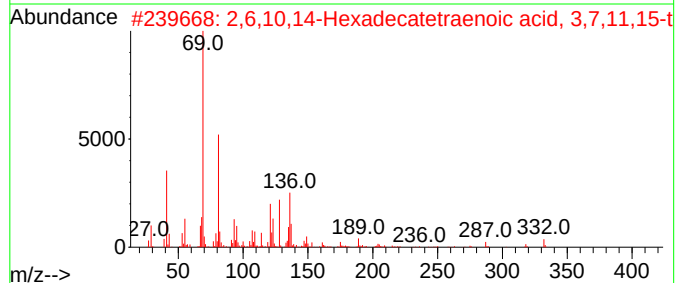
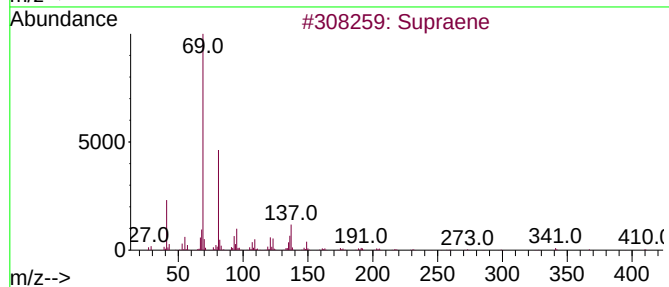
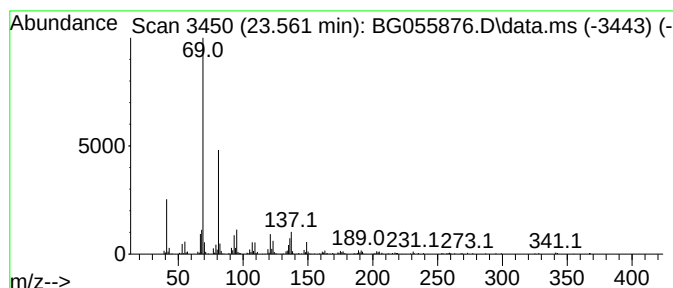
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.561	12.23 ng	394090	Perylene-d12	25.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58
5			5,9-Undecadien-1-yne, 6,10-dimet...	176	C13H20	100451-98-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120222\
Data File : BG055876.D
Acq On : 2 Dec 2022 16:25
Operator : CG/JU
Sample : N5830-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP1-1201

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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-...	5.247	14.2	ng	133815	1	8.202	189000	20.0
Isopropyl myris...	17.444	2.8	ng	76724	4	17.568	553082	20.0
n-Hexadecanoic ...	18.431	6.6	ng	183628	4	17.568	553082	20.0
1-Nonadecene	21.504	6.5	ng	195533	5	21.857	596831	20.0
Supraene	23.561	12.2	ng	394090	6	25.235	644551	20.0