

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
 Data File : BG055446.D
 Acq On : 3 Nov 2022 20:50
 Operator : CG/JU
 Sample : N5306-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20221174-COMP-09-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: BG055446.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.274	333	338	348	rVB	25501	38419	1.88%	0.420%
2	5.762	414	421	436	rBV	247754	405332	19.85%	4.434%
3	7.383	689	697	710	rBV	193675	340343	16.67%	3.723%
4	8.235	835	842	853	rBV	97386	165236	8.09%	1.807%
5	9.410	1034	1042	1053	rBV	323973	566565	27.74%	6.197%
6	10.809	1273	1280	1298	rBV	157678	277001	13.56%	3.030%
7	11.061	1316	1323	1334	rBV	138284	245135	12.00%	2.681%
8	13.476	1727	1734	1741	rBV	936539	1486335	72.78%	16.258%
9	14.851	1960	1968	1976	rVB	254346	380037	18.61%	4.157%
10	16.332	2213	2220	2233	rBV	781122	1202923	58.90%	13.158%
11	17.583	2427	2433	2440	rBV	330186	489743	23.98%	5.357%
12	18.206	2532	2539	2547	rBV	54725	78573	3.85%	0.859%
13	18.435	2573	2578	2587	rBV2	30535	52962	2.59%	0.579%
14	19.363	2732	2736	2740	rVB	70994	78992	3.87%	0.864%
15	20.156	2865	2871	2879	rVB	1566861	2042218	100.00%	22.339%
16	21.461	3087	3093	3110	rBV7	24162	93772	4.59%	1.026%
17	21.854	3153	3160	3168	rBV	333078	561082	27.47%	6.137%
18	23.547	3443	3448	3456	rBV	21573	45568	2.23%	0.498%
19	25.227	3725	3734	3747	rVB2	205030	591846	28.98%	6.474%

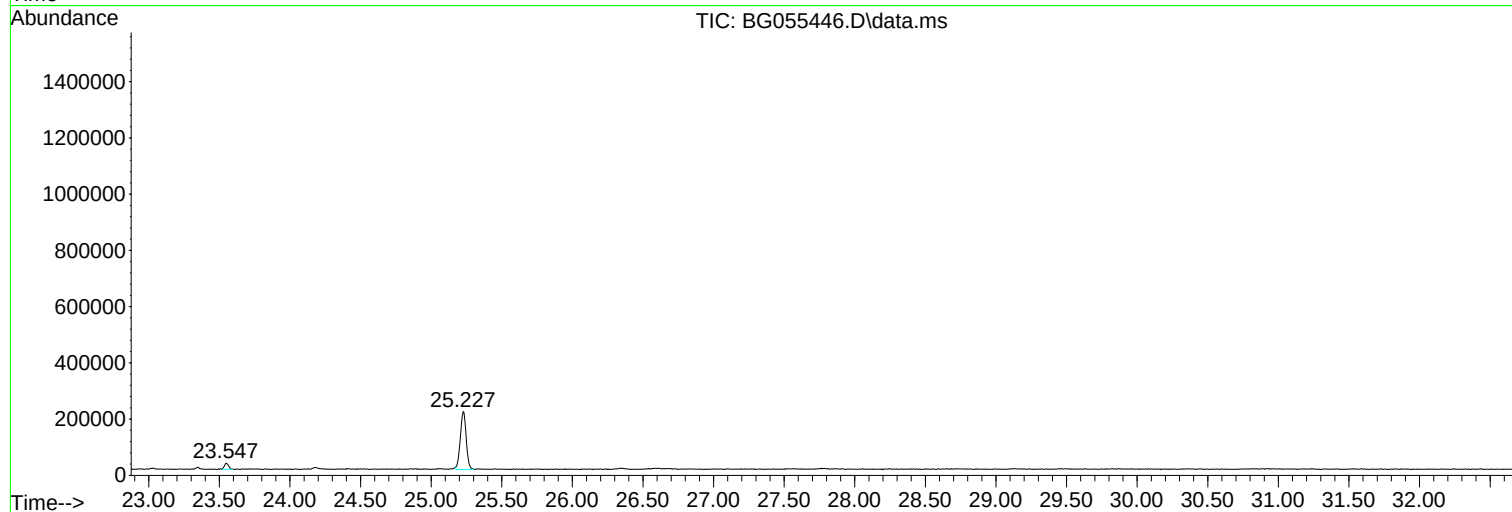
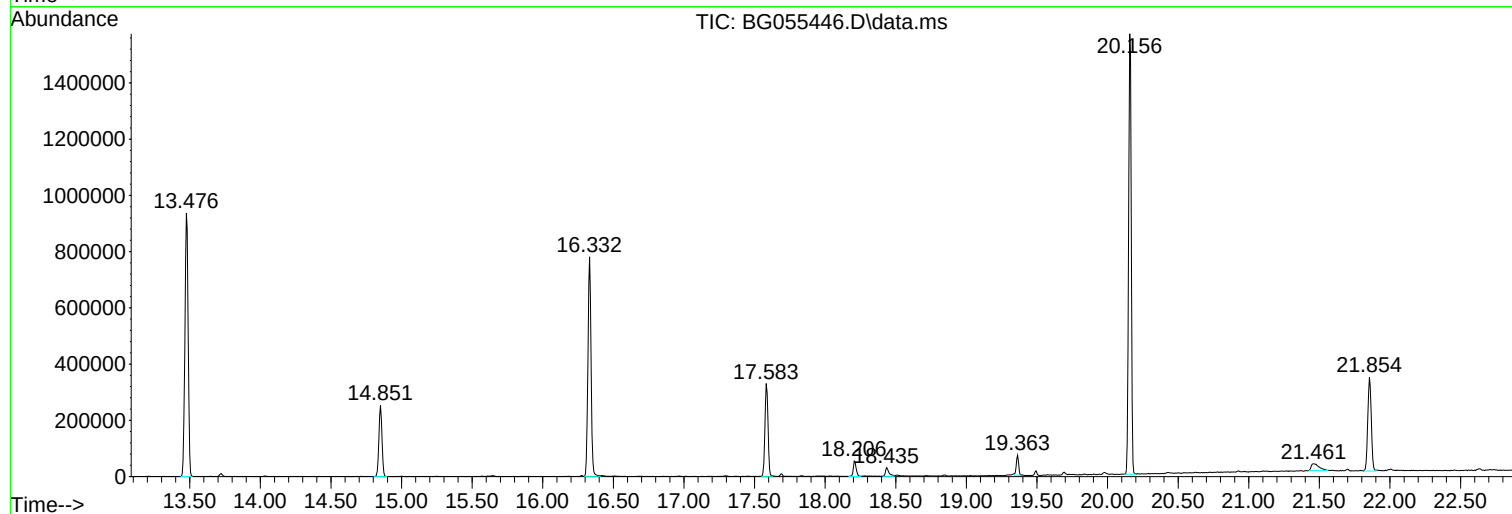
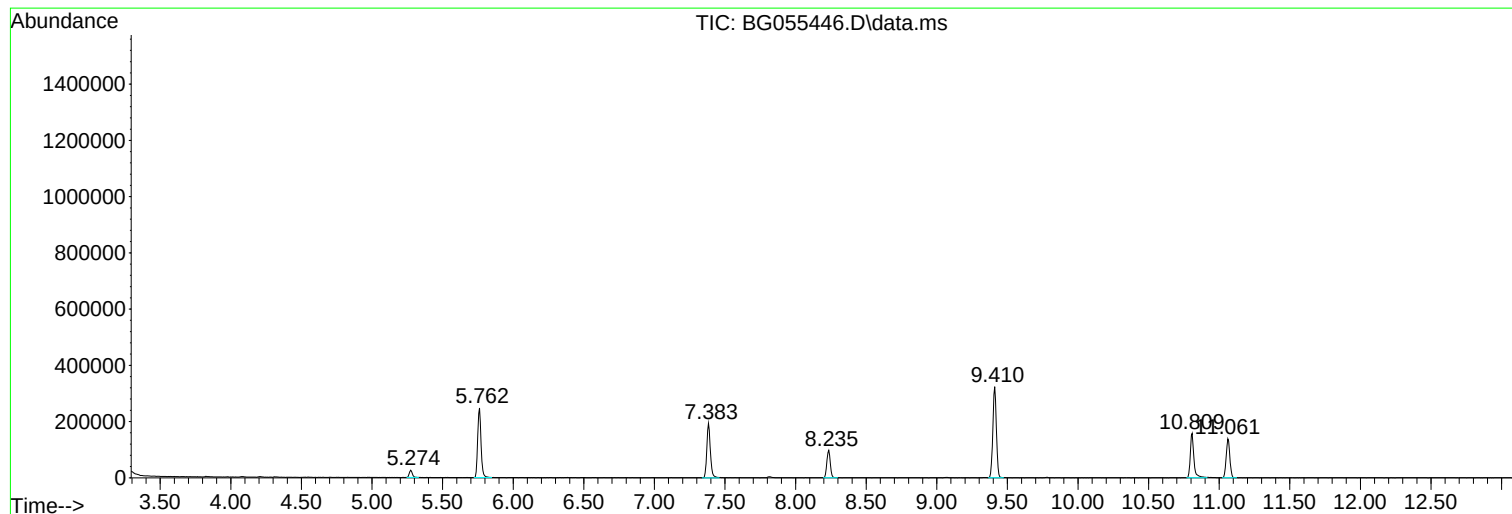
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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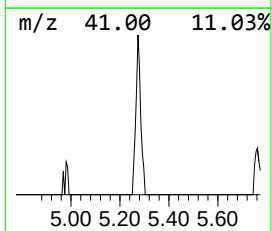
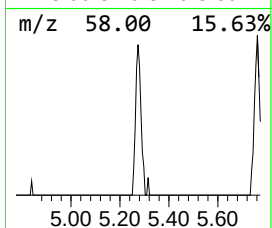
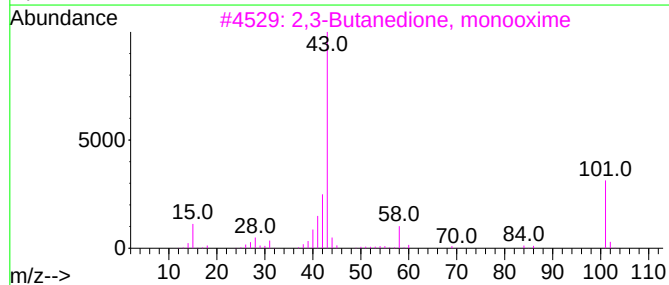
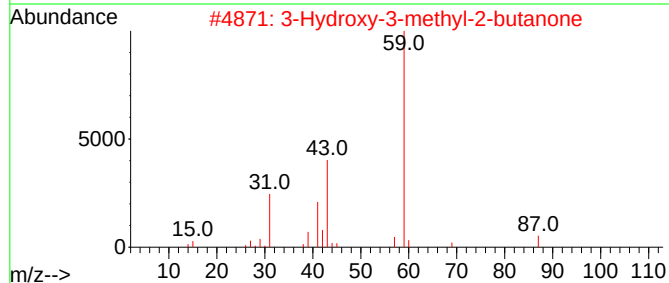
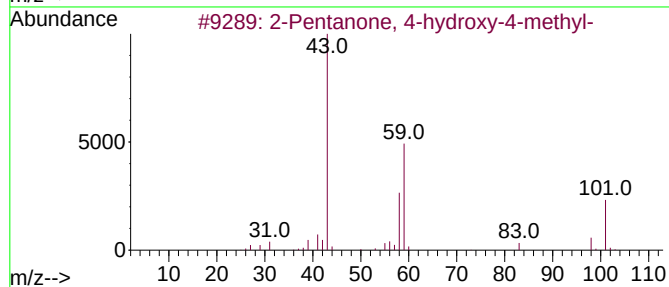
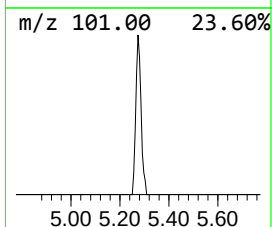
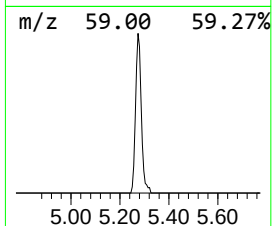
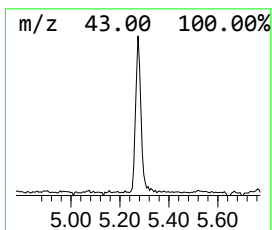
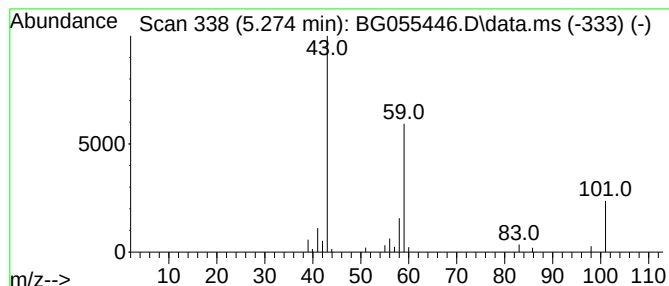
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.274	4.65 ng	38419	1,4-Dichlorobenzene-d4	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	3-Heptanol	116	C7H16O	000589-82-2	9		
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9		



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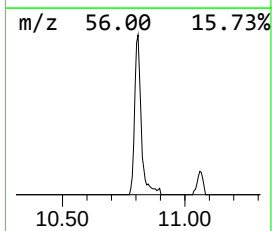
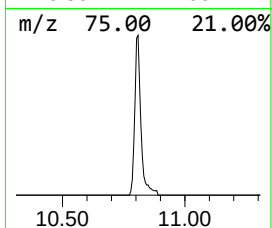
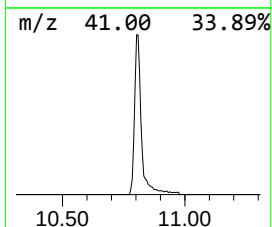
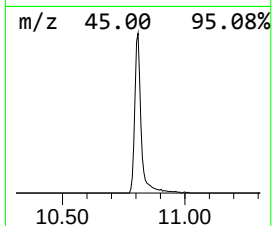
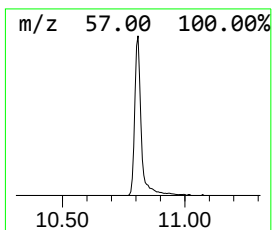
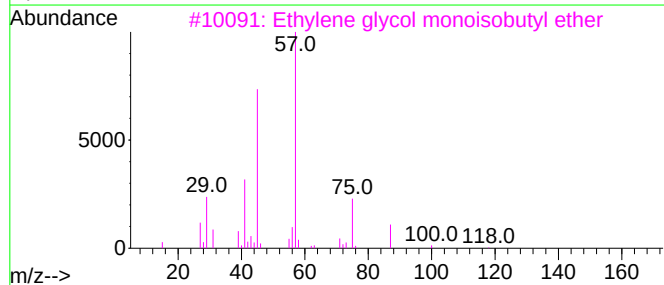
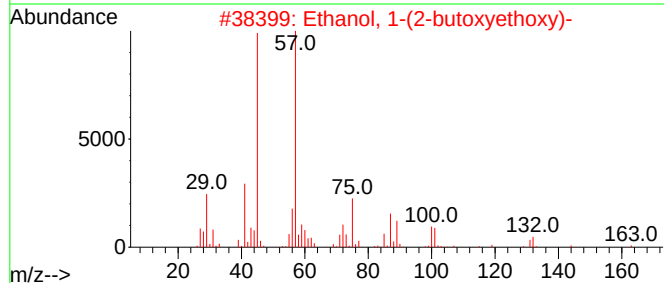
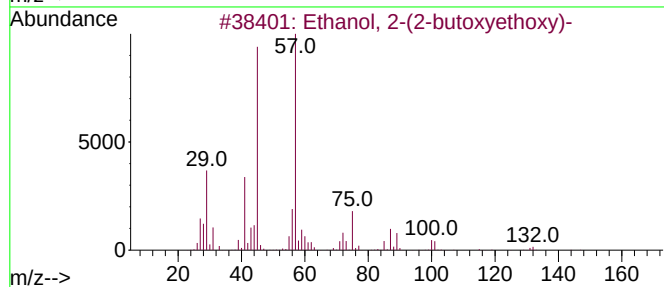
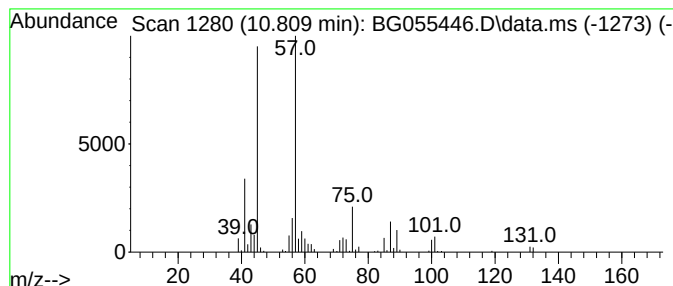
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.809	22.60 ng	277001	Naphthalene-d8	11.061	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	74
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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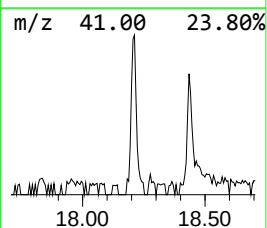
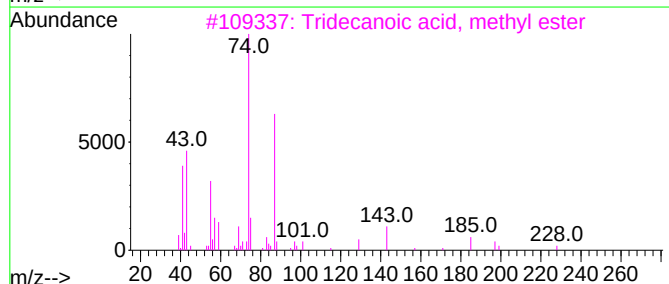
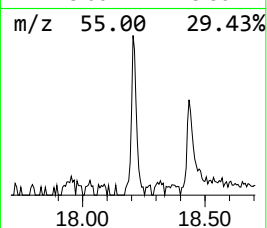
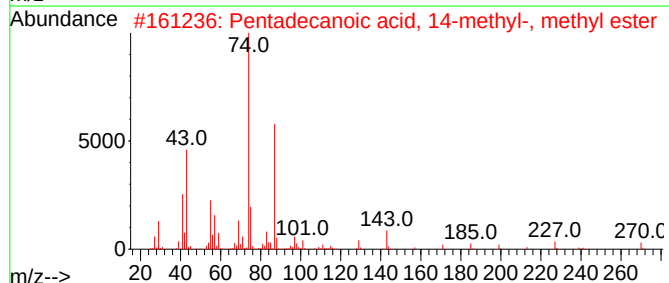
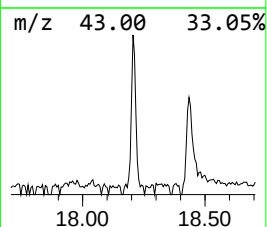
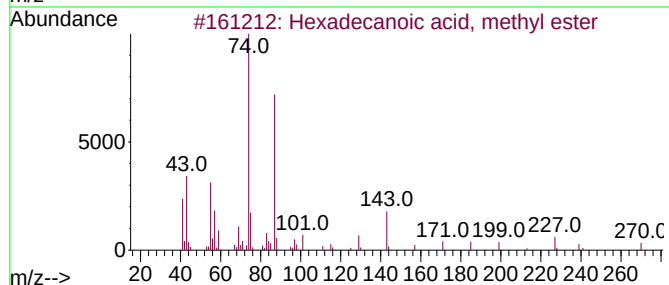
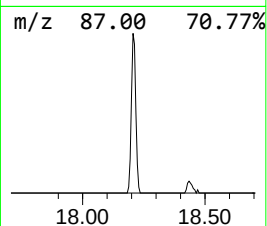
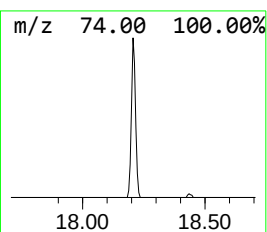
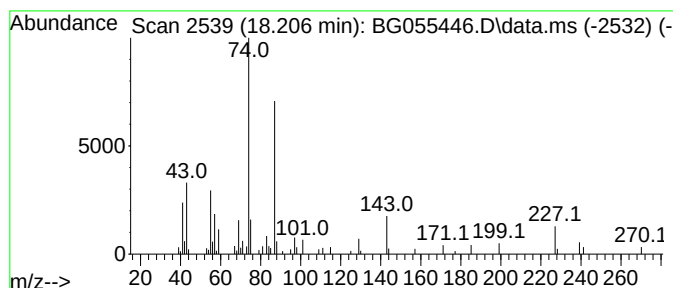
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Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.206	3.21 ng	78573	Phenanthrene-d10	17.583

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5			Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	80



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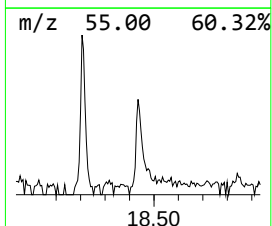
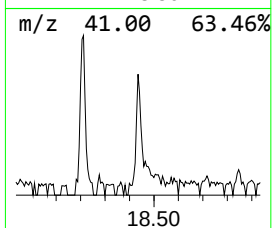
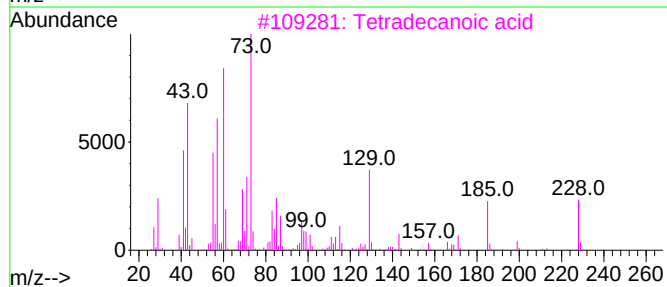
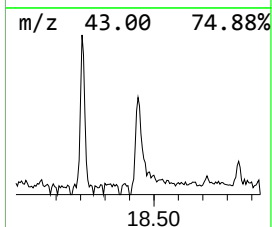
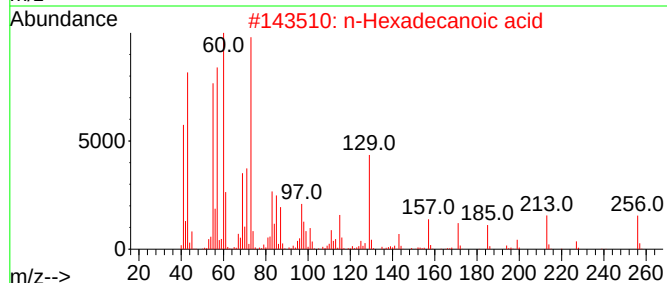
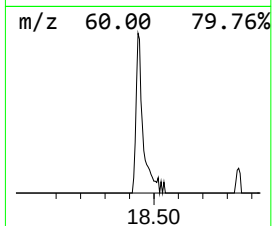
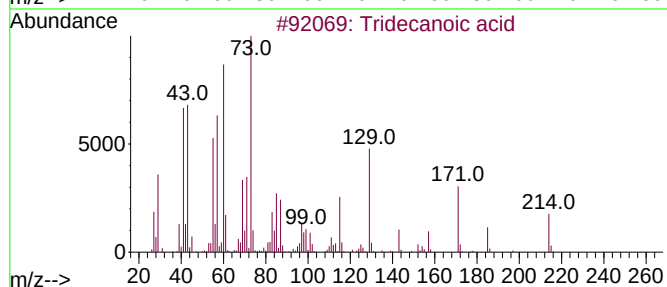
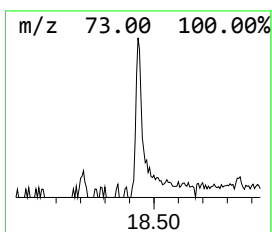
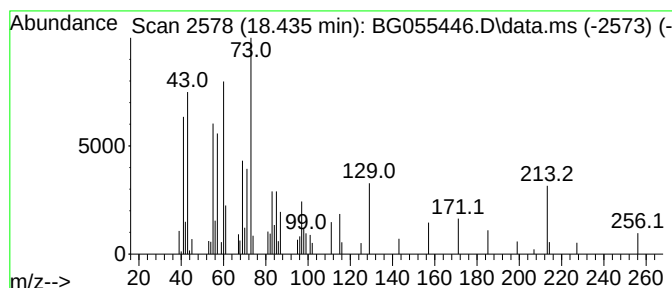
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Peak Number 4 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.435	2.16 ng	52962	Phenanthrene-d10	17.583

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	64



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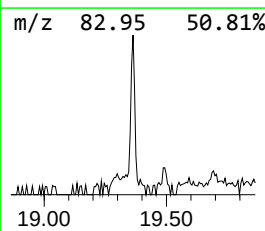
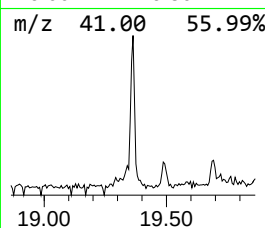
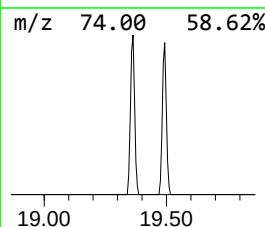
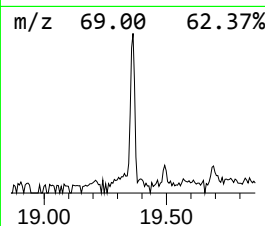
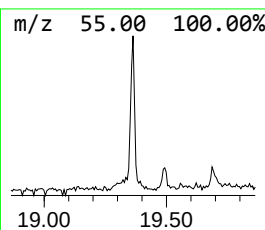
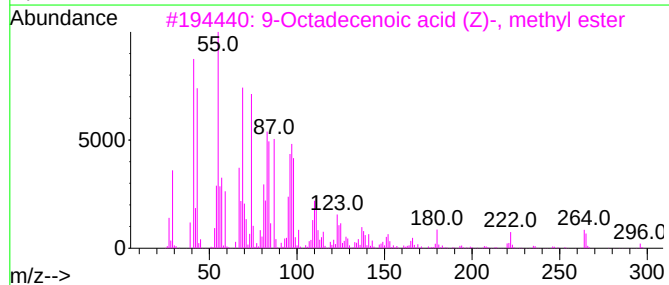
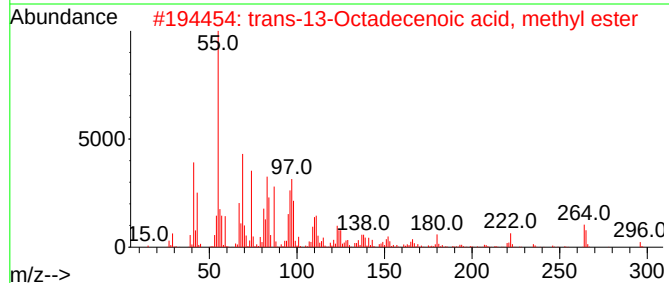
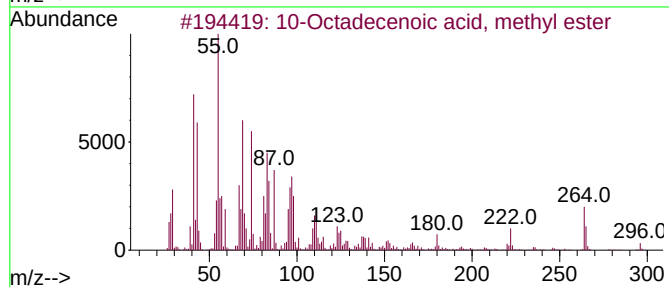
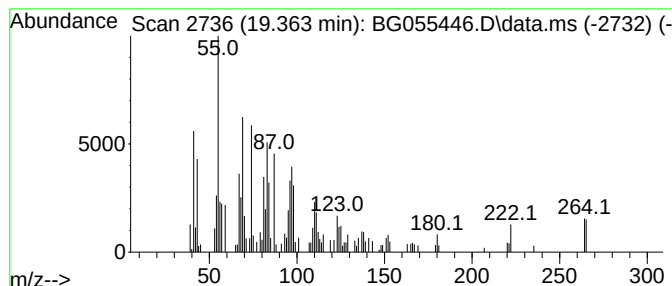
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Peak Number 5 10-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.363	3.23 ng	78992	Phenanthrene-d10	17.583

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
2			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
3			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91
4			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	91
5			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91



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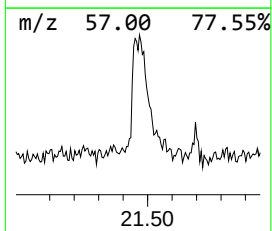
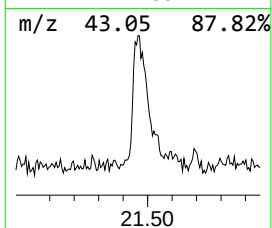
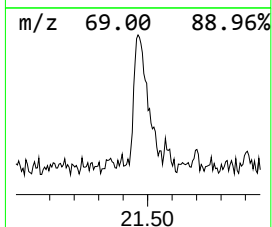
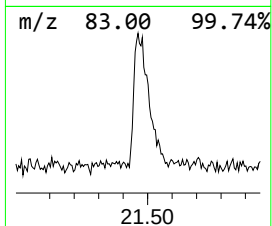
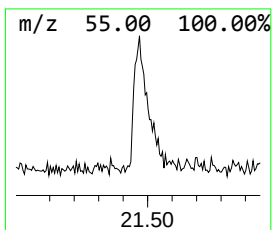
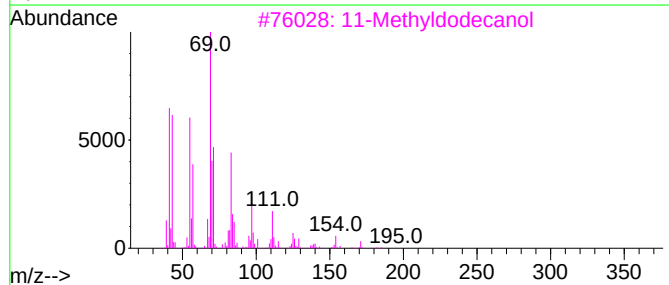
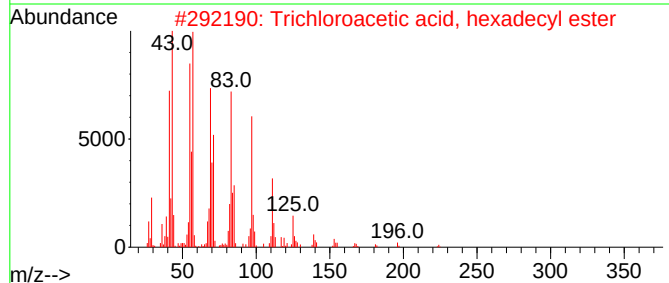
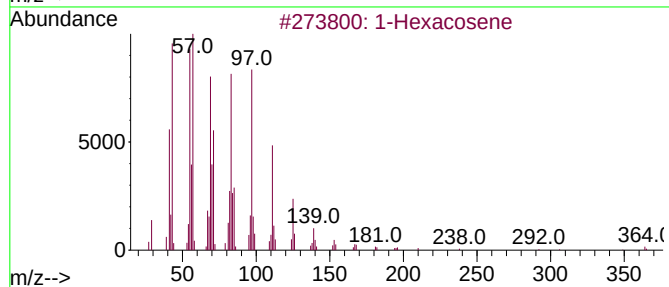
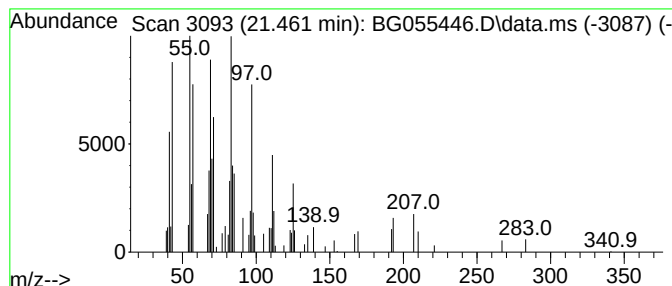
Instrument :
BNA_G
ClientSampleId :
20221174-COMP-09-MODIFIED-ELUTRIATE

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 1-Hexacosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.461	3.34 ng	93772	Chrysene-d12		21.855	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Hexacosene		364	C26H52	018835-33-1	90
2	Trichloroacetic acid, hexadecyl ...		386	C18H33Cl13O2	074339-54-1	87
3	11-Methyldodecanol		200	C13H28O	085763-57-1	87
4	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	87
5	Trichloroacetic acid, pentadecyl...		372	C17H31Cl13O2	074339-53-0	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055446.D
Acq On : 3 Nov 2022 20:50
Operator : CG/JU
Sample : N5306-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221174-COMP-09-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-...	5.274	4.7	ng	38419	1	8.235	165236	20.0
Ethanol, 2-(2-b...	10.809	22.6	ng	277001	2	11.061	245135	20.0
Hexadecanoic ac...	18.206	3.2	ng	78573	4	17.583	489743	20.0
Tridecanoic acid	18.435	2.2	ng	52962	4	17.583	489743	20.0
10-Octadecenoic...	19.363	3.2	ng	78992	4	17.583	489743	20.0
1-Hexacosene	21.461	3.3	ng	93772	5	21.855	561082	20.0