

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
 Data File : BG055443.D
 Acq On : 3 Nov 2022 18:44
 Operator : CG/JU
 Sample : N5306-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20221167-COMP-02-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: BG055443.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	332	338	350	rBV	23511	39994	2.05%	0.447%
2	5.762	415	421	439	rBV	228248	400482	20.48%	4.480%
3	7.384	690	697	711	rBV	174108	315201	16.12%	3.526%
4	8.236	835	842	853	rVB	99088	168458	8.61%	1.885%
5	9.411	1033	1042	1056	rBV	288717	517866	26.48%	5.794%
6	10.809	1273	1280	1298	rBV	163250	290983	14.88%	3.255%
7	11.062	1315	1323	1333	rBV	135554	242220	12.39%	2.710%
8	13.477	1726	1734	1746	rBV	866775	1330692	68.05%	14.887%
9	13.723	1768	1776	1786	rBV	60192	92241	4.72%	1.032%
10	14.851	1960	1968	1977	rVB	241725	369007	18.87%	4.128%
11	16.332	2213	2220	2233	rBV	687586	1061797	54.30%	11.879%
12	17.584	2427	2433	2439	rBV	321904	479282	24.51%	5.362%
13	18.212	2535	2540	2547	rBV2	45144	70719	3.62%	0.791%
14	18.435	2574	2578	2587	rBV2	40626	67900	3.47%	0.760%
15	19.364	2732	2736	2740	rVB	103222	116592	5.96%	1.304%
16	19.493	2750	2758	2763	rBV	42845	49091	2.51%	0.549%
17	20.157	2865	2871	2877	rBV	1533361	1955431	100.00%	21.877%
18	20.433	2911	2918	2921	rBV7	11192	23220	1.19%	0.260%
19	20.768	2972	2975	2981	rVB3	31469	37142	1.90%	0.416%
20	21.455	3087	3092	3106	rBV7	32663	112686	5.76%	1.261%
21	21.696	3130	3133	3138	rVB2	18663	24787	1.27%	0.277%
22	21.855	3153	3160	3167	rBV	346199	554741	28.37%	6.206%
23	23.547	3444	3448	3455	rVB2	21089	42274	2.16%	0.473%
24	25.227	3724	3734	3748	rVB2	191085	575587	29.44%	6.439%

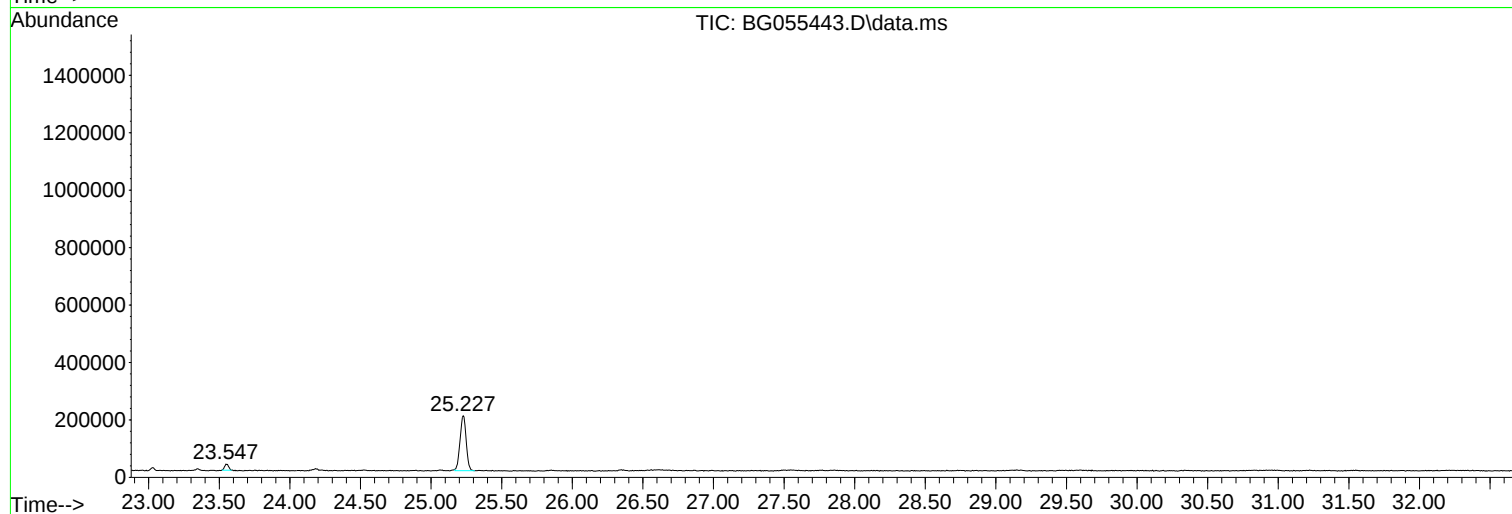
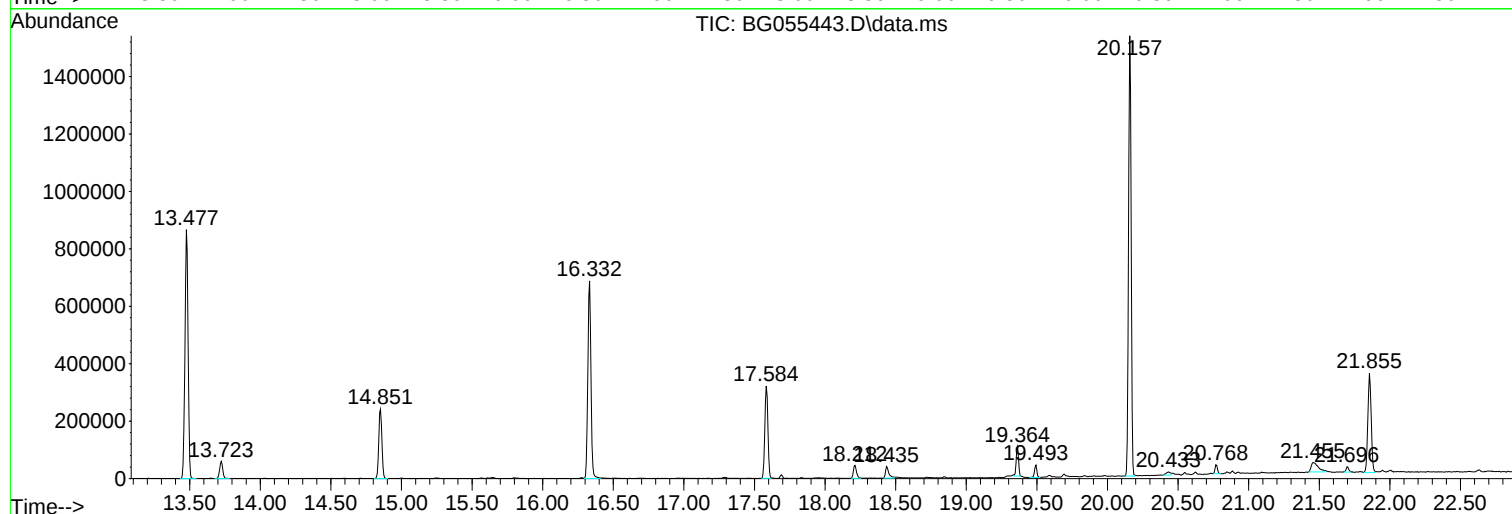
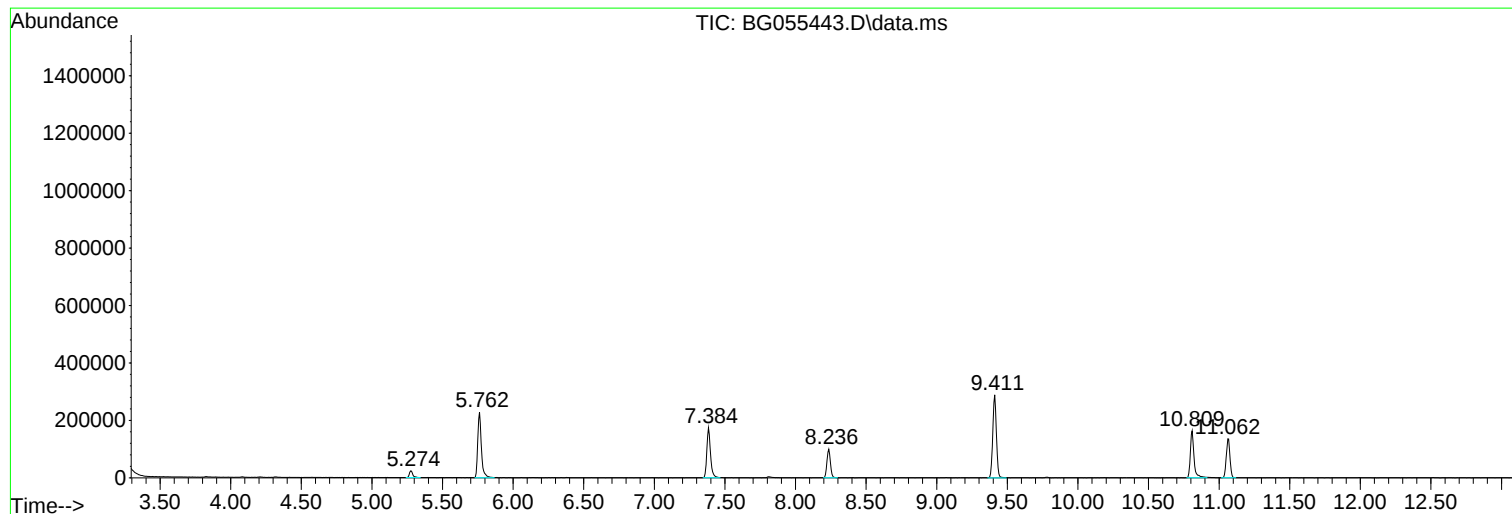
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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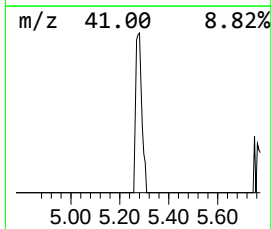
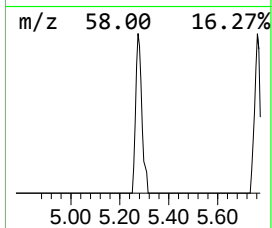
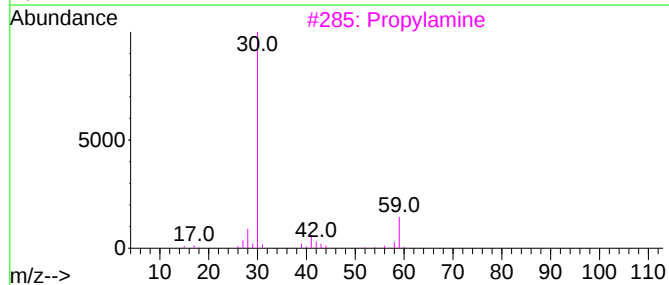
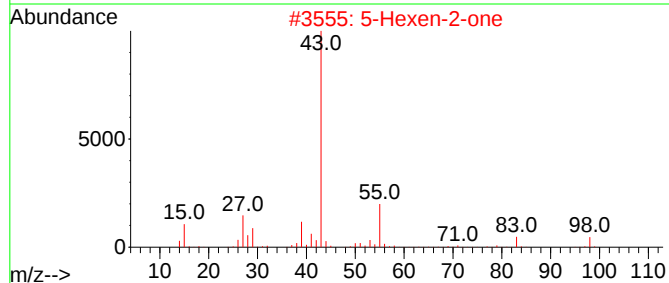
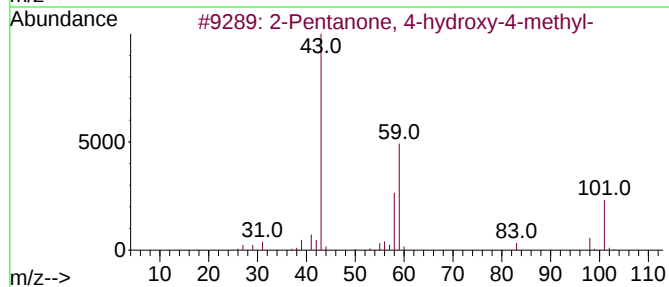
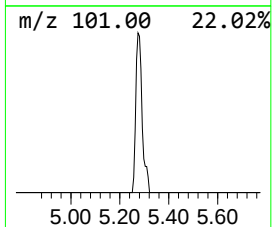
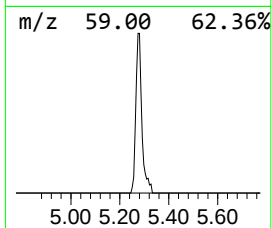
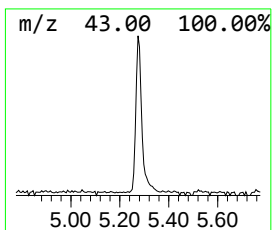
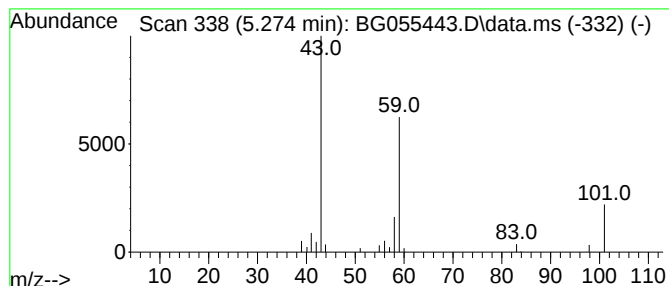
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.274	4.75 ng	39994	1,4-Dichlorobenzene-d4	8.236

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		5-Hexen-2-one	98	C6H10O	000109-49-9	12
3		Propylamine	59	C3H9N	000107-10-8	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9



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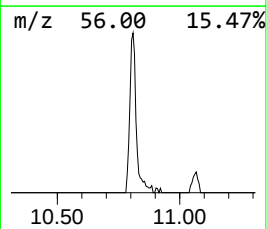
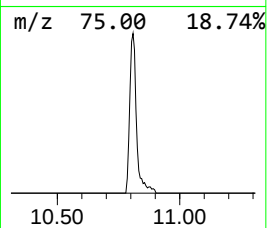
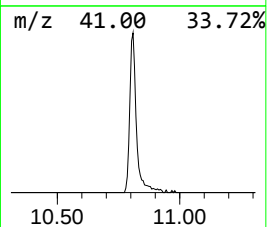
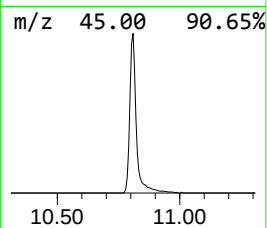
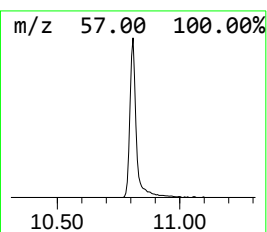
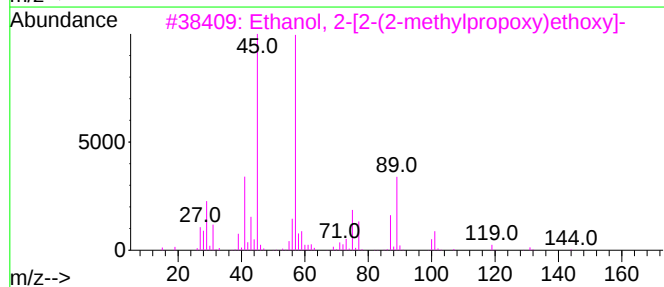
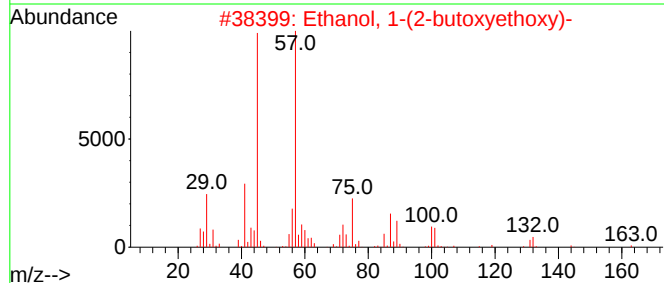
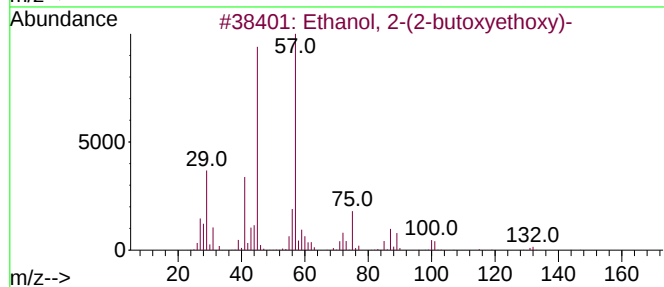
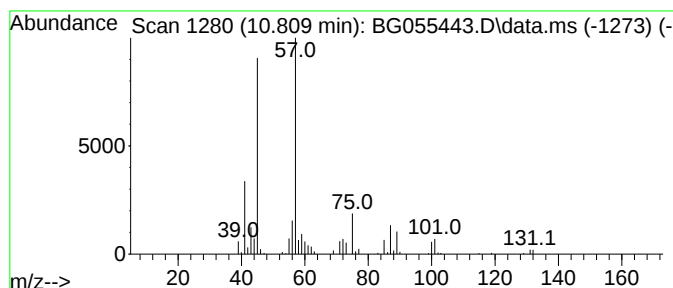
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.809	24.03 ng	290983	Naphthalene-d8	11.062	
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	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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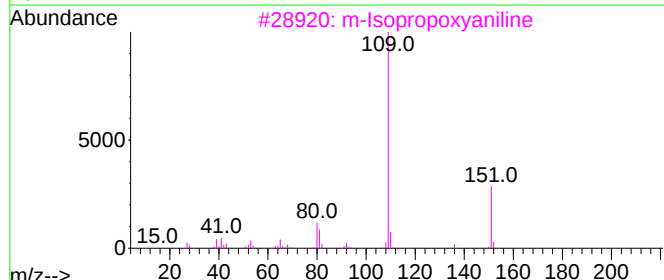
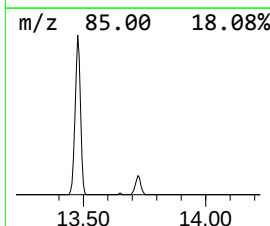
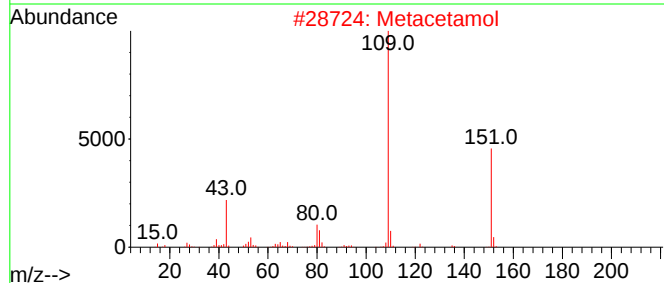
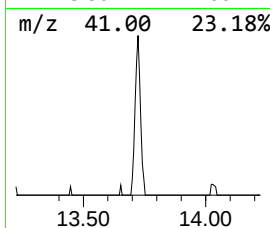
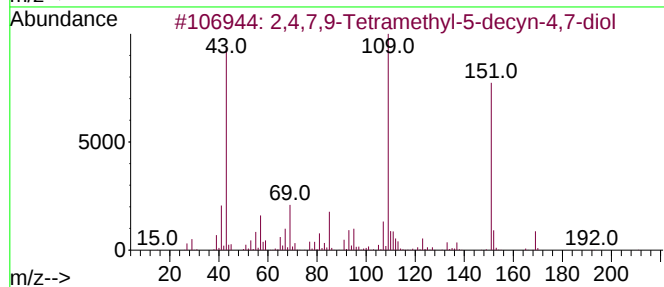
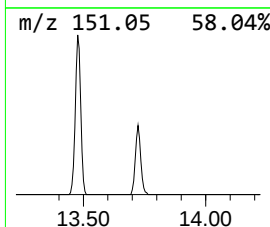
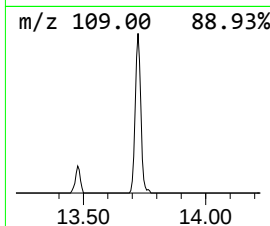
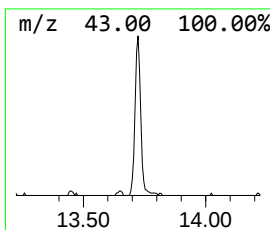
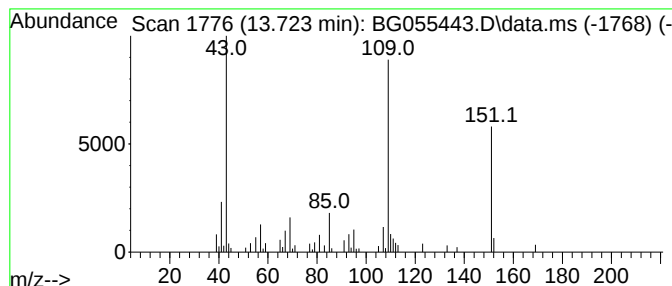
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.723	5.00 ng	92241	Acenaphthene-d10	14.851

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91	
2	Metacetamol	151	C8H9NO2	000621-42-1	64	
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	64	
4	Acetaminophen	151	C8H9NO2	000103-90-2	59	
5	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59	



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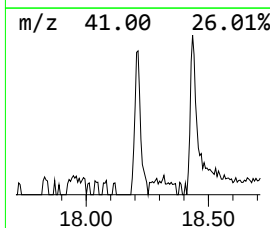
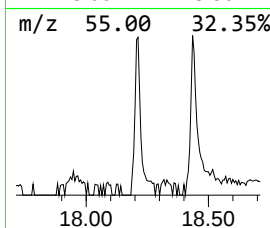
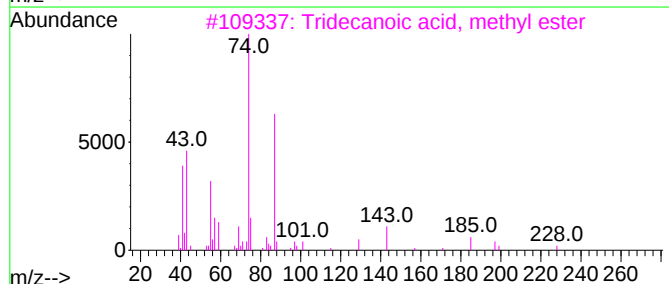
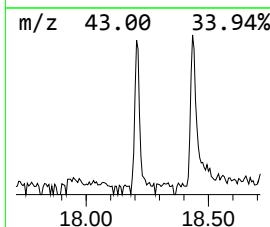
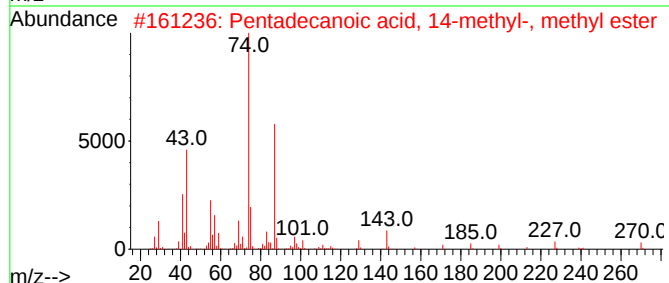
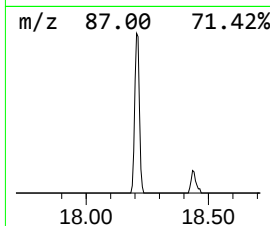
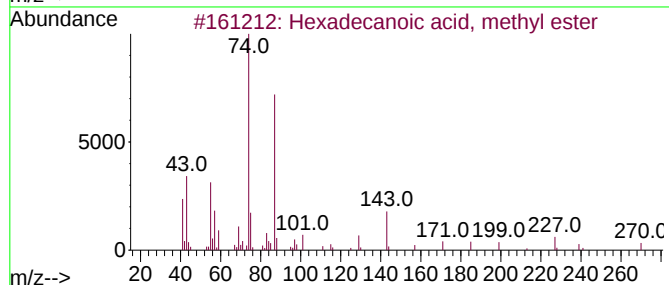
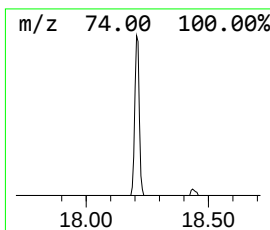
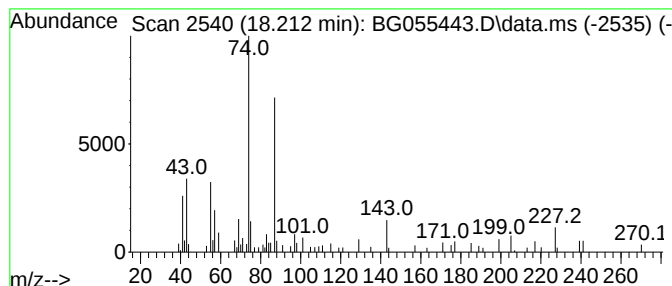
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Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.212	2.95 ng	70719	Phenanthrene-d10	17.584

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	89
4			Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	74
5			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	74



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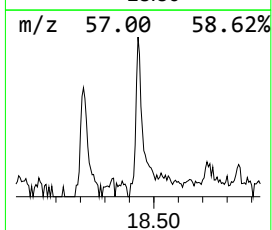
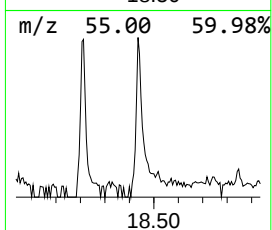
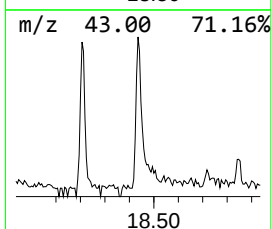
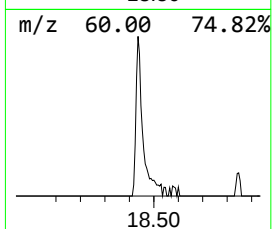
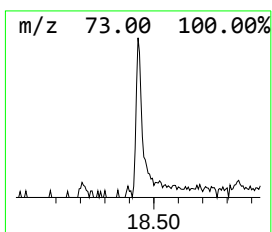
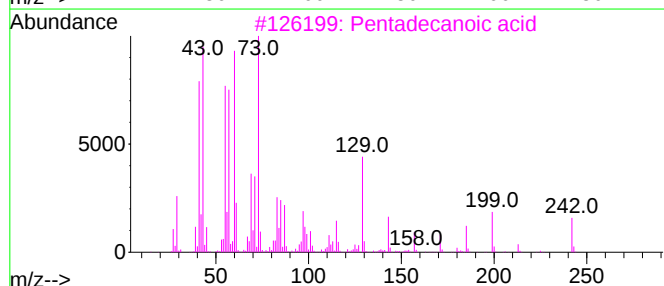
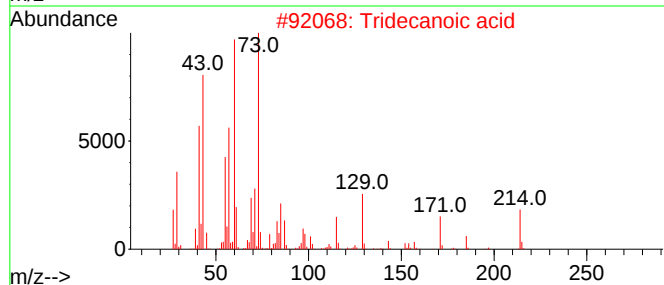
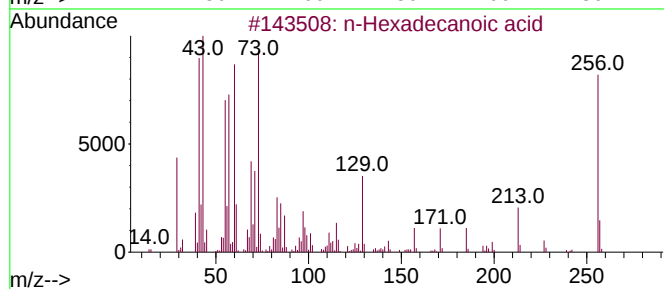
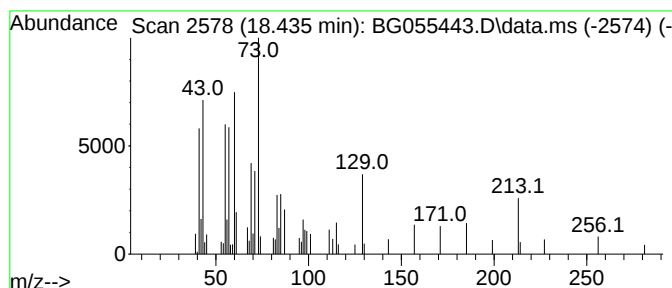
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.435	2.83 ng	67900	Phenanthrene-d10	17.584

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	59



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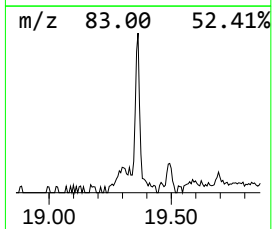
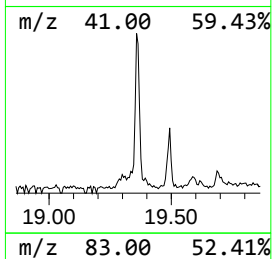
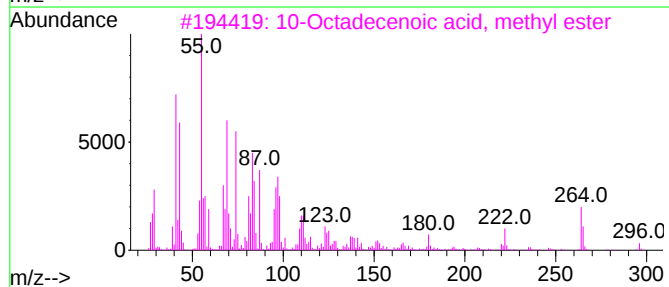
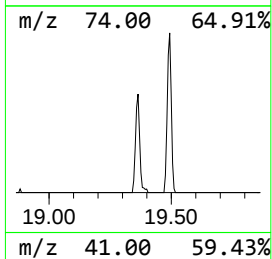
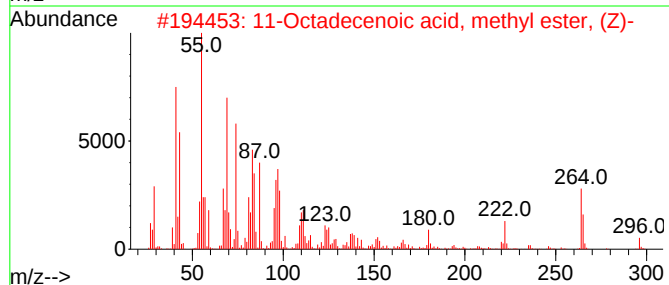
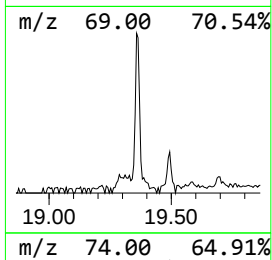
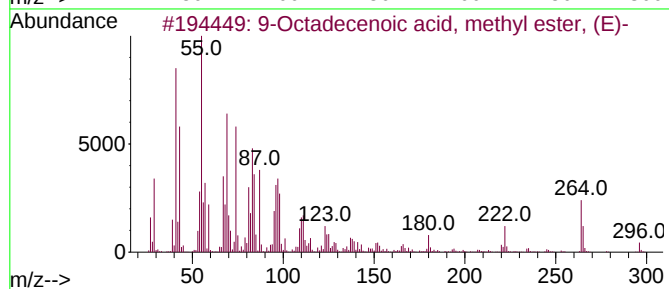
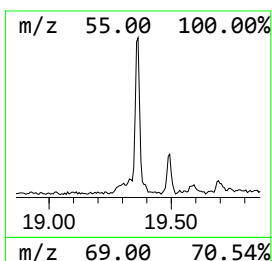
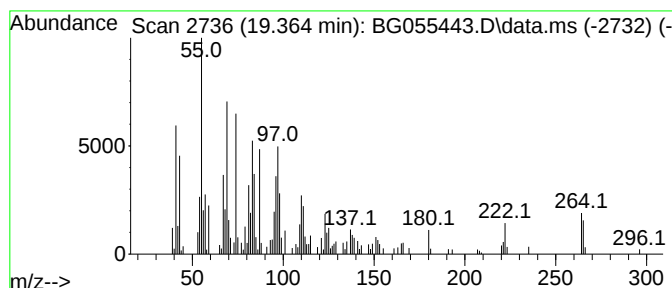
Instrument :
BNA_G
ClientSampleId :
20221167-COMP-02-MODIFIED-ELUTRIATE

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 9-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.364	4.87 ng	116592	Phenanthrene-d10	17.584	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
2	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055443.D
Acq On : 3 Nov 2022 18:44
Operator : CG/JU
Sample : N5306-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221167-COMP-02-MODIFIED-ELUTRIATE

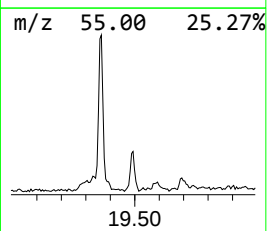
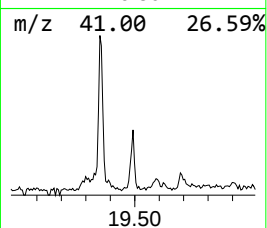
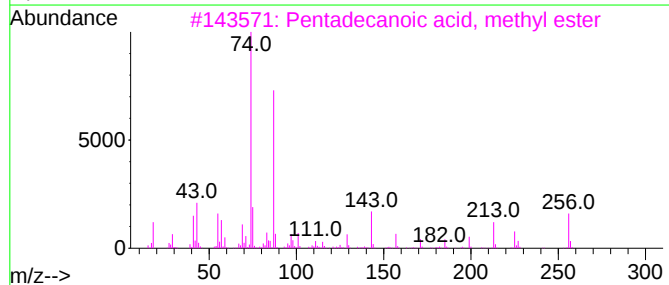
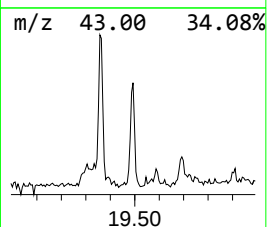
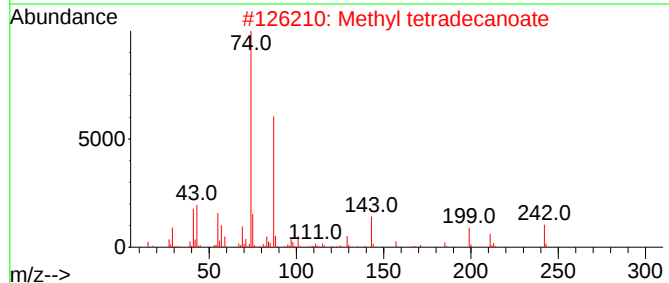
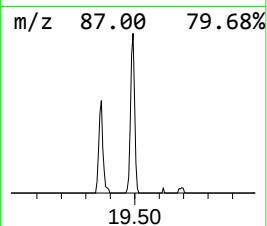
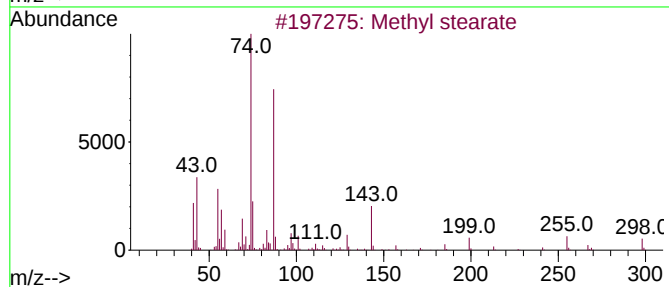
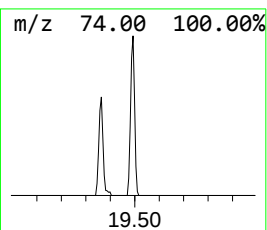
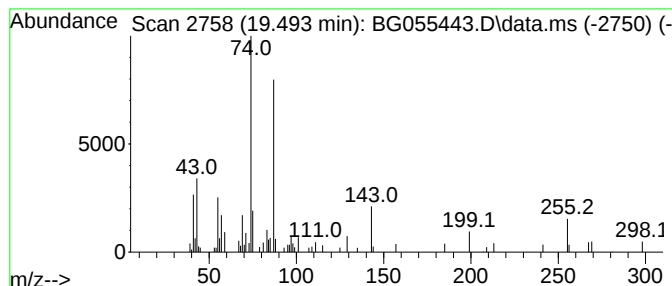
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Methyl stearate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.493	2.05 ng	49091	Phenanthrene-d10	17.584

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	97
2			Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	80
5			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055443.D
Acq On : 3 Nov 2022 18:44
Operator : CG/JU
Sample : N5306-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221167-COMP-02-MODIFIED-ELUTRIATE

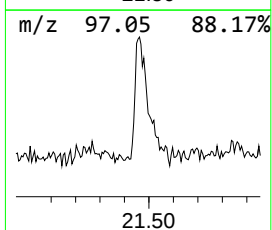
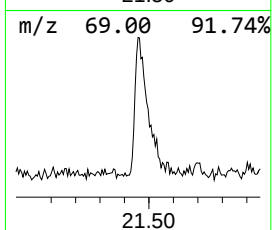
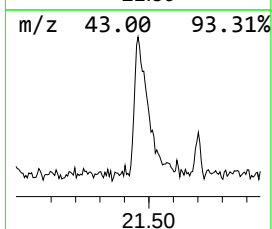
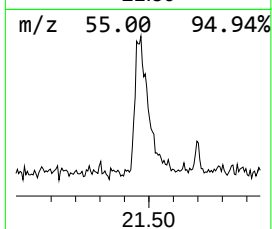
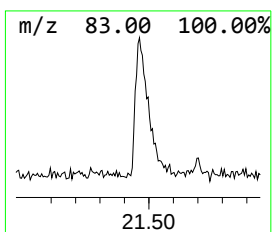
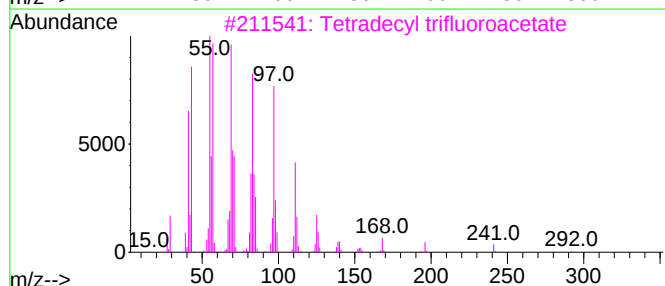
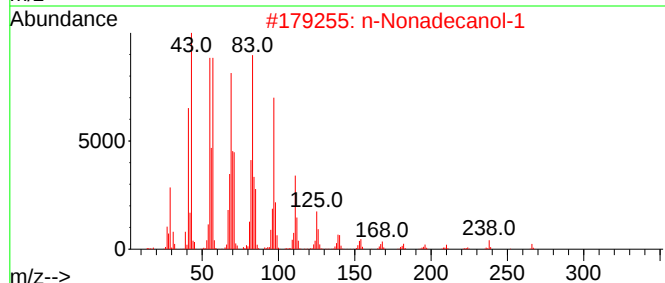
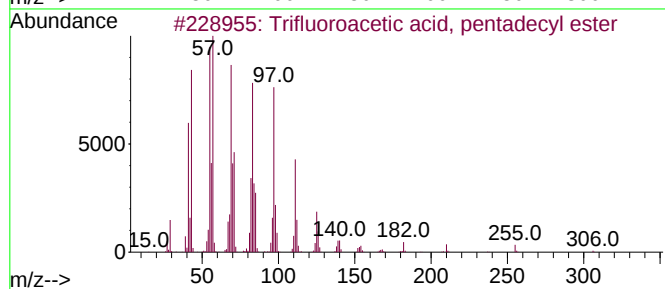
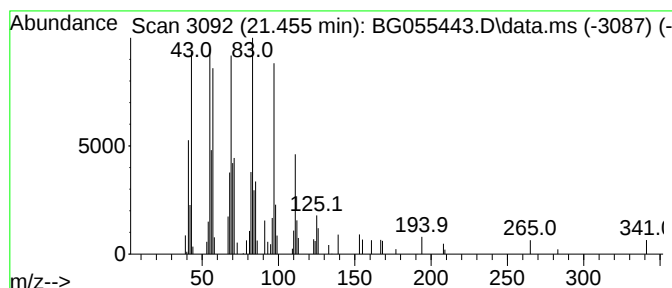
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trifluoroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.455	4.06 ng	112686	Chrysene-d12	21.855

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	95
4			n-Heptadecanol-1	256	C17H36O	001454-85-9	94
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055443.D
Acq On : 3 Nov 2022 18:44
Operator : CG/JU
Sample : N5306-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221167-COMP-02-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	4.8	ng	39994	1	8.236	168458	20.0
Ethanol, 2-(2-b...	10.809	24.0	ng	290983	2	11.062	242220	20.0
2,4,7,9-Tetrame...	13.723	5.0	ng	92241	3	14.851	369007	20.0
Hexadecanoic ac...	18.212	3.0	ng	70719	4	17.584	479282	20.0
n-Hexadecanoic ...	18.435	2.8	ng	67900	4	17.584	479282	20.0
9-Octadecenoic ...	19.364	4.9	ng	116592	4	17.584	479282	20.0
Methyl stearate	19.493	2.0	ng	49091	4	17.584	479282	20.0
Trifluoroacetic...	21.455	4.1	ng	112686	5	21.855	554741	20.0