

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
 Data File : BG055581.D
 Acq On : 12 Nov 2022 1:09
 Operator : CG/JU
 Sample : N5530-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-13

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-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055581.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.330	3	7	12	rBV	155454	231068	7.45%	1.304%
2	5.328	341	347	359	rBV	221510	353701	11.41%	1.996%
3	5.804	420	428	447	rBV	956086	1612119	52.01%	9.098%
4	7.408	692	701	718	rBV	986673	1758409	56.73%	9.924%
5	8.271	842	848	861	rBV	216034	388140	12.52%	2.191%
6	9.446	1039	1048	1057	rBV	593301	1072208	34.59%	6.051%
7	10.851	1280	1287	1296	rBV	53888	92191	2.97%	0.520%
8	11.103	1323	1330	1338	rVB	319605	558509	18.02%	3.152%
9	13.518	1733	1741	1748	rBV	1604720	2497723	80.58%	14.097%
10	14.511	1905	1910	1918	rBV3	19353	32551	1.05%	0.184%
11	14.893	1967	1975	1982	rVB	497848	792733	25.58%	4.474%
12	16.374	2220	2227	2236	rBV	1324852	2053501	66.25%	11.590%
13	17.631	2434	2441	2447	rBV	591803	906428	29.24%	5.116%
14	18.489	2583	2587	2594	rBV	133050	199388	6.43%	1.125%
15	19.752	2798	2802	2807	rBV2	66474	98252	3.17%	0.555%
16	20.216	2876	2881	2887	rVB	2330584	3099603	100.00%	17.494%
17	21.538	3102	3106	3113	rBV2	104339	169341	5.46%	0.956%
18	21.932	3168	3173	3181	rVB2	509461	865836	27.93%	4.887%
19	25.363	3750	3757	3777	rVB3	261616	936860	30.23%	5.287%

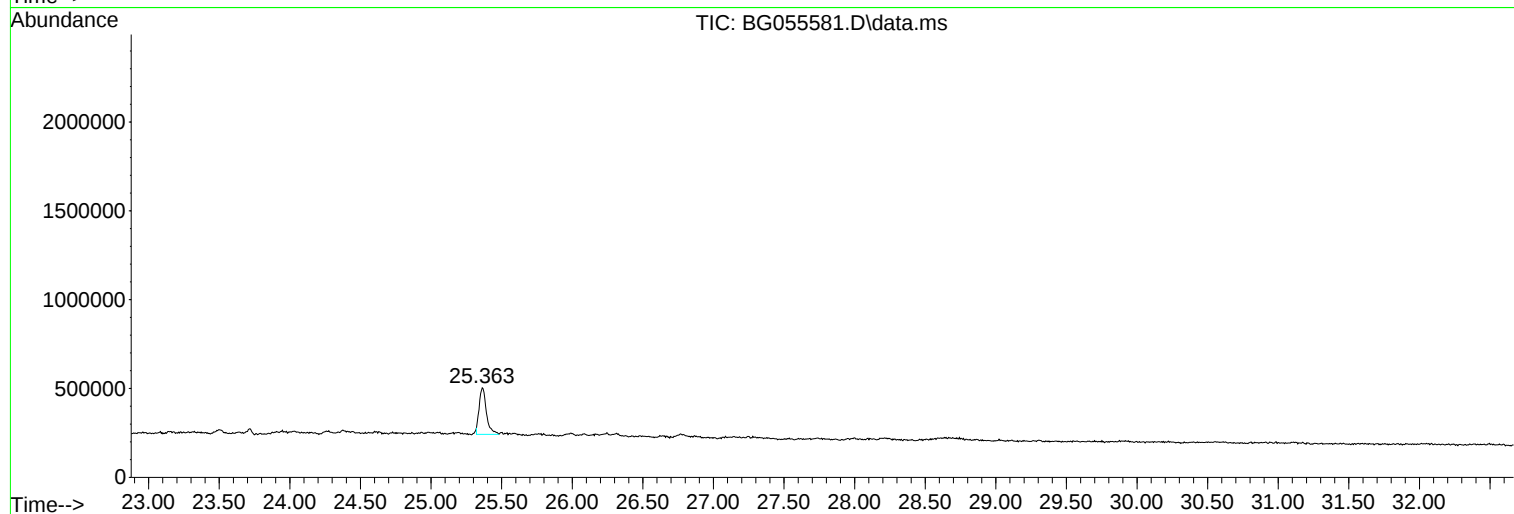
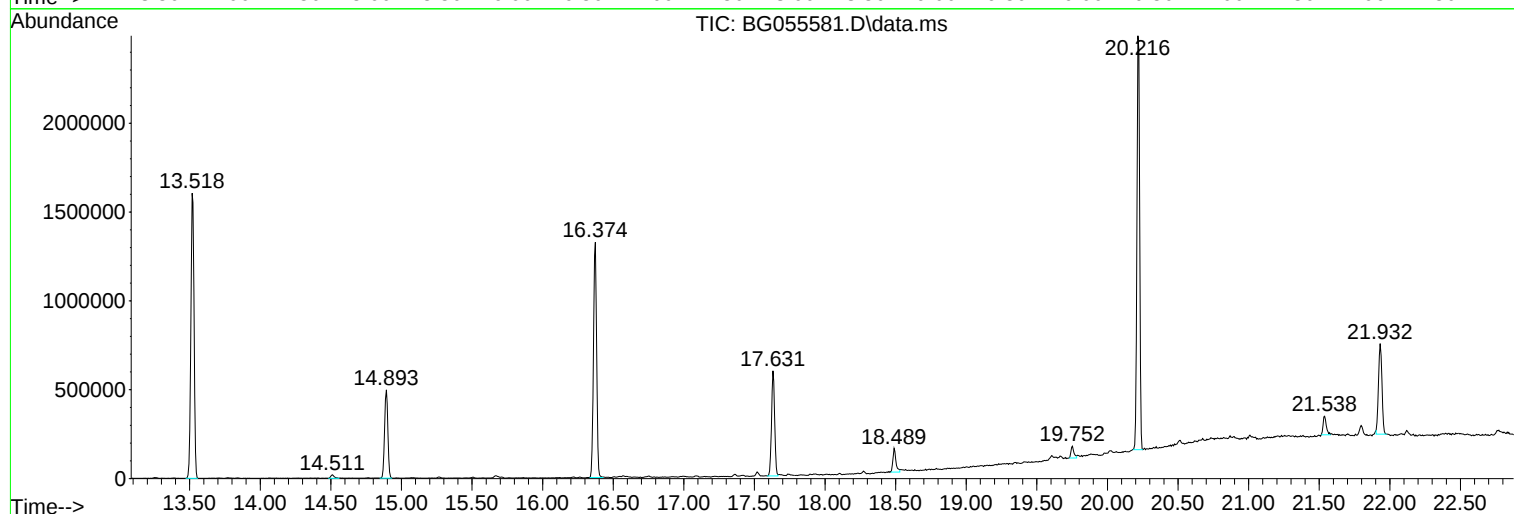
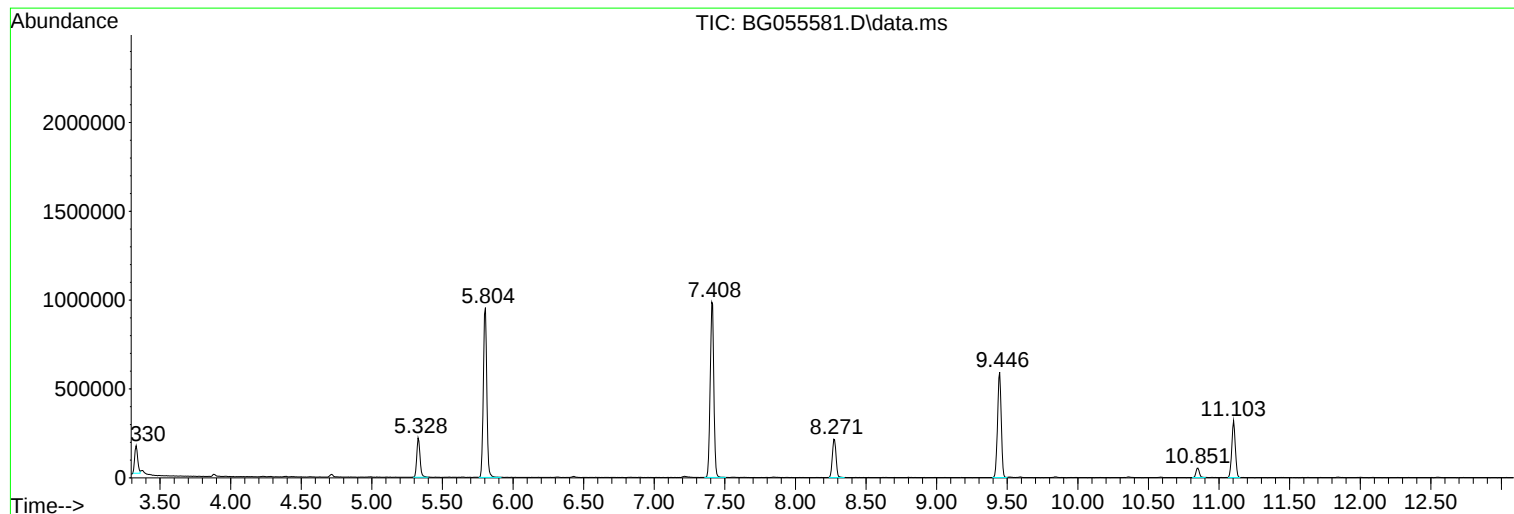
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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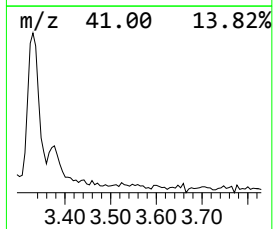
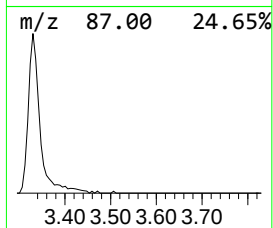
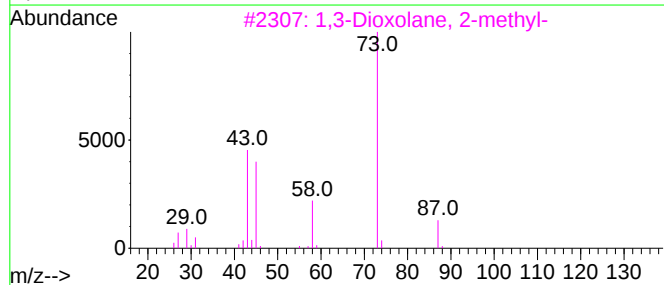
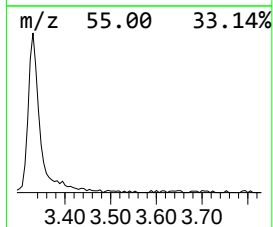
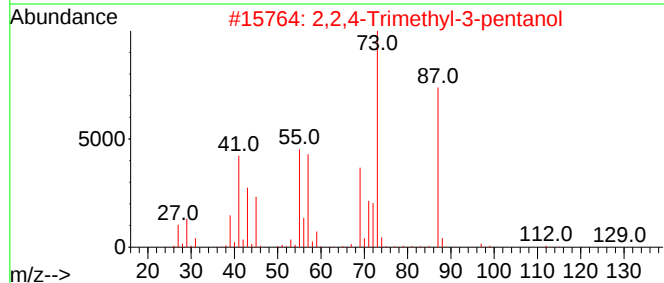
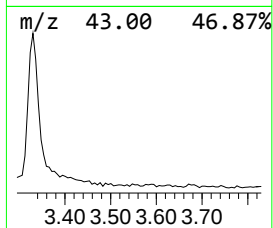
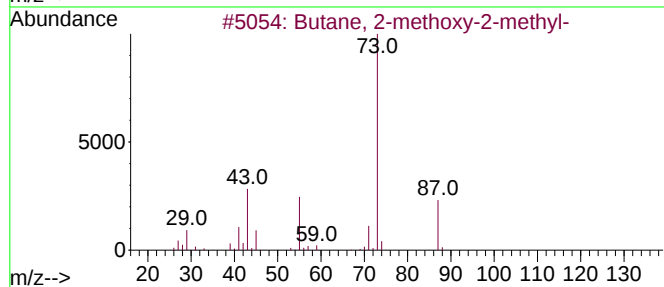
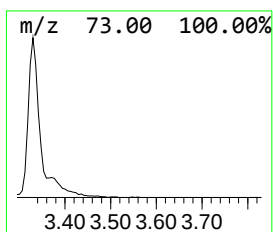
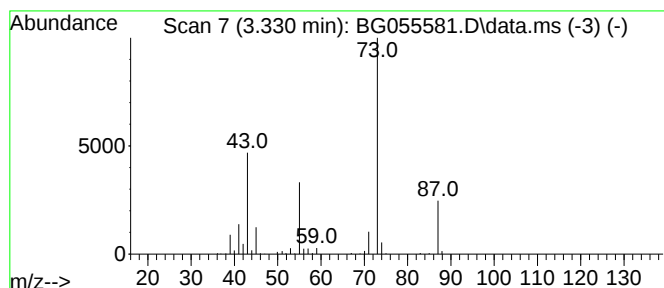
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.330	11.91 ng	231068	1,4-Dichlorobenzene-d4	8.271

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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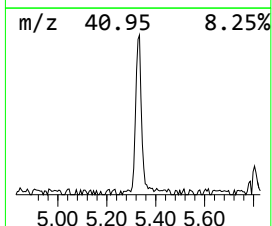
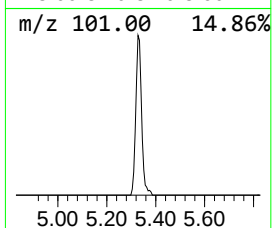
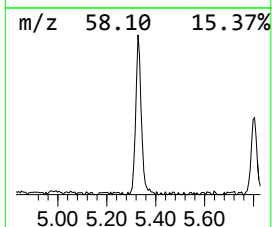
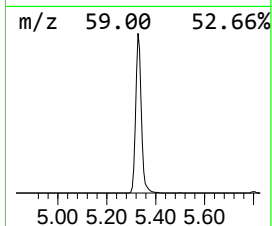
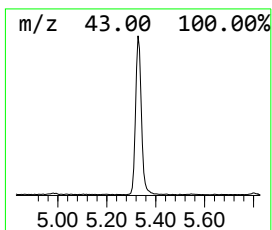
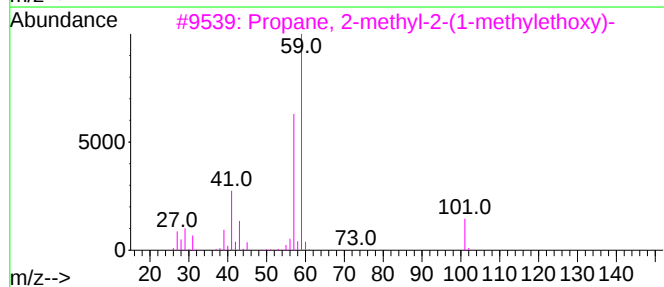
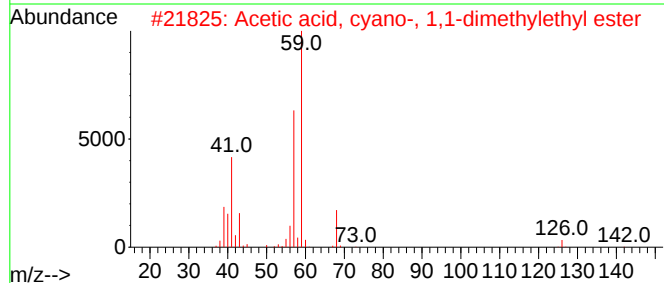
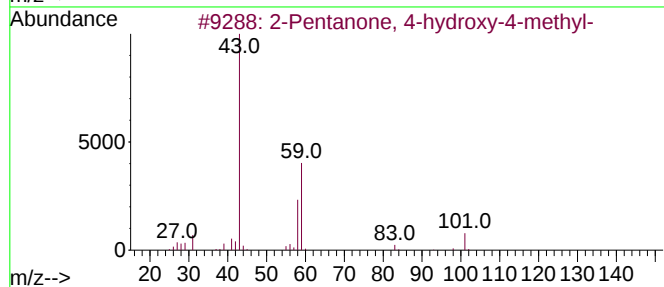
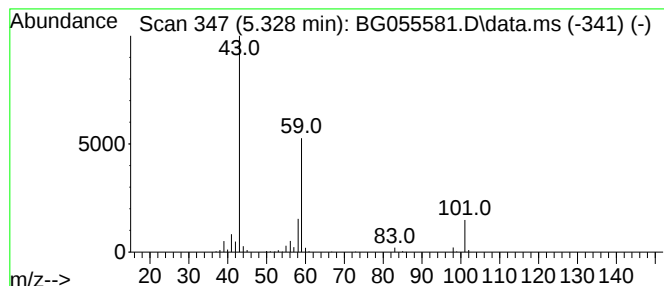
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.328	18.23 ng	353701	1,4-Dichlorobenzene-d4	8.271

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25



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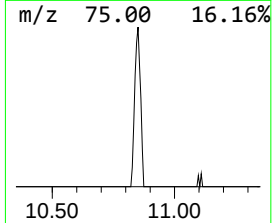
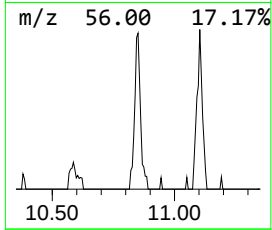
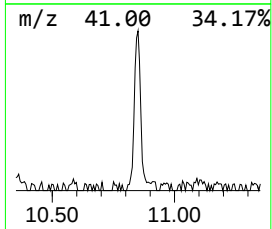
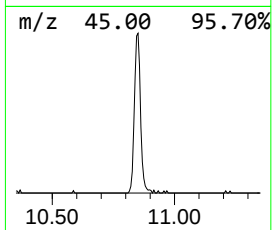
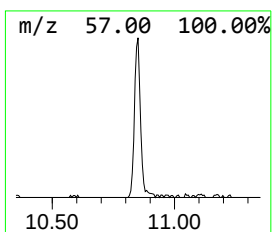
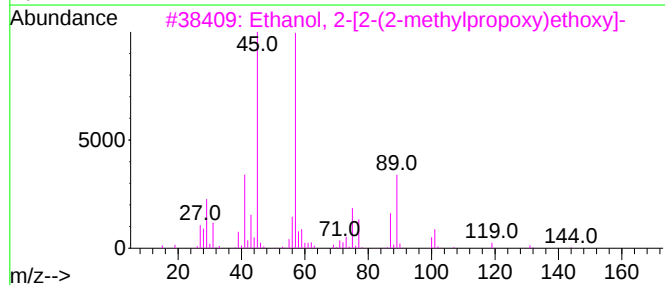
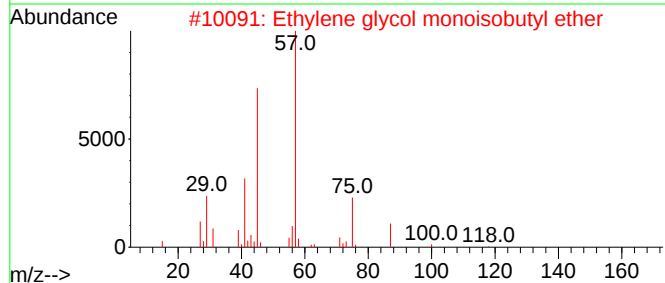
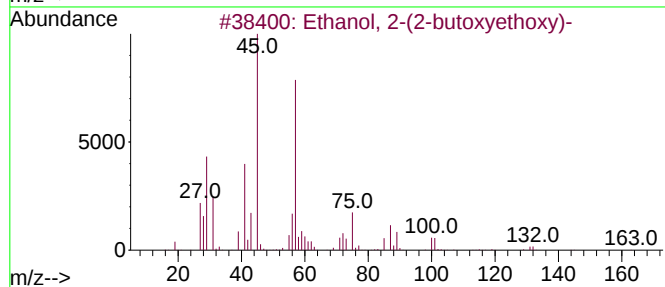
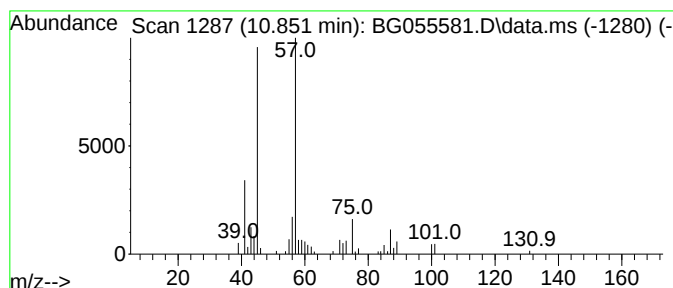
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.851	3.30 ng	92191	Naphthalene-d8	11.103	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
5	1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	47



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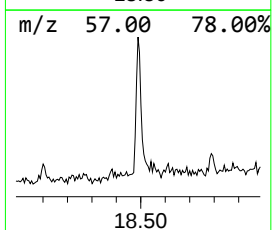
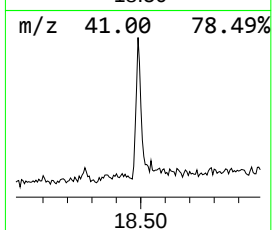
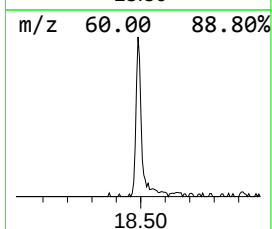
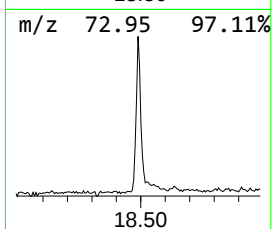
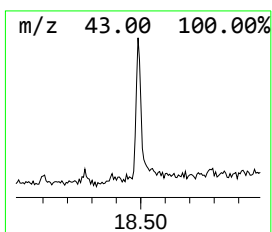
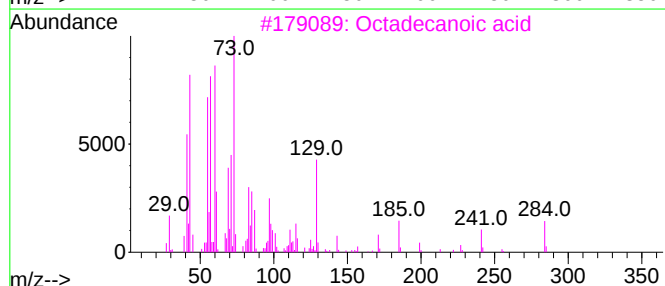
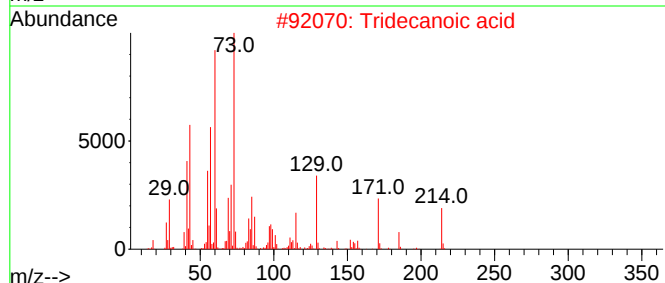
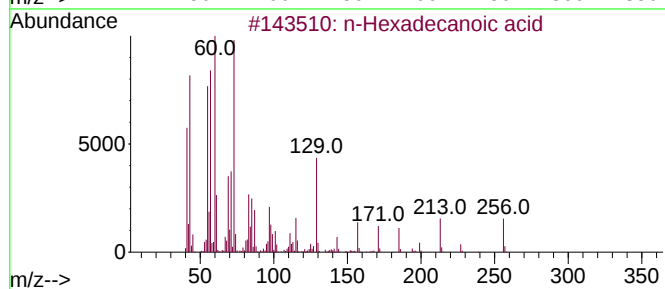
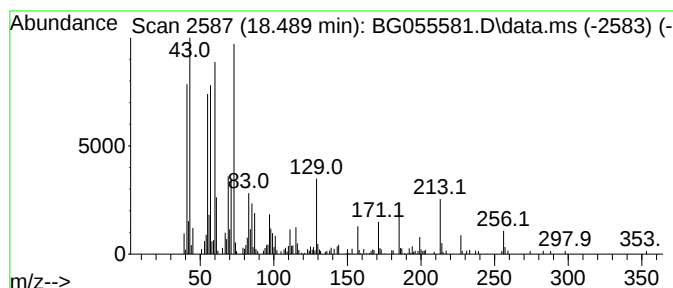
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.489	4.40 ng	199388	Phenanthrene-d10	17.631

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	89
3		Octadecanoic acid	284	C18H36O2	000057-11-4	81
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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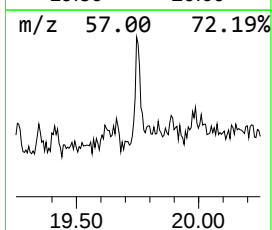
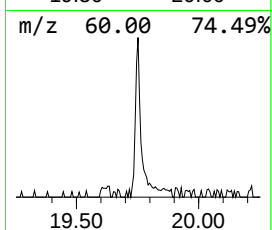
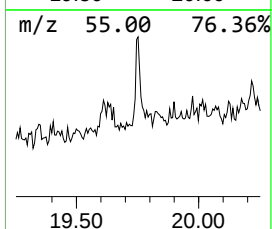
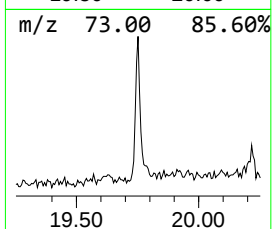
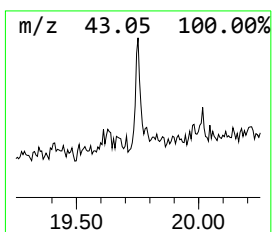
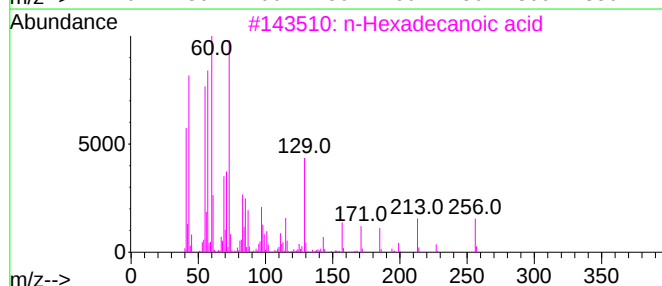
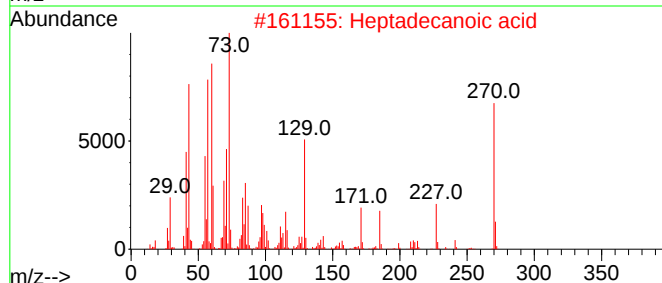
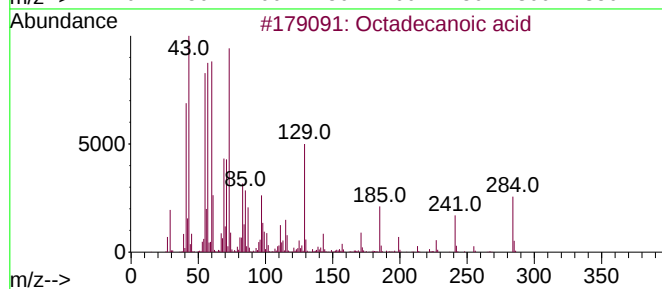
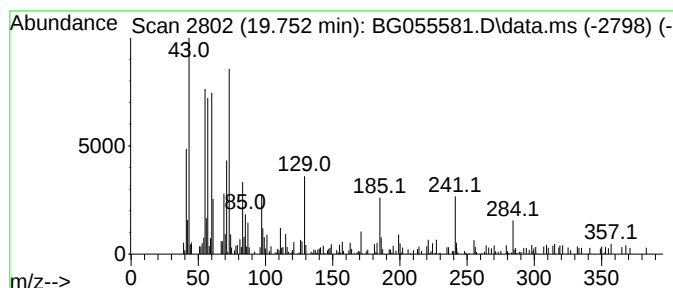
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.752	2.17 ng	98252	Phenanthrene-d10	17.631

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			Heptadecanoic acid	270	C17H34O2	000506-12-7	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			Tetracosanoic acid	368	C24H48O2	000557-59-5	64



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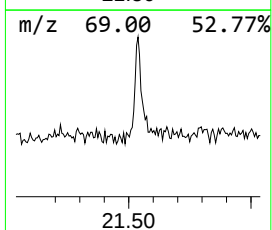
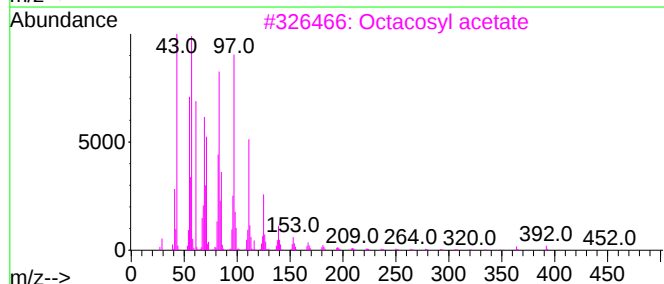
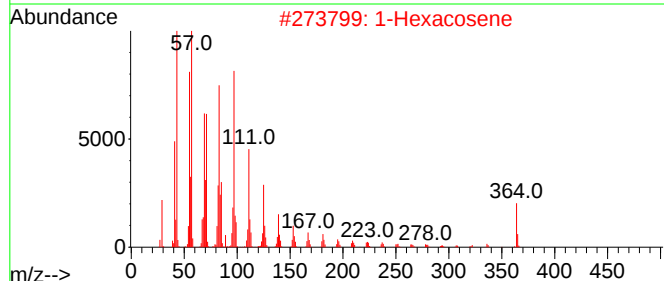
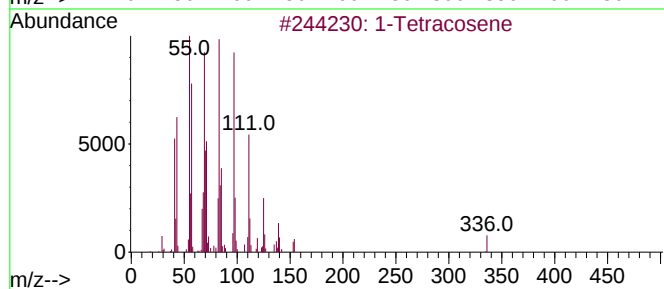
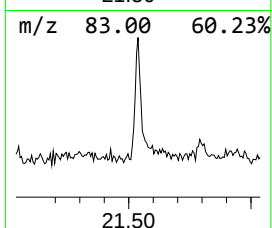
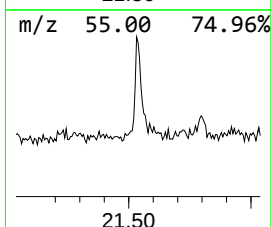
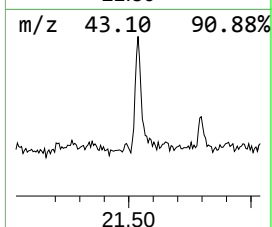
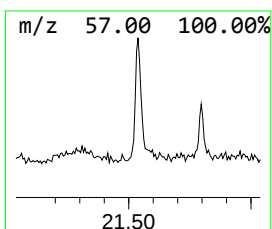
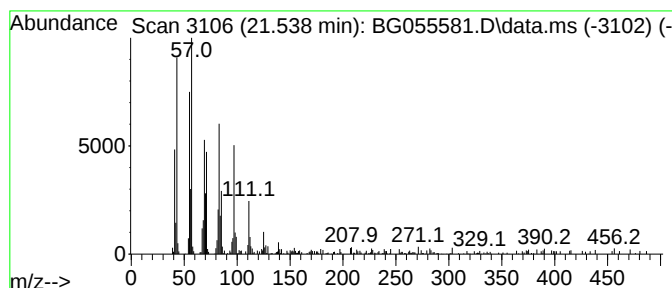
Instrument :
BNA_G
ClientSampleId :
SB-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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-Tetracosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.538	3.91 ng	169341	Chrysene-d12	21.932	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	97
2	1-Hexacosene	364	C26H52	018835-33-1	93
3	Octacosyl acetate	452	C30H60O2	018206-97-8	90
4	17-Pentatriacontene	491	C35H70	006971-40-0	90
5	Heneicosyl trifluoroacetate	408	C23H43F3O2	1000351-76-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055581.D
Acq On : 12 Nov 2022 1:09
Operator : CG/JU
Sample : N5530-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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
Butane, 2-metho...	3.330	11.9	ng	231068	1	8.271	388140	20.0
2-Pentanone, 4-...	5.328	18.2	ng	353701	1	8.271	388140	20.0
Ethanol, 2-(2-b...	10.851	3.3	ng	92191	2	11.103	558509	20.0
n-Hexadecanoic ...	18.489	4.4	ng	199388	4	17.631	906428	20.0
Octadecanoic acid	19.752	2.2	ng	98252	4	17.631	906428	20.0
1-Tetracosene	21.538	3.9	ng	169341	5	21.932	865836	20.0