

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040921\
 Data File : BG048653.D
 Acq On : 9 Apr 2021 20:24
 Operator : CG/JU
 Sample : M1990-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 ELEVATOR-PIT-STANDING-WATER

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-BG033021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048653.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.636	384	391	398	rBV	134961	218234	10.84%	2.641%
2	7.246	658	665	678	rVB	70223	154124	7.66%	1.865%
3	8.092	801	809	816	rBV	99112	168681	8.38%	2.042%
4	8.333	843	850	857	rBV	107290	190456	9.46%	2.305%
5	8.415	857	864	872	rVB	406206	685218	34.05%	8.294%
6	9.261	1000	1008	1016	rBV	304395	540804	26.87%	6.546%
7	10.013	1129	1136	1141	rBV	33395	53173	2.64%	0.644%
8	10.078	1141	1147	1151	rVV2	31567	50126	2.49%	0.607%
9	10.918	1283	1290	1296	rBV2	124837	228600	11.36%	2.767%
10	13.362	1695	1706	1715	rBV	818829	1262567	62.74%	15.282%
11	14.179	1841	1845	1855	rBV2	18120	31754	1.58%	0.384%
12	14.743	1936	1941	1948	rVB	195175	302016	15.01%	3.656%
13	15.019	1983	1988	1993	rBV3	13917	22186	1.10%	0.269%
14	16.229	2188	2194	2204	rBV	451341	697264	34.65%	8.439%
15	17.492	2403	2409	2417	rBV	246120	368690	18.32%	4.463%
16	18.374	2553	2559	2565	rBV2	107485	161239	8.01%	1.952%
17	19.643	2772	2775	2781	rVB4	53407	69317	3.44%	0.839%
18	20.101	2848	2853	2862	rBV	1506326	2012513	100.00%	24.359%
19	21.417	3072	3077	3085	rBV3	64736	127768	6.35%	1.546%
20	21.787	3134	3140	3147	rVB	233458	389676	19.36%	4.717%
21	23.515	3431	3434	3443	rVB3	39083	80526	4.00%	0.975%
22	25.125	3696	3708	3720	rBV3	146068	447000	22.21%	5.410%

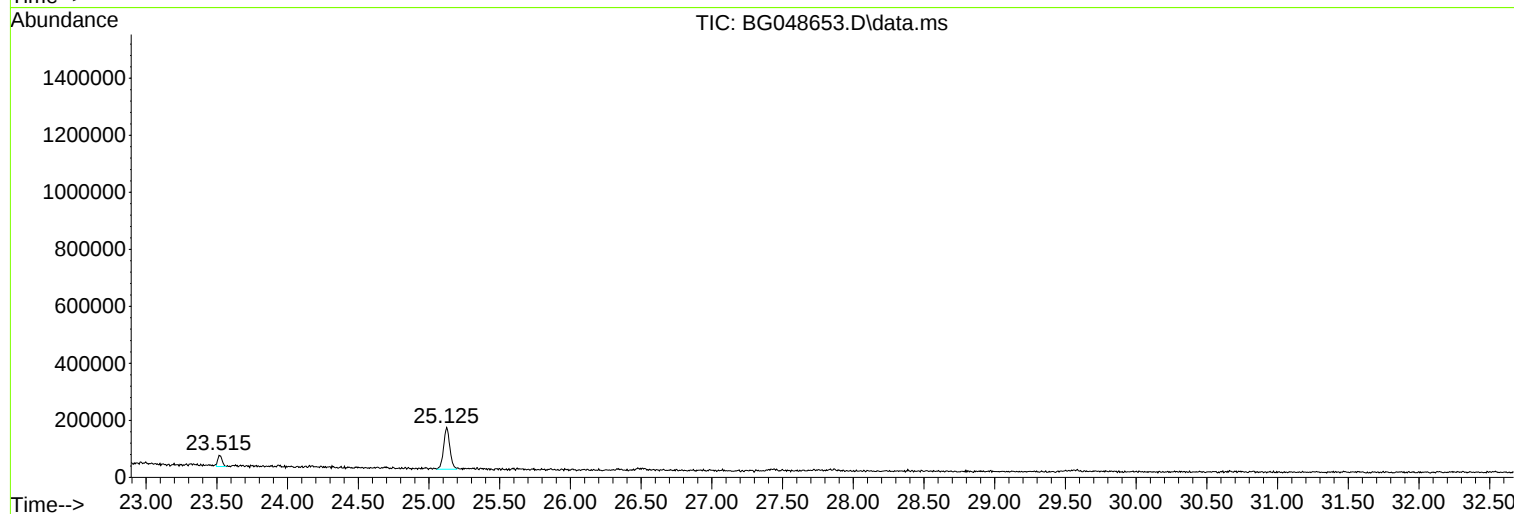
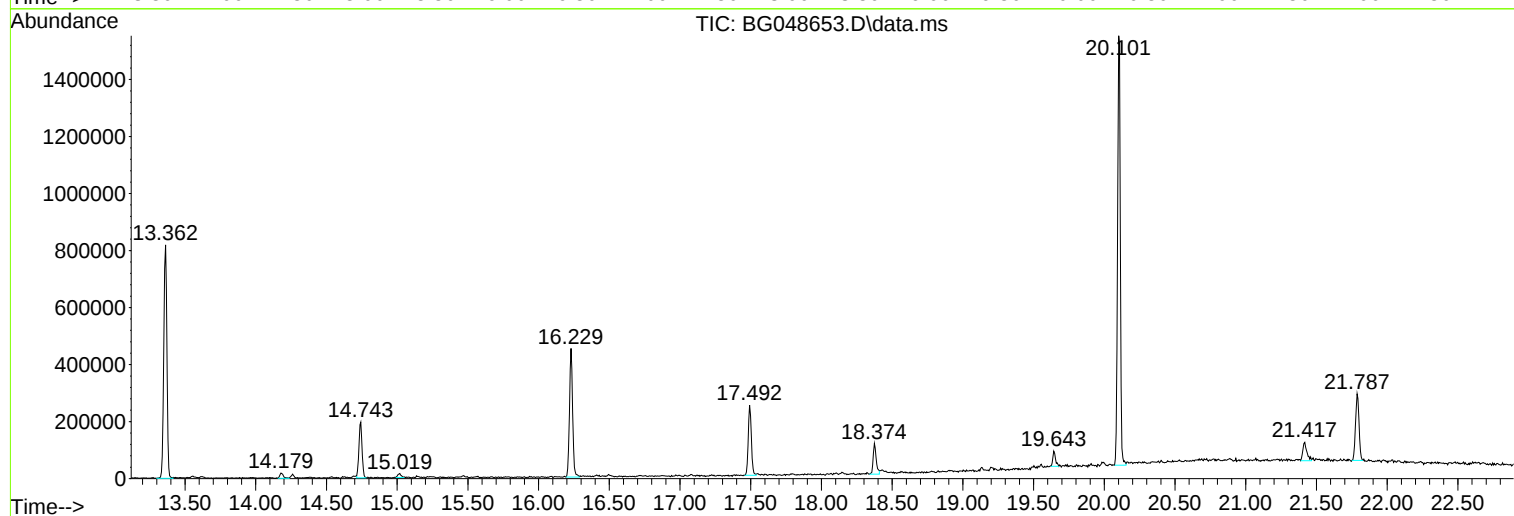
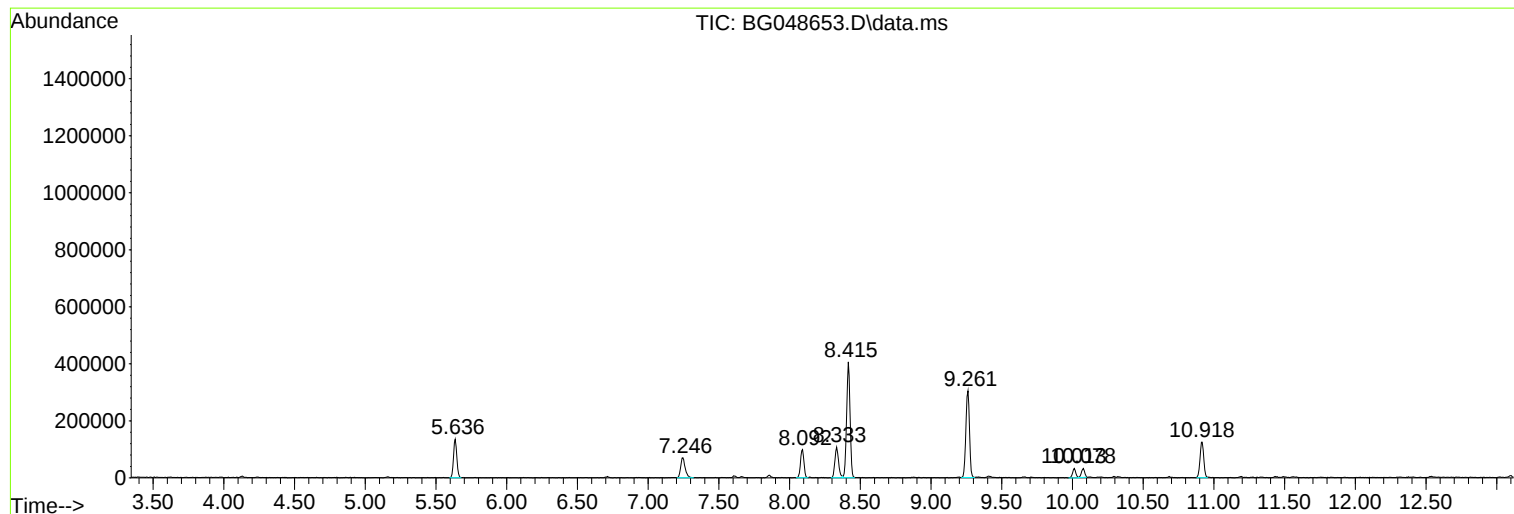
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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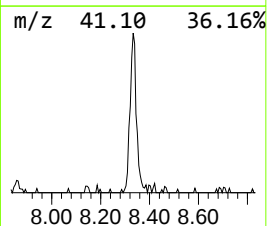
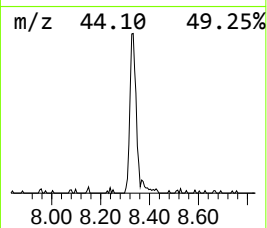
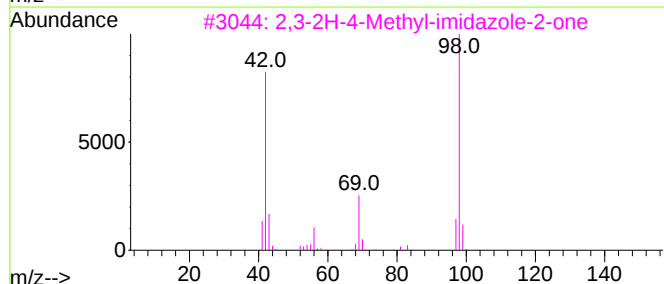
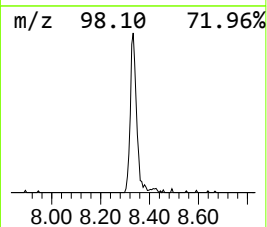
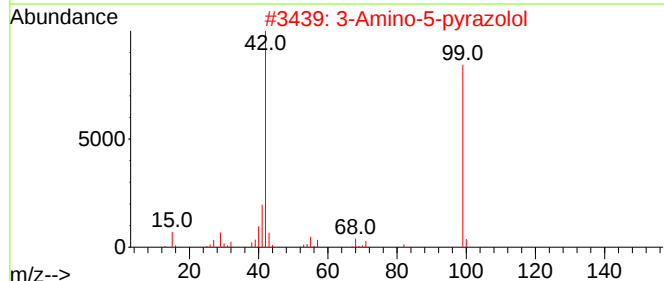
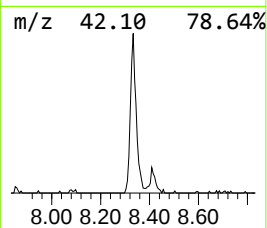
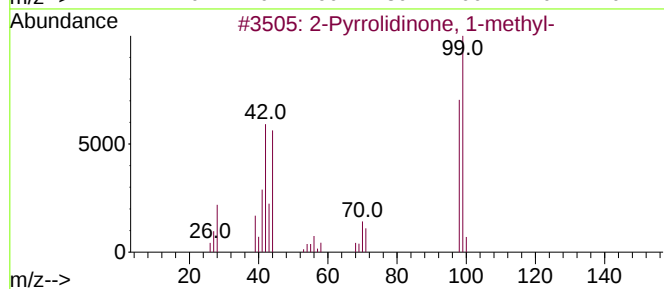
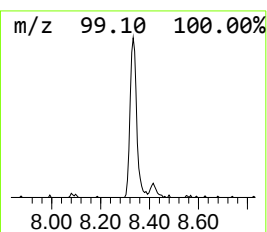
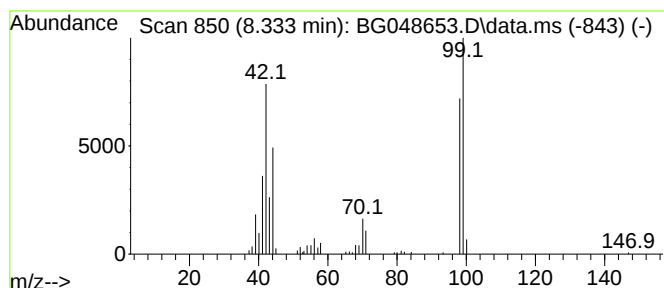
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pyrrolidinone, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.333	22.58 ng	190456	1,4-Dichlorobenzene-d4	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrrolidinone, 1-methyl-			99	C5H9NO	000872-50-4	87
2	3-Amino-5-pyrazolol			99	C3H5N3O	006126-22-3	47
3	2,3-2H-4-Methyl-imidazole-2-one			98	C4H6N2O	039799-77-4	38
4	2-Amino-4-methyl-oxazole			98	C4H6N2O	035629-70-0	38
5	4-Piperidone			99	C5H9NO	041661-47-6	38



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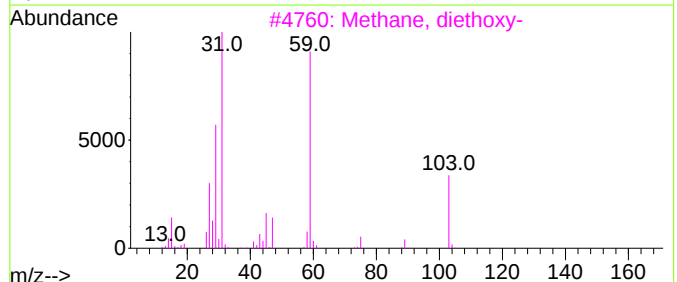
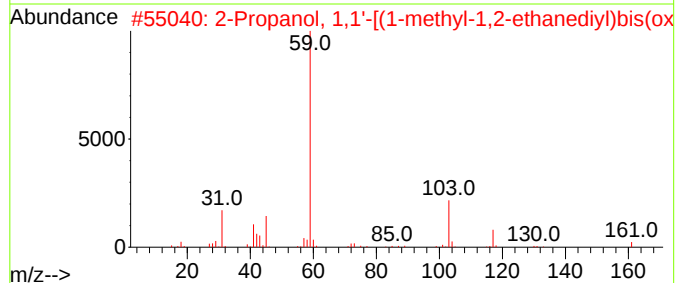
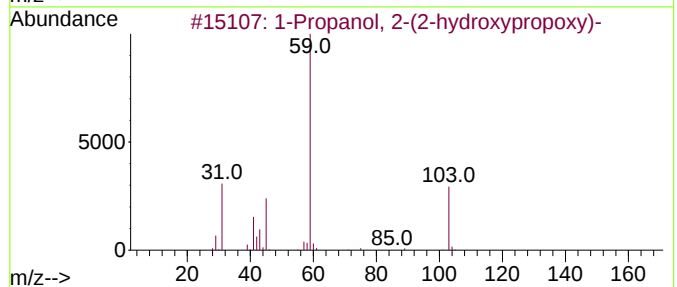
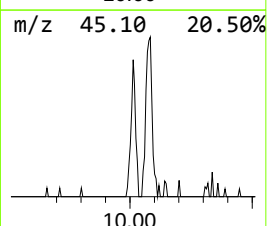
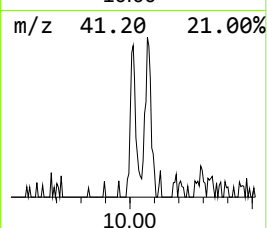
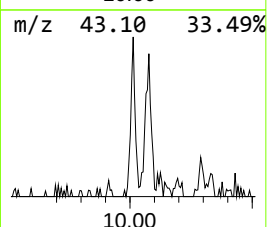
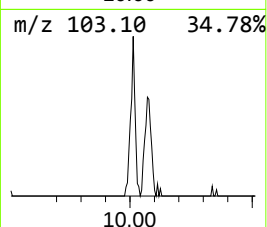
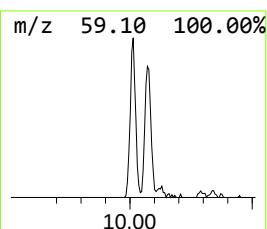
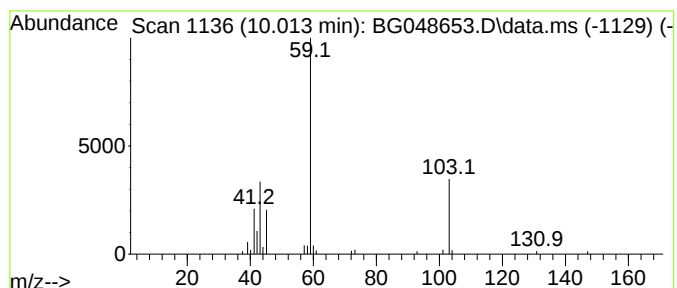
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Peak Number 3 1-Propanol, 2-(2-hydroxypro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.013	4.65 ng	53173	Naphthalene-d8	10.918

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
2			2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	72
3			Methane, diethoxy-	104	C5H12O2	000462-95-3	72
4			2-Butanol, 3,3'-oxybis-	162	C8H18O3	054305-61-2	72
5			1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	64



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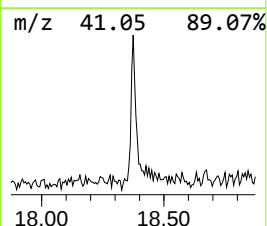
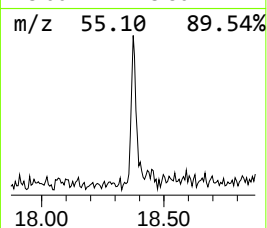
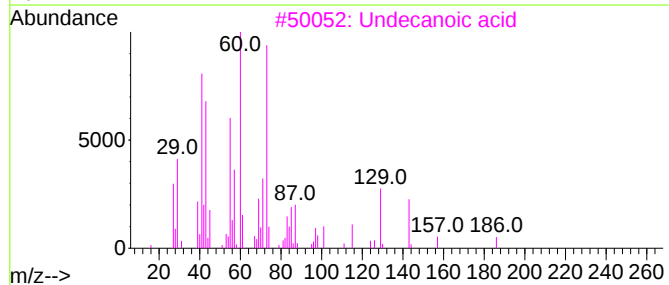
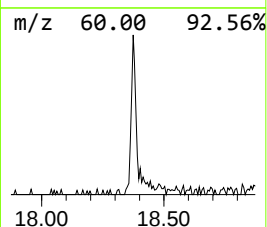
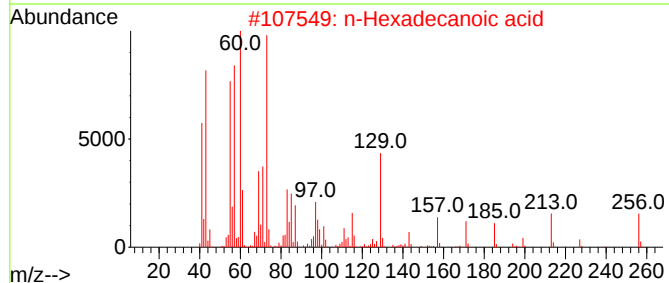
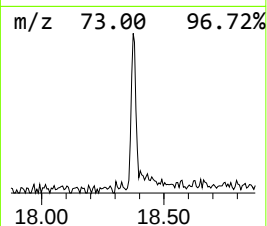
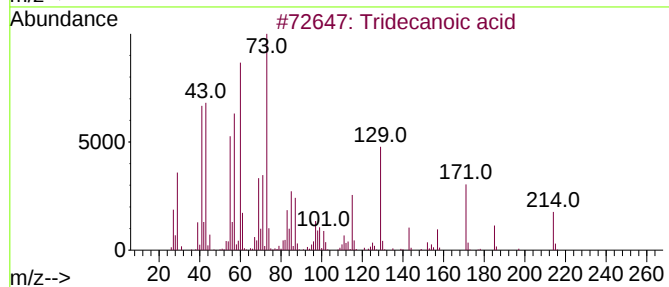
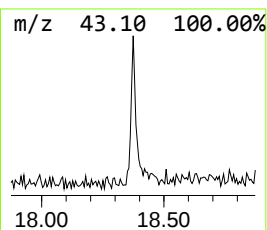
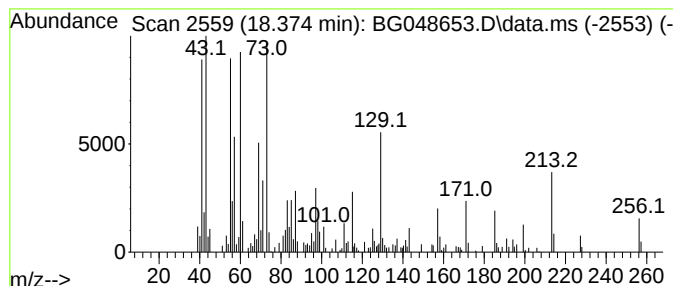
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.374	8.75 ng	161239	Phenanthrene-d10	17.493

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	96
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3			Undecanoic acid	186	C11H22O2	000112-37-8	60
4			n-Decanoic acid	172	C10H20O2	000334-48-5	55
5			Dodecanoic acid	200	C12H24O2	000143-07-7	52



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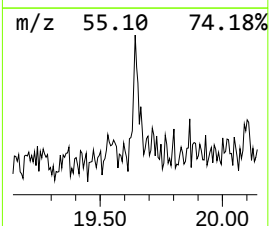
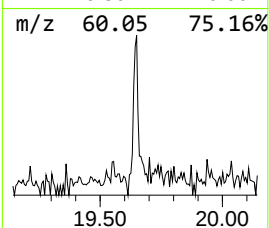
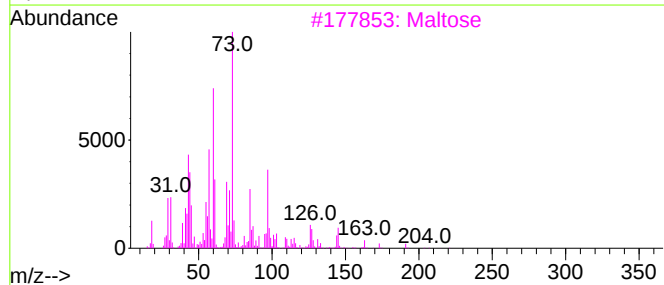
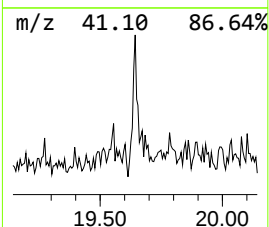
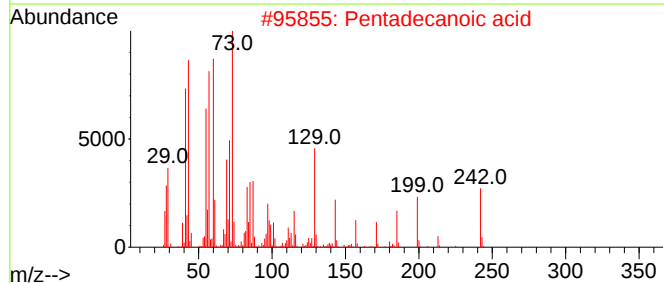
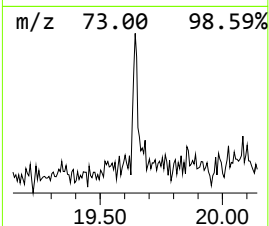
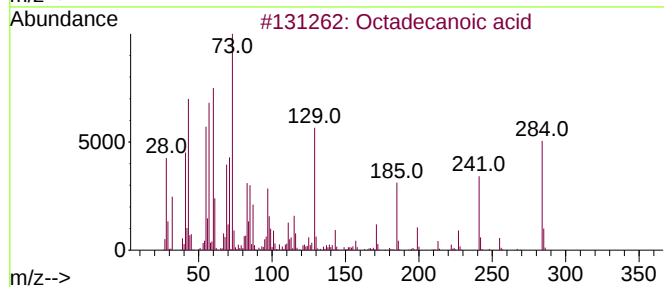
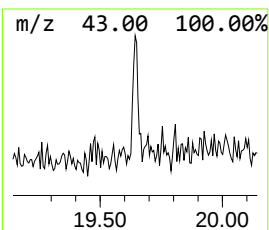
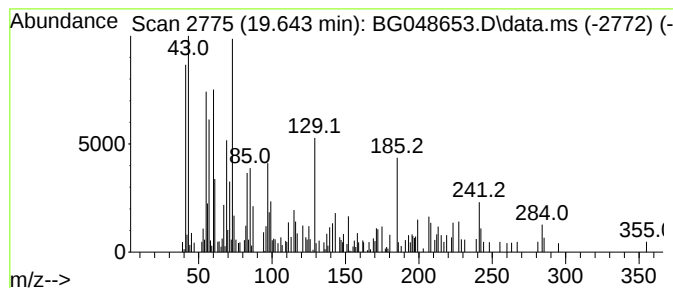
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Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.643	3.56 ng	69317	Chrysene-d12	21.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	52
3			Maltose	342	C12H22O11	000069-79-4	38
4			n-Decanoic acid	172	C10H20O2	000334-48-5	27
5			Lactose	342	C12H22O11	000063-42-3	14



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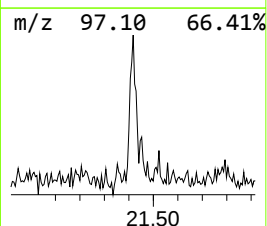
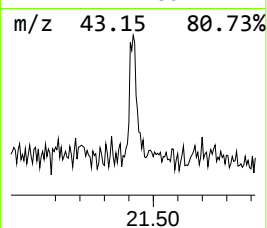
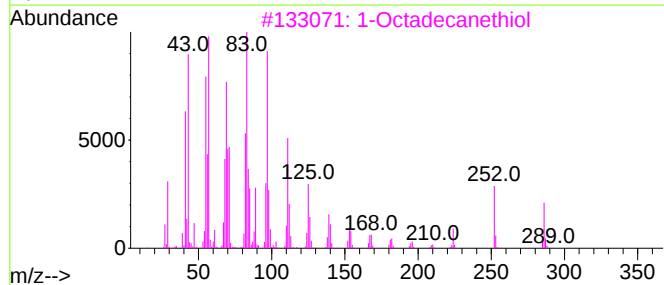
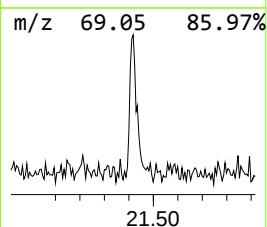
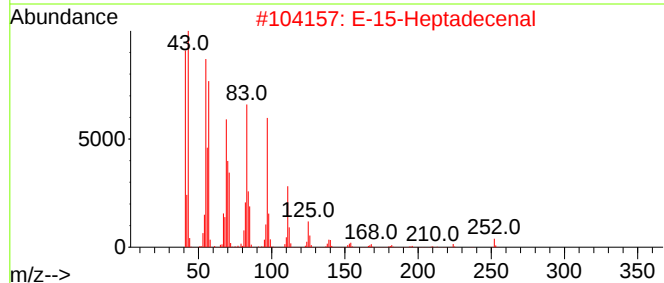
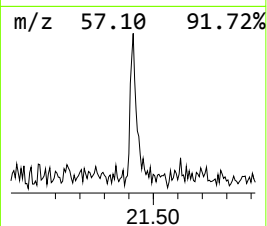
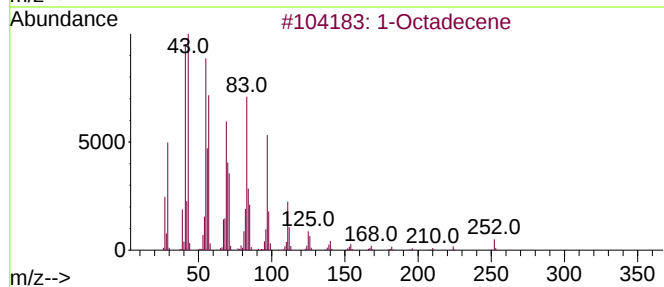
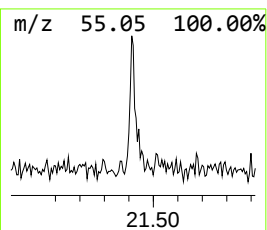
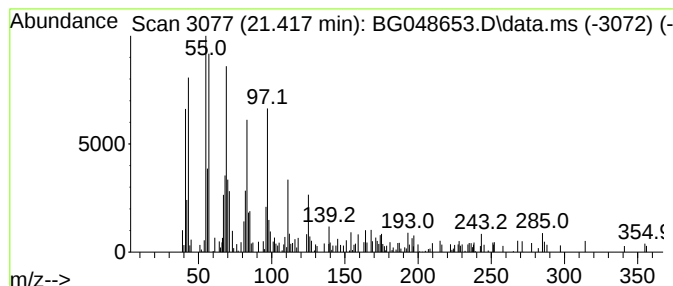
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Octadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.417	6.56 ng	127768	Chrysene-d12	21.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecene	252	C18H36	000112-88-9	93
2			E-15-Heptadecenal	252	C17H32O	1000130-97-9	91
3			1-Octadecanethiol	286	C18H38S	002885-00-9	90
4			Cyclopentane, 1-butyl-2-pentyl-	196	C14H28	061142-52-7	76
5			1-Heneicosanol	312	C21H44O	015594-90-8	60



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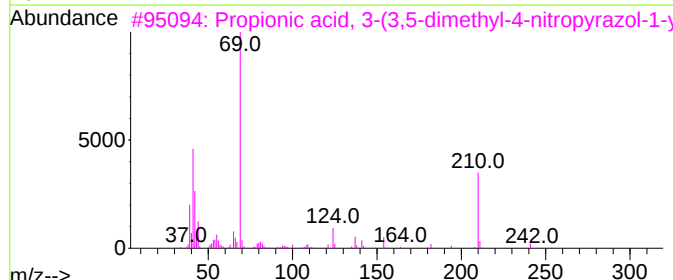
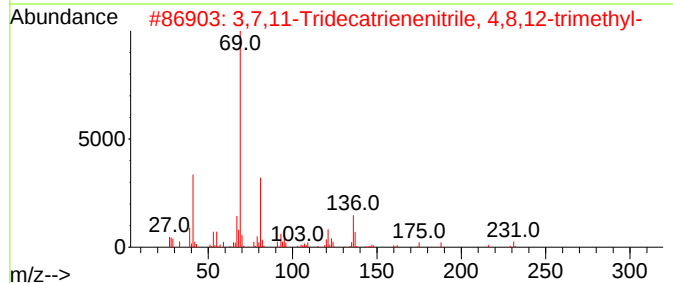
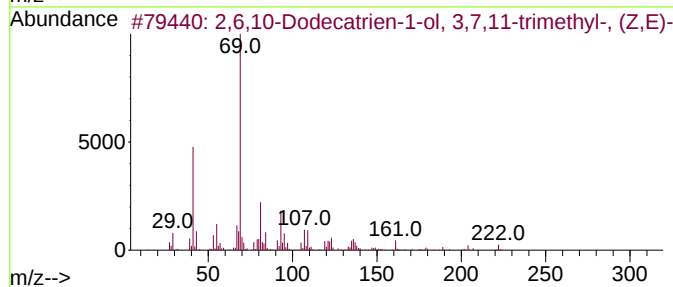
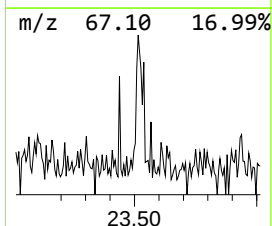
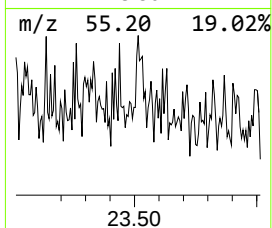
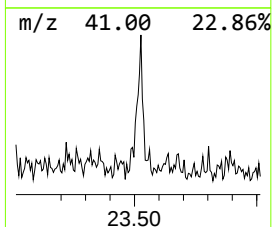
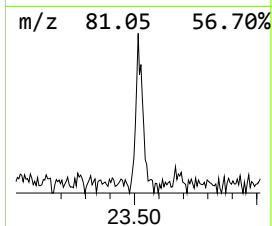
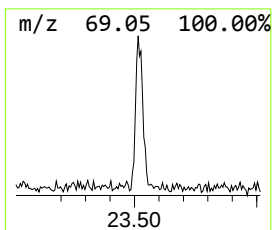
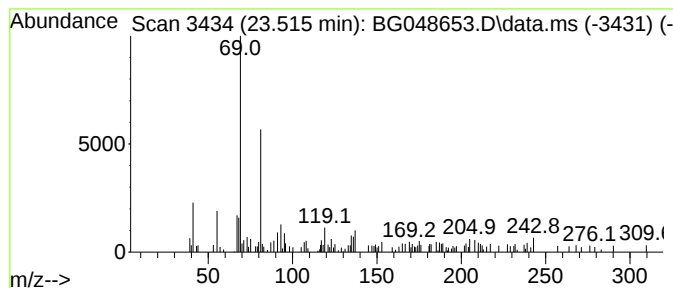
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.515	3.60 ng	80526	Perylene-d12	25.125

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	003790-71-4	58		
2	3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	58		
3	Propionic acid, 3-(3,5-dimethyl-...	241	C9H15N5O3	1000304-09-4	53		
4	Farnesol isomer a	222	C15H26O	1000108-92-4	50		
5	trans-Farnesol	222	C15H26O	000106-28-5	50		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040921\
Data File : BG048653.D
Acq On : 9 Apr 2021 20:24
Operator : CG/JU
Sample : M1990-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ELEVATOR-PIT-STANDING-WATER

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pyrrolidinone...	8.333	22.6	ng	190456	1	8.086	168681	20.0
1-Propanol, 2-(...	10.013	4.7	ng	53173	2	10.918	228600	20.0
2-(2-(2-(2-M...	10.078	4.4	ng	50126	2	10.918	228600	20.0
Tridecanoic acid	18.374	8.8	ng	161239	4	17.493	368690	20.0
Octadecanoic acid	19.643	3.6	ng	69317	5	21.788	389676	20.0
1-Octadecene	21.417	6.6	ng	127768	5	21.788	389676	20.0
2,6,10-Dodecatr...	23.515	3.6	ng	80526	6	25.125	447000	20.0