

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
 Data File : BG055593.D
 Acq On : 12 Nov 2022 17:19
 Operator : CG/JU
 Sample : N5431-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20221178-COMP-13-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-BG110922.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055593.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.326	3	6	27	rVB	618623	937528	27.38%	5.712%
2	4.706	235	241	247	rBV	26013	37708	1.10%	0.230%
3	5.323	340	346	355	rVB	52818	84850	2.48%	0.517%
4	5.793	418	426	436	rBV	368410	592989	17.32%	3.613%
5	7.397	691	699	707	rBV	277725	471716	13.78%	2.874%
6	8.267	840	847	854	rBV	218577	367500	10.73%	2.239%
7	9.436	1039	1046	1057	rVB	480822	844824	24.68%	5.147%
8	11.093	1321	1328	1337	rBV	298782	539260	15.75%	3.285%
9	13.514	1732	1740	1748	rVB	1321766	2025285	59.16%	12.339%
10	14.888	1967	1974	1982	rVB	518565	830111	24.25%	5.057%
11	16.363	2219	2225	2236	rBV	1197688	1863250	54.42%	11.352%
12	17.626	2433	2440	2449	rBV	743820	1132665	33.08%	6.901%
13	18.273	2545	2550	2555	rBV2	63068	82011	2.40%	0.500%
14	18.484	2582	2586	2597	rBV	104931	173042	5.05%	1.054%
15	19.424	2739	2746	2754	rVB2	54251	78775	2.30%	0.480%
16	19.630	2774	2781	2789	rBV10	14303	34385	1.00%	0.209%
17	19.747	2797	2801	2808	rBV2	39076	60563	1.77%	0.369%
18	20.212	2874	2880	2887	rBV	2491776	3423588	100.00%	20.858%
19	21.534	3101	3105	3117	rBV2	45250	98739	2.88%	0.602%
20	21.927	3165	3172	3179	rVB	736775	1237688	36.15%	7.540%
21	23.702	3469	3474	3481	rVB2	61363	125644	3.67%	0.765%
22	25.347	3744	3754	3771	rVB3	426074	1371958	40.07%	8.358%

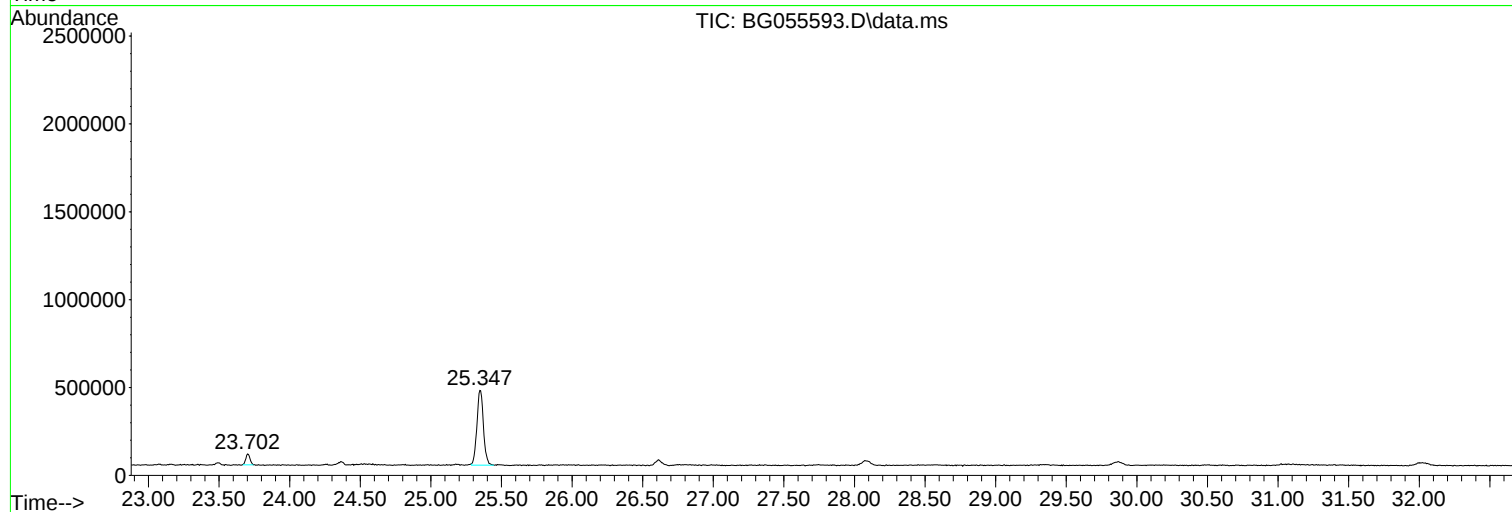
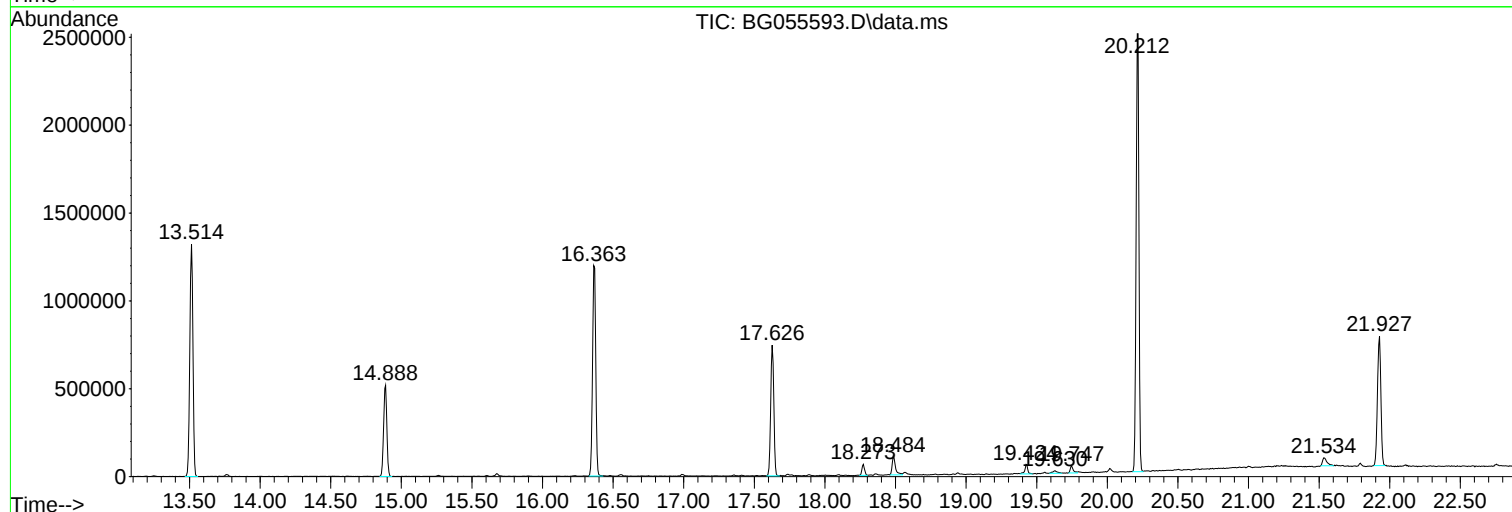
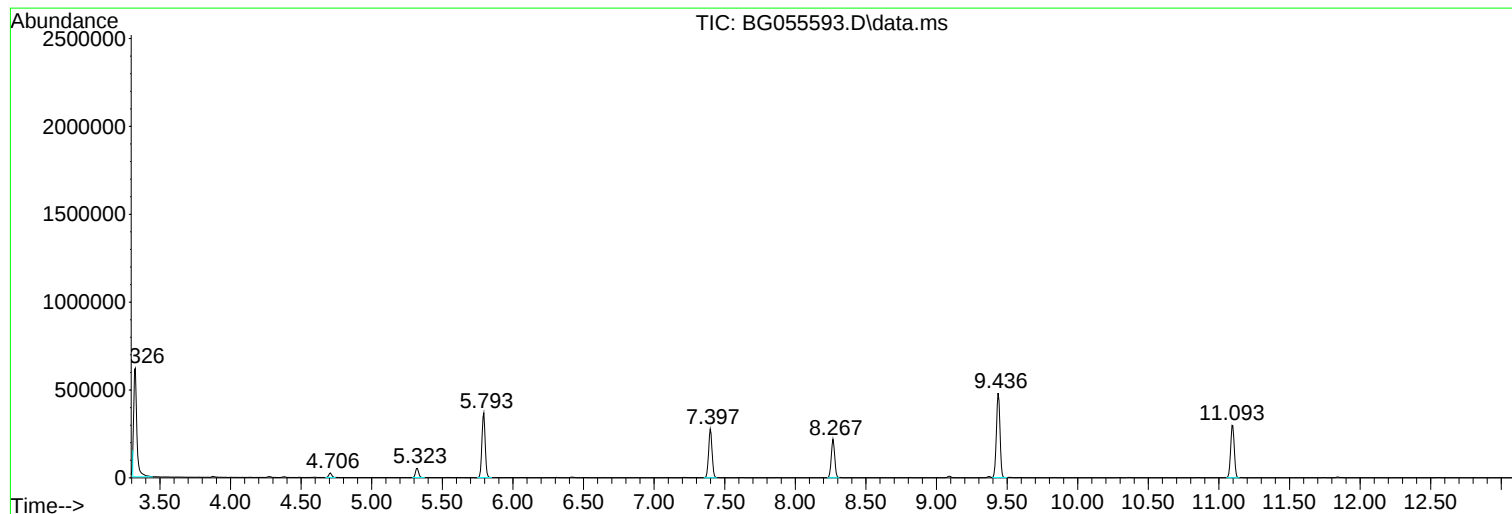
Sum of corrected areas: 16414079

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055593.D
Acq On : 12 Nov 2022 17:19
Operator : CG/JU
Sample : N5431-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221178-COMP-13-MODIFIED-ELUTRIATE

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055593.D
Acq On : 12 Nov 2022 17:19
Operator : CG/JU
Sample : N5431-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221178-COMP-13-MODIFIED-ELUTRIATE

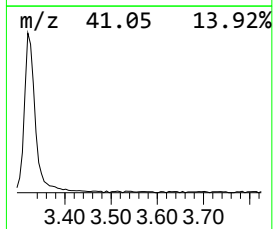
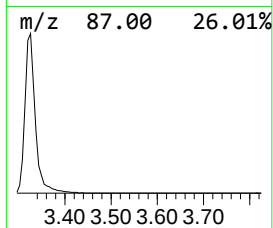
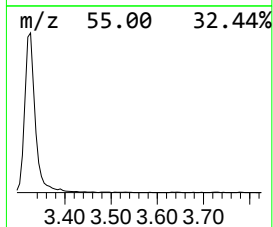
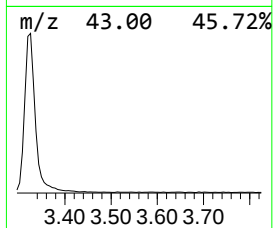
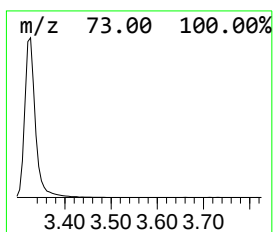
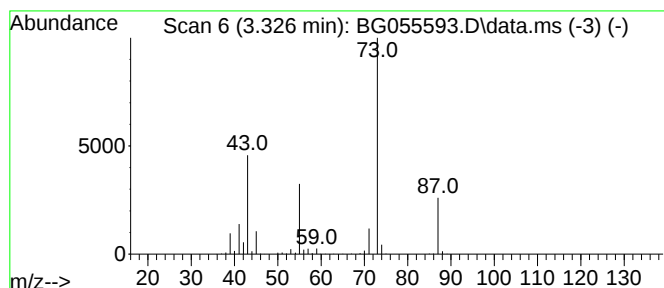
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.326	51.02 ng	937528	1,4-Dichlorobenzene-d4	8.267

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055593.D
Acq On : 12 Nov 2022 17:19
Operator : CG/JU
Sample : N5431-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221178-COMP-13-MODIFIED-ELUTRIATE

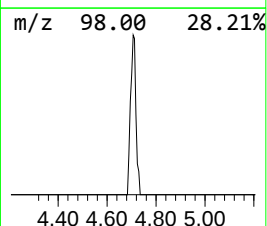
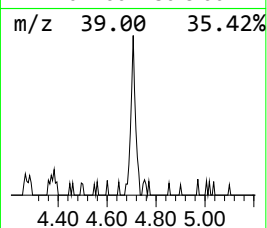
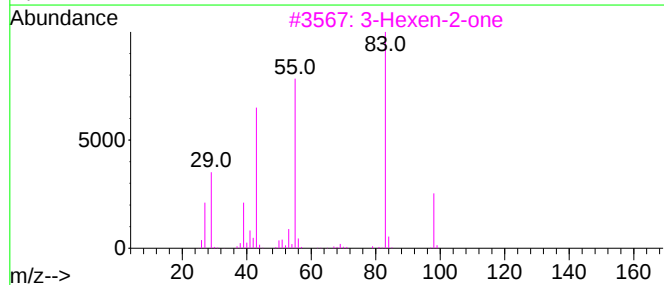
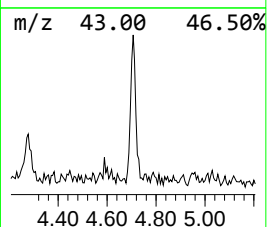
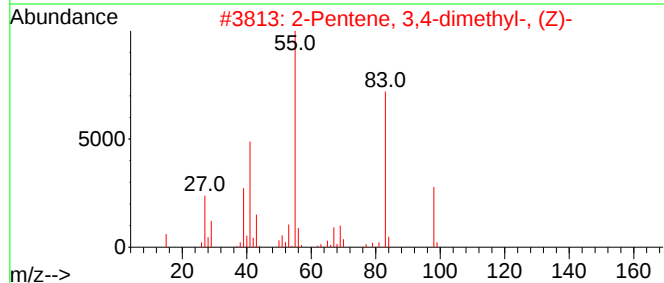
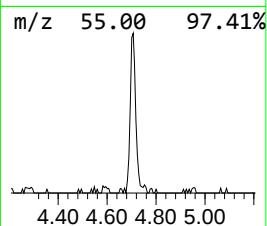
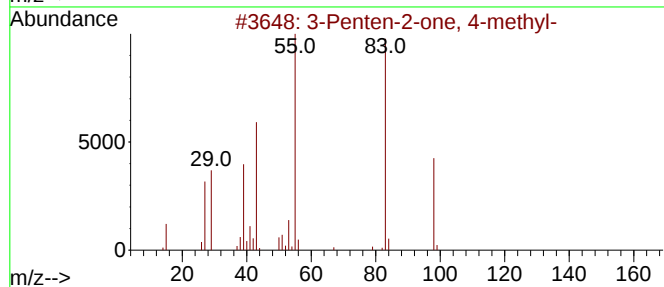
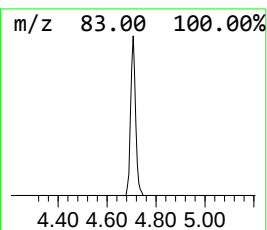
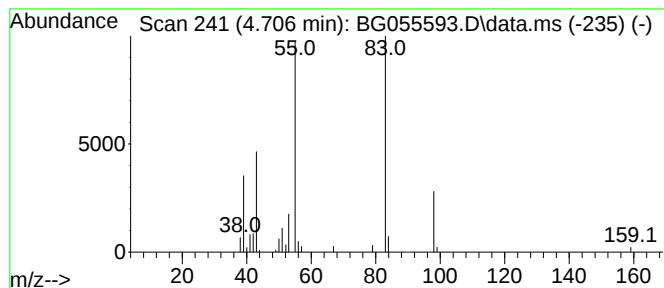
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.706	2.05 ng	37708	1,4-Dichlorobenzene-d4	8.267

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
3		3-Hexen-2-one	98	C6H10O	000763-93-9	86
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055593.D
Acq On : 12 Nov 2022 17:19
Operator : CG/JU
Sample : N5431-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221178-COMP-13-MODIFIED-ELUTRIATE

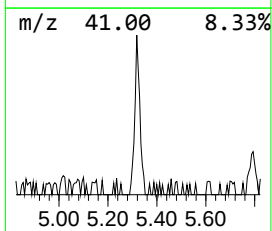
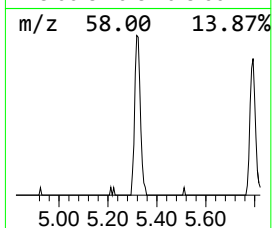
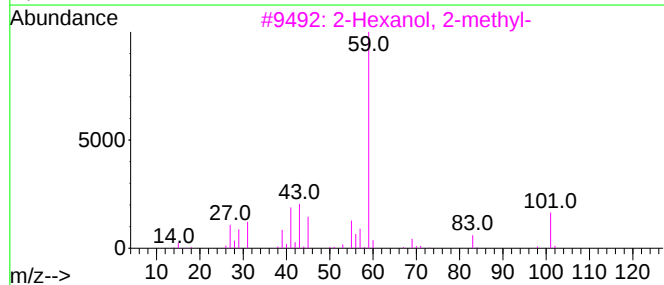
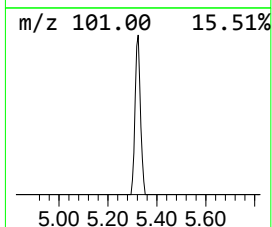
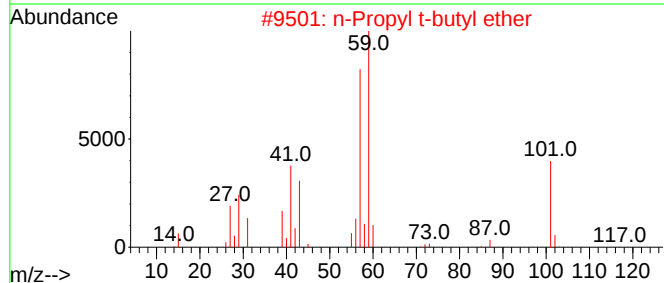
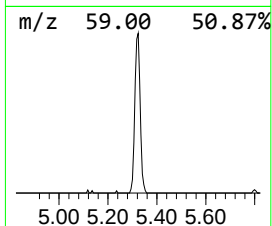
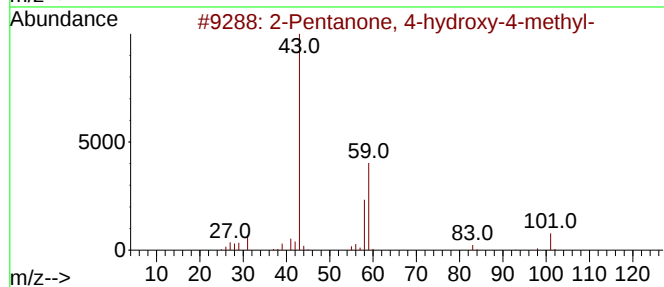
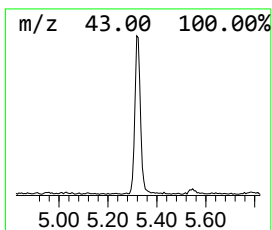
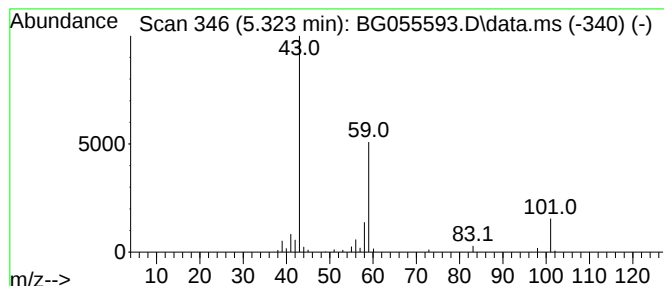
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.323	4.62 ng	84850	1,4-Dichlorobenzene-d4	8.267

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055593.D
Acq On : 12 Nov 2022 17:19
Operator : CG/JU
Sample : N5431-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221178-COMP-13-MODIFIED-ELUTRIATE

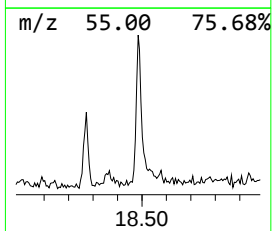
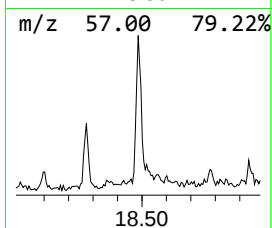
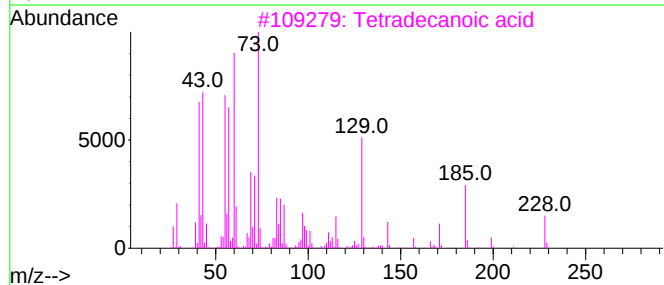
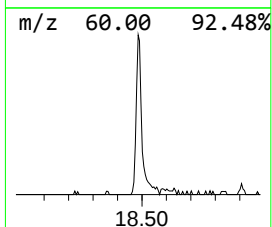
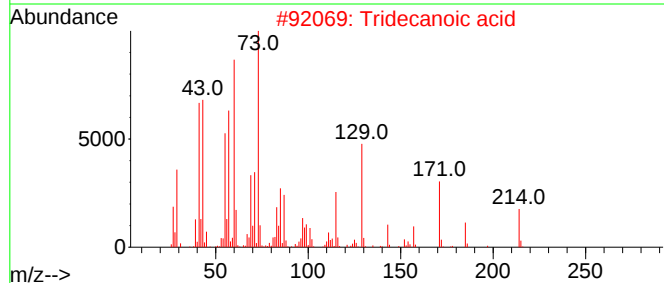
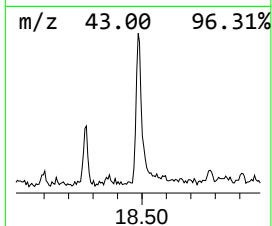
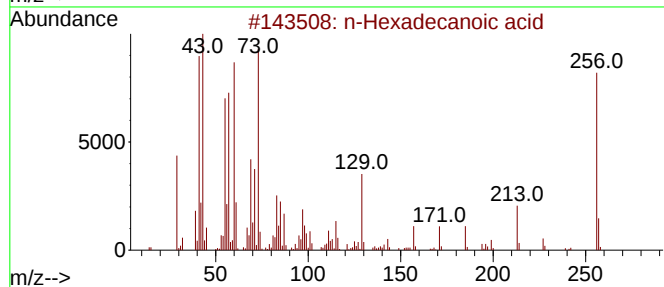
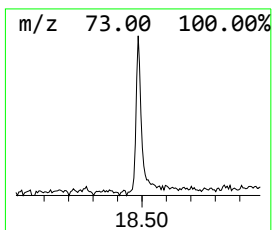
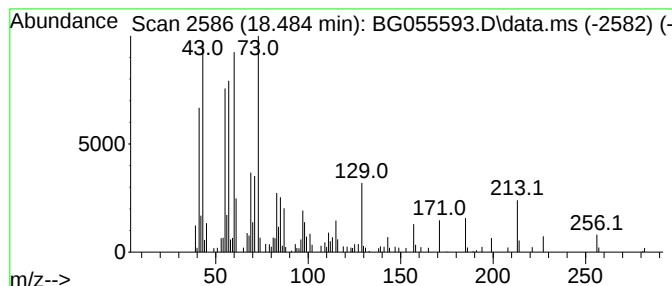
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.484	3.06 ng	173042	Phenanthrene-d10	17.626

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Nonanoic acid	158	C9H18O2	000112-05-0	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111222\
Data File : BG055593.D
Acq On : 12 Nov 2022 17:19
Operator : CG/JU
Sample : N5431-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221178-COMP-13-MODIFIED-ELUTRIATE

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.326	51.0	ng	937528	1	8.267	367500	20.0
3-Penten-2-one,...	4.706	2.0	ng	37708	1	8.267	367500	20.0
2-Pentanone, 4-...	5.323	4.6	ng	84850	1	8.267	367500	20.0
n-Hexadecanoic ...	18.484	3.1	ng	173042	4	17.626	1132670	20.0