LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055444.D
Acq On : 3 Nov 2022 19:26
Operator : CG/JU
Sample : N5306-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221168-COMP-03-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: BG055444.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	331	338	350	rBV	19719	32201	1.56%	0.363%
2	5.761	414	421	438	rBV	202395	348898	16.86%	3.932%
3	7.383	689	697	710	rBV	163975	302939	14.64%	3.414%
4	8.235	835	842	849	rBV	93374	155787	7.53%	1.756%
5	9.410	1034	1042	1058	rVB	276006	489269	23.64%	5.514%
6	10.808	1273	1280	1298	rBV	262914	443200	21.42%	4.994%
7	11.061	1316	1323	1332	rBV	127040	227493	10.99%	2.564%
8	13.476	1724	1734	1742	rBV	829981	1276957	61.71%	14.390%
9	13.723	1770	1776	1786	rBV	43799	66490	3.21%	0.749%
10	14.851	1960	1968	1979	rBB	227913	354751	17.14%	3.998%
11	16.331	2214	2220	2234	rBV	664636	1017319	49.16%	11.464%
12	17.583	2427	2433	2440	rBV	304352	456450	22.06%	5.144%
13	18.211	2534	2540	2546	rBV	72132	101215	4.89%	1.141%
14	18.435	2573	2578	2585	rBV2	30246	49959	2.41%	0.563%
15	19.363	2732	2736	2740	rVB	141113	151577	7.32%	1.708%
16	19.492	2750	2758	2763	rBV	46277	52801	2.55%	0.595%
17	20.162	2866	2872	2877	rBV	1538884	2069379	100.00%	23.320%
18	21.461	3087	3093	3109	rBV5	38759	141789	6.85%	1.598%
19	21.854	3154	3160	3168	rBV2	310798	518103	25.04%	5.839%
20	23.552	3443	3449	3457	rBV	30518	60155	2.91%	0.678%
21	25.227	3724	3734	3751	rVB2	185690	557102	26.92%	6.278%

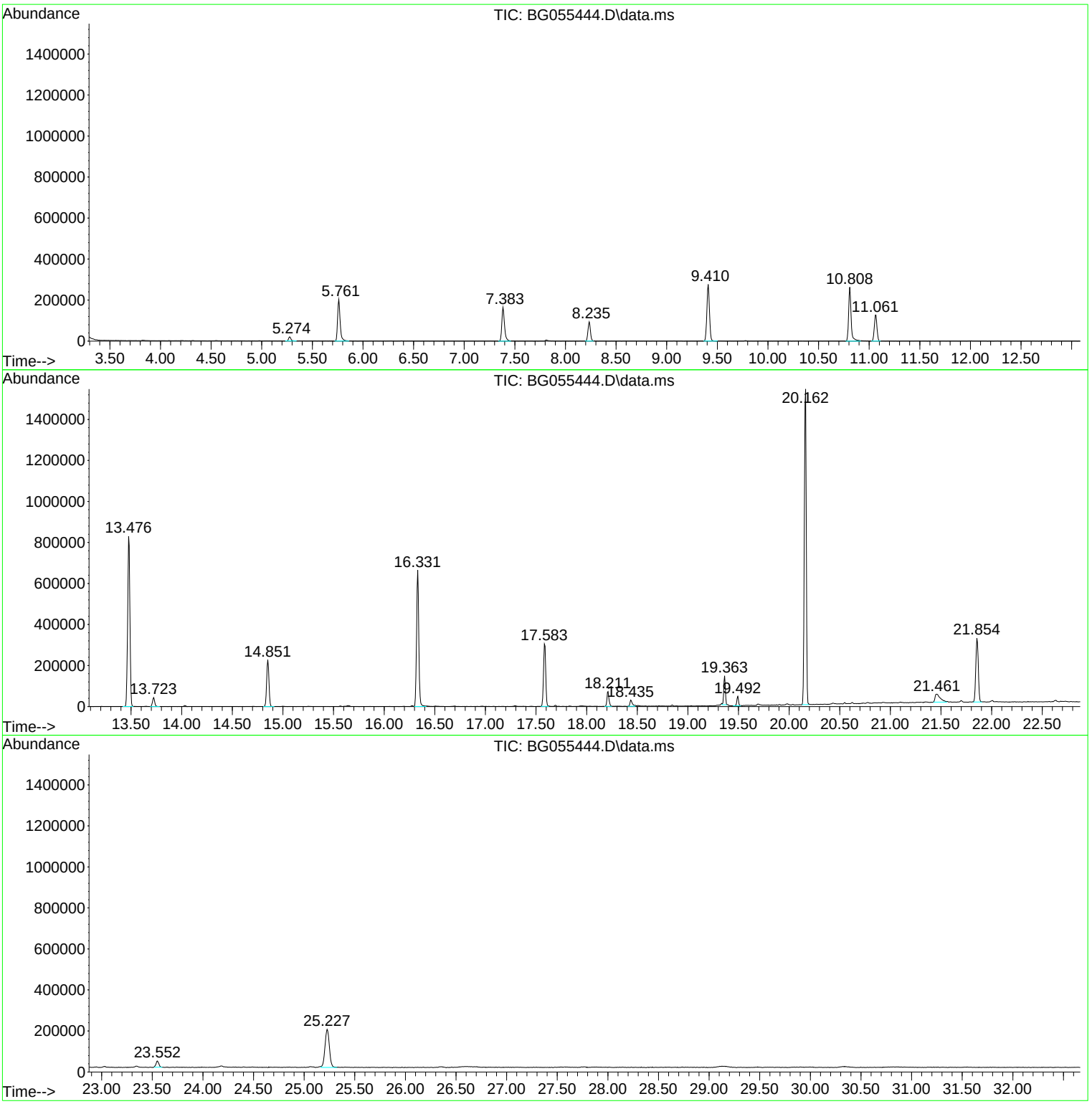
Sum of corrected areas: 8873834

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055444.D
Acq On : 3 Nov 2022 19:26
Operator : CG/JU
Sample : N5306-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221168-COMP-03-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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055444.D
Acq On : 3 Nov 2022 19:26
Operator : CG/JU
Sample : N5306-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221168-COMP-03-MODIFIED-ELUTRIATE

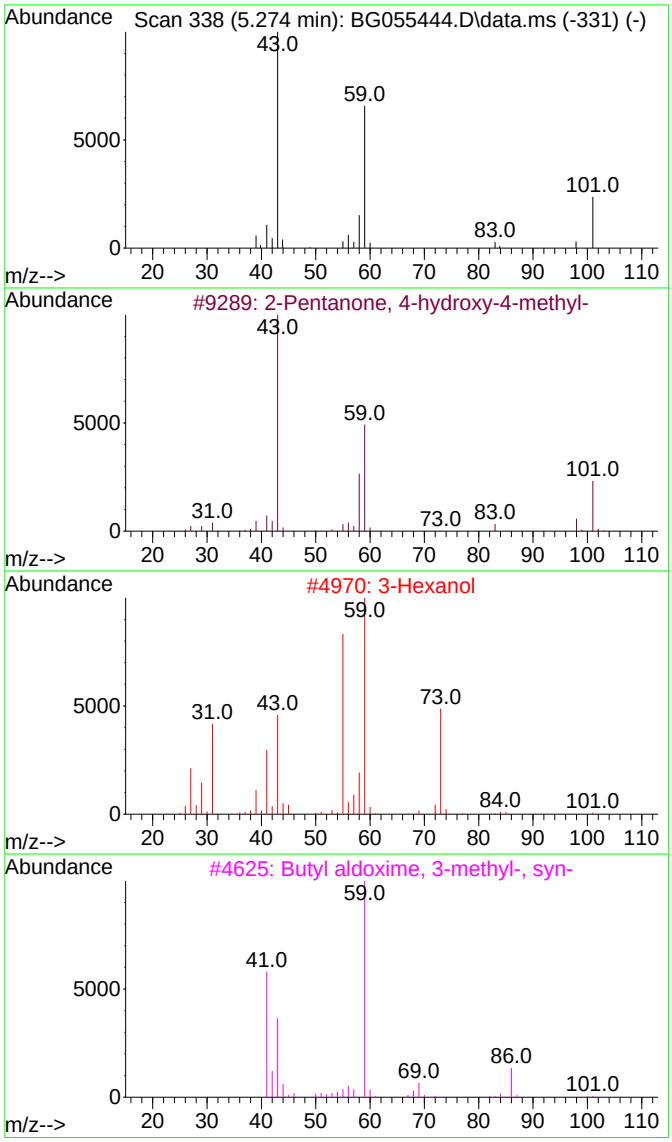
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

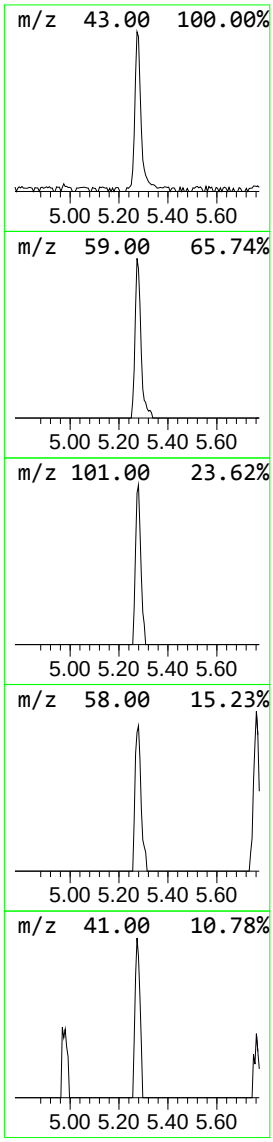
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.274	4.13 ng	32201	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-Hexanol	102	C6H14O	000623-37-0	33
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	23
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055444.D
Acq On : 3 Nov 2022 19:26
Operator : CG/JU
Sample : N5306-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221168-COMP-03-MODIFIED-ELUTRIATE

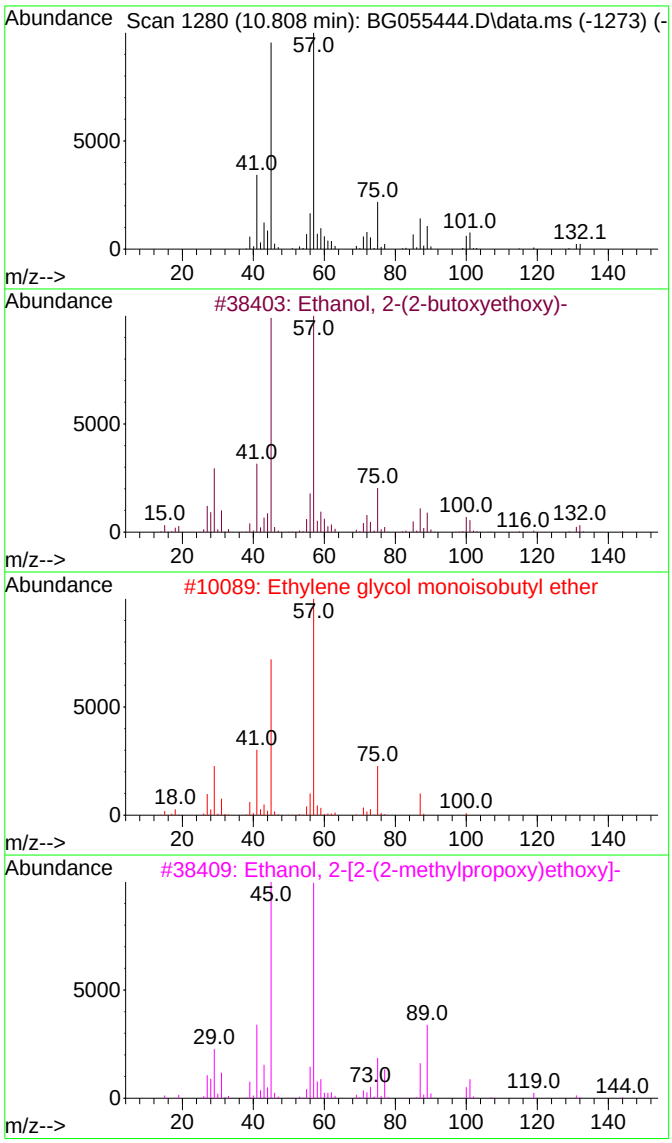
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

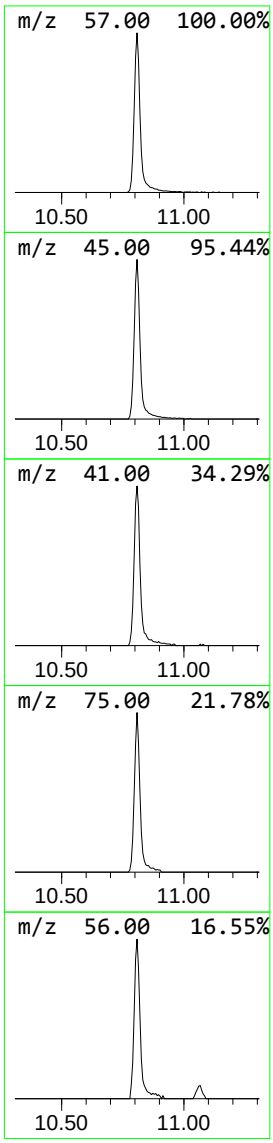
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.808	38.96 ng	443200	Naphthalene-d8	11.067

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055444.D
Acq On : 3 Nov 2022 19:26
Operator : CG/JU
Sample : N5306-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221168-COMP-03-MODIFIED-ELUTRIATE

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

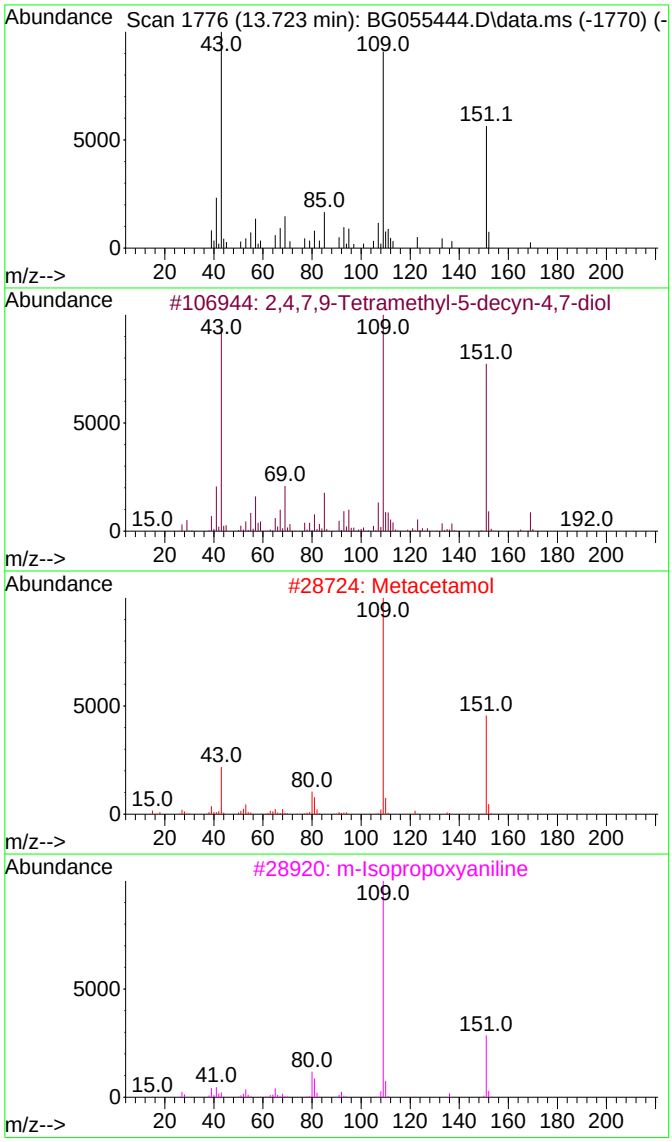
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

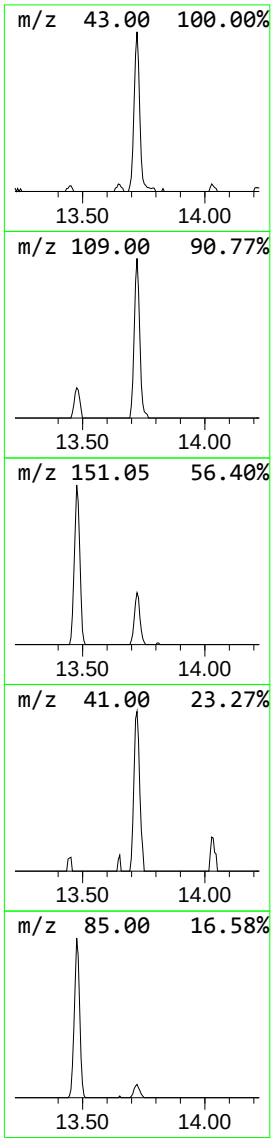
****

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.723	3.75 ng	66490	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	58
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	58
4	Acetaminophen	151	C8H9NO2	000103-90-2	53
5	(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055444.D
Acq On : 3 Nov 2022 19:26
Operator : CG/JU
Sample : N5306-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221168-COMP-03-MODIFIED-ELUTRIATE

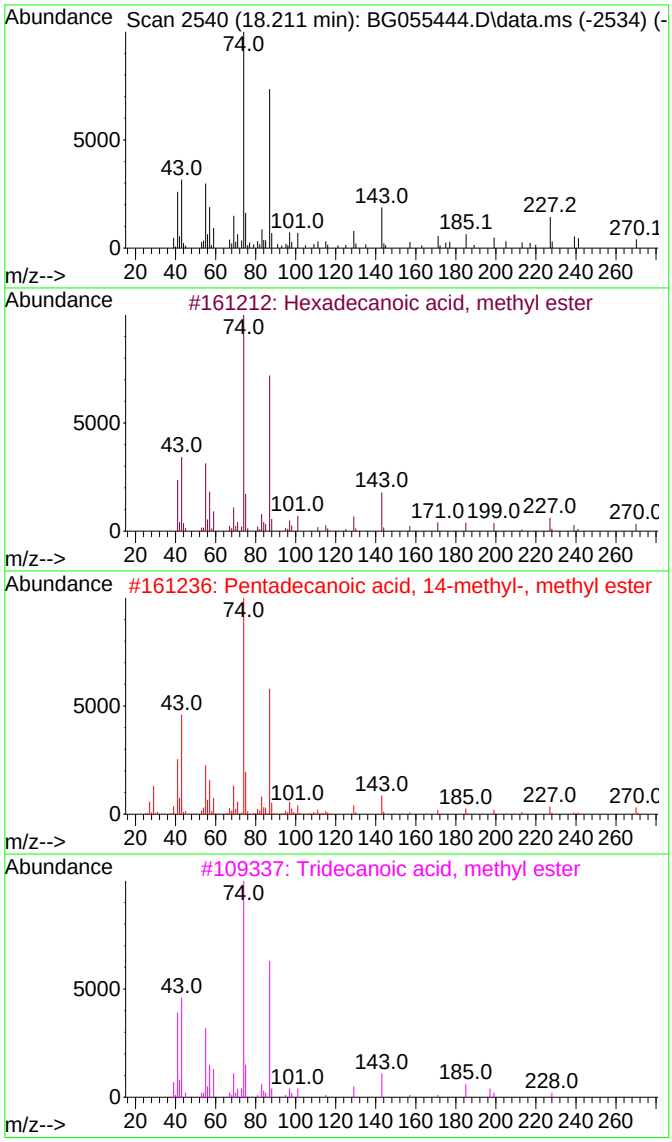
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

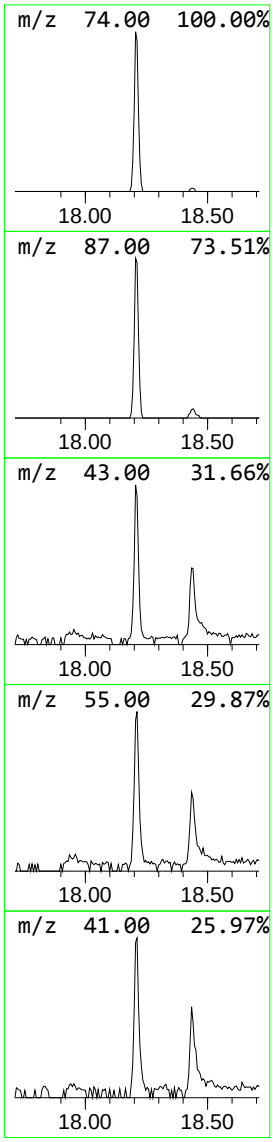
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.211	4.43 ng	101215	Phenanthrene-d10	17.583

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	93
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055444.D
Acq On : 3 Nov 2022 19:26
Operator : CG/JU
Sample : N5306-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221168-COMP-03-MODIFIED-ELUTRIATE

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

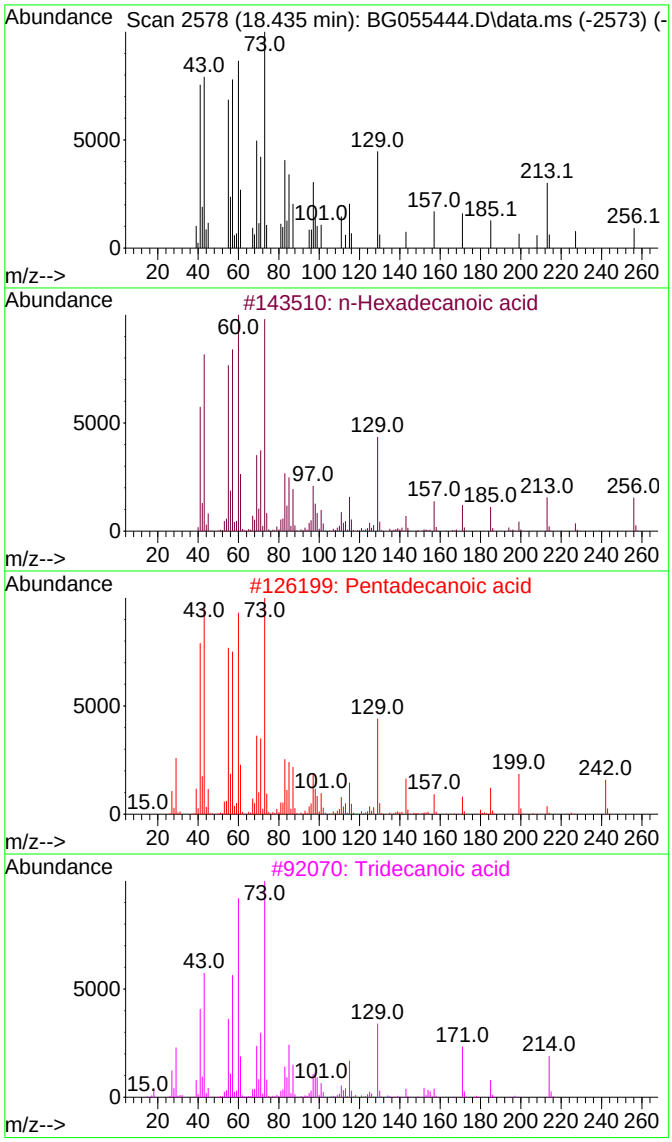
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

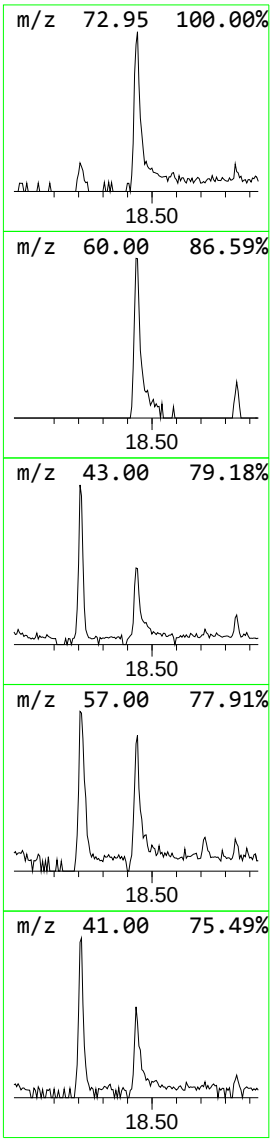
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.435	2.19 ng	49959	Phenanthrene-d10	17.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055444.D
Acq On : 3 Nov 2022 19:26
Operator : CG/JU
Sample : N5306-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221168-COMP-03-MODIFIED-ELUTRIATE

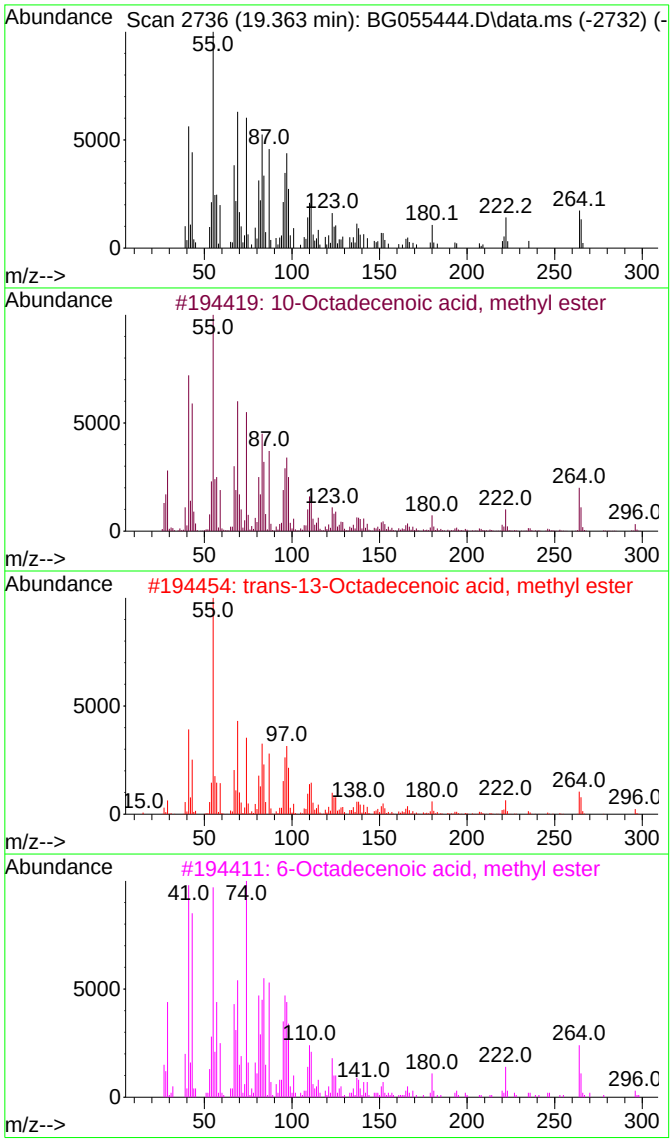
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

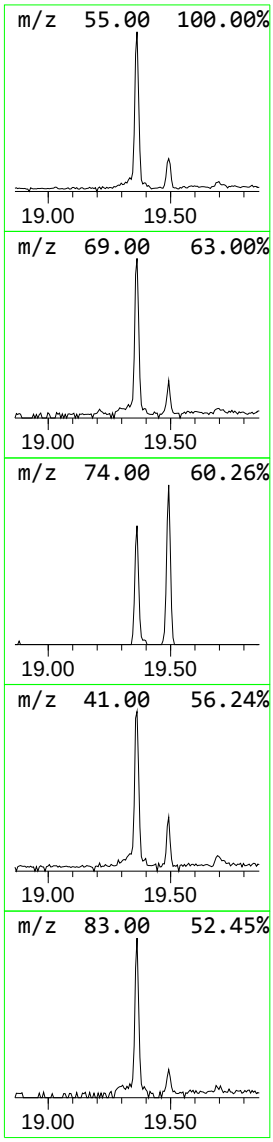
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 10-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.363	6.64 ng	151577	Phenanthrene-d10	17.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	95
2	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	94
3	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	93
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055444.D
Acq On : 3 Nov 2022 19:26
Operator : CG/JU
Sample : N5306-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221168-COMP-03-MODIFIED-ELUTRIATE

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

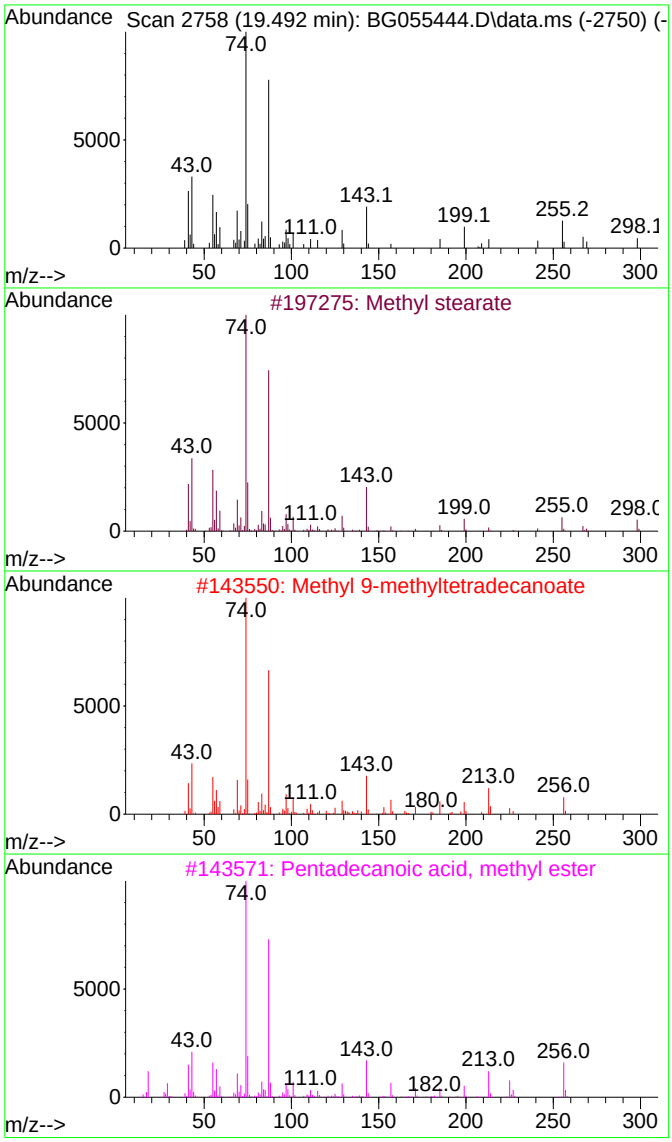
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

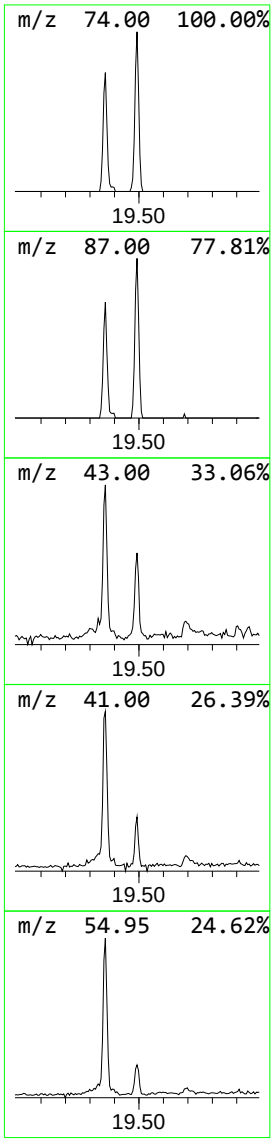
****

Peak Number 7 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.492	2.31 ng	52801	Phenanthrene-d10	17.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	86
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	83
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055444.D
Acq On : 3 Nov 2022 19:26
Operator : CG/JU
Sample : N5306-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221168-COMP-03-MODIFIED-ELUTRIATE

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

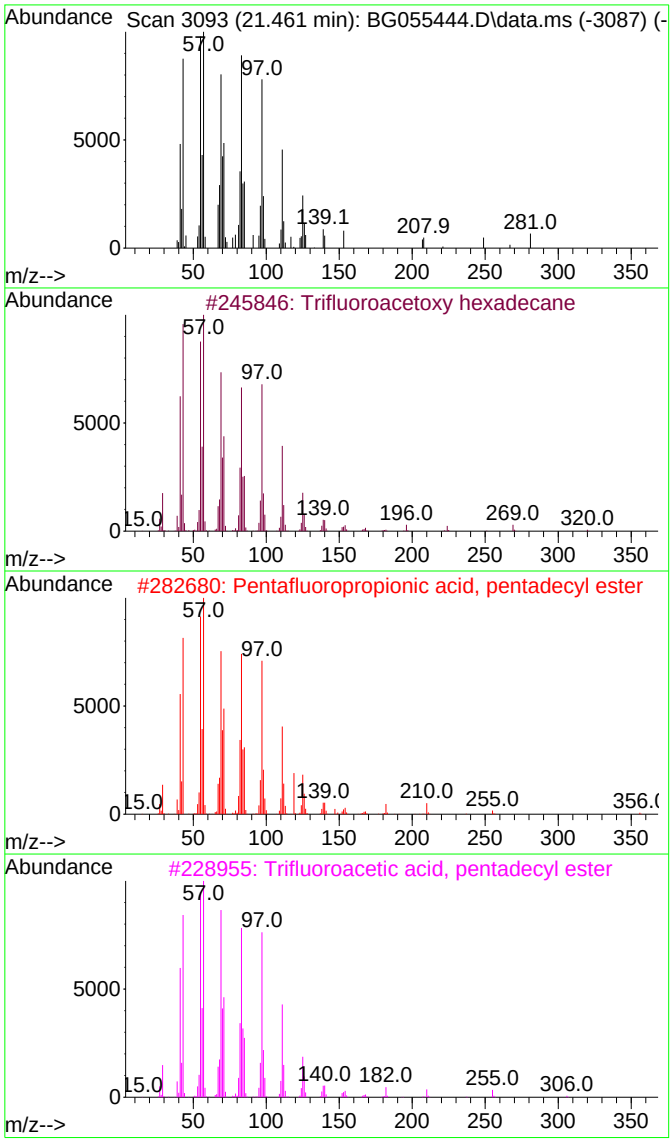
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

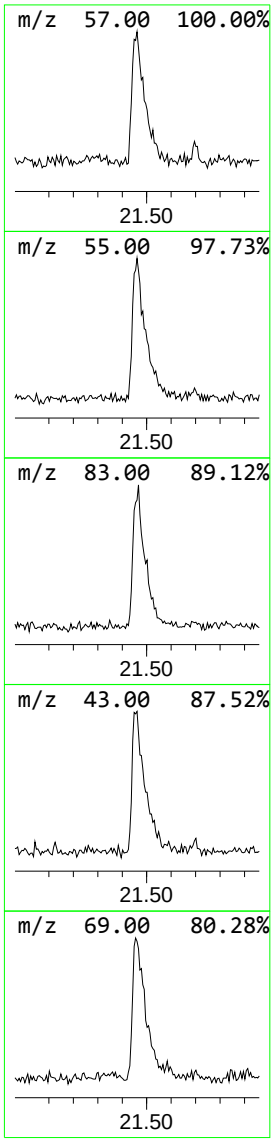
****

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.461	5.47 ng	141789	Chrysene-d12	21.854

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
5	Behenic alcohol	326	C22H46O	000661-19-8	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055444.D
Acq On : 3 Nov 2022 19:26
Operator : CG/JU
Sample : N5306-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221168-COMP-03-MODIFIED-ELUTRIATE

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

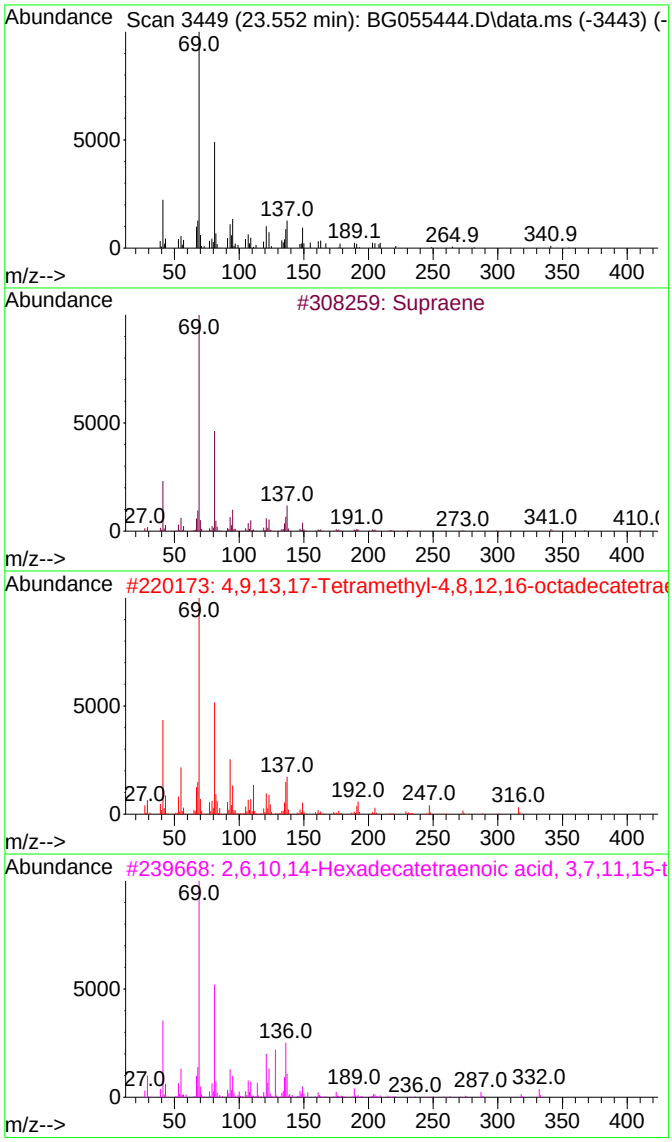
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

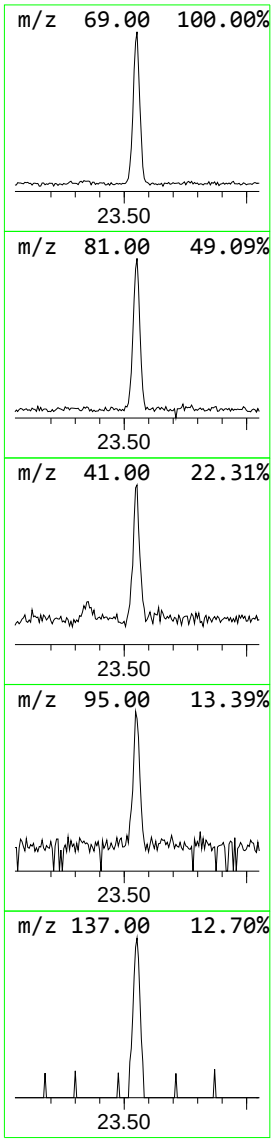
****

Peak Number 9 Supraene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.552	2.16 ng	60155	Perylene-d12	25.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055444.D
Acq On : 3 Nov 2022 19:26
Operator : CG/JU
Sample : N5306-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221168-COMP-03-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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.274	4.1	ng	32201	1	8.235	155787	20.0
Ethanol, 2-(2-b...	10.808	39.0	ng	443200	2	11.067	227493	20.0
2,4,7,9-Tetrame...	13.723	3.8	ng	66490	3	14.851	354751	20.0
Hexadecanoic ac...	18.211	4.4	ng	101215	4	17.583	456450	20.0
n-Hexadecanoic ...	18.435	2.2	ng	49959	4	17.583	456450	20.0
10-Octadecenoic...	19.363	6.6	ng	151577	4	17.583	456450	20.0
Methyl stearate	19.492	2.3	ng	52801	4	17.583	456450	20.0
Trifluoroacetox...	21.461	5.5	ng	141789	5	21.854	518103	20.0
Supraene	23.552	2.2	ng	60155	6	25.227	557102	20.0