LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081221\
Data File : BG049827.D
Acq On : 12 Aug 2021 21:20
Operator : CG/JU
Sample : M3341-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 228-344

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-BG080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049827.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.032	844	850	858	rBV	140614	249086	1.29%	0.534%
2	10.857	1319	1331	1338	rBV	202133	373656	1.93%	0.801%
3	13.301	1737	1747	1755	rVB	187690	296105	1.53%	0.635%
4	14.687	1975	1983	1990	rVB	313425	485382	2.51%	1.040%
5	16.179	2230	2237	2245	rVB	144763	219281	1.13%	0.470%
6	17.442	2445	2452	2458	rBV	325199	511880	2.64%	1.097%
7	17.965	2537	2541	2547	rVB	175965	231563	1.20%	0.496%
8	18.100	2557	2564	2569	rBV	3924700	4861968	25.12%	10.420%
9	18.335	2598	2604	2614	rBV	130952	221127	1.14%	0.474%
10	19.246	2751	2759	2762	rBV	8740556	14828719	76.61%	31.781%
11	19.287	2762	2766	2774	rVB	14840927	19355375	100.00%	41.483%
12	19.399	2780	2785	2791	rVB	2204514	2609400	13.48%	5.592%
13	19.487	2797	2800	2811	rVB3	220102	382009	1.97%	0.819%
14	20.051	2892	2896	2903	rVB	262262	384427	1.99%	0.824%
15	20.374	2945	2951	2958	rVB2	238699	379943	1.96%	0.814%
16	20.485	2966	2970	2973	rBV	181714	211015	1.09%	0.452%
17	21.126	3074	3079	3085	rVB4	102315	218332	1.13%	0.468%
18	21.731	3176	3182	3199	rVB	264654	524464	2.71%	1.124%
19	25.015	3736	3741	3750	rVB3	121034	315233	1.63%	0.676%

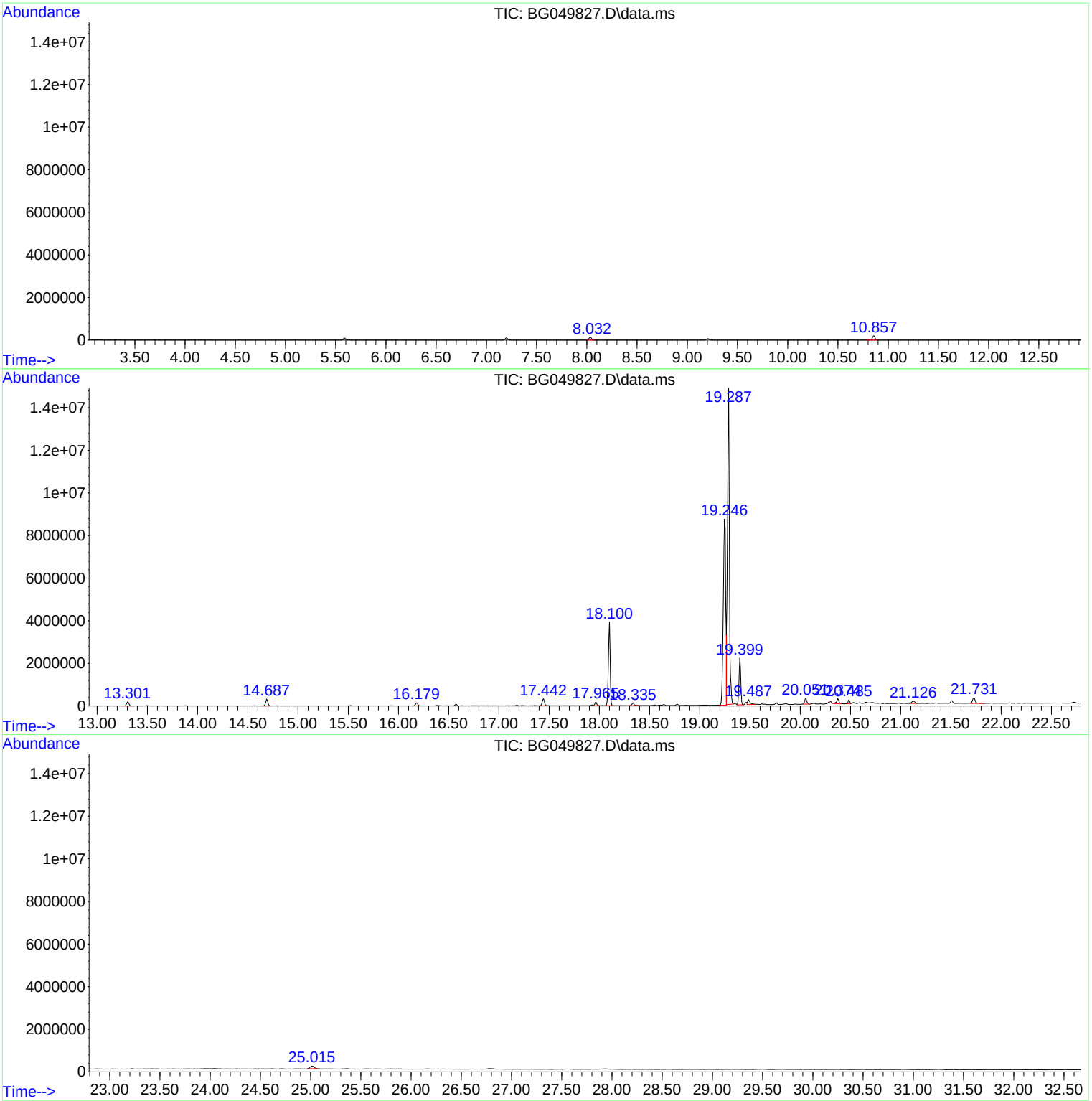
Sum of corrected areas: 46658965

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081221\
Data File : BG049827.D
Acq On : 12 Aug 2021 21:20
Operator : CG/JU
Sample : M3341-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
228-344

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.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\BG081221\
Data File : BG049827.D
Acq On : 12 Aug 2021 21:20
Operator : CG/JU
Sample : M3341-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 228-344

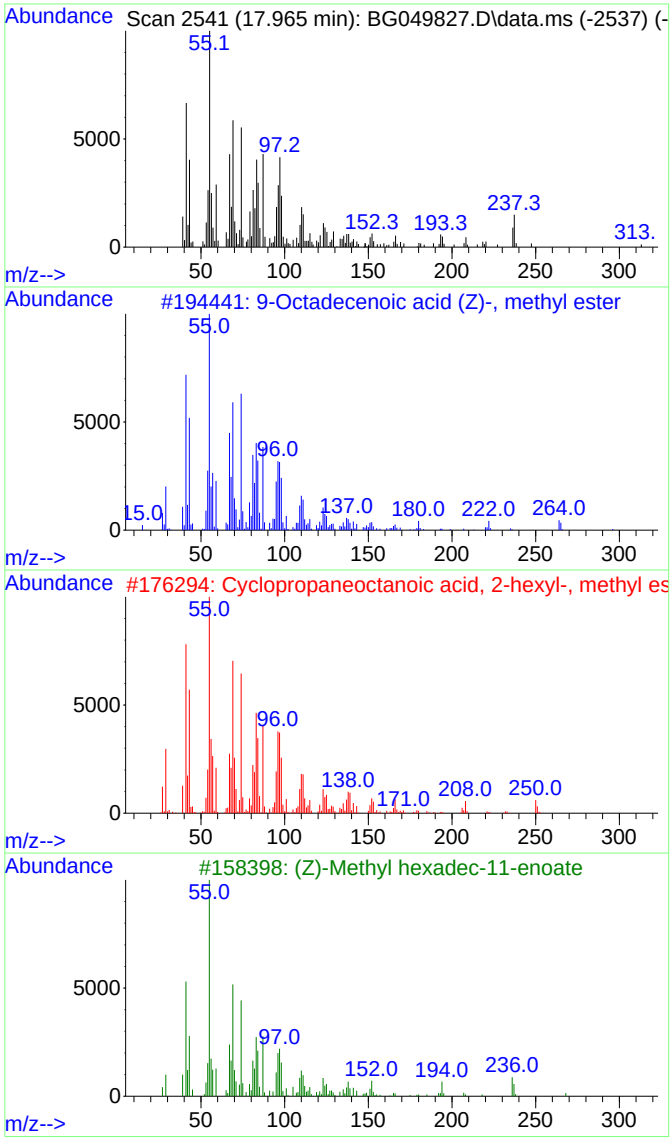
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

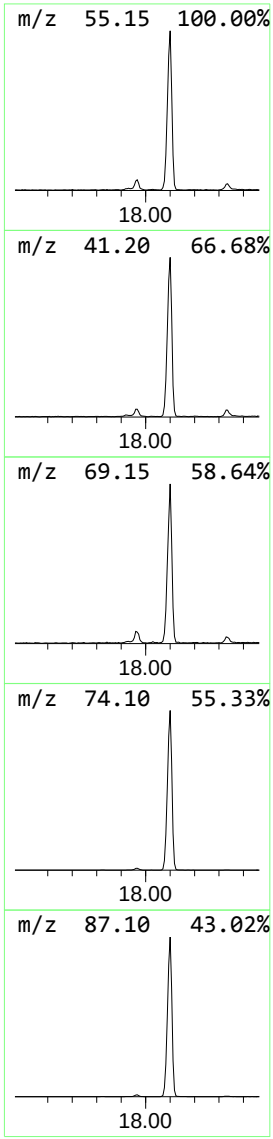
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 9-Octadecenoic acid (Z)-, m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.965	9.05 ng	231563	Phenanthrene-d10	17.442

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	87
2	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	76
3	(Z)-Methyl hexadec-11-enoate	268	C17H32O2	000822-05-9	72
4	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	72
5	cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081221\
Data File : BG049827.D
Acq On : 12 Aug 2021 21:20
Operator : CG/JU
Sample : M3341-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 228-344

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

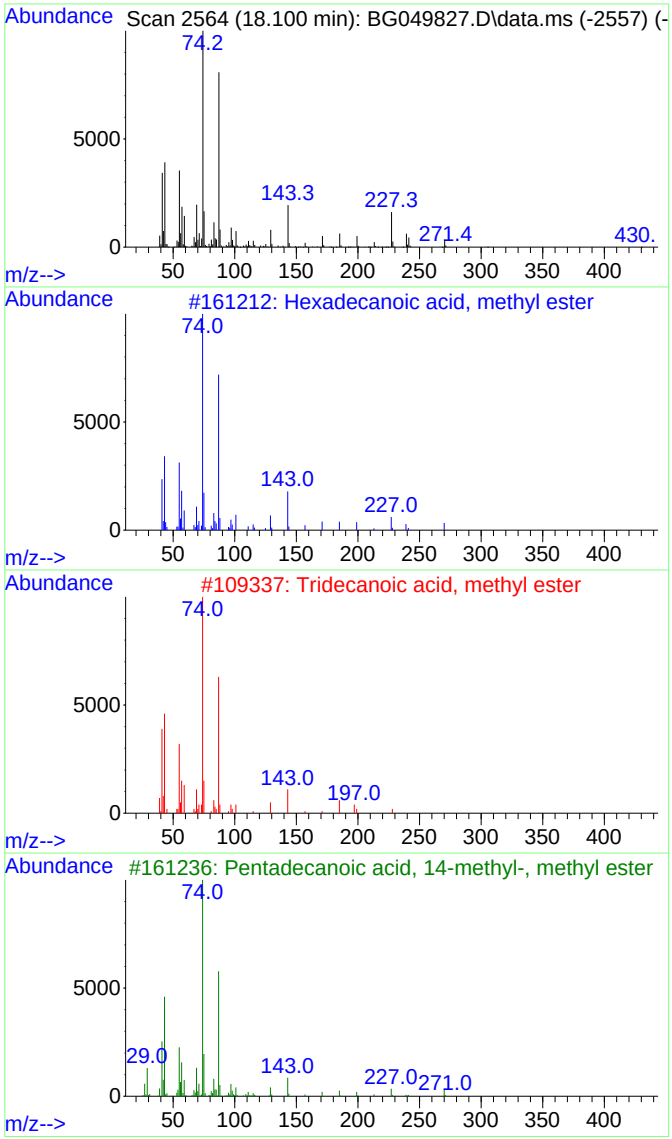
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

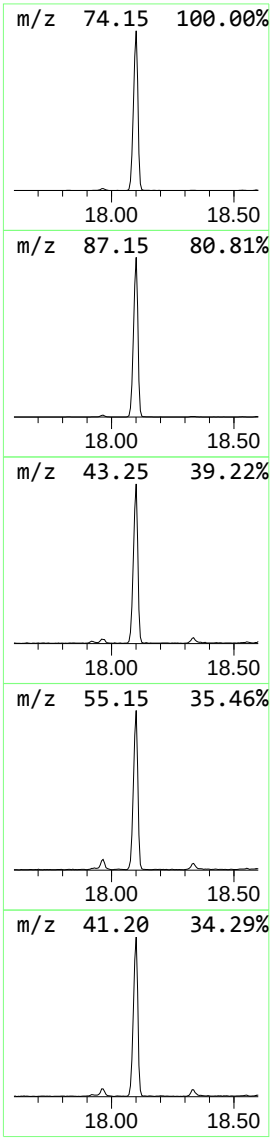
****

Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.100	189.97 ng	4861970	Phenanthrene-d10	17.442

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	95
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	83
5	Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	83





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Data File : BG049827.D
Acq On : 12 Aug 2021 21:20
Operator : CG/JU
Sample : M3341-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 228-344

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

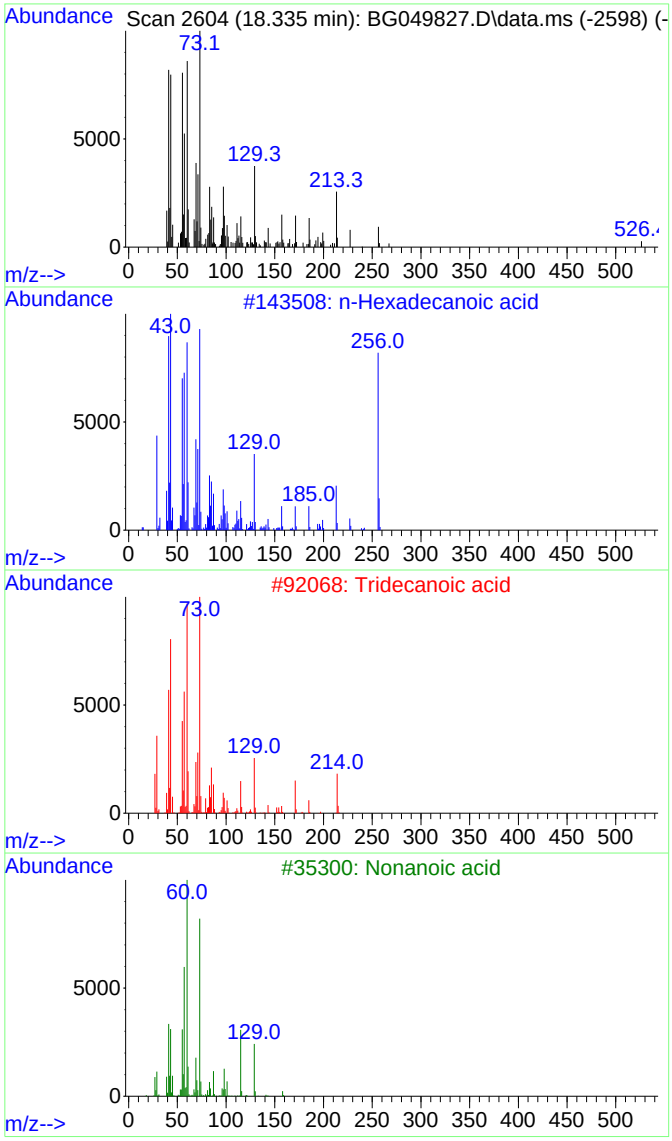
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

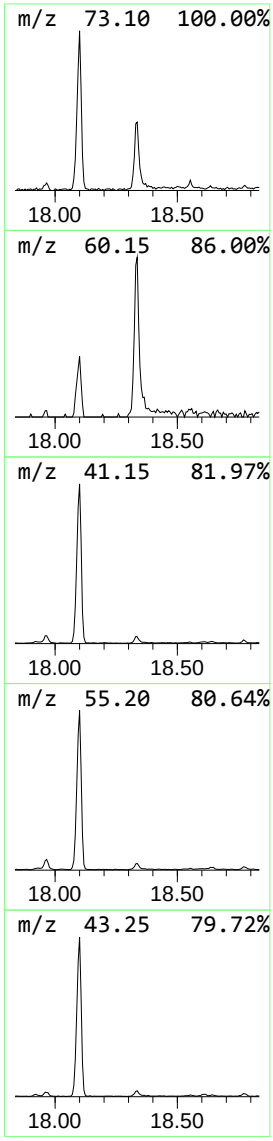
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.335	8.64 ng	221127	Phenanthrene-d10	17.442

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	70
3	Nonanoic acid	158	C9H18O2	000112-05-0	60
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081221\
Data File : BG049827.D
Acq On : 12 Aug 2021 21:20
Operator : CG/JU
Sample : M3341-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 228-344

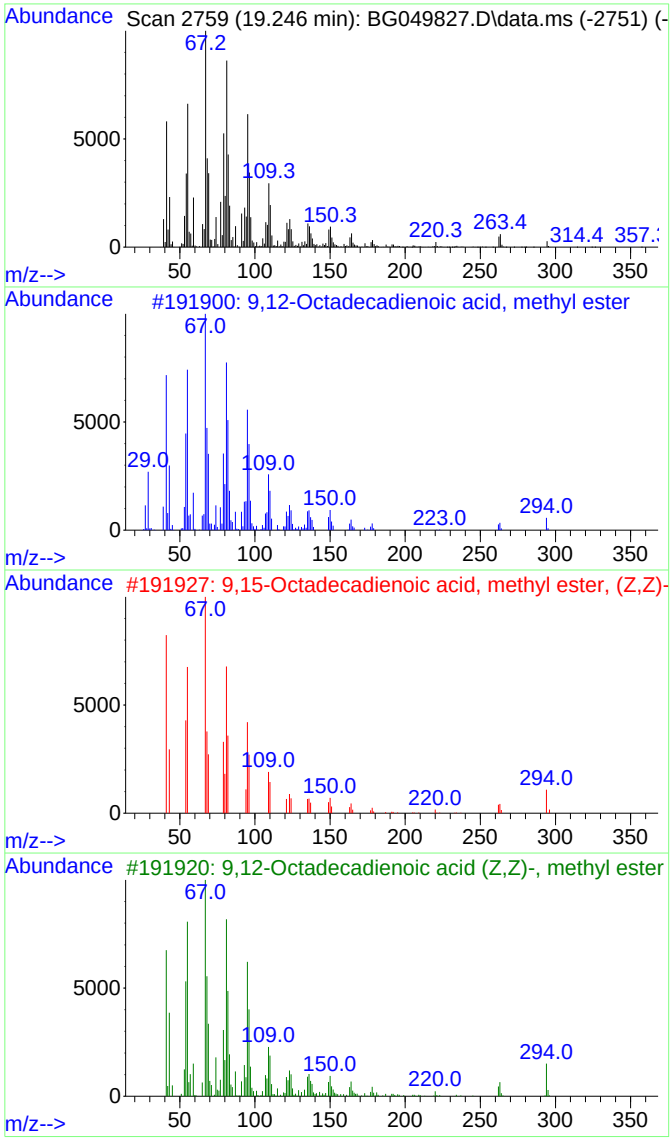
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

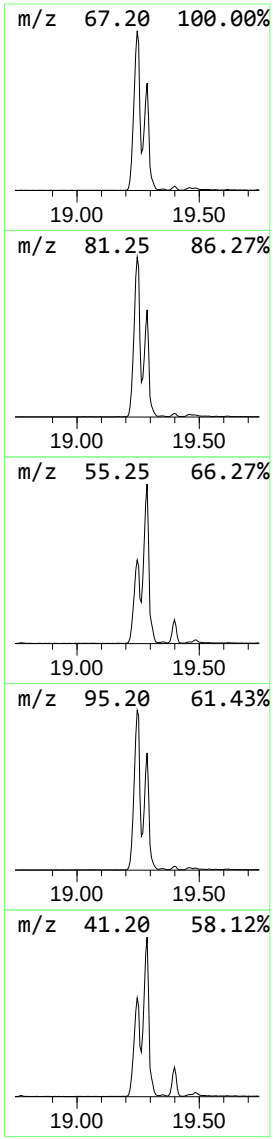
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.246	579.38 ng	14828700	Phenanthrene-d10	17.442

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	98
5	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	96





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081221\
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Acq On : 12 Aug 2021 21:20
Operator : CG/JU
Sample : M3341-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 228-344

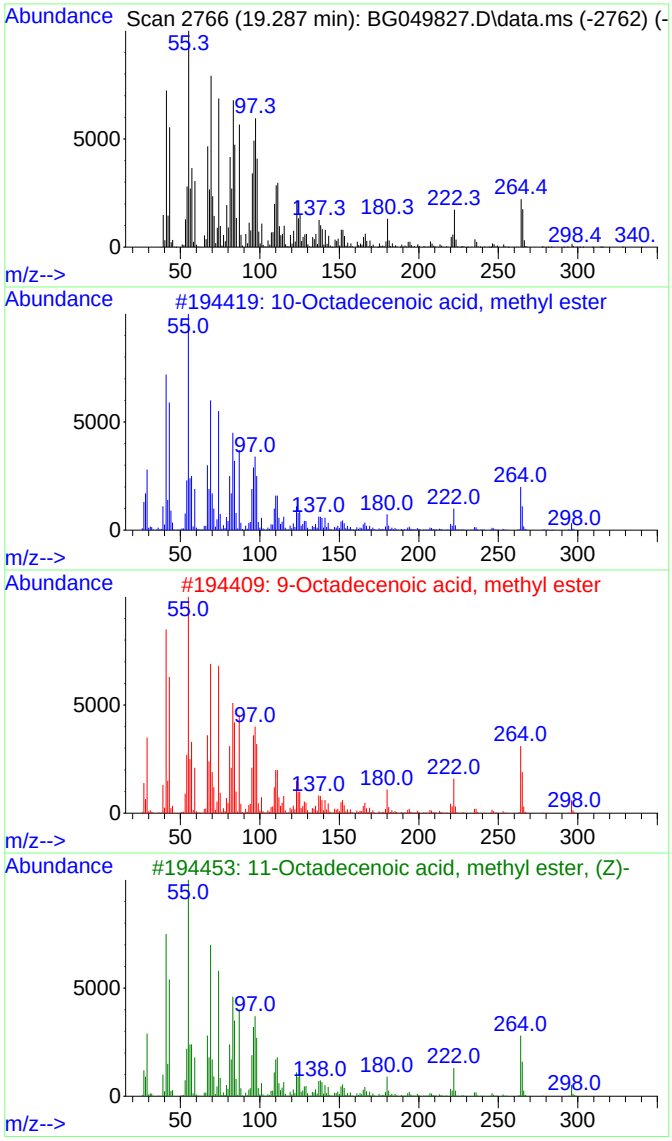
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

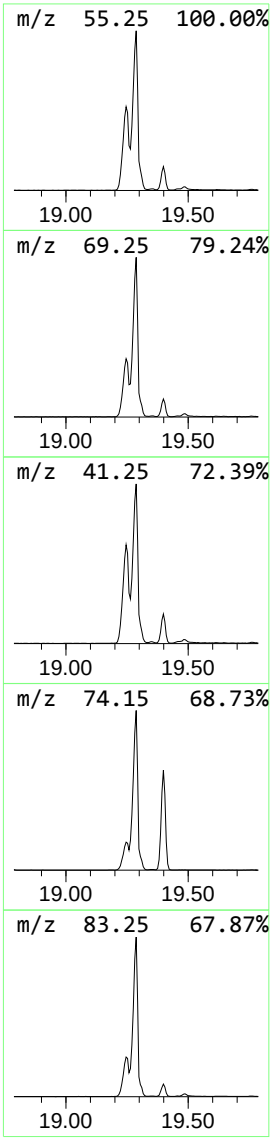
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 10-Octadecenoic acid, methy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.287	756.25 ng	19355400	Phenanthrene-d10	17.442

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
2	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
3	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
5	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99





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Operator : CG/JU
Sample : M3341-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 228-344

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

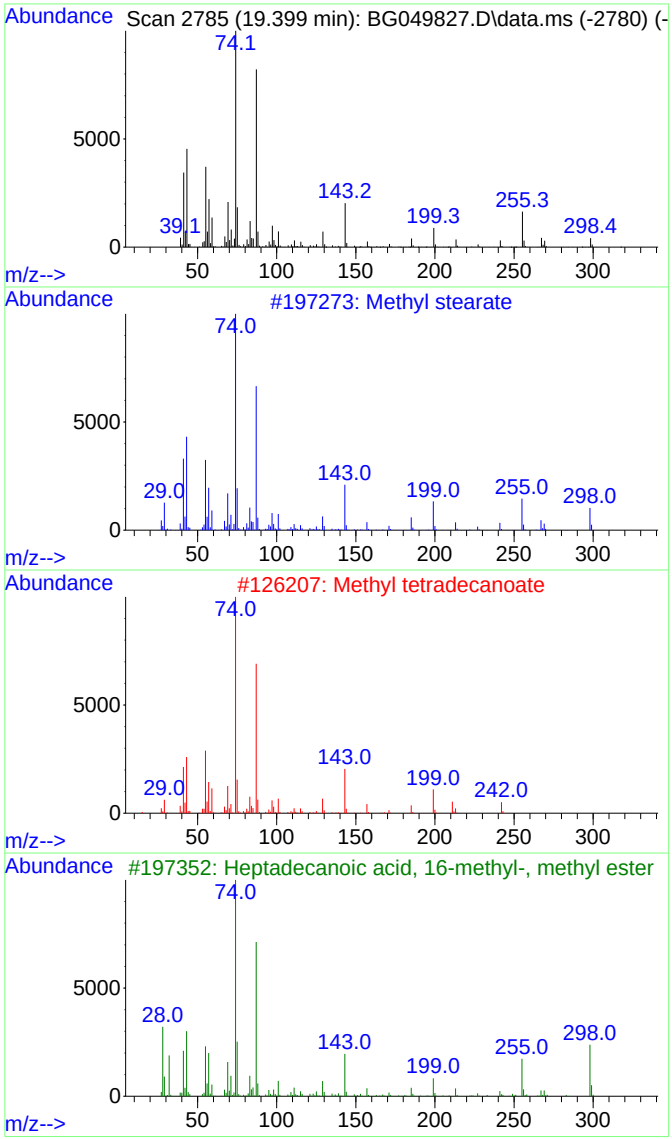
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

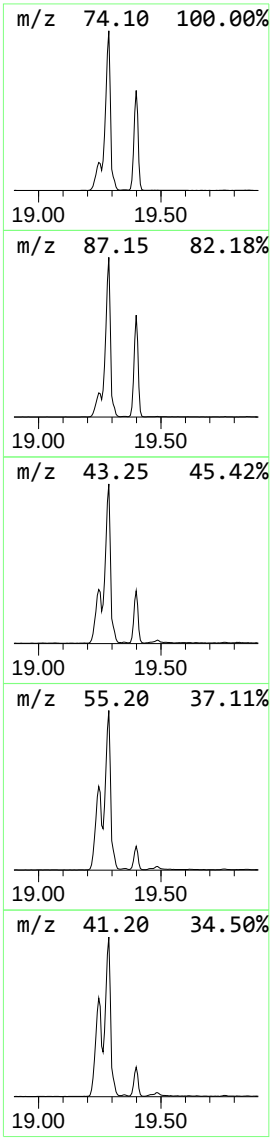
****

Peak Number 6 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.399	101.95 ng	2609400	Phenanthrene-d10	17.442

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	90
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	89
4	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	83





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Operator : CG/JU
Sample : M3341-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 228-344

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

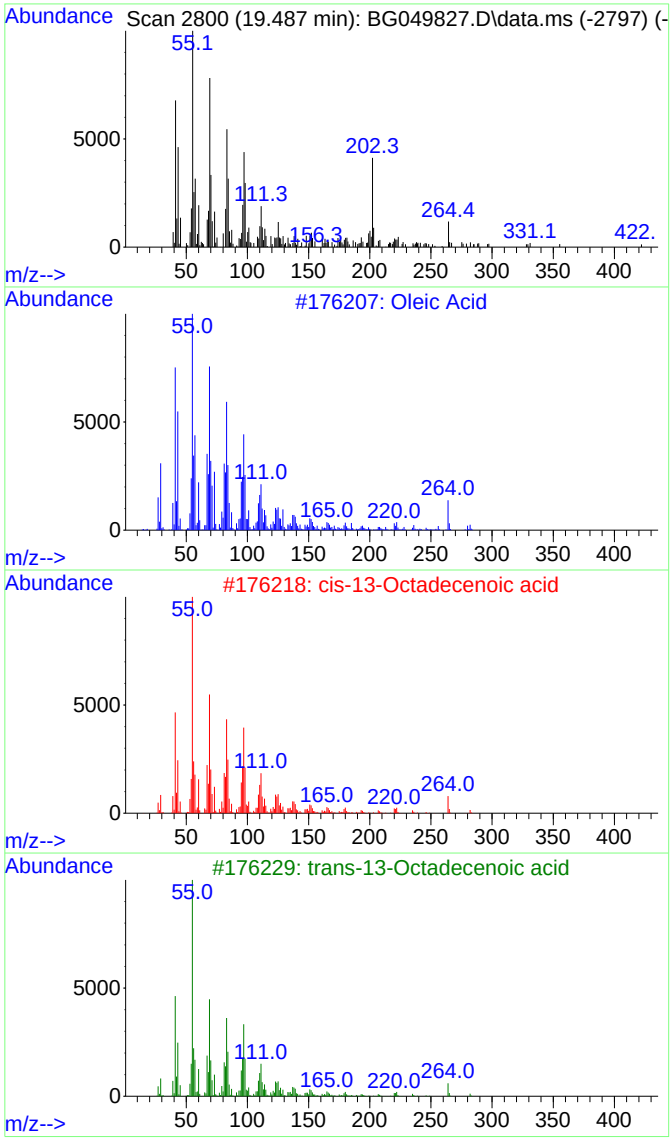
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

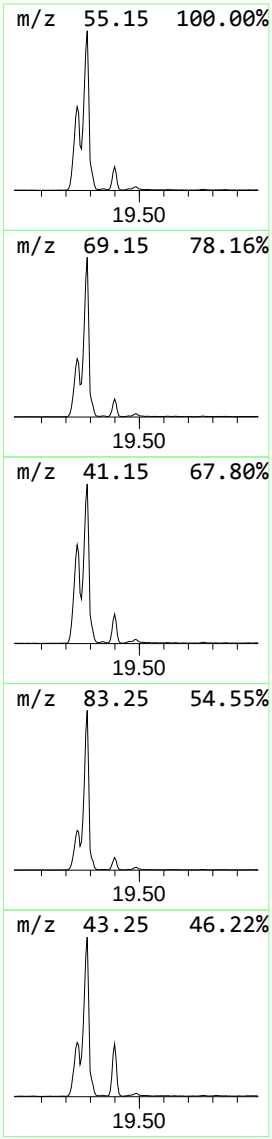
****

Peak Number 7 Oleic Acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.487	14.93 ng	382009	Phenanthrene-d10	17.442

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	91
2	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	90
3	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	89
4	cis-Vaccenic acid	282	C18H34O2	000506-17-2	59
5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	52





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Operator : CG/JU
Sample : M3341-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 228-344

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

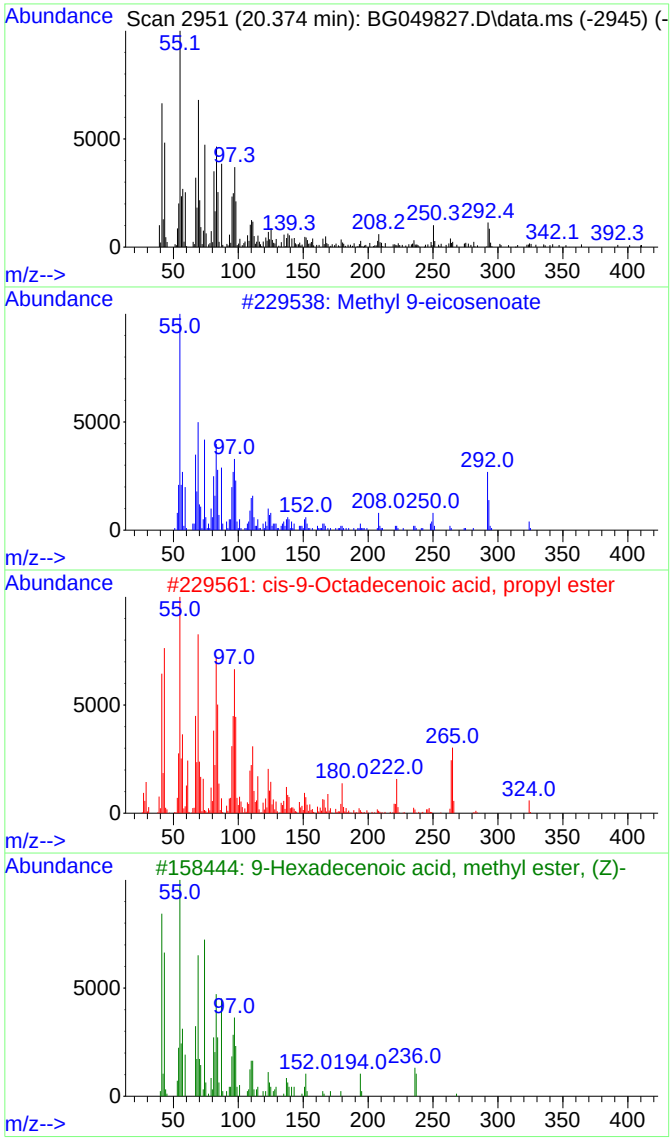
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

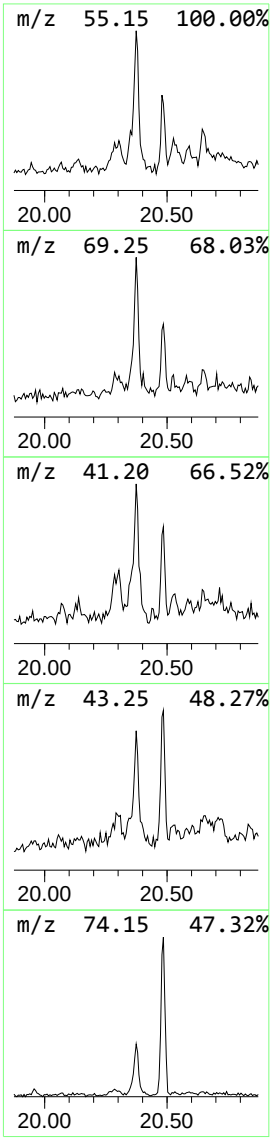
****

Peak Number 8 Methyl 9-eicosenoate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.374	14.49 ng	379943	Chrysene-d12	21.725

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	93
2	cis-9-Octadecenoic acid, propyl ...	324	C21H40O2	1000405-15-0	91
3	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	90
4	cis-Vaccenic acid	282	C18H34O2	000506-17-2	89
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	87





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Sample : M3341-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 228-344

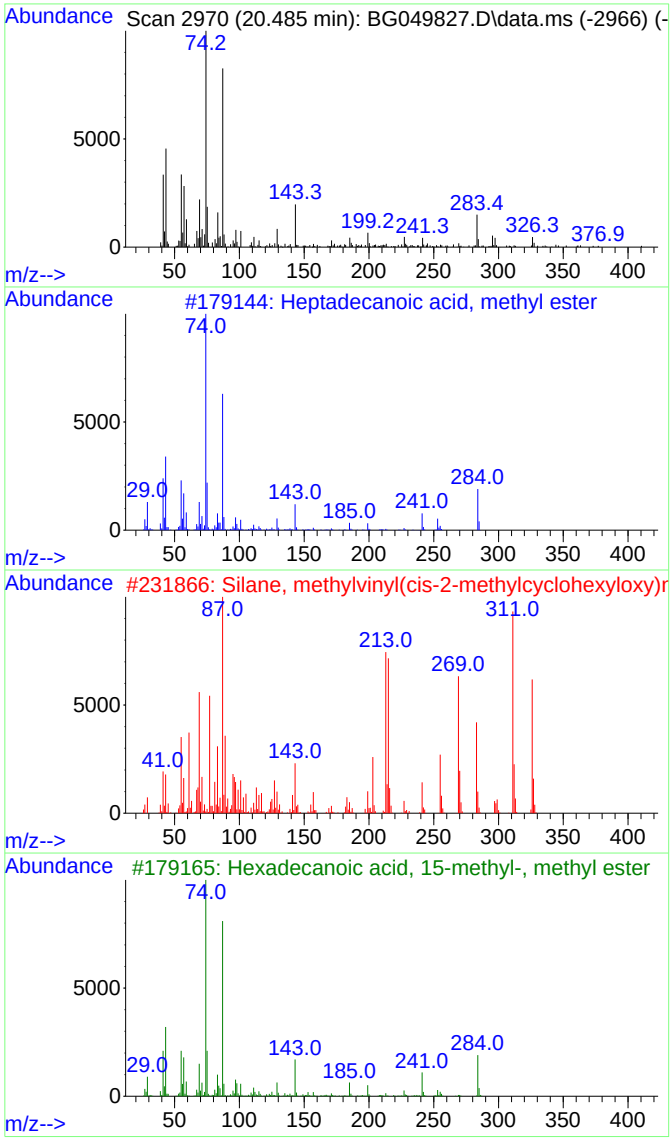
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

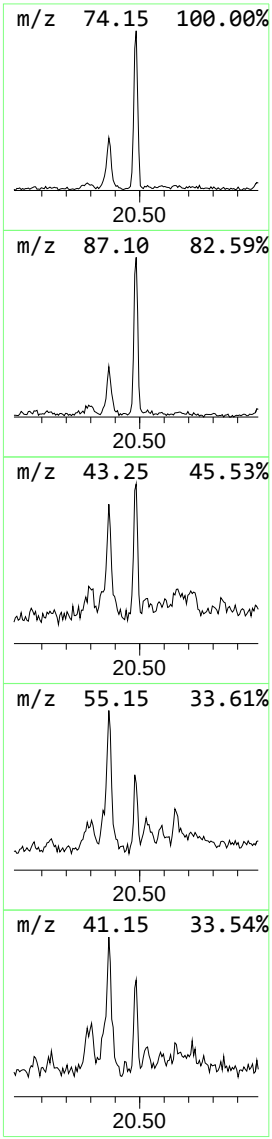
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Heptadecanoic acid, methyl ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.485	8.05 ng	211015	Chrysene-d12	21.725

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
2	Silane, methylvinyl(cis-2-methyl...	326	C19H38O2Si	1000421-05-3	90
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	90
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
5	Methyl stearate	298	C19H38O2	000112-61-8	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081221\
Data File : BG049827.D
Acq On : 12 Aug 2021 21:20
Operator : CG/JU
Sample : M3341-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 228-344

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

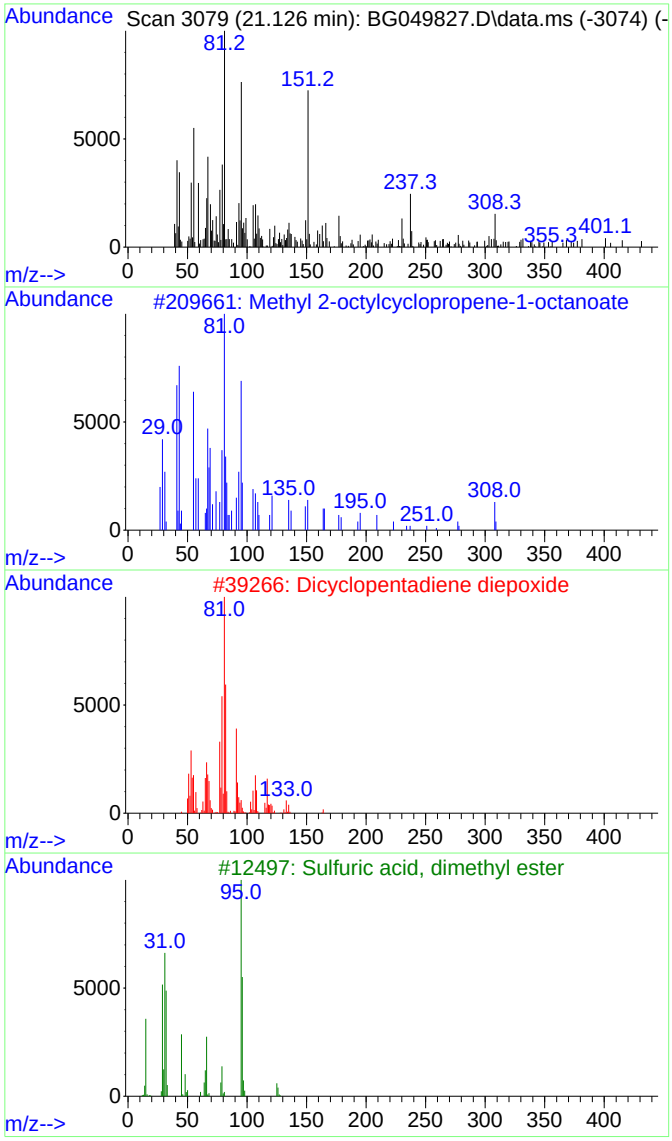
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

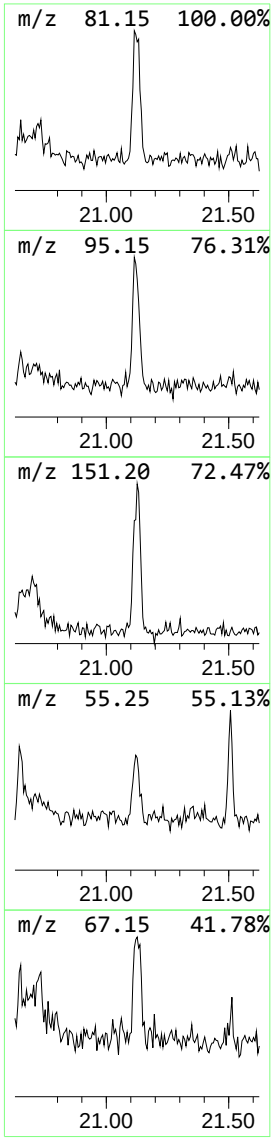
****

Peak Number 10 unknown21.126 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.126	8.33 ng	218332	Chrysene-d12	21.725

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 2-octylcyclopropene-1-oct...	308	C20H36O2	003220-60-8	47
2	Dicyclopentadiene diepoxide	164	C10H12O2	000081-21-0	46
3	Sulfuric acid, dimethyl ester	126	C2H6O4S	000077-78-1	35
4	1,3,7-Octatriene, 2,7-dimethyl-	136	C10H16	036638-38-7	25
5	Trifluoroacetyl-.alpha.-fenchol	250	C12H17F3O2	031076-73-0	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081221\
Data File : BG049827.D
Acq On : 12 Aug 2021 21:20
Operator : CG/JU
Sample : M3341-01 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 228-344

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.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
9-Octadecenoic ...	17.965	9.1	ng	231563	4	17.442	511880	20.0
Hexadecanoic ac...	18.100	190.0	ng	4861970	4	17.442	511880	20.0
n-Hexadecanoic ...	18.335	8.6	ng	221127	4	17.442	511880	20.0
9,12-Octadecadi...	19.246	579.4	ng	14828700	4	17.442	511880	20.0
10-Octadecenoic...	19.287	756.3	ng	19355400	4	17.442	511880	20.0
Methyl stearate	19.399	102.0	ng	2609400	4	17.442	511880	20.0
Oleic Acid	19.487	14.9	ng	382009	4	17.442	511880	20.0
Methyl 9-eicose...	20.374	14.5	ng	379943	5	21.725	524464	20.0
Heptadecanoic a...	20.485	8.1	ng	211015	5	21.725	524464	20.0
unknown21.126	21.126	8.3	ng	218332	5	21.725	524464	20.0