LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028472.D
Acq On : 20 Jan 2021 17:42
Operator : CG/JU
Sample : M1161-01 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TR-05-011521

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_M\Methods\8270-BM012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028472.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.034	811	824	830	rBV	129685	209508	1.34%	0.577%
2	10.851	1297	1303	1309	rVB	165932	276525	1.77%	0.762%
3	14.674	1947	1953	1960	rVB	224385	337830	2.16%	0.931%
4	17.398	2410	2416	2421	rBV	257859	359533	2.30%	0.991%
5	18.057	2521	2528	2532	rBV	3710807	4845429	31.01%	13.354%
6	18.274	2560	2565	2578	rBV2	99551	175273	1.12%	0.483%
7	19.204	2714	2723	2725	rBV	7055491	15624406	100.00%	43.062%
8	19.233	2725	2728	2736	rVV3	6835800	10643799	68.12%	29.335%
9	19.345	2742	2747	2752	rVB	1932320	2160101	13.83%	5.953%
10	19.992	2852	2857	2861	rBV	134127	175226	1.12%	0.483%
11	20.421	2927	2930	2933	rBV	179363	197195	1.26%	0.543%
12	20.462	2933	2937	2943	rVV4	118864	210936	1.35%	0.581%
13	20.521	2943	2947	2951	rVV	121992	163303	1.05%	0.450%
14	21.356	3086	3089	3096	rVB	188428	211094	1.35%	0.582%
15	21.527	3114	3118	3123	rBV	300418	353629	2.26%	0.975%
16	23.815	3503	3507	3513	rVB2	189278	339378	2.17%	0.935%

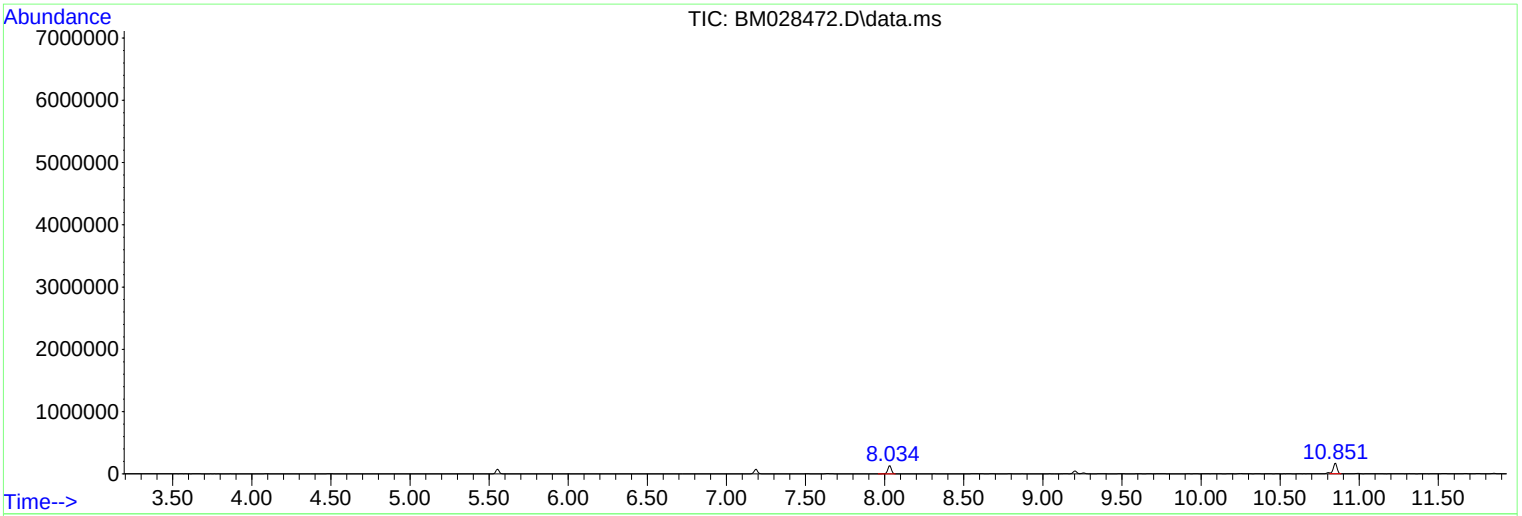
Sum of corrected areas: 36283165

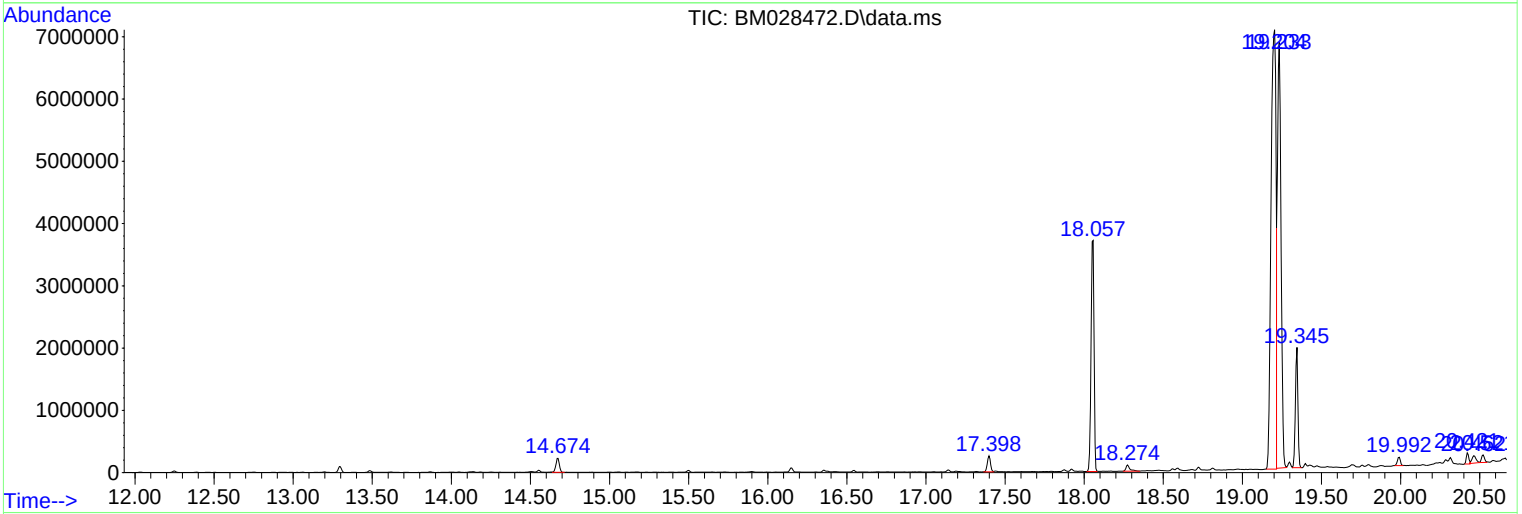
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028472.D
Acq On : 20 Jan 2021 17:42
Operator : CG/JU
Sample : M1161-01 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

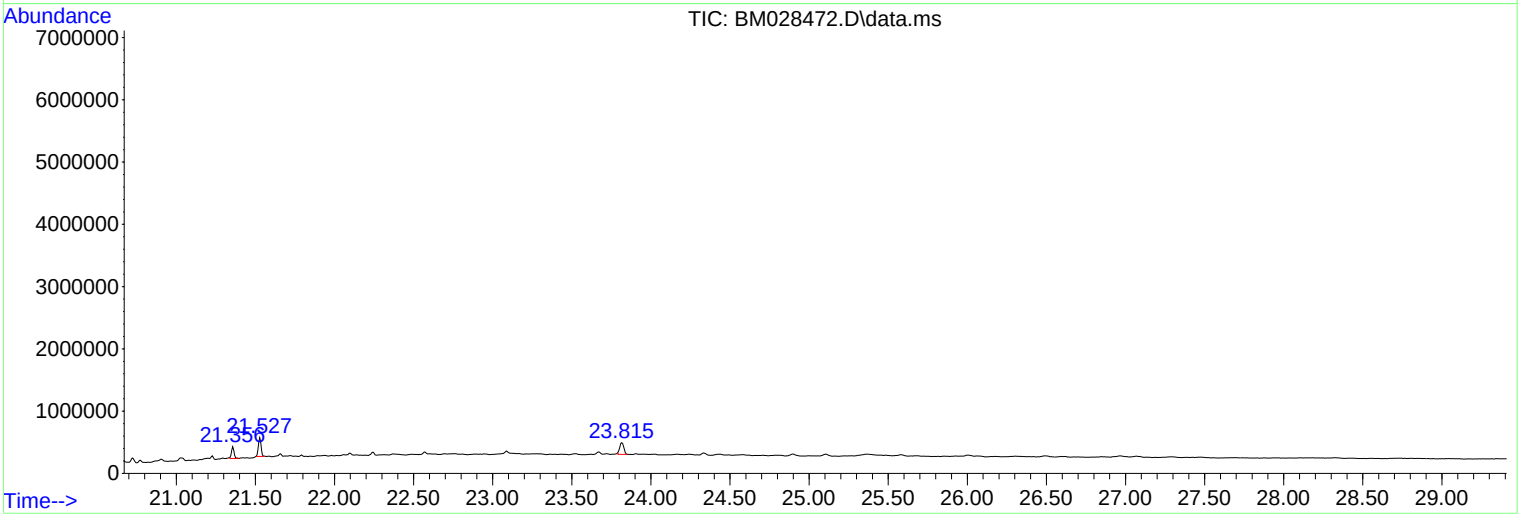
Instrument :
BNA_M
ClientSampleId :
TR-05-011521

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028472.D
Acq On : 20 Jan 2021 17:42
Operator : CG/JU
Sample : M1161-01 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TR-05-011521

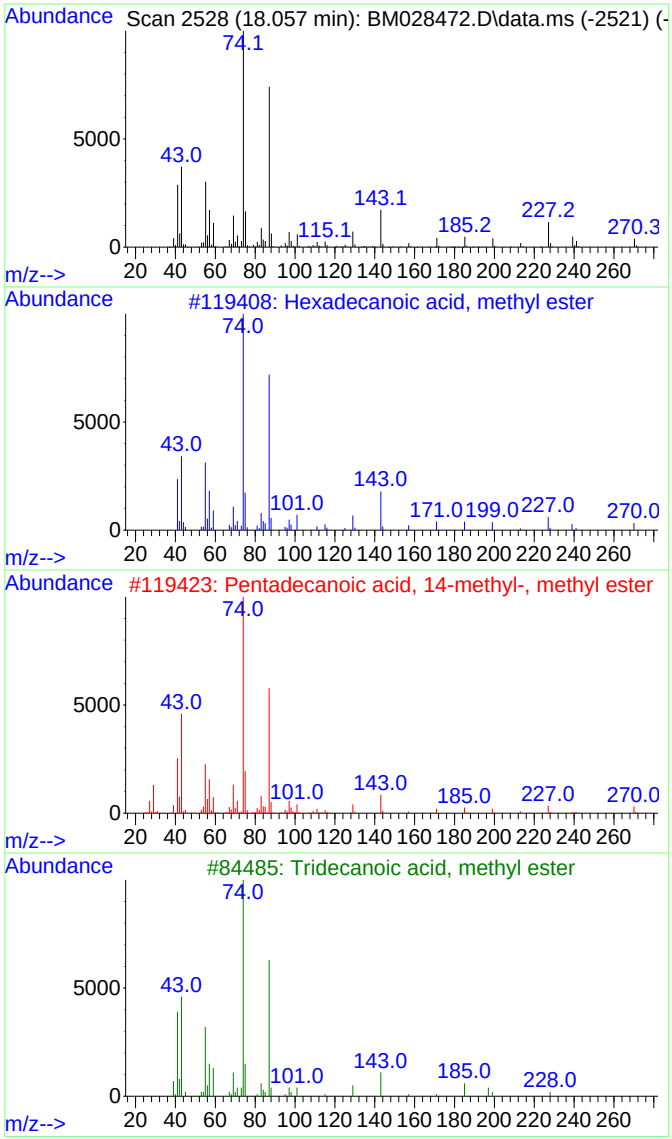
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

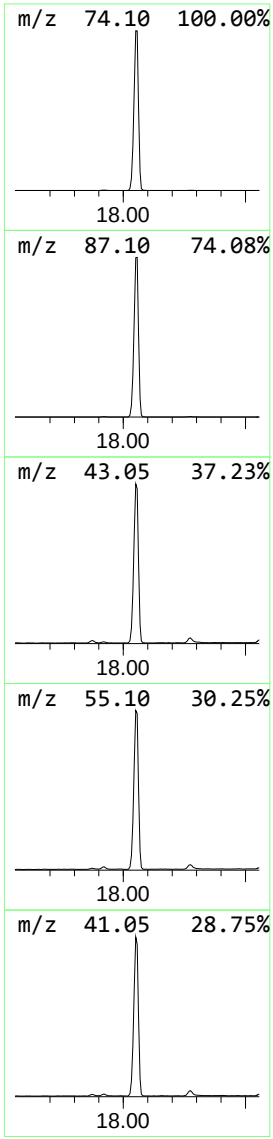
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.057	269.54 ng	4845430	Phenanthrene-d10	17.398

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	95
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028472.D
Acq On : 20 Jan 2021 17:42
Operator : CG/JU
Sample : M1161-01 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TR-05-011521

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

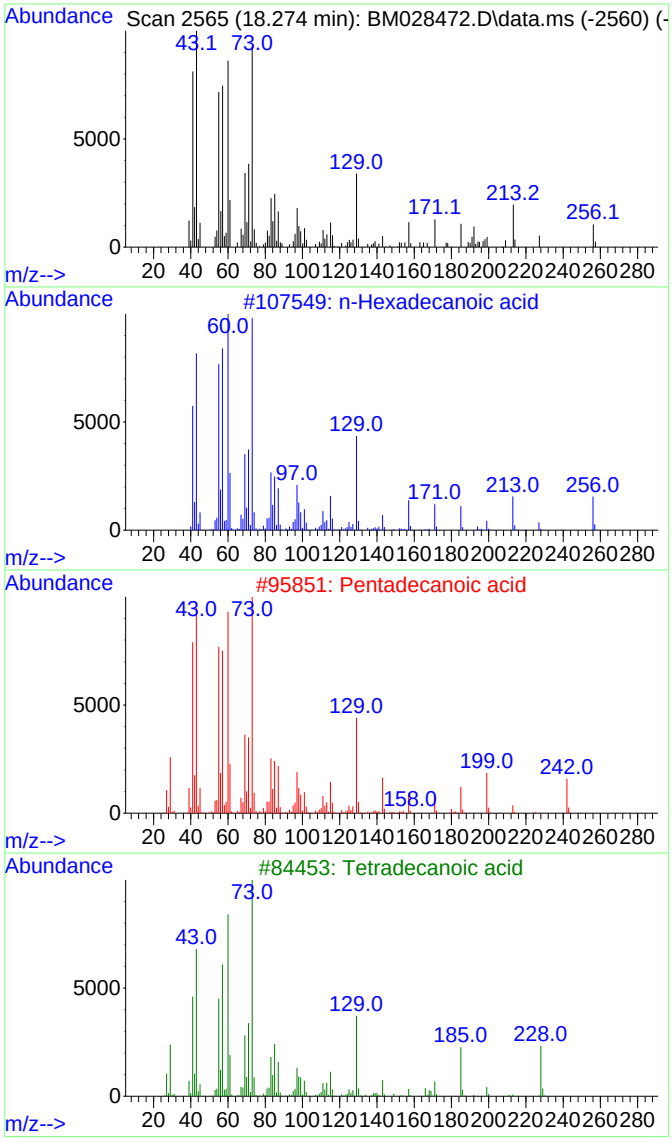
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

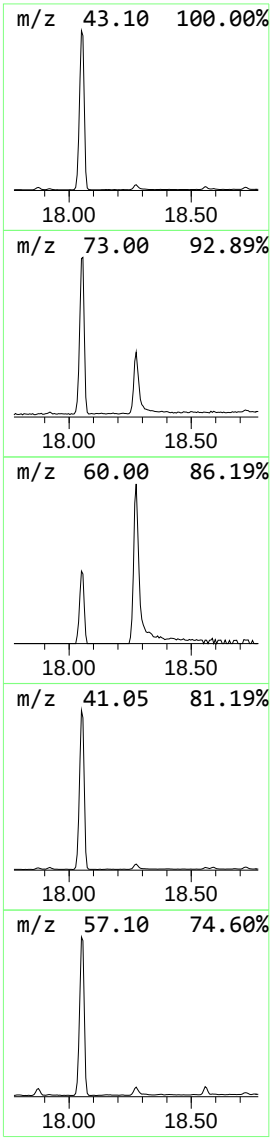
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.274	9.75 ng	175273	Phenanthrene-d10	17.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	Isoamyl nitrite	117	C5H11NO2	000110-46-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028472.D
Acq On : 20 Jan 2021 17:42
Operator : CG/JU
Sample : M1161-01 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TR-05-011521

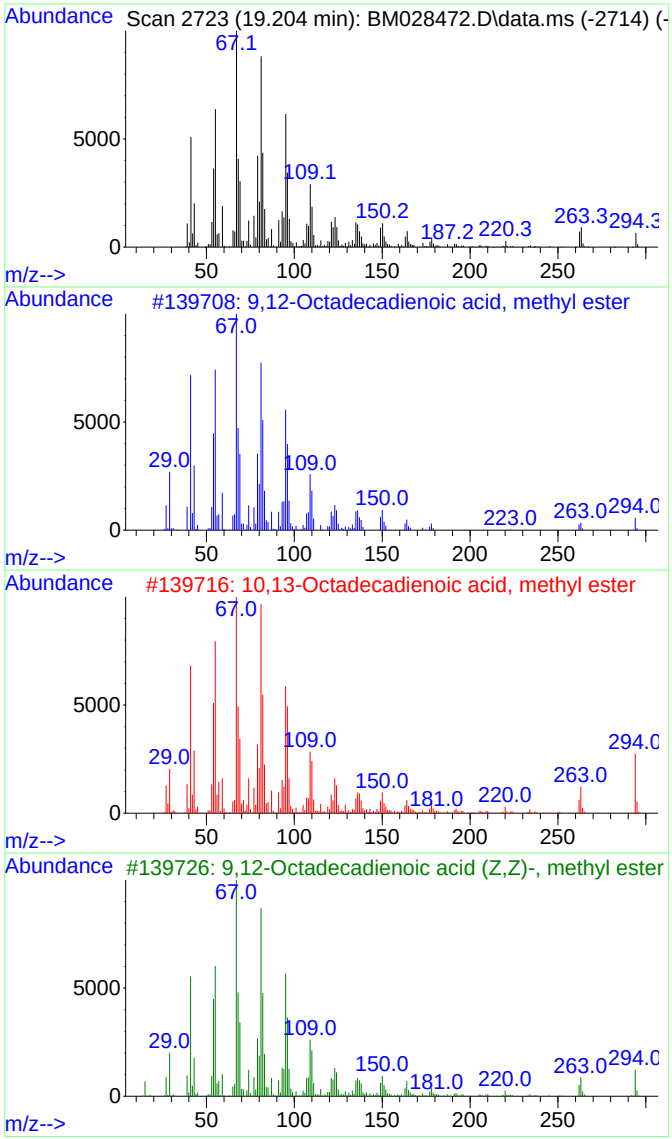
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

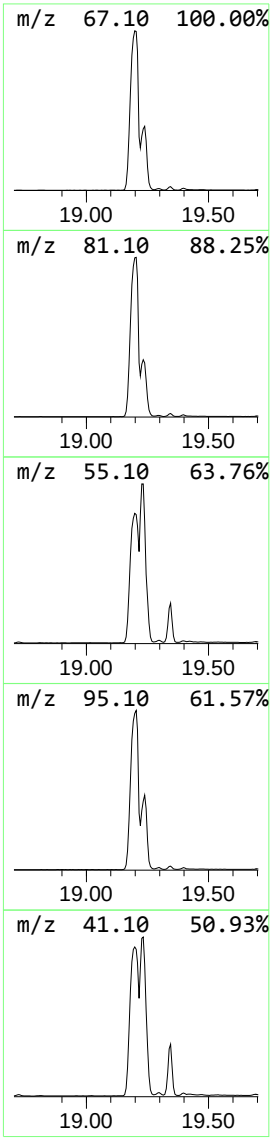
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.204	869.15 ng	15624400	Phenanthrene-d10	17.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028472.D
Acq On : 20 Jan 2021 17:42
Operator : CG/JU
Sample : M1161-01 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TR-05-011521

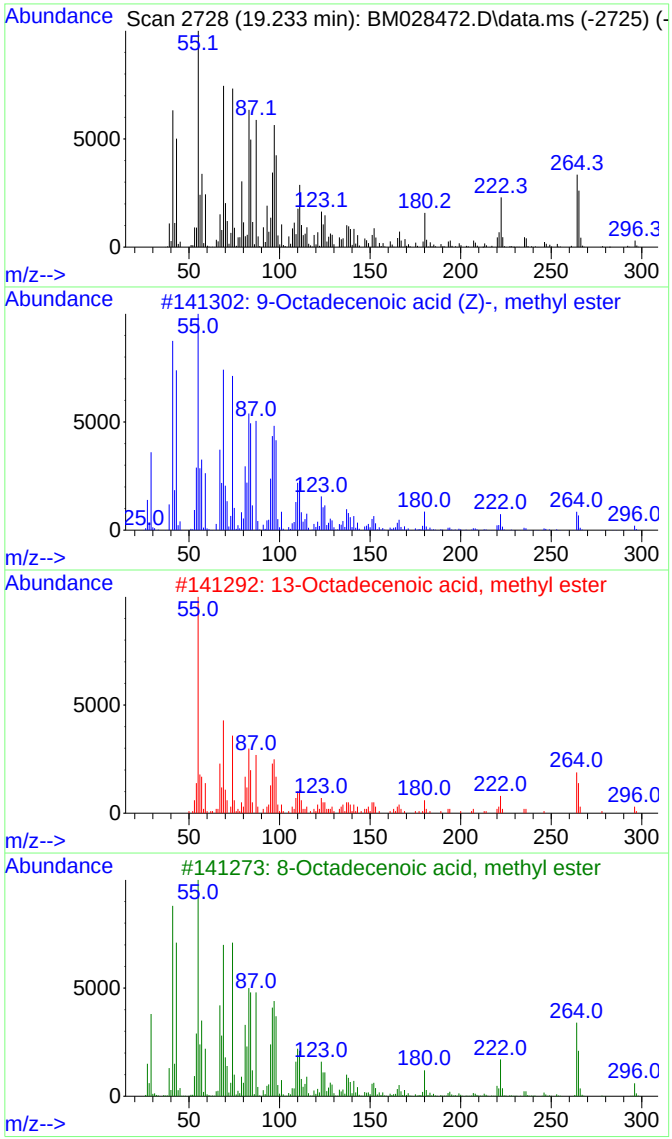
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

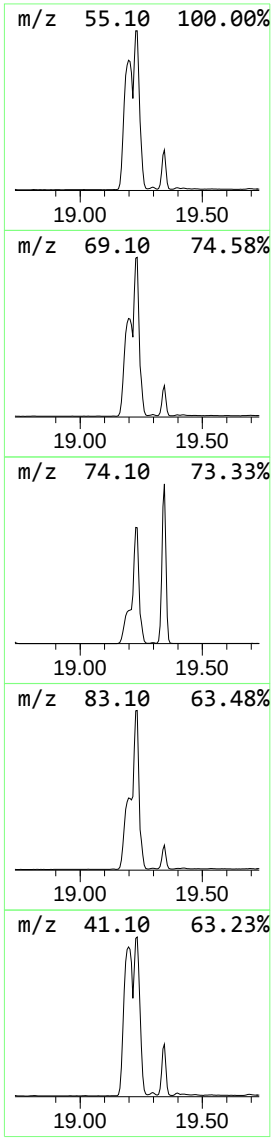
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.233	592.09 ng	10643800	Phenanthrene-d10	17.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	87
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	81
3	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	74
4	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	70
5	3-Octadecenoic acid, methyl ester	296	C19H36O2	056599-33-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028472.D
Acq On : 20 Jan 2021 17:42
Operator : CG/JU
Sample : M1161-01 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TR-05-011521

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

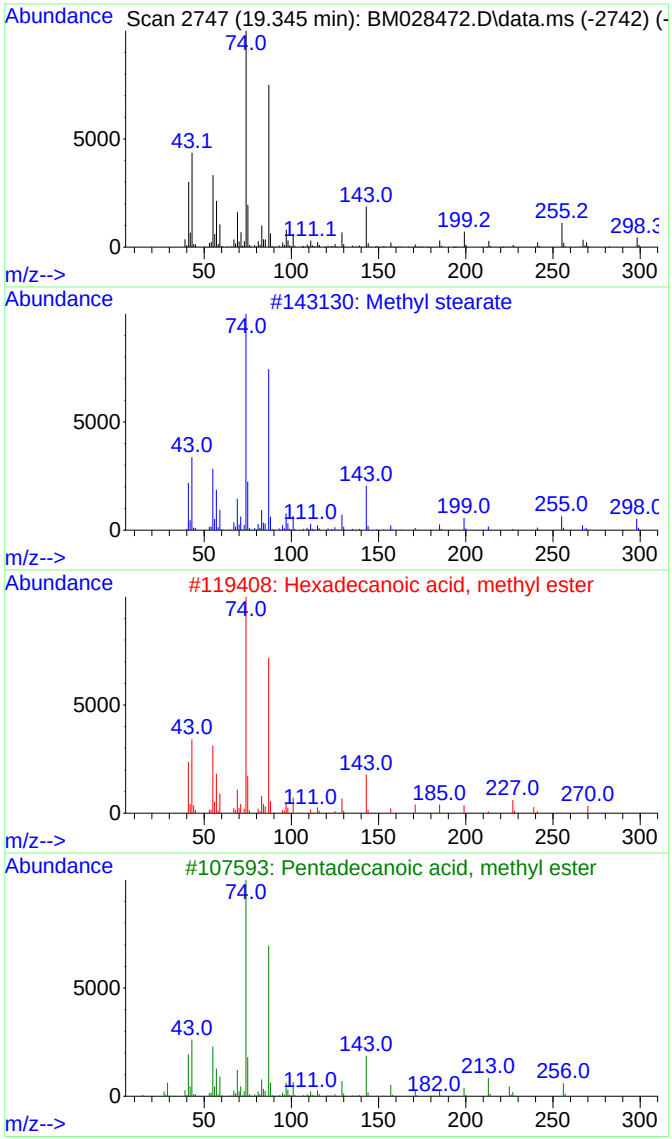
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

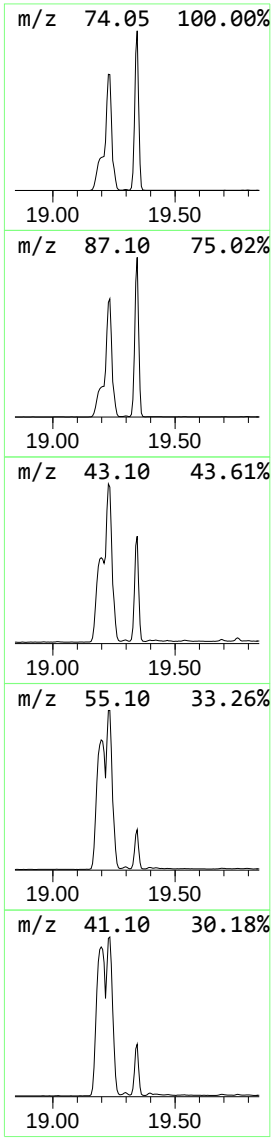
****

Peak Number 5 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.345	120.16 ng	2160100	Phenanthrene-d10	17.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	99
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	90
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	89
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028472.D
Acq On : 20 Jan 2021 17:42
Operator : CG/JU
Sample : M1161-01 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TR-05-011521

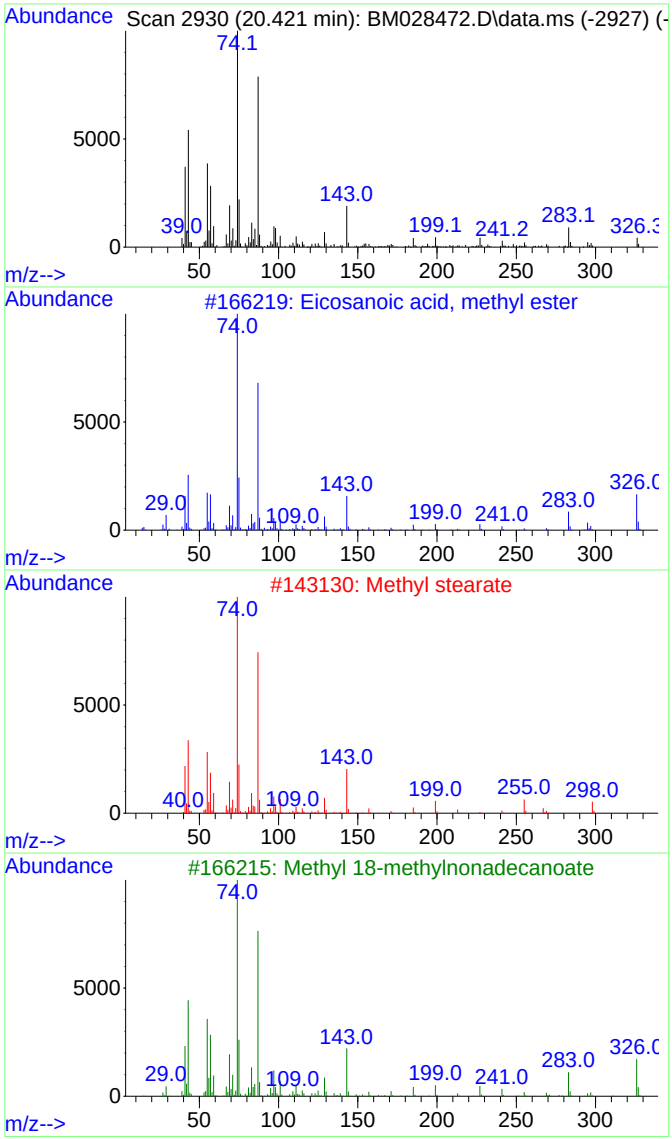
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

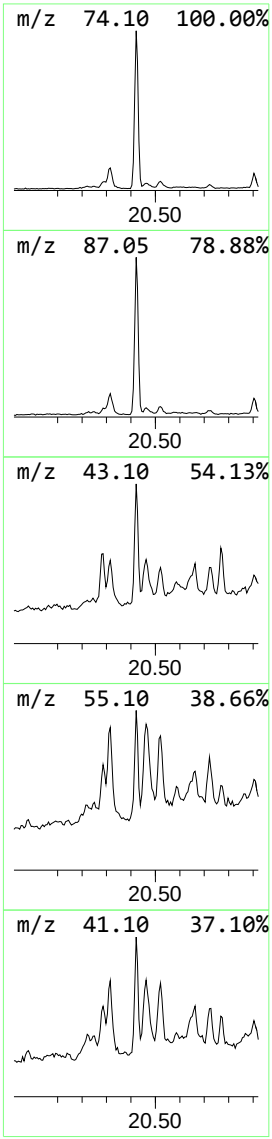
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Eicosanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.421	11.15 ng	197195	Chrysene-d12	21.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	97
2	Methyl stearate	298	C19H38O2	000112-61-8	95
3	Methyl 18-methylnonadecanoate	326	C21H42O2	1000352-20-6	94
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028472.D
Acq On : 20 Jan 2021 17:42
Operator : CG/JU
Sample : M1161-01 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TR-05-011521

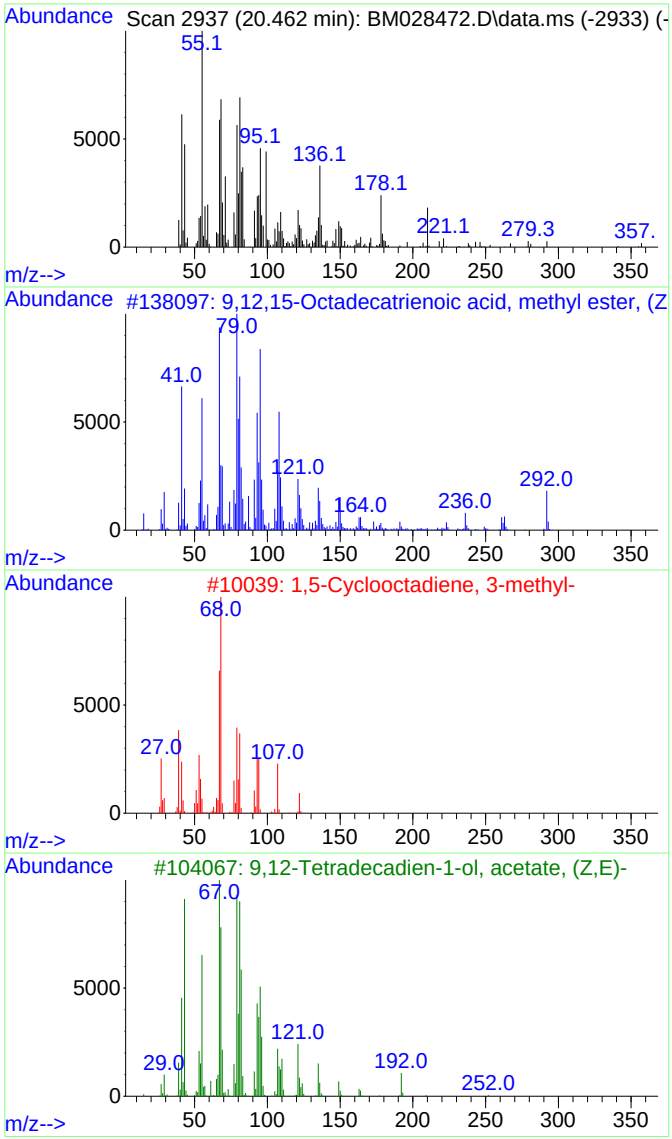
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

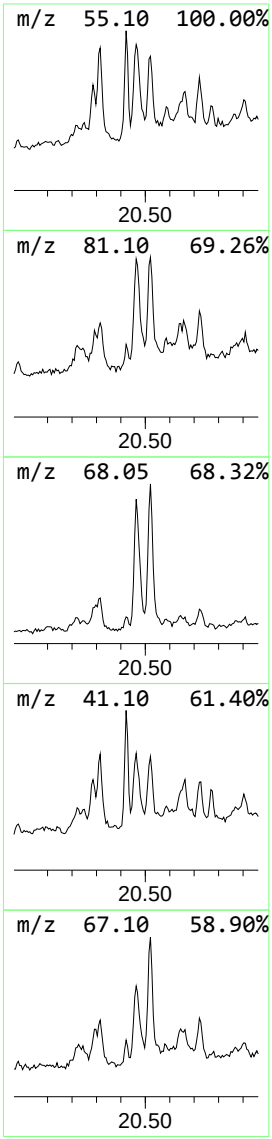
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 9,12,15-Octadecatrienoic ac... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.462	11.93 ng	210936	Chrysene-d12	21.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	50
2	1,5-Cyclooctadiene, 3-methyl-	122	C9H14	056564-88-6	46
3	9,12-Tetradecadien-1-ol, acetate...	252	C16H28O2	031654-77-0	38
4	9-Oxabicyclo[3.3.1]non-6-en-2-ol...	140	C8H12O2	029946-76-7	38
5	2-Isopropenyl-5-methyl-6-hepten-...	168	C11H20O	013066-55-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028472.D
Acq On : 20 Jan 2021 17:42
Operator : CG/JU
Sample : M1161-01 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TR-05-011521

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

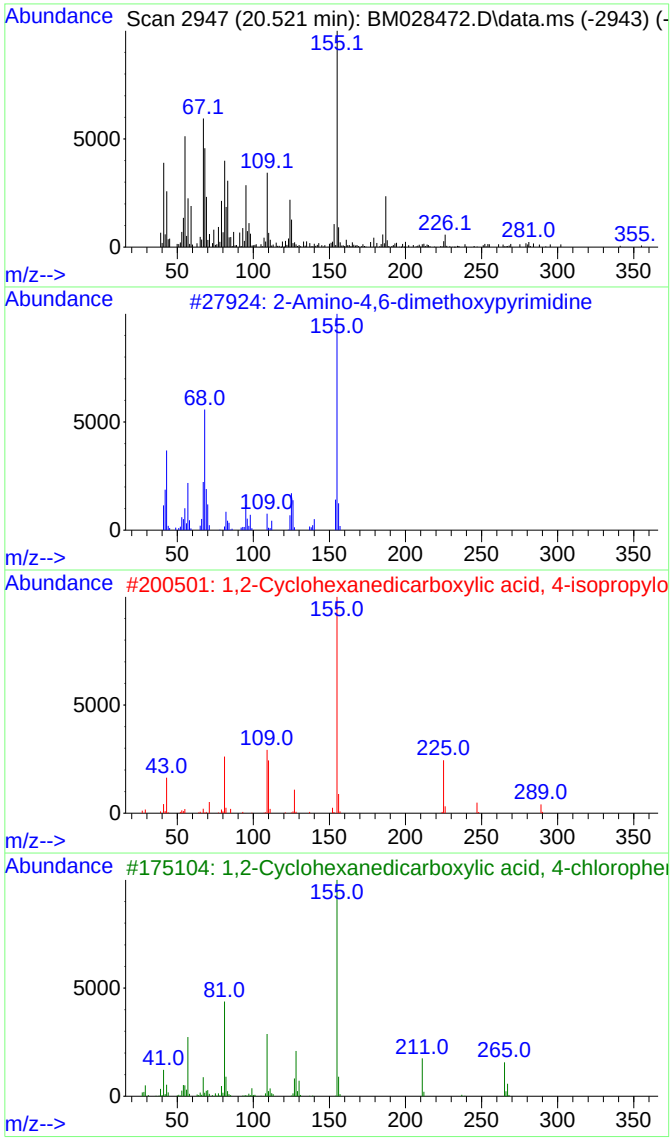
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

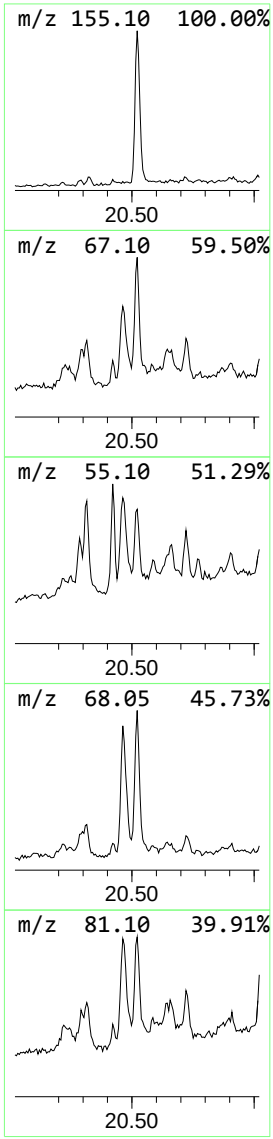
****

Peak Number 8 unknown20.521 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.521	9.24 ng	163303	Chrysene-d12	21.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-4,6-dimethoxypyrimidine	155	C6H9N3O2	036315-01-2	43
2	1,2-Cyclohexanedicarboxylic acid...	376	C22H32O5	1000339-57-5	27
3	1,2-Cyclohexanedicarboxylic acid...	338	C18H23ClO4	1000339-68-0	27
4	1,2-Cyclohexanedicarboxylic acid...	352	C19H25ClO4	1000339-68-2	27
5	1,2-Cyclohexanedicarboxylic acid...	372	C18H22Cl2O4	1000339-79-8	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028472.D
Acq On : 20 Jan 2021 17:42
Operator : CG/JU
Sample : M1161-01 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TR-05-011521

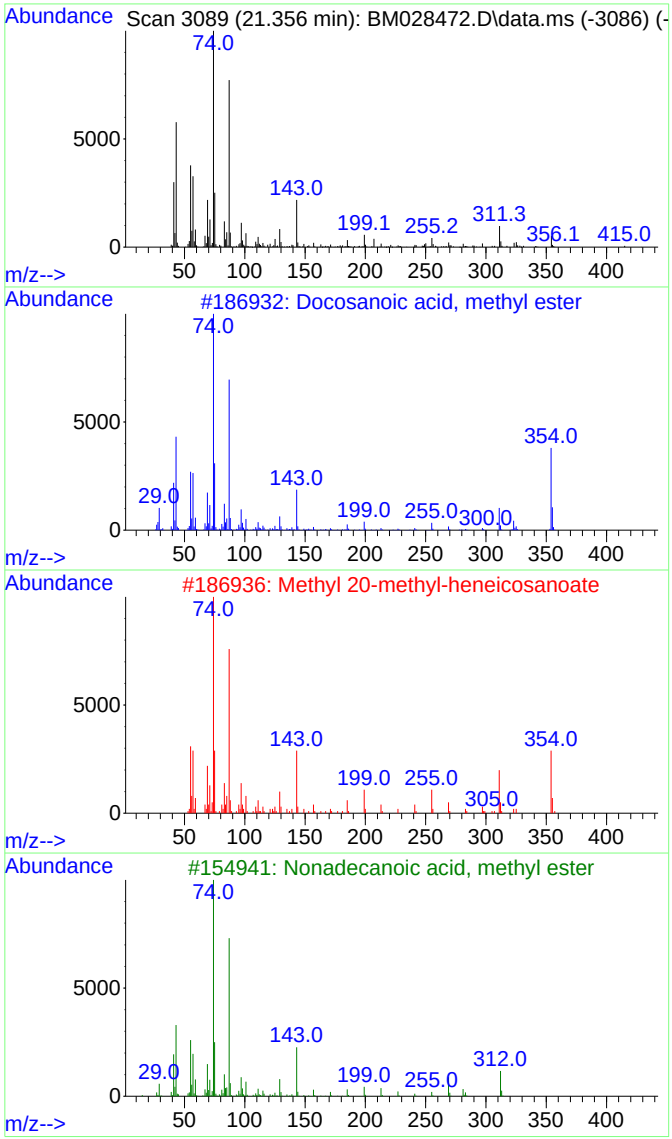
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

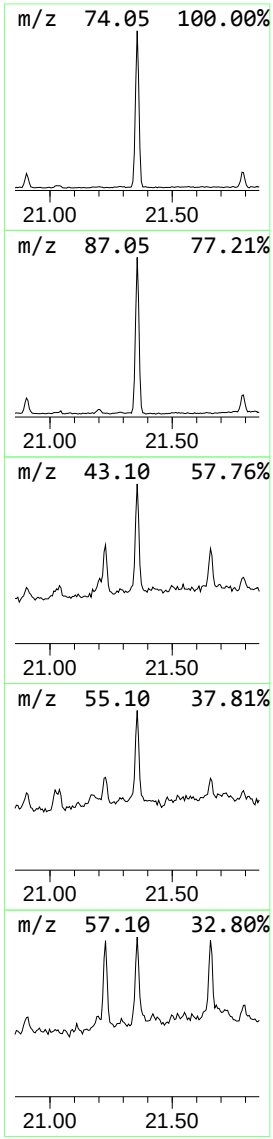
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Docosanoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.356	11.94 ng	211094	Chrysene-d12	21.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	97
2	Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	94
3	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	93
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
5	Hexacosanoic acid, methyl ester	410	C27H54O2	005802-82-4	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028472.D
Acq On : 20 Jan 2021 17:42
Operator : CG/JU
Sample : M1161-01 5X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TR-05-011521

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexadecanoic ac...	18.057	269.5	ng	4845430	4	17.398	359533	20.0
n-Hexadecanoic ...	18.274	9.8	ng	175273	4	17.398	359533	20.0
9,12-Octadecadi...	19.204	869.1	ng	15624400	4	17.398	359533	20.0
9-Octadecenoic ...	19.233	592.1	ng	10643800	4	17.398	359533	20.0
Methyl stearate	19.345	120.2	ng	2160100	4	17.398	359533	20.0
Eicosanoic acid...	20.421	11.2	ng	197195	5	21.527	353629	20.0
9,12,15-Octadec...	20.462	11.9	ng	210936	5	21.527	353629	20.0
unknown20.521	20.521	9.2	ng	163303	5	21.527	353629	20.0
Docosanoic acid...	21.356	11.9	ng	211094	5	21.527	353629	20.0