LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055682.D
Acq On : 18 Nov 2022 2:10
Operator : CG/JU
Sample : N5638-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JC-3-111522

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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055682.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.785	417	425	434	rBV	373832	640269	1.29%	0.545%
2	7.401	691	700	709	rBV	379571	680213	1.37%	0.579%
3	13.500	1731	1738	1749	rVB	644138	993118	1.99%	0.846%
4	14.874	1964	1972	1978	rVB	400538	637917	1.28%	0.543%
5	16.355	2219	2224	2232	rVB	488037	737959	1.48%	0.629%
6	17.618	2433	2439	2443	rBV	463584	756305	1.52%	0.644%
7	17.659	2443	2446	2452	rVB	362367	508645	1.02%	0.433%
8	18.270	2542	2550	2555	rBV	9849934	17405330	34.95%	14.825%
9	18.523	2582	2593	2604	rBV2	1991869	3967060	7.97%	3.379%
10	19.446	2734	2750	2751	rBV4	12017663	49800656	100.00%	42.417%
11	19.563	2765	2770	2774	rVB	8589879	11549837	23.19%	9.837%
12	19.639	2775	2783	2785	rBV	4813798	9765785	19.61%	8.318%
13	19.663	2785	2787	2796	rVV2	4390089	6470391	12.99%	5.511%
14	19.757	2800	2803	2810	rVB	559601	710752	1.43%	0.605%
15	20.033	2841	2850	2858	rVB	926716	2195054	4.41%	1.870%
16	20.215	2877	2881	2886	rVB	1107850	1461928	2.94%	1.245%
17	20.521	2925	2933	2941	rVB2	936103	1886868	3.79%	1.607%
18	20.627	2947	2951	2955	rBV2	998380	1246446	2.50%	1.062%
19	20.879	2988	2994	3001	rVB4	269533	634537	1.27%	0.540%
20	21.290	3058	3064	3070	rVB4	467806	953760	1.92%	0.812%
21	21.684	3126	3131	3137	rVB	915453	1274720	2.56%	1.086%
22	21.907	3163	3169	3176	rBV2	775192	2063624	4.14%	1.758%
23	21.972	3177	3180	3193	rVB	584406	1066506	2.14%	0.908%

Sum of corrected areas: 117407680

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
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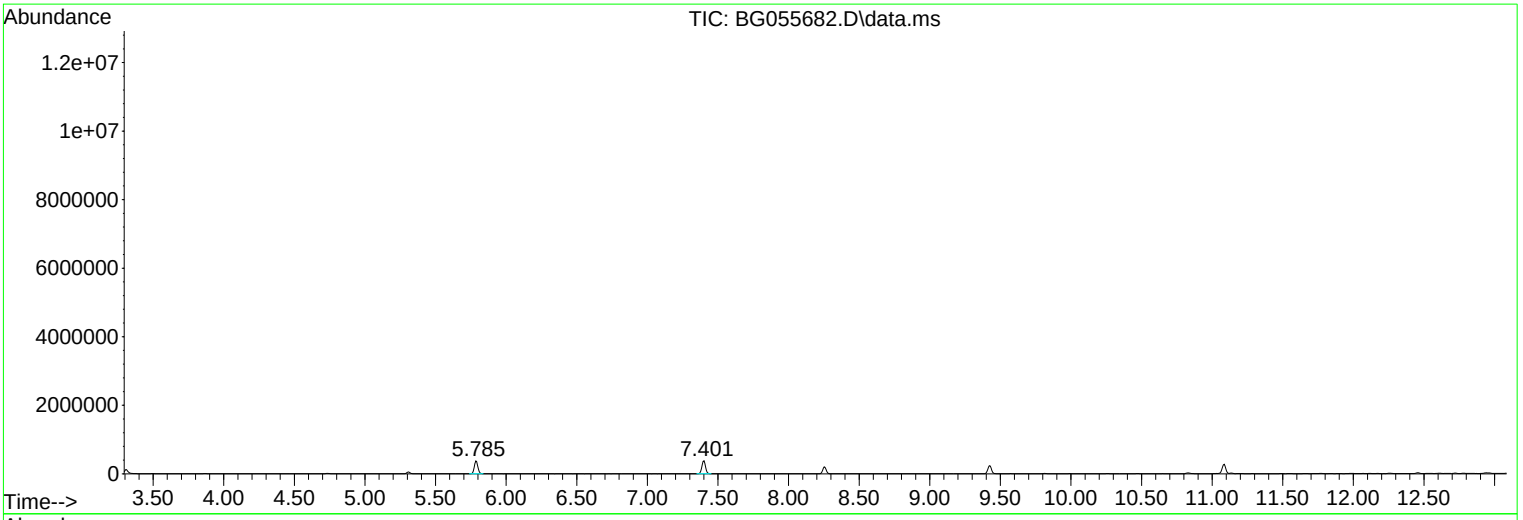
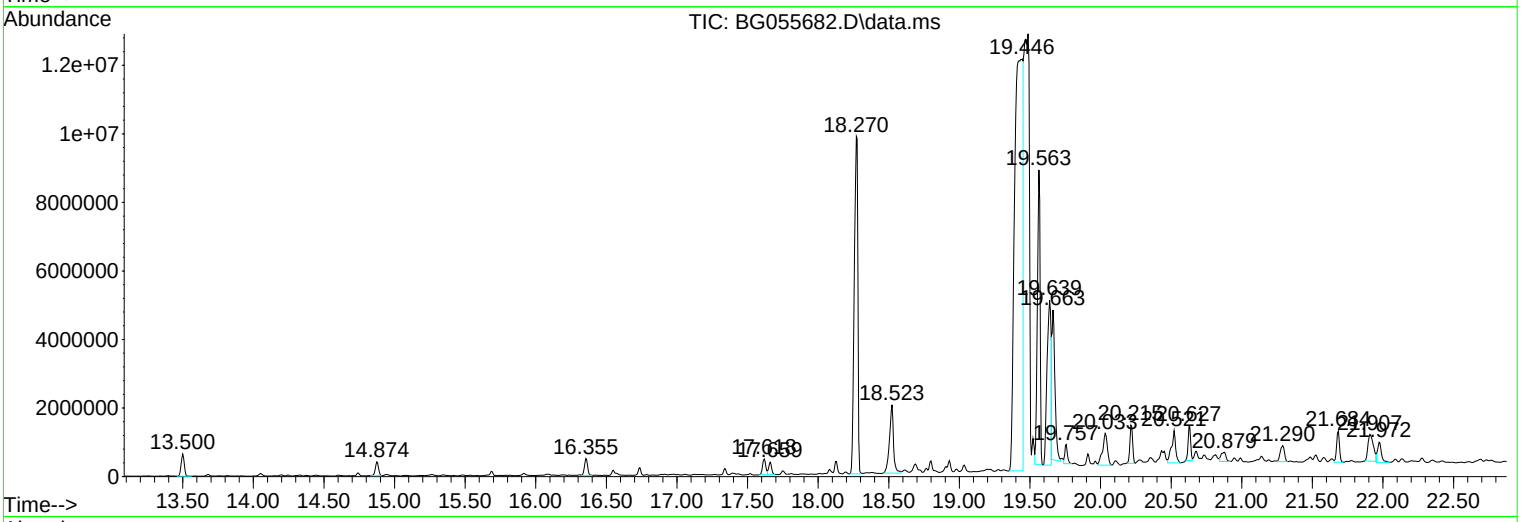
Operator : CG/JU
Sample : N5638-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

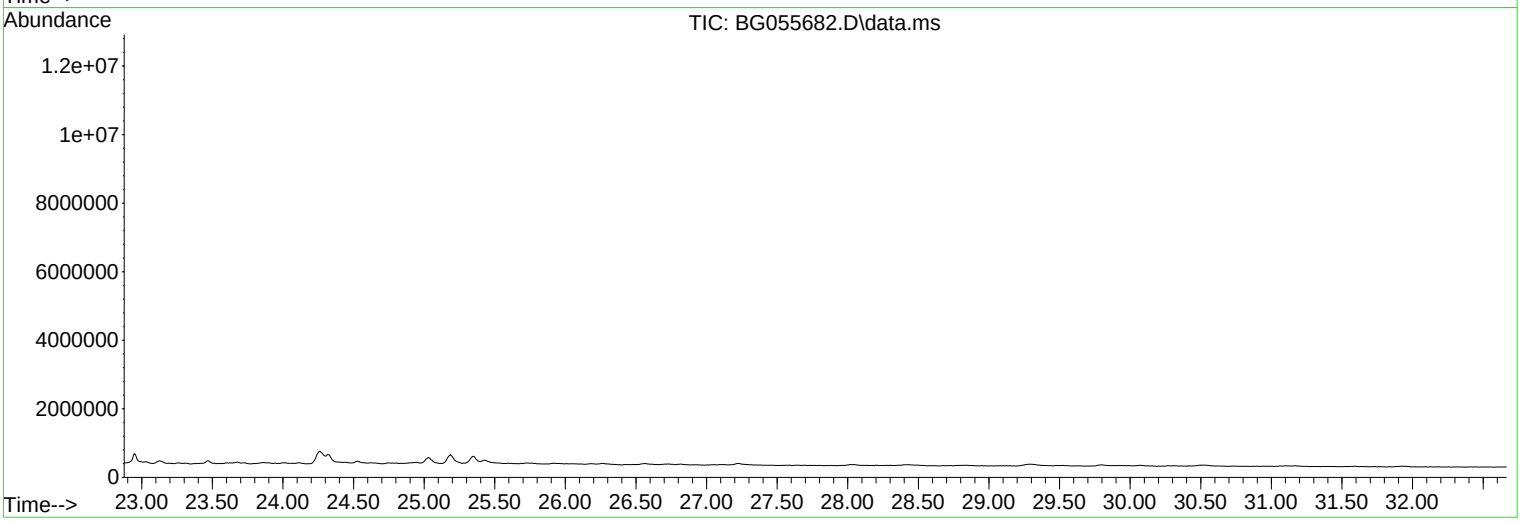
Instrument :
BNA_G
ClientSampleId :
JC-3-111522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Operator : CG/JU
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

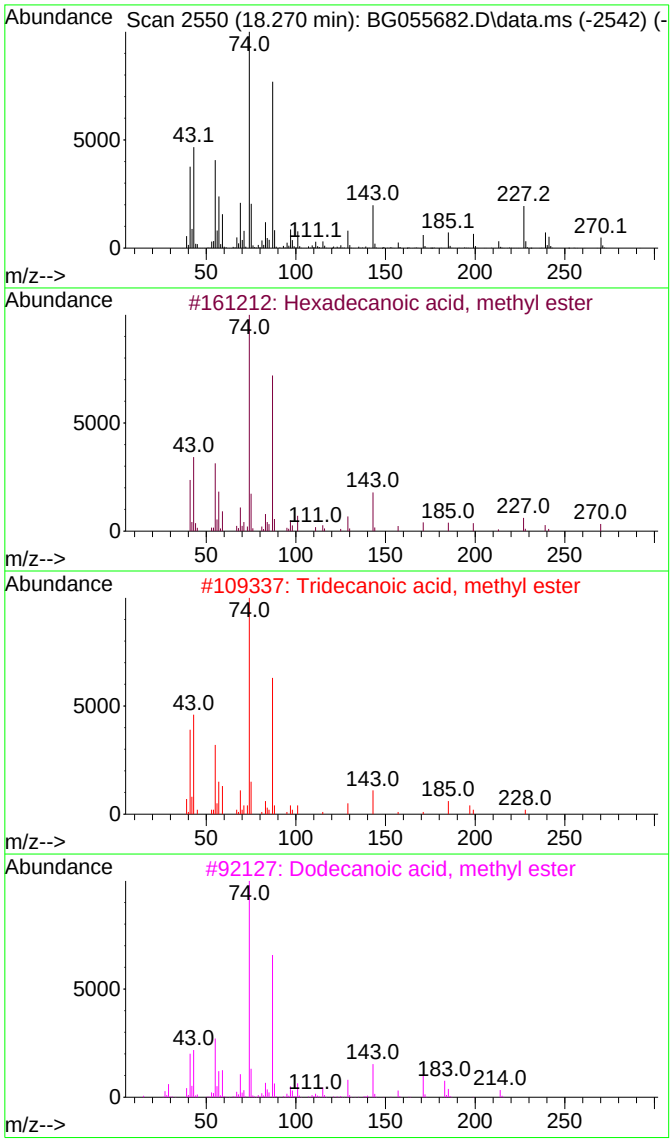
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

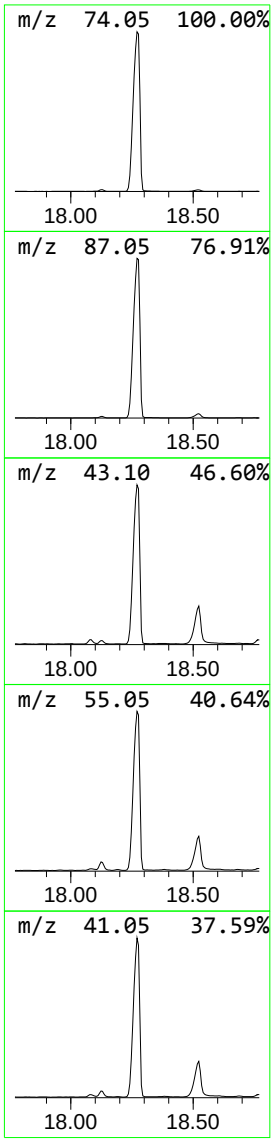
****

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.270	460.27 ng	17405300	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
3	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	81
4	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	81
5	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055682.D
Acq On : 18 Nov 2022 2:10
Operator : CG/JU
Sample : N5638-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JC-3-111522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

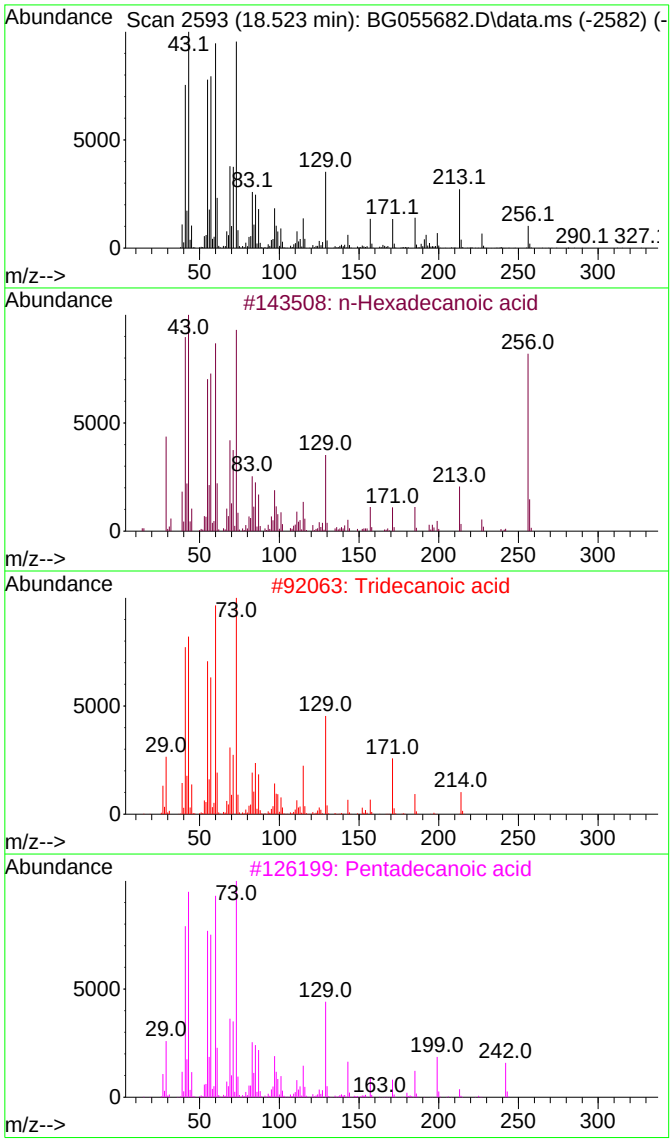
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

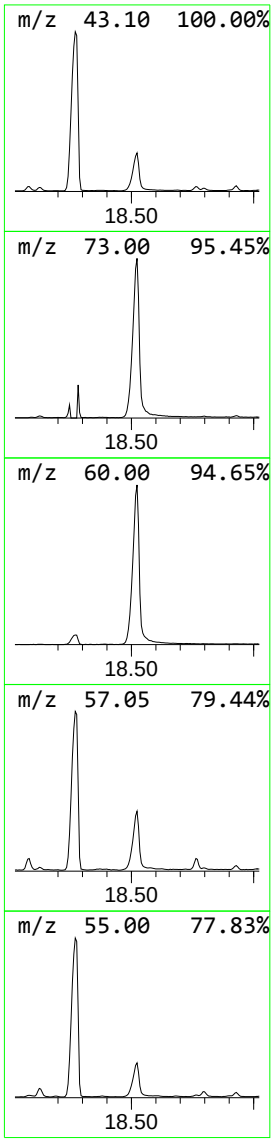
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.523	104.91 ng	3967060	Phenanthrene-d10	17.618

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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055682.D
Acq On : 18 Nov 2022 2:10
Operator : CG/JU
Sample : N5638-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JC-3-111522

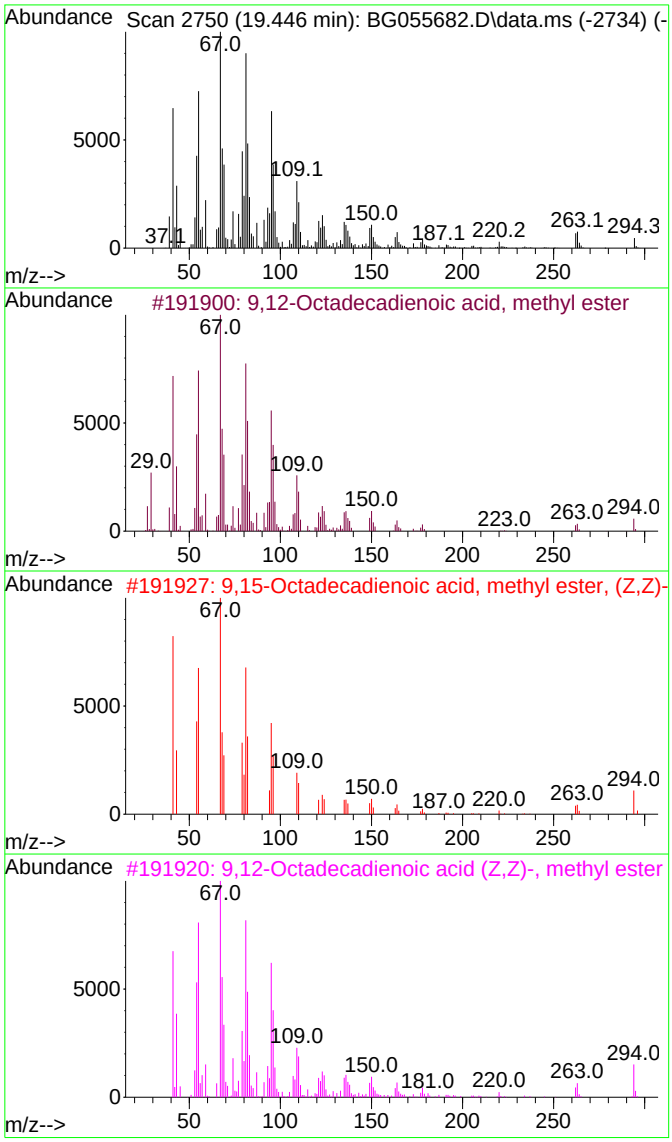
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

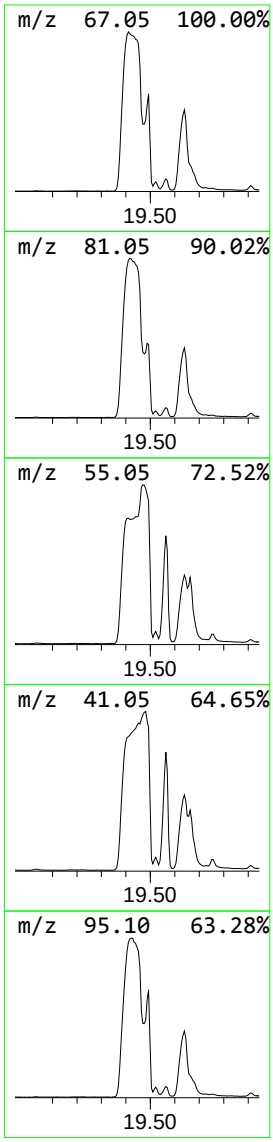
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.446	1316.95 ng	49800700	Phenanthrene-d10	17.618

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	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	98
5	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98





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Acq On : 18 Nov 2022 2:10
Operator : CG/JU
Sample : N5638-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JC-3-111522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

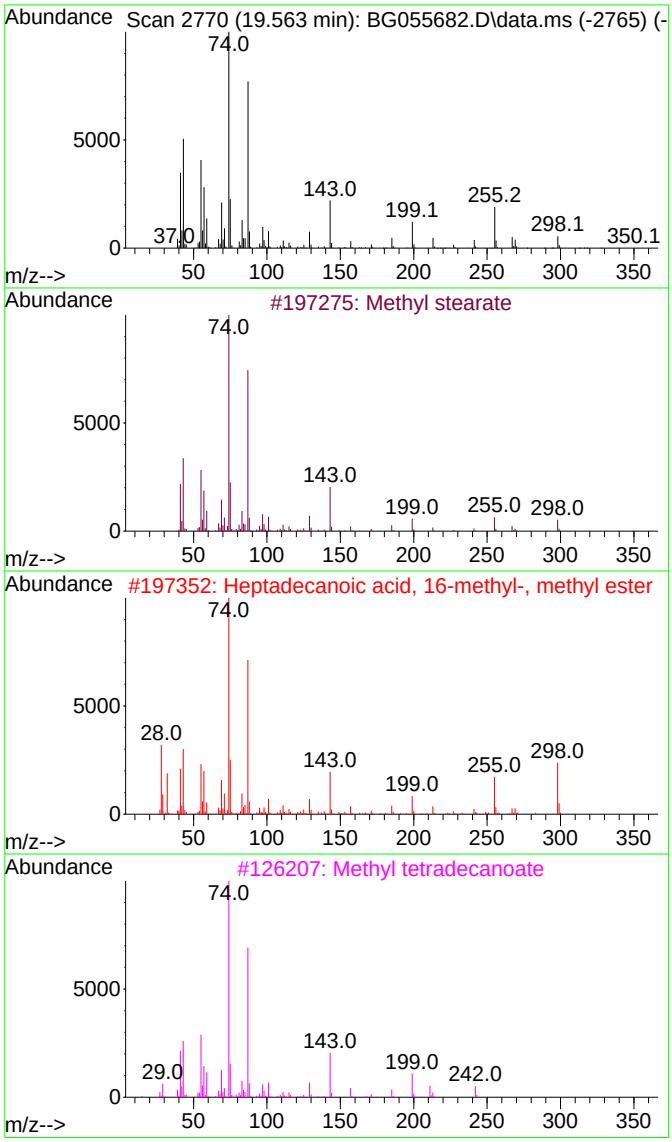
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

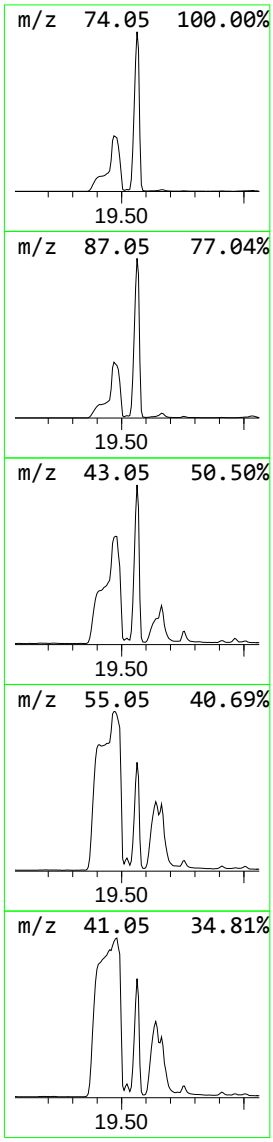
****

Peak Number 4 Methyl stearate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.563	305.43 ng	11549800	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
4	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	87
5	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055682.D
Acq On : 18 Nov 2022 2:10
Operator : CG/JU
Sample : N5638-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JC-3-111522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

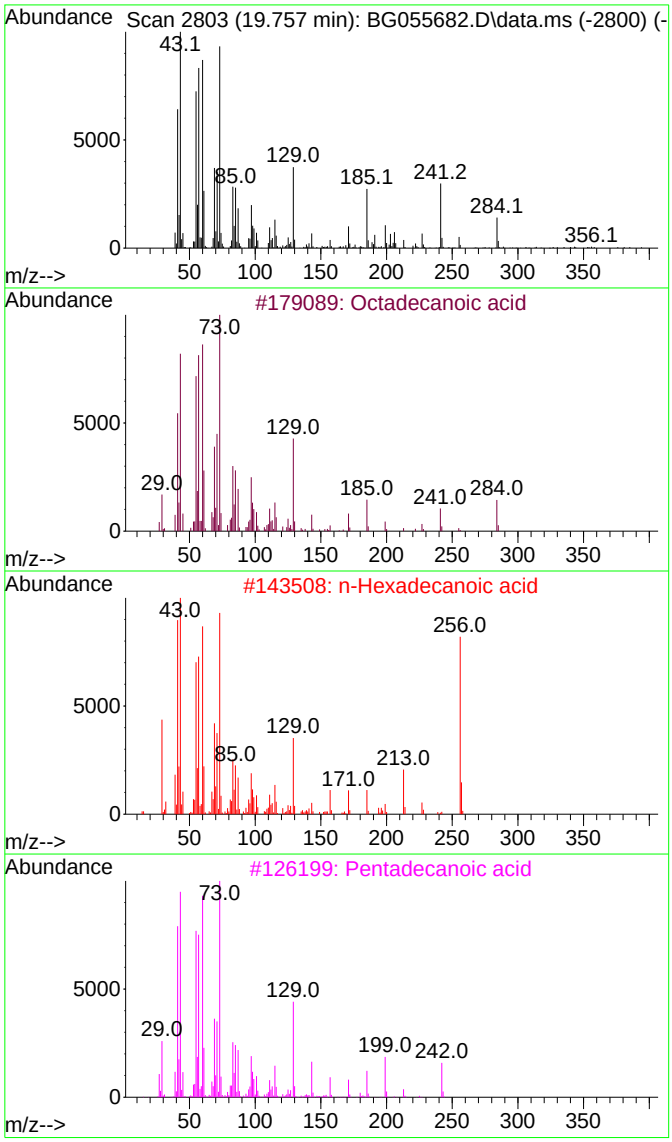
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

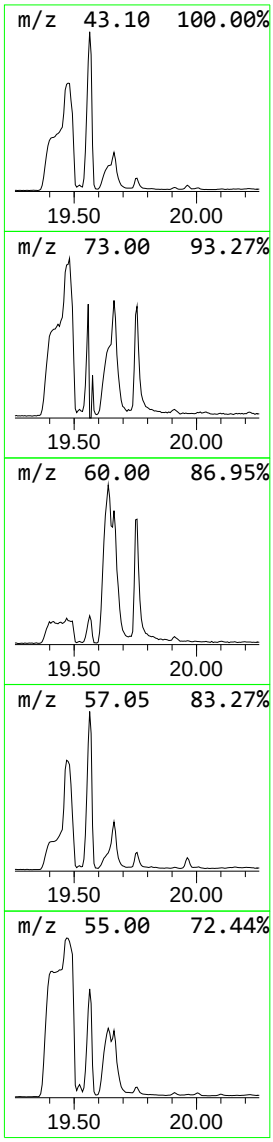
****

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.757	18.80 ng	710752	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JC-3-111522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

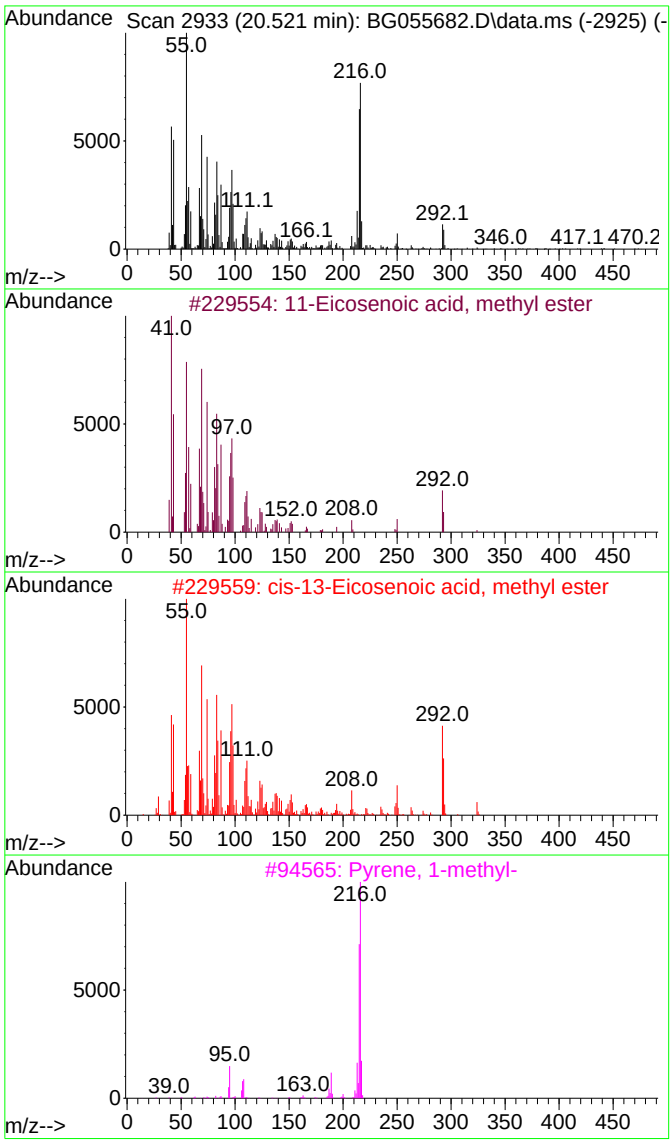
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

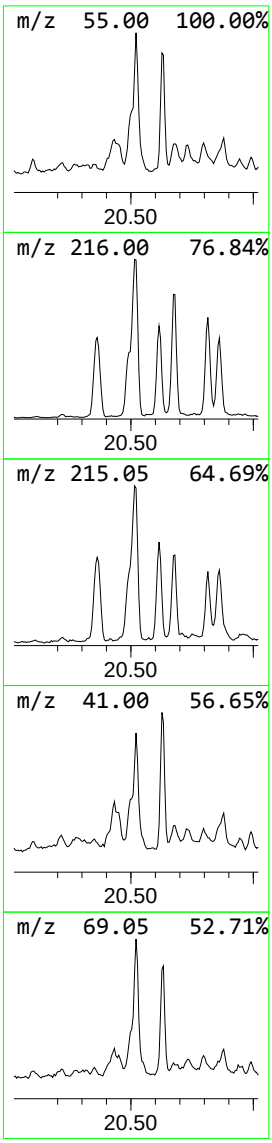
****

Peak Number 6 11-Eicosenoic acid, methyl ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.521	18.29 ng	1886870	Chrysene-d12	21.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	98
2	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	70
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	66
4	cis-Methyl 11-eicosenoate	324	C21H40O2	002390-09-2	55
5	Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055682.D
Acq On : 18 Nov 2022 2:10
Operator : CG/JU
Sample : N5638-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JC-3-111522

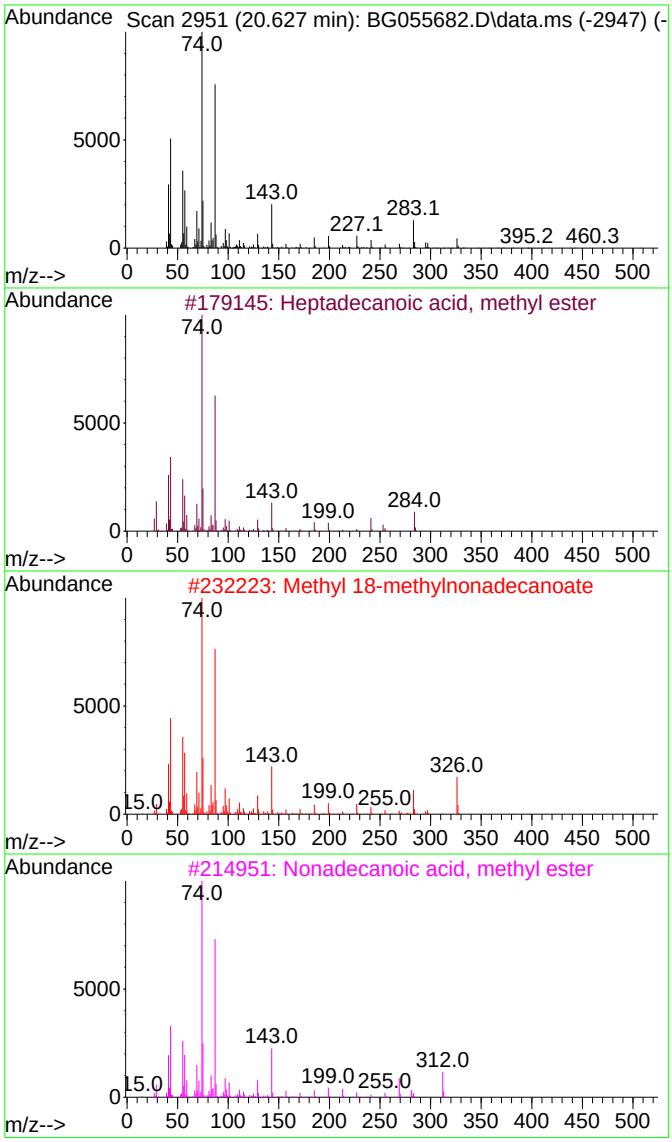
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

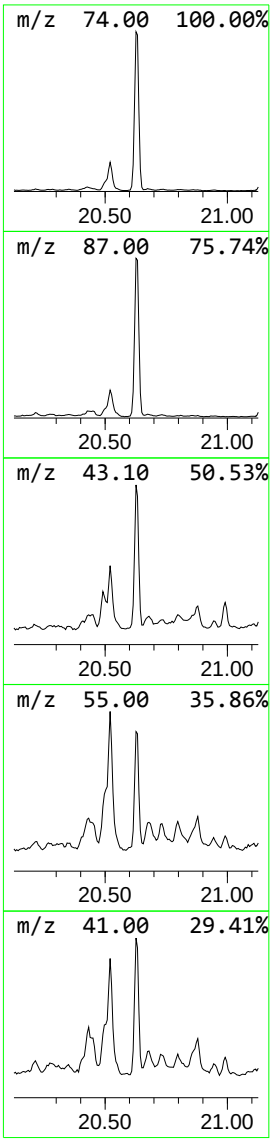
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heptadecanoic acid, methyl ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.627	12.08 ng	1246450	Chrysene-d12	21.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93
2	Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	91
3	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	90
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	90
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87





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BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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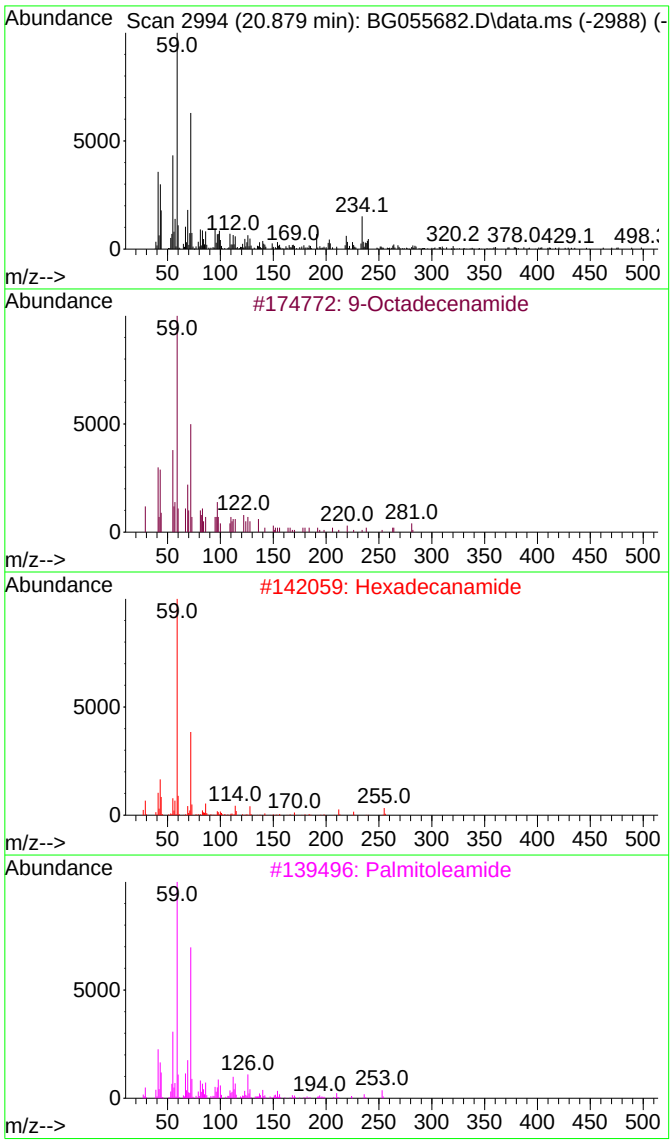
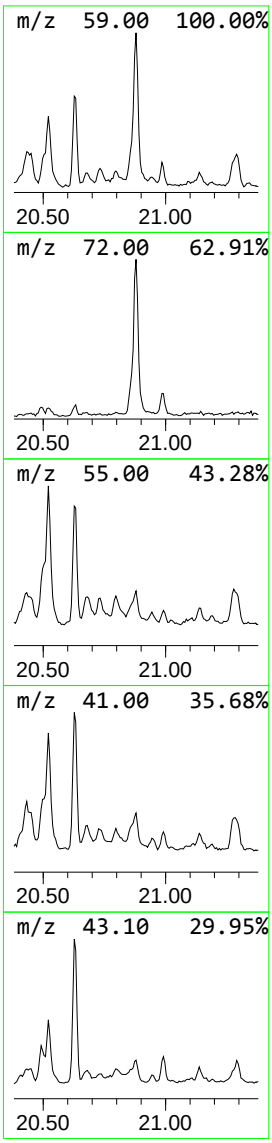
****

Peak Number 8 9-Octadecenamide Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.879	6.15 ng	634537	Chrysene-d12	21.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide	281	C18H35NO	003322-62-1	80
2	Hexadecanamide	255	C16H33NO	000629-54-9	72
3	Palmitoleamide	253	C16H31NO	106010-22-4	72
4	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	60
5	Octadecanamide	283	C18H37NO	000124-26-5	58





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Data File : BG055682.D
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Operator : CG/JU
Sample : N5638-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JC-3-111522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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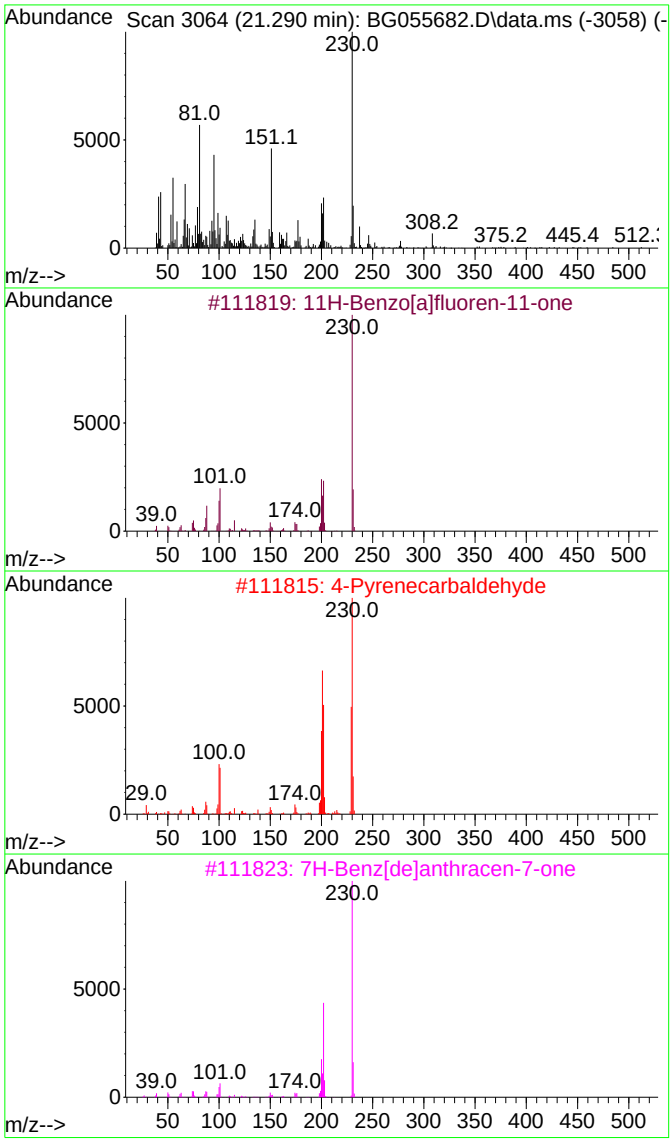
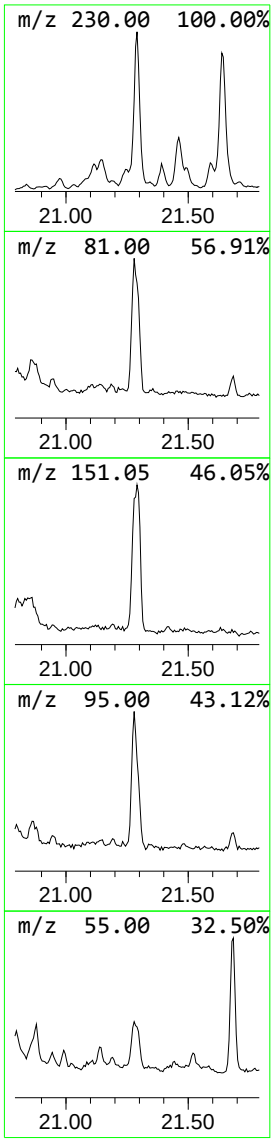
Peak Number 9 11H-Benzo[a]fluoren-11-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.291	9.24 ng	953760	Chrysene-d12	21.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	91
2	4-Pyrenecarbaldehyde	230	C17H10O	022245-51-8	49
3	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	45
4	o-Terphenyl	230	C18H14	000084-15-1	38
5	m-Terphenyl	230	C18H14	000092-06-8	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055682.D
Acq On : 18 Nov 2022 2:10
Operator : CG/JU
Sample : N5638-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JC-3-111522

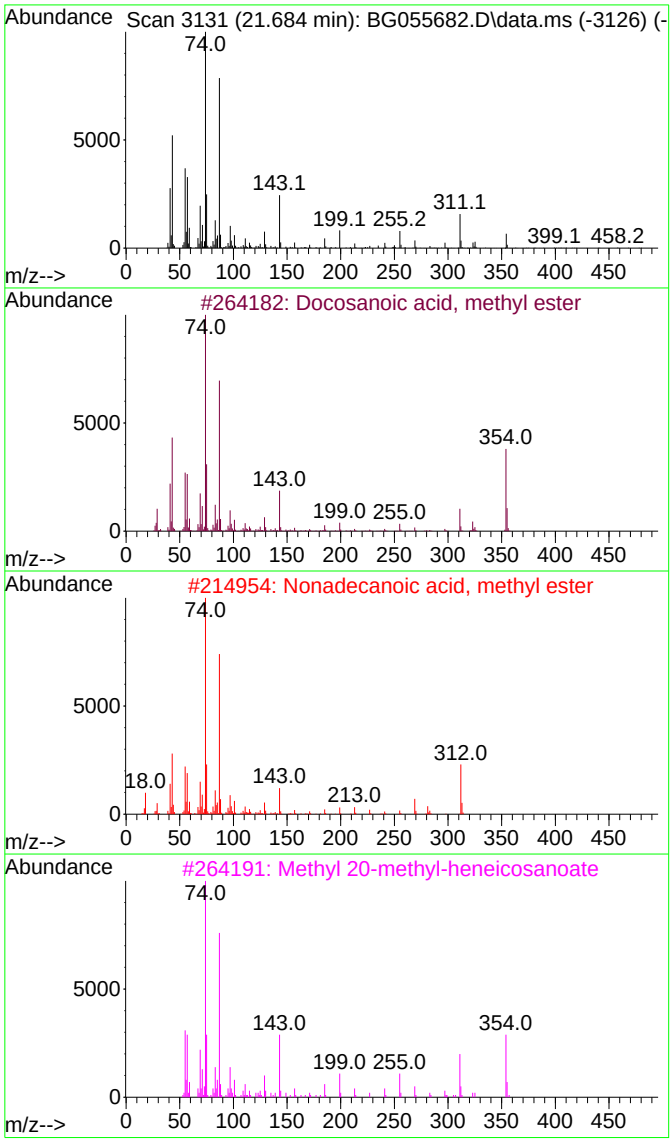
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

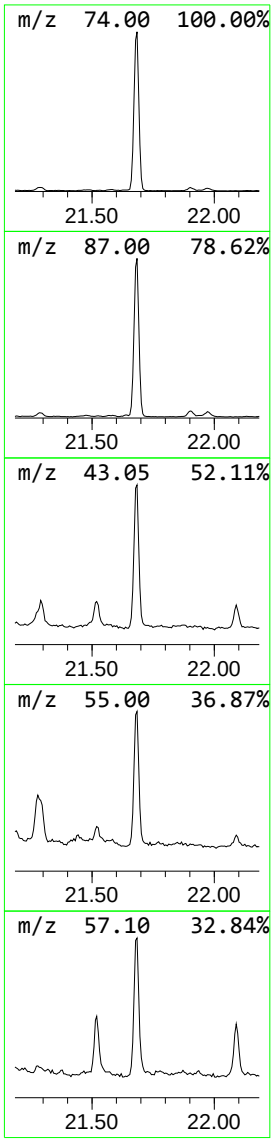
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Docosanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.684	12.35 ng	1274720	Chrysene-d12	21.925

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	98
2	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	97
3	Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	95
4	Methyl stearate	298	C19H38O2	000112-61-8	87
5	Octadecanoic acid, 10-methyl-, m...	312	C20H40O2	002490-19-9	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111722\
Data File : BG055682.D
Acq On : 18 Nov 2022 2:10
Operator : CG/JU
Sample : N5638-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JC-3-111522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.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
Hexadecanoic ac...	18.270	460.3	ng	17405300	4	17.618	756305	20.0
n-Hexadecanoic ...	18.523	104.9	ng	3967060	4	17.618	756305	20.0
9,12-Octadecadi...	19.446	1317.0	ng	49800700	4	17.618	756305	20.0
Methyl stearate	19.563	305.4	ng	11549800	4	17.618	756305	20.0
Octadecanoic acid	19.757	18.8	ng	710752	4	17.618	756305	20.0
11-Eicosenoic a...	20.521	18.3	ng	1886870	5	21.925	2063620	20.0
Heptadecanoic a...	20.627	12.1	ng	1246450	5	21.925	2063620	20.0
9-Octadecenamide	20.879	6.2	ng	634537	5	21.925	2063620	20.0
11H-Benzo[a]flu...	21.291	9.2	ng	953760	5	21.925	2063620	20.0
Docosanoic acid...	21.684	12.4	ng	1274720	5	21.925	2063620	20.0