LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044048.D
Acq On : 14 Jan 2020 22:42
Operator : JU
Sample : L1004-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BU-RO-229

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-BG123019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.141	3	9	23	rVB	190101	405136	1.23%	0.371%
2	5.532	409	416	430	rBV	848342	1409144	4.27%	1.291%
3	7.119	677	686	701	rBV	908254	1612040	4.89%	1.477%
4	7.483	741	748	761	rBV	910751	1598942	4.85%	1.465%
5	7.947	820	827	836	rBV	504780	883757	2.68%	0.810%
6	8.270	870	882	892	rBV	688151	1236261	3.75%	1.133%
7	9.105	1014	1024	1034	rBV	513317	954421	2.89%	0.875%
8	10.750	1295	1304	1310	rBV	716865	1320698	4.00%	1.210%
9	13.206	1715	1722	1733	rVB	1283273	2094272	6.35%	1.919%
10	14.581	1947	1956	1962	rBV	1065308	1701770	5.16%	1.559%
11	16.067	2203	2209	2217	rBV	976119	1521856	4.61%	1.395%
12	17.324	2417	2423	2427	rBV	1127702	1749269	5.30%	1.603%
13	17.365	2427	2430	2436	rVB	573088	790551	2.40%	0.724%
14	18.012	2533	2540	2545	rBV	7883007	10853046	32.89%	9.946%
15	19.157	2727	2735	2737	rBV	18519161	32995499	100.00%	30.236%
16	19.193	2737	2741	2749	rVV2	19054327	30193557	91.51%	27.669%
17	19.310	2756	2761	2767	rVB	4896810	5916733	17.93%	5.422%
18	19.375	2767	2772	2779	rBV	618447	994729	3.01%	0.912%
19	19.739	2826	2834	2843	rVB	590688	1123394	3.40%	1.029%
20	19.945	2863	2869	2874	rBV	1988114	2731163	8.28%	2.503%
21	20.286	2924	2927	2932	rVB	484795	586665	1.78%	0.538%
22	20.397	2942	2946	2949	rBV	489550	582924	1.77%	0.534%
23	20.432	2949	2952	2957	rVV3	325624	488923	1.48%	0.448%
24	20.491	2958	2962	2966	rVV	301325	395846	1.20%	0.363%
25	21.243	3087	3090	3098	rVB4	247849	388746	1.18%	0.356%
26	21.402	3113	3117	3122	rBV	362400	439642	1.33%	0.403%
27	21.578	3140	3147	3152	rBV3	1119443	2214299	6.71%	2.029%
28	24.727	3675	3683	3702	rVB2	572338	1941723	5.88%	1.779%

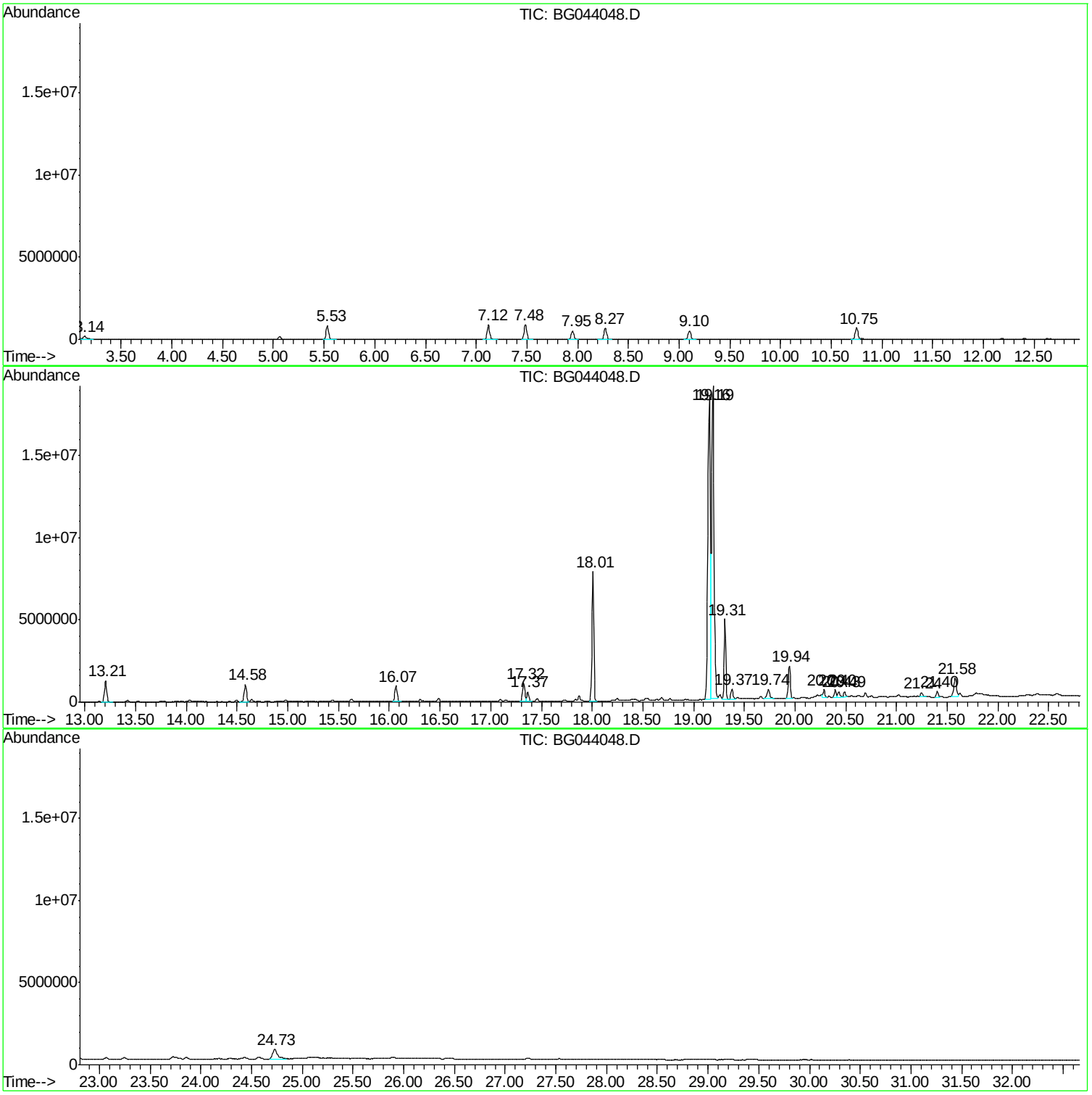
Sum of corrected areas: 109125006

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044048.D
Acq On : 14 Jan 2020 22:42
Operator : JU
Sample : L1004-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BU-RO-229

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044048.D
Acq On : 14 Jan 2020 22:42
Operator : JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

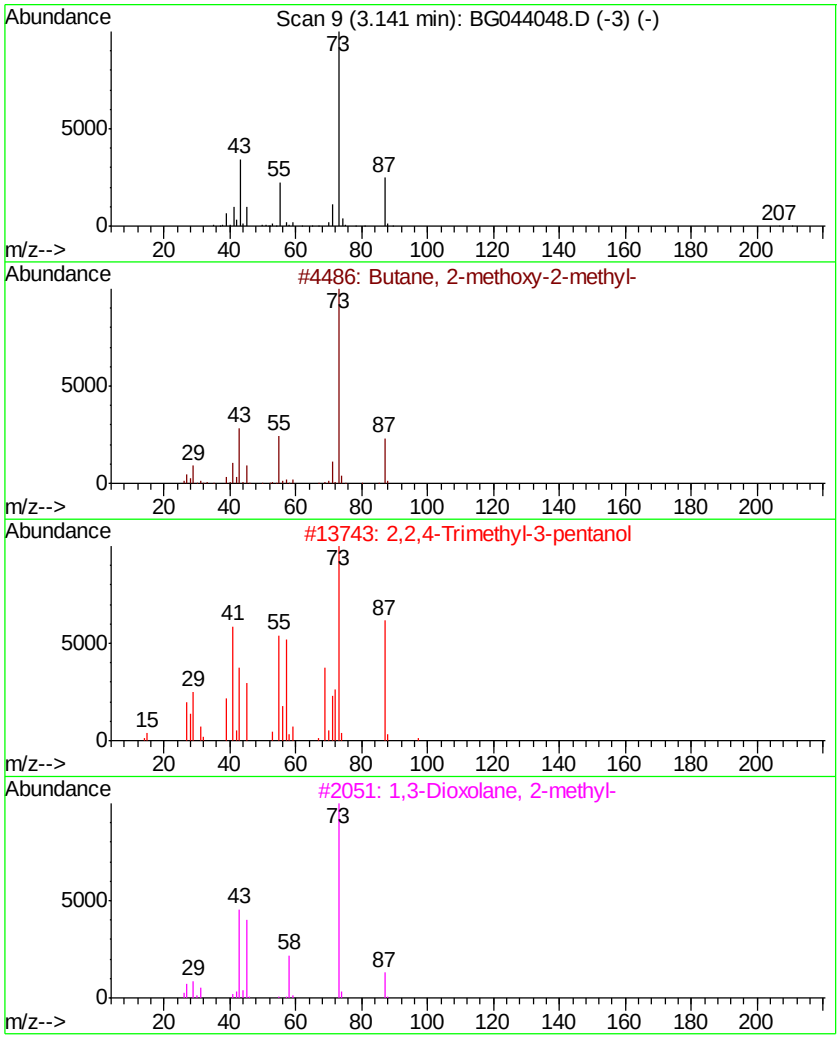
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

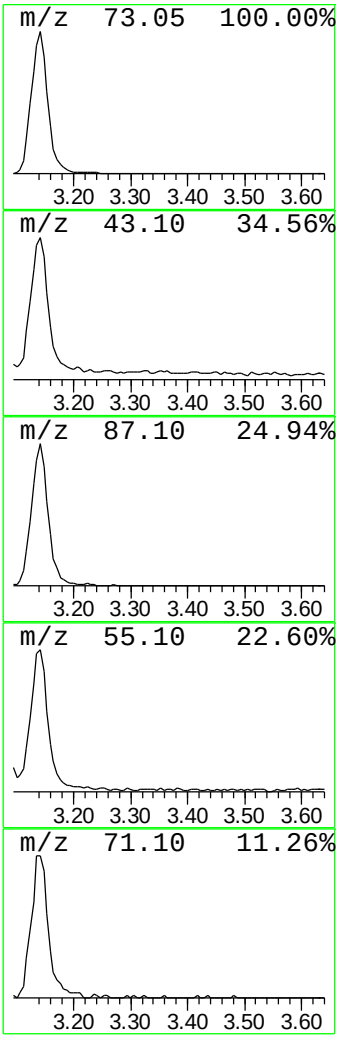
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.14	9.17 ng	405136	1,4-Dichlorobenzene-d4	7.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	64
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044048.D
Acq On : 14 Jan 2020 22:42
Operator : JU
Sample : L1004-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BU-RO-229

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

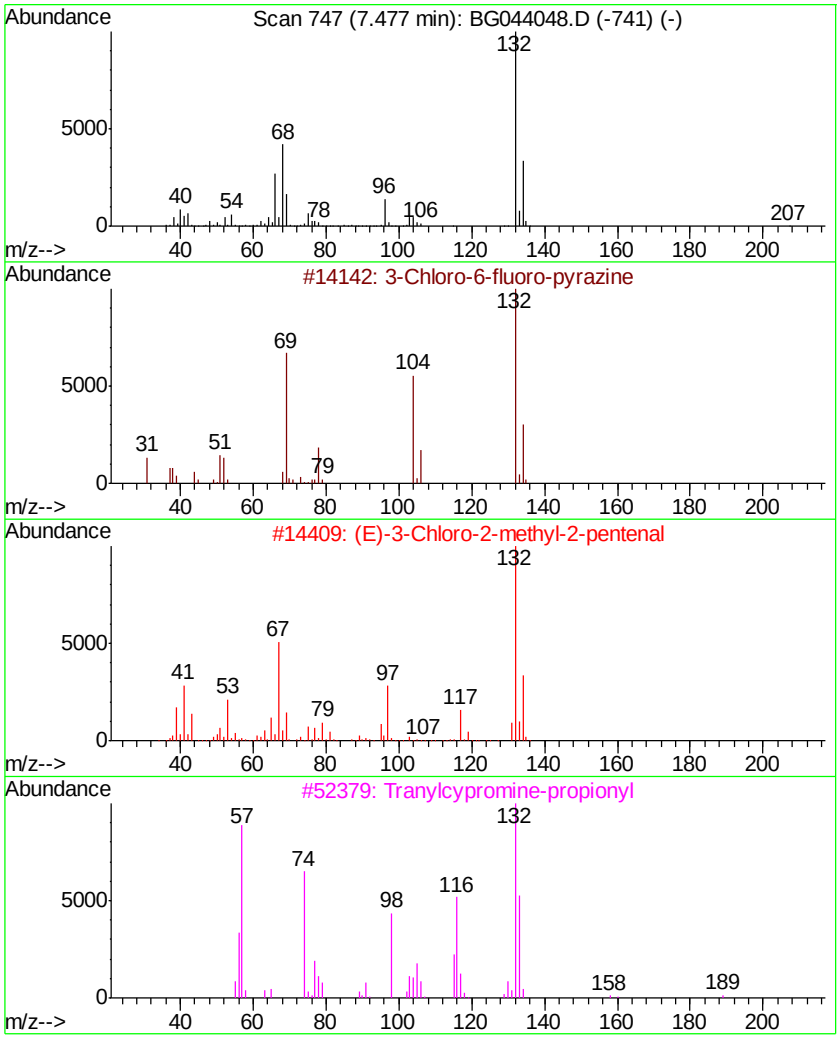
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

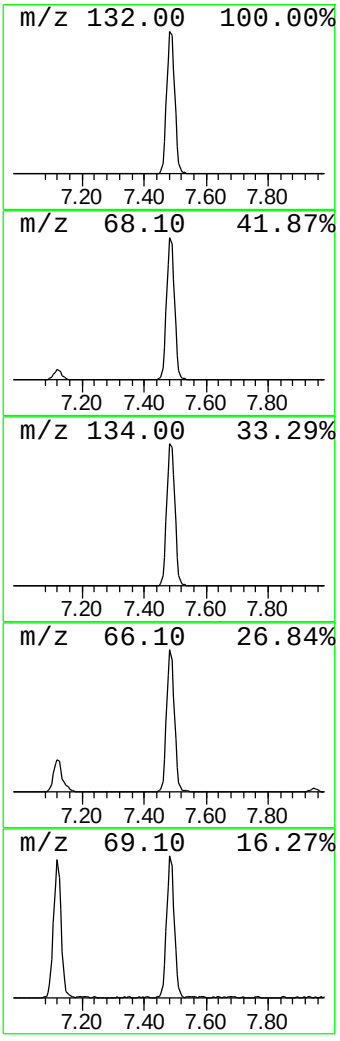
****

Peak Number 2 unknown7.48 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	36.19 ng	1598940	1,4-Dichlorobenzene-d4	7.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044048.D
Acq On : 14 Jan 2020 22:42
Operator : JU
Sample : L1004-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BU-RO-229

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

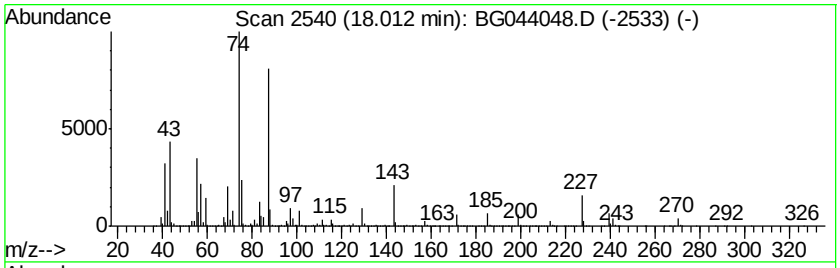
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

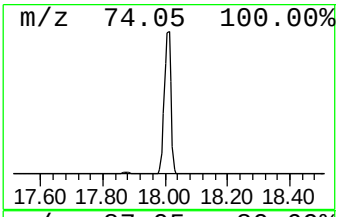
****

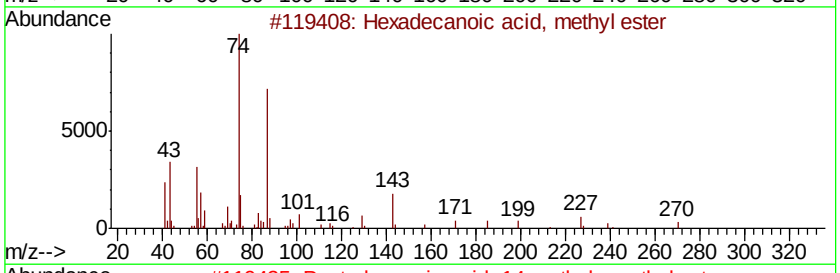
Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 3

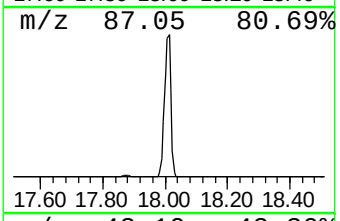
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.01	124.09 ng	10853000	Phenanthrene-d10	17.32

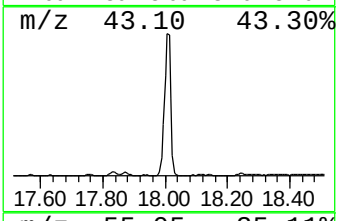
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	89
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	83
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	83

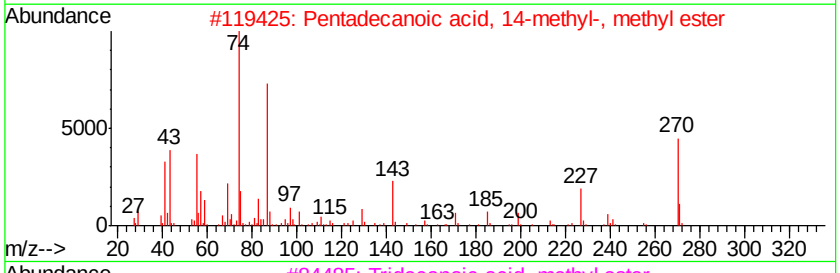


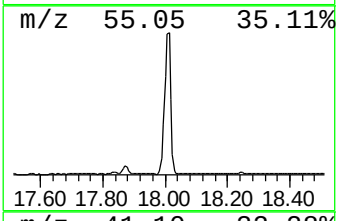


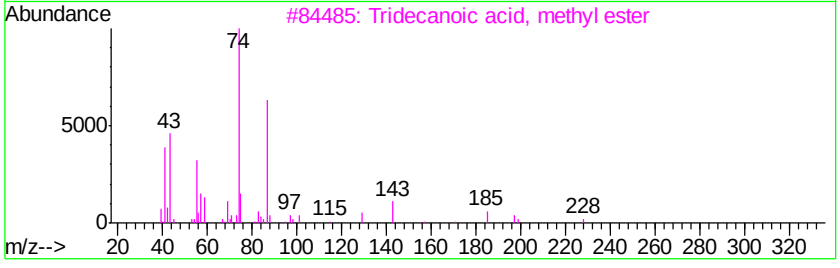


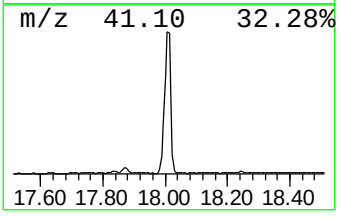












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044048.D
Acq On : 14 Jan 2020 22:42
Operator : JU
Sample : L1004-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BU-RO-229

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

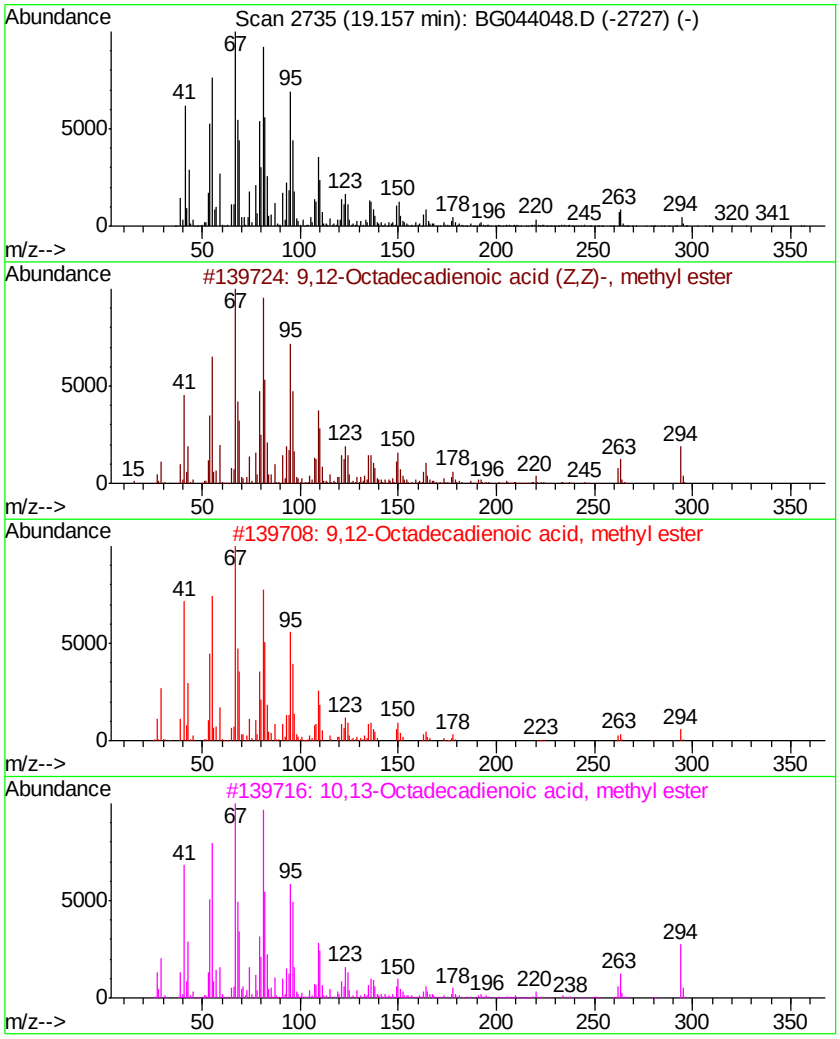
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

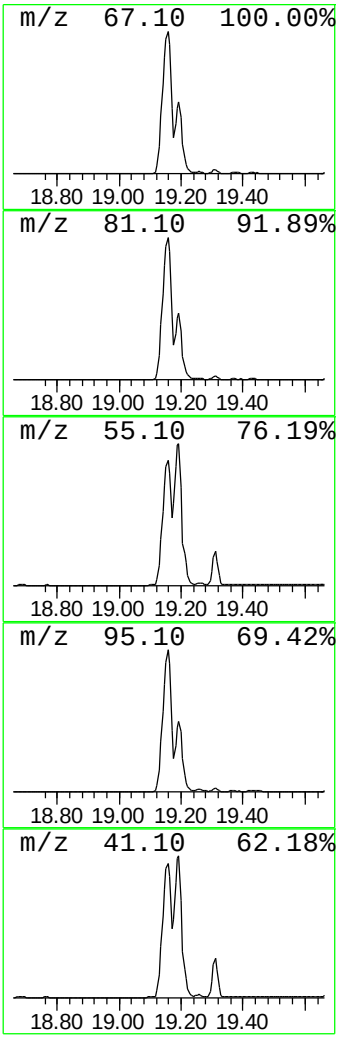
****

Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.16	377.25 ng	32995500	Phenanthrene-d10	17.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	97
3	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	97
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	97
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	95





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044048.D
Acq On : 14 Jan 2020 22:42
Operator : JU
Sample : L1004-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BU-RO-229

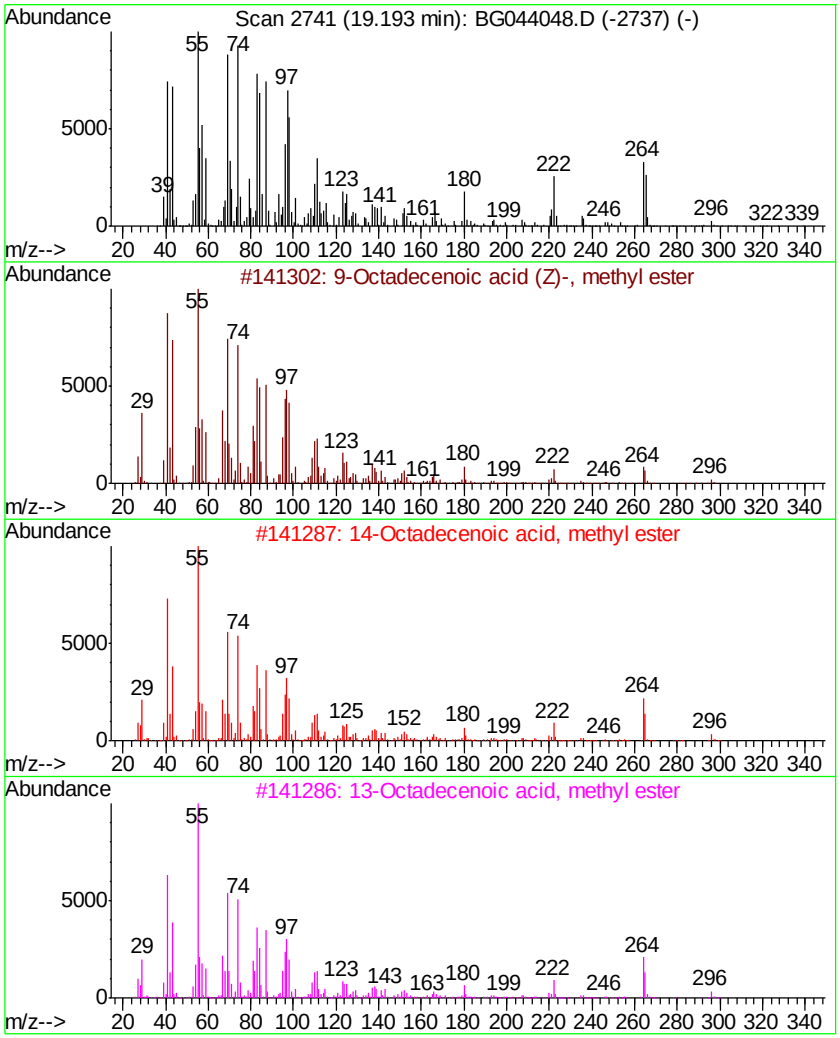
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

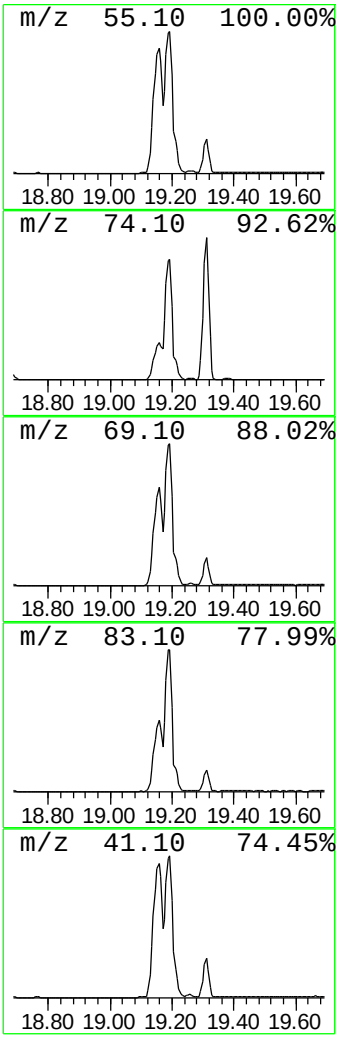
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.19	345.21 ng	30193600	Phenanthrene-d10	17.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	93
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	93
4	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	93
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044048.D
Acq On : 14 Jan 2020 22:42
Operator : JU
Sample : L1004-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BU-RO-229

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

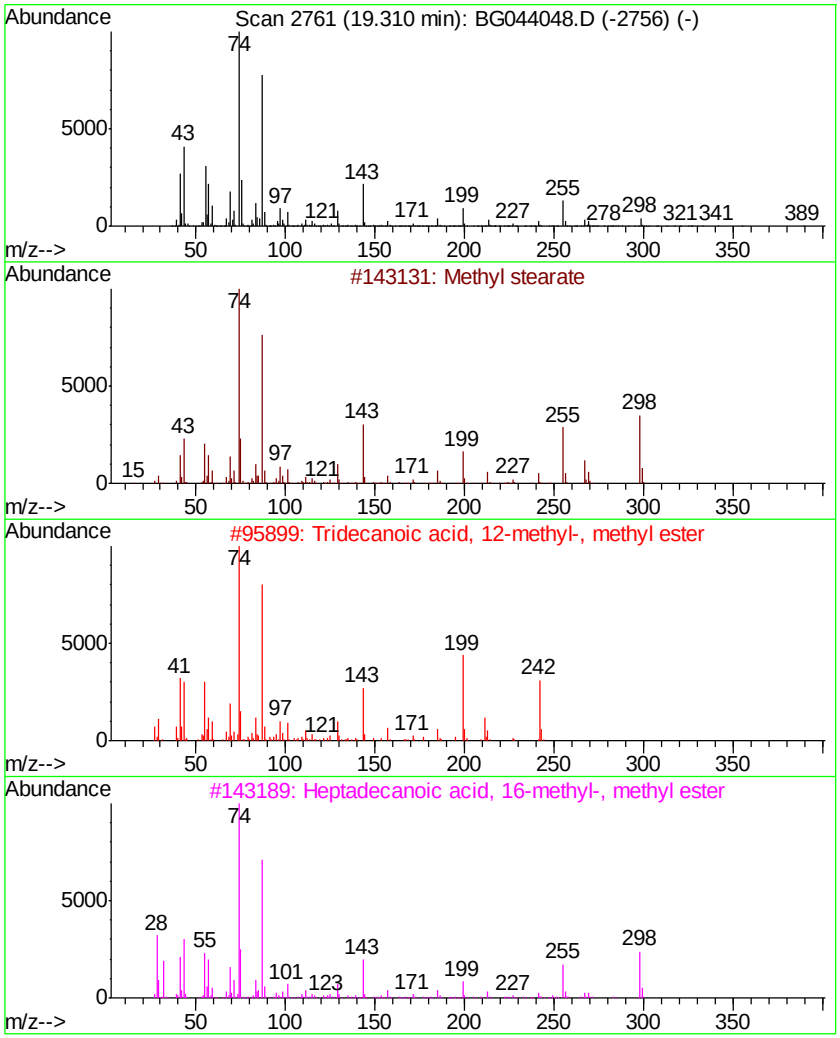
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

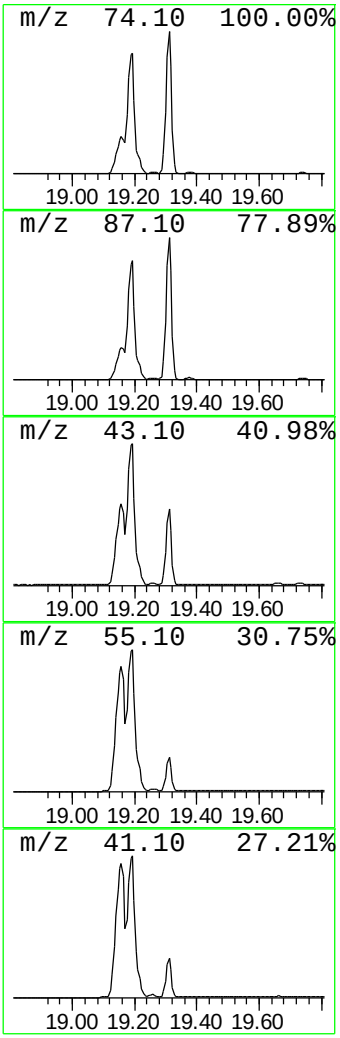
****

Peak Number 7 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.31	67.65 ng	5916730	Phenanthrene-d10	17.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	94
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044048.D
Acq On : 14 Jan 2020 22:42
Operator : JU
Sample : L1004-07 2X
Misc :
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Instrument : BNA_G
ClientSampleId : BU-RO-229

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

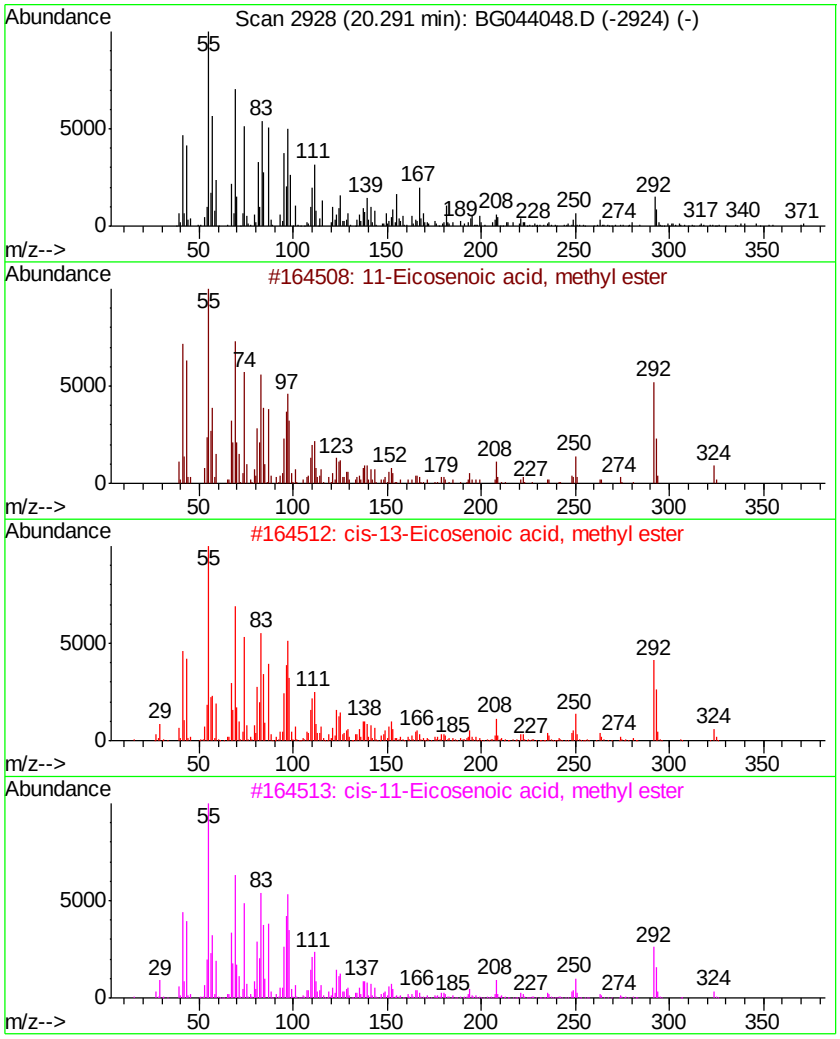
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

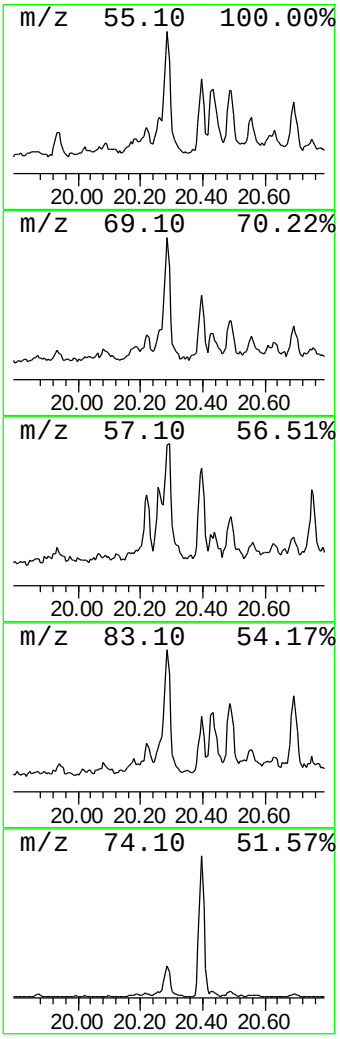
****

Peak Number 8 11-Eicosenoic acid, methyl ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.29	5.30 ng	586665	Chrysene-d12	21.58

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	1000333-52-1	97
3	cis-11-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-63-8	68
4	cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	68
5	Methyl 9-heptadecenoate or 9-17:1	282	C18H34O2	1000336-38-0	58





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044048.D
Acq On : 14 Jan 2020 22:42
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Sample : L1004-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BU-RO-229

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

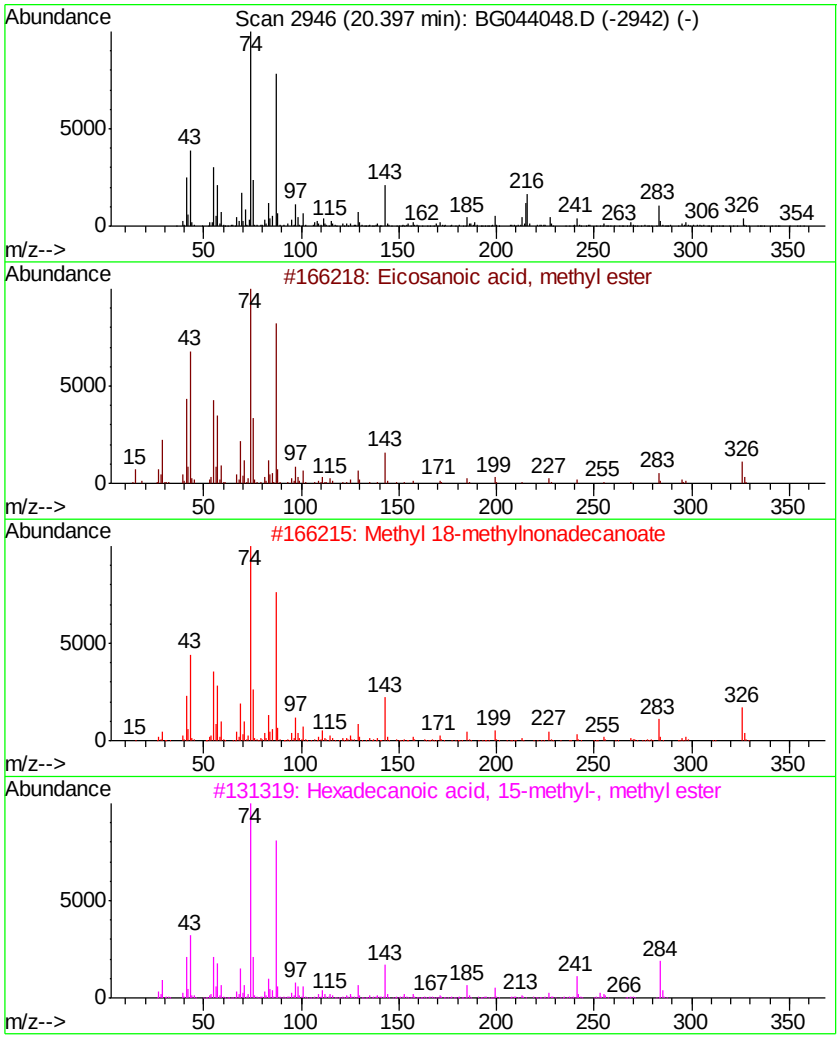
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

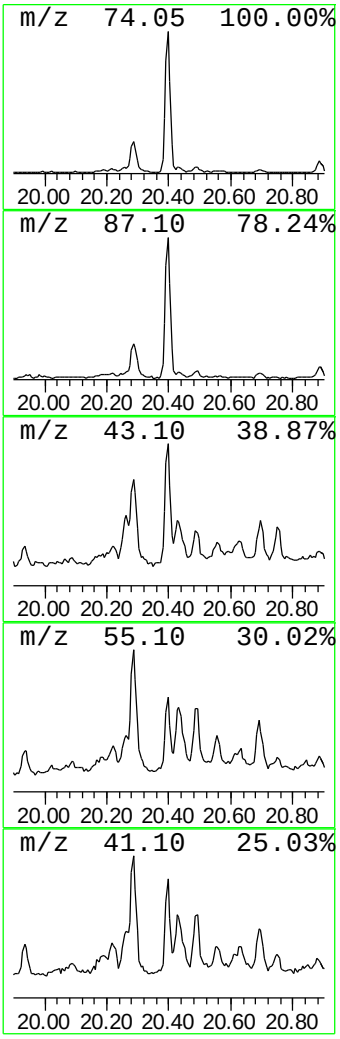
****

Peak Number 9 Eicosanoic acid, methyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.40	5.27 ng	582924	Chrysene-d12	21.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	97
2	Methyl 18-methylnonadecanoate	326	C21H42O2	1000352-20-6	97
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	95
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
5	Hexadecanoic acid, 14-methyl-, m...	284	C18H36O2	002490-49-5	91





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Data File : BG044048.D
Acq On : 14 Jan 2020 22:42
Operator : JU
Sample : L1004-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BU-RO-229

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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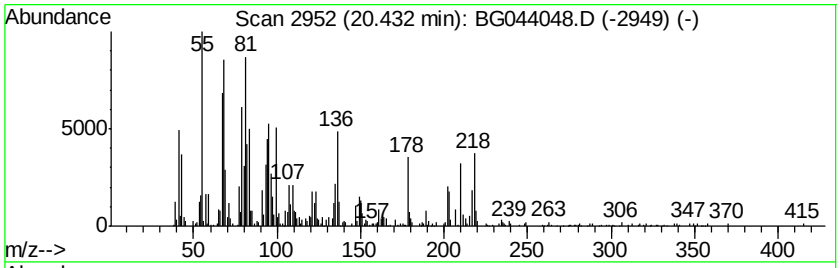
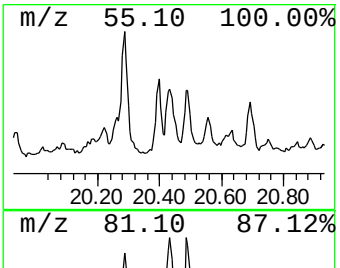
Peak Number 10 8,10-Dodecadien-1-ol, aceta... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.43	4.42 ng	488923	Chrysene-d12	21.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8,10-Dodecadien-1-ol, acetate, (...	224	C14H24O2	053880-51-6	55
2	13-Tetradece-11-yn-1-ol	208	C14H24O	1000131-00-4	52
3	9-Octadecynoic acid, methyl ester	294	C19H34O2	001120-32-7	46
4	Cyclopentanepropanol, 2-methylene-	140	C9H16O	053544-48-2	44
5	1,2,3,4,4a,5,6,8a-Octahydro-naph...	136	C10H16	031244-58-3	43





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Data File : BG044048.D
Acq On : 14 Jan 2020 22:42
Operator : JU
Sample : L1004-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BU-RO-229

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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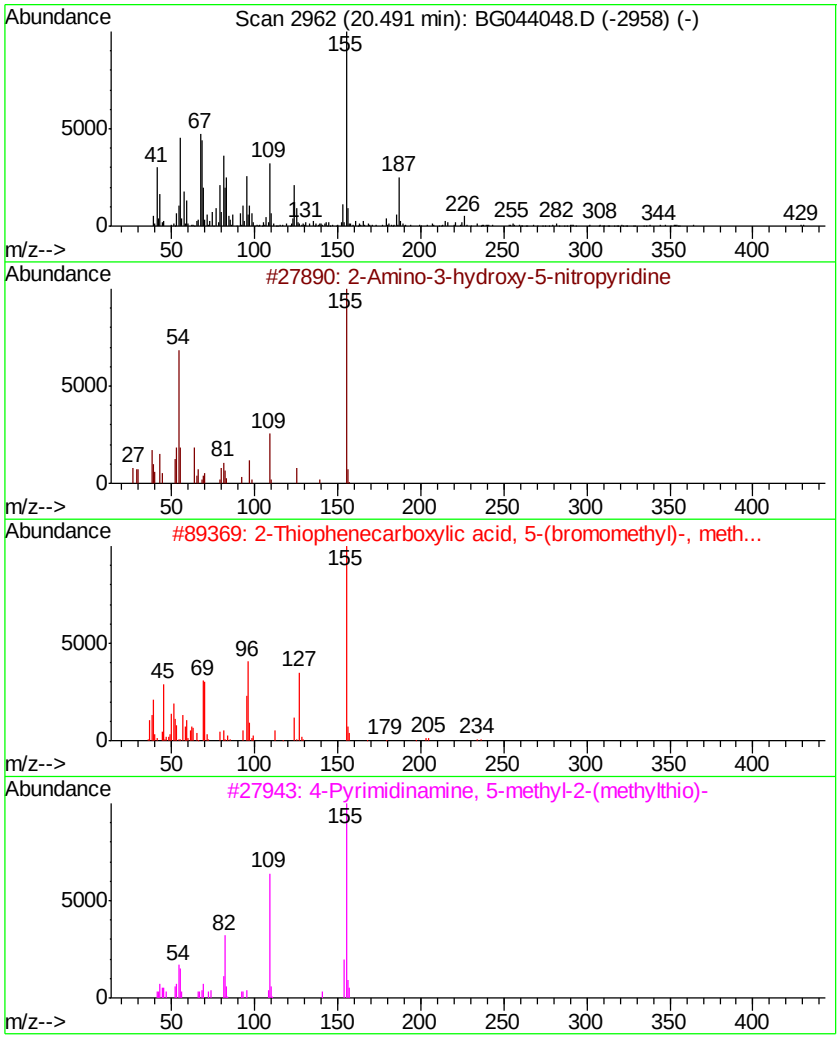
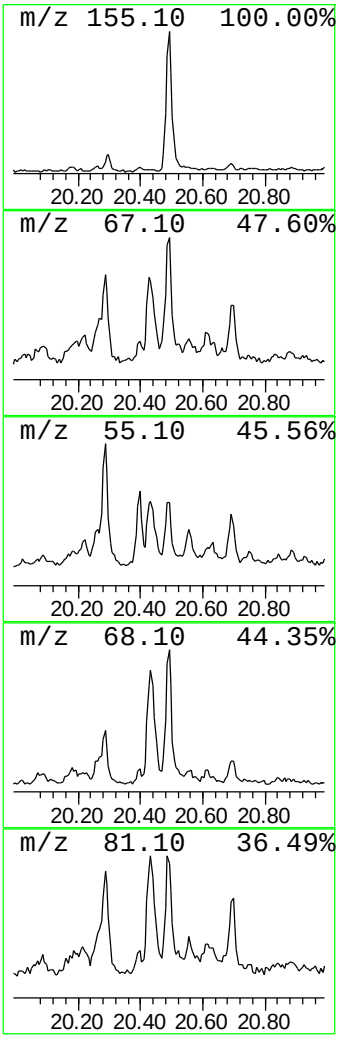
Peak Number 11 unknown20.49 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.49	3.58 ng	395846	Chrysene-d12	21.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-3-hydroxy-5-nitropyridine	155	C5H5N3O3	1000289-29-0	38
2	2-Thiophenecarboxylic acid, 5-(b...	234	C7H7BrO2S	1000362-74-6	38
3	4-Pyrimidinamine, 5-methyl-2-(me...	155	C6H9N3S	054308-64-4	27
4	1,2-Cyclohexanedicarboxylic acid...	372	C18H22Cl2O4	1000339-84-2	27
5	Cyclohexanol, 1-butyl-4-(1,1-dim...	212	C14H28O	053188-79-7	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044048.D
Acq On : 14 Jan 2020 22:42
Operator : JU
Sample : L1004-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BU-RO-229

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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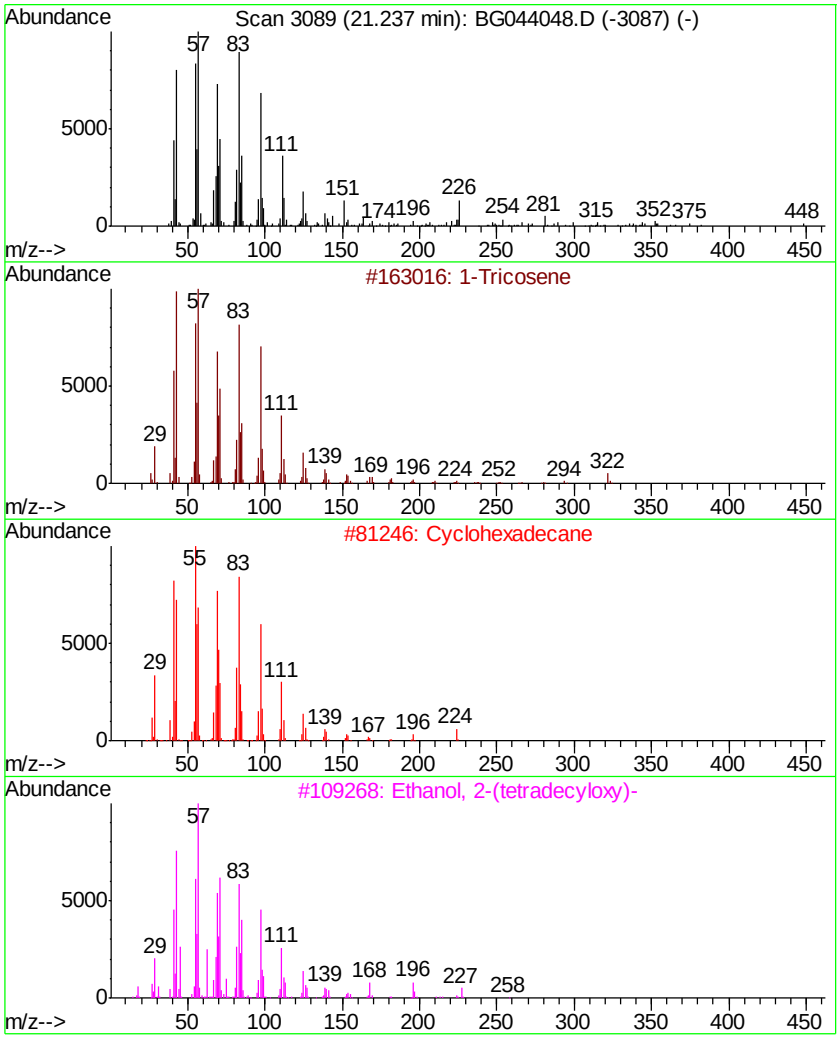
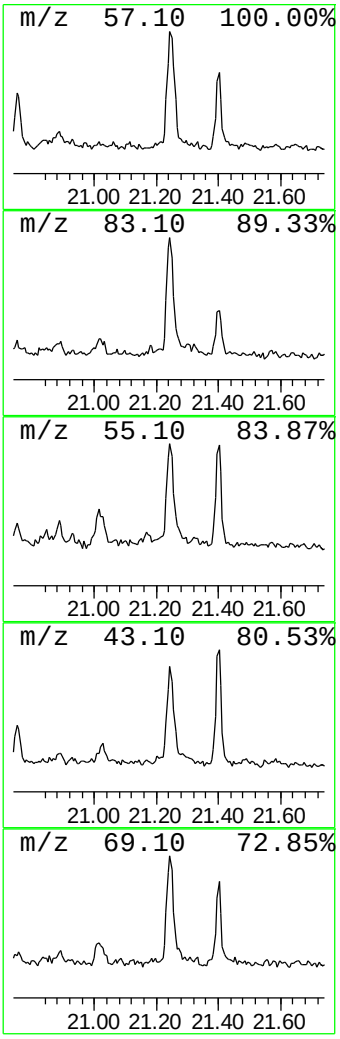
Peak Number 12 1-Tricosene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.24	3.51 ng	388746	Chrysene-d12	21.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	95
2	Cyclohexadecane	224	C16H32	000295-65-8	91
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
4	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	90
5	Tetracosyl trifluoroacetate	450	C26H49F3O2	1000351-76-4	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011420\
Data File : BG044048.D
Acq On : 14 Jan 2020 22:42
Operator : JU
Sample : L1004-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BU-RO-229

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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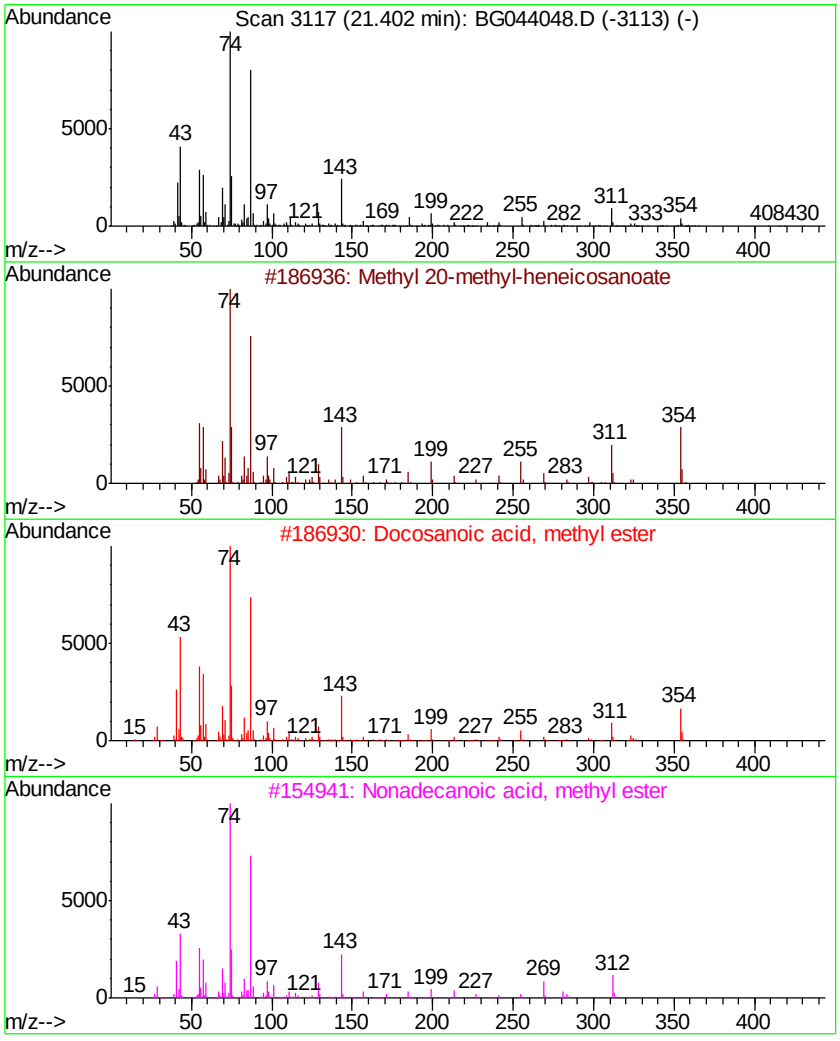
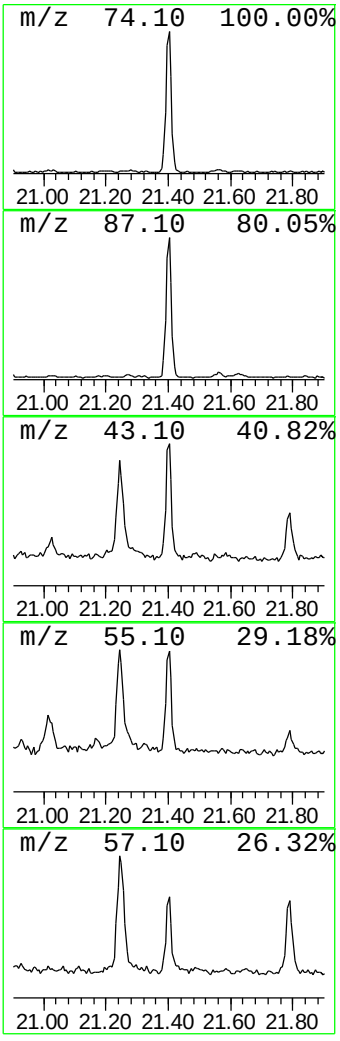
Peak Number 13 Methyl 20-methyl-heneicosan... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	3.97 ng	439642	Chrysene-d12	21.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	99
2	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	99
3	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	90
4	Hexacosanoic acid, methyl ester	410	C27H54O2	005802-82-4	90
5	Methyl stearate	298	C19H38O2	000112-61-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG011420\
Data File : BG044048.D
Acq On : 14 Jan 2020 22:42
Operator : JU
Sample : L1004-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BU-RO-229

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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
Butane, 2-methoxy...	3.14	9.2	ng	405136	1	7.95	883757	20.0
unknown7.48	7.48	36.2	ng	1598940	1	7.95	883757	20.0
Hexadecanoic acid...	18.01	124.1	ng	10853000	4	17.32	1749270	20.0
9,12-Octadecadien...	19.16	377.3	ng	32995500	4	17.32	1749270	20.0
9-Octadecenoic ac...	19.19	345.2	ng	30193600	4	17.32	1749270	20.0
Methyl stearate	19.31	67.7	ng	5916730	4	17.32	1749270	20.0
11-Eicosenoic aci...	20.29	5.3	ng	586665	5	21.58	2214300	20.0
Eicosanoic acid, ...	20.40	5.3	ng	582924	5	21.58	2214300	20.0
8,10-Dodecadien-1...	20.43	4.4	ng	488923	5	21.58	2214300	20.0
unknown20.49	20.49	3.6	ng	395846	5	21.58	2214300	20.0
1-Tricosene	21.24	3.5	ng	388746	5	21.58	2214300	20.0
Methyl 20-methyl-...	21.40	4.0	ng	439642	5	21.58	2214300	20.0