LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
Data File : BF128278.D
Acq On : 16 May 2022 20:15
Operator : CG\JU
Sample : N2855-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-051322

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_F\Methods\8270-BF050922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128278.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.510	544	548	564	rBV	1520265	1528764	4.01%	2.174%
2	6.516	715	719	722	rBV	1699827	1494961	3.92%	2.126%
3	6.887	778	782	785	rBV	534068	464063	1.22%	0.660%
4	7.451	874	878	881	rBV	1094115	977978	2.57%	1.391%
5	8.169	996	1000	1003	rBV	653383	516302	1.35%	0.734%
6	9.239	1178	1182	1186	rBV	1662998	1512976	3.97%	2.152%
7	9.928	1295	1299	1302	rVB	623268	522559	1.37%	0.743%
8	10.716	1430	1433	1437	rBV	1038164	883283	2.32%	1.256%
9	11.416	1548	1552	1555	rBV	655448	556002	1.46%	0.791%
10	11.810	1613	1619	1622	rBV	8501122	10812964	28.38%	15.379%
11	11.957	1637	1644	1648	rBV	489048	583914	1.53%	0.830%
12	12.545	1729	1744	1745	rBV5	10080756	38104560	100.00%	54.196%
13	12.610	1752	1755	1758	rVB	6762333	6099346	16.01%	8.675%
14	12.657	1758	1763	1771	rBV2	1125877	2304160	6.05%	3.277%
15	13.016	1818	1824	1826	rBV	1613088	1507606	3.96%	2.144%
16	13.239	1860	1862	1869	rVB	575589	633523	1.66%	0.901%
17	13.316	1872	1875	1881	rBV	856555	719597	1.89%	1.023%
18	13.986	1985	1989	1992	rBV	795023	701914	1.84%	0.998%
19	14.068	2000	2003	2009	rVB	443165	384476	1.01%	0.547%

Sum of corrected areas: 70308948

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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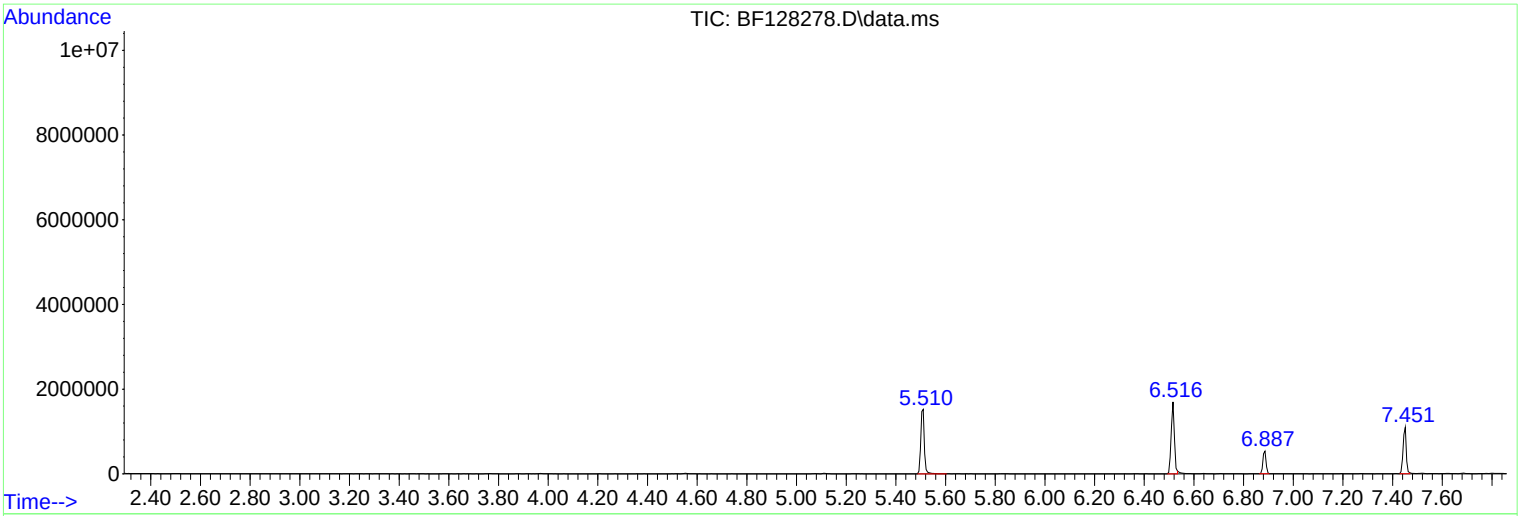
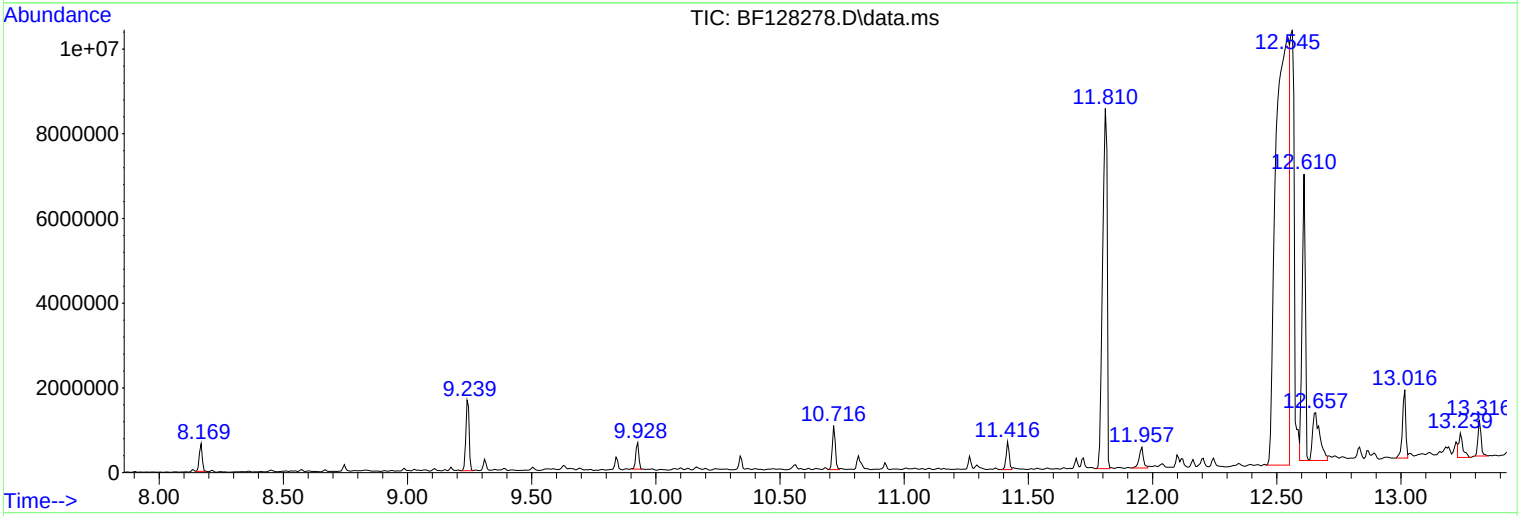
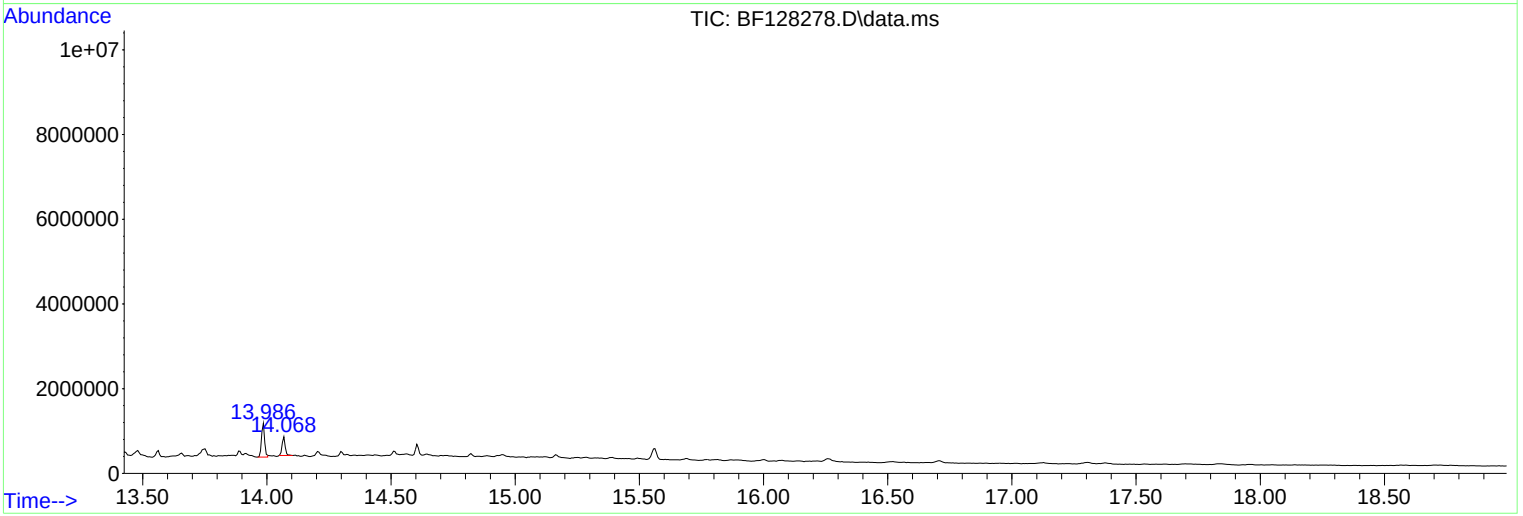
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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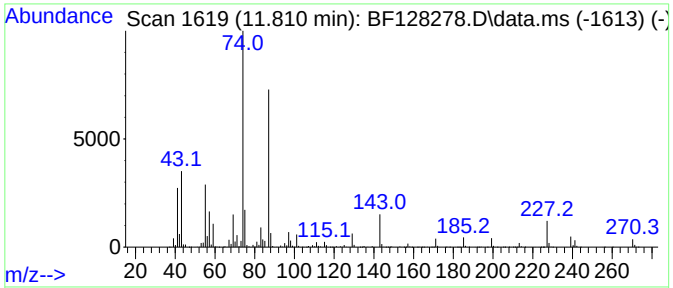
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

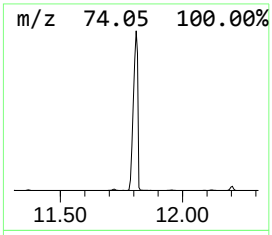
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

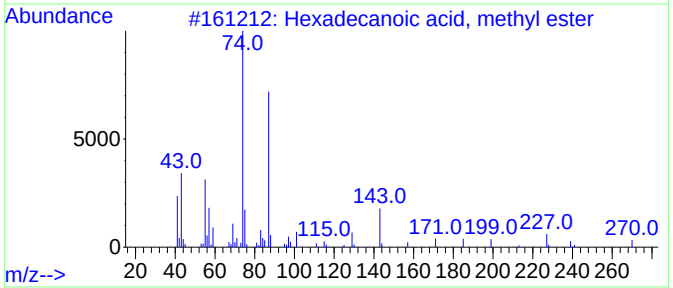
****
Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 2

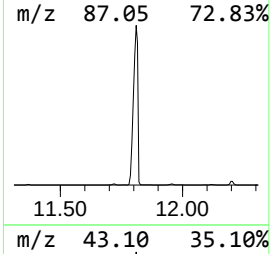
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	388.95 ng	10813000	Phenanthrene-d10	11.416

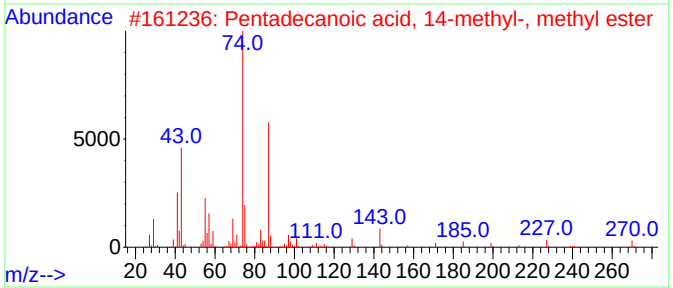
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	89
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	74

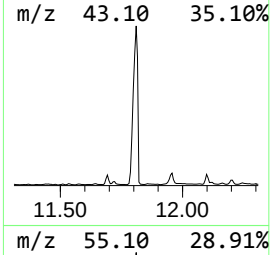


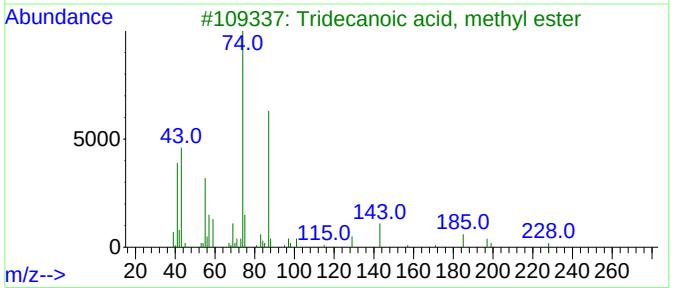


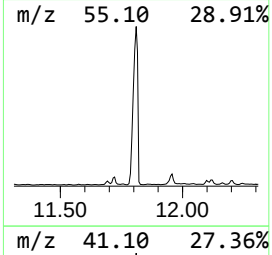


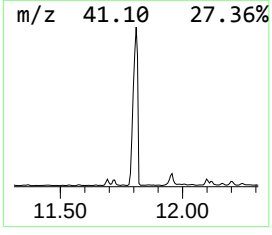












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Acq On : 16 May 2022 20:15
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Sample : N2855-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-051322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

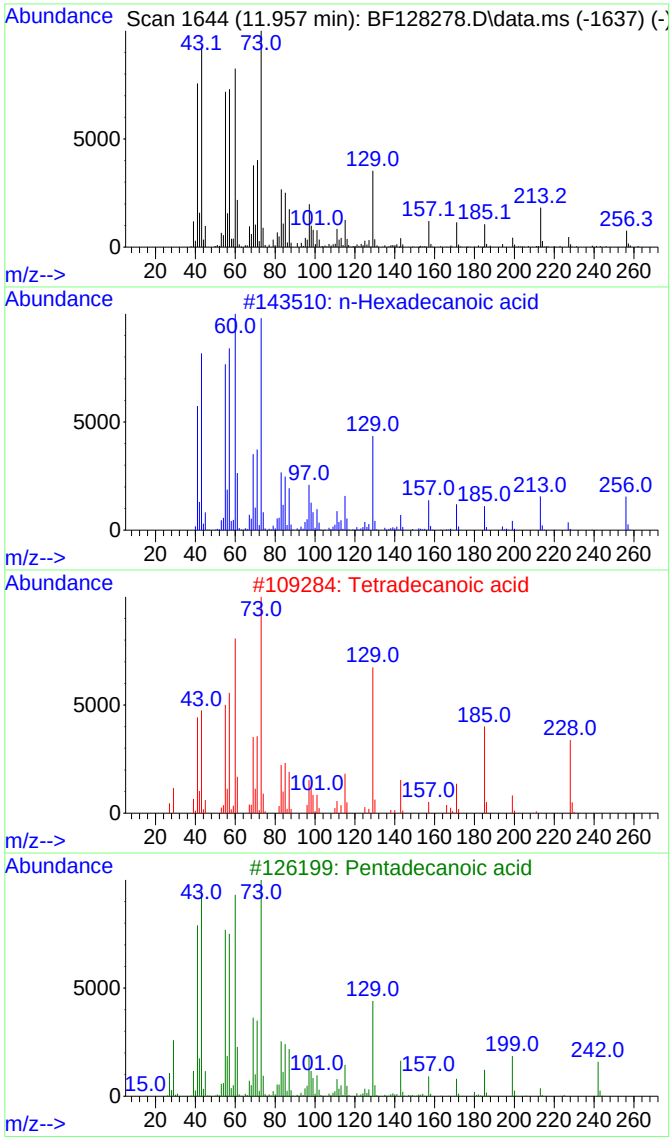
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

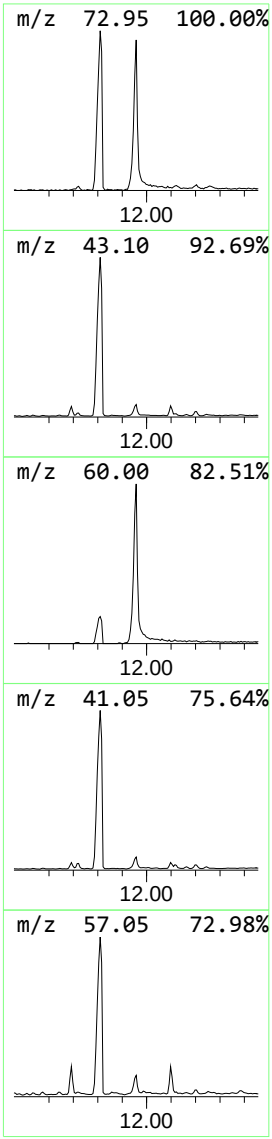
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	21.00 ng	583914	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	53





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Acq On : 16 May 2022 20:15
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

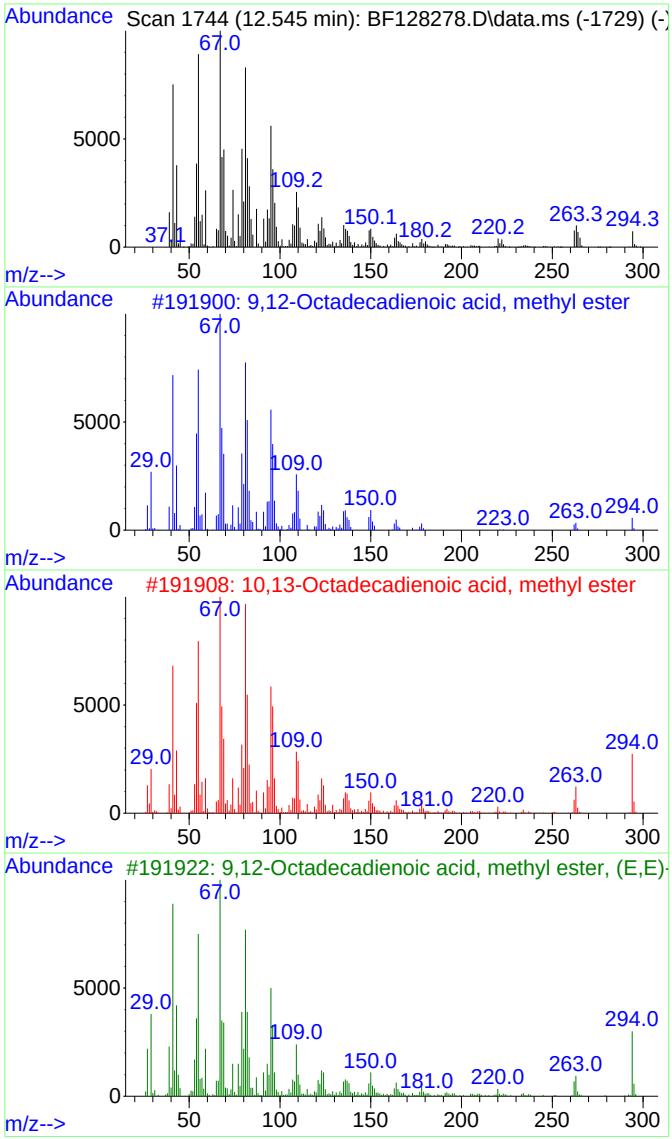
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

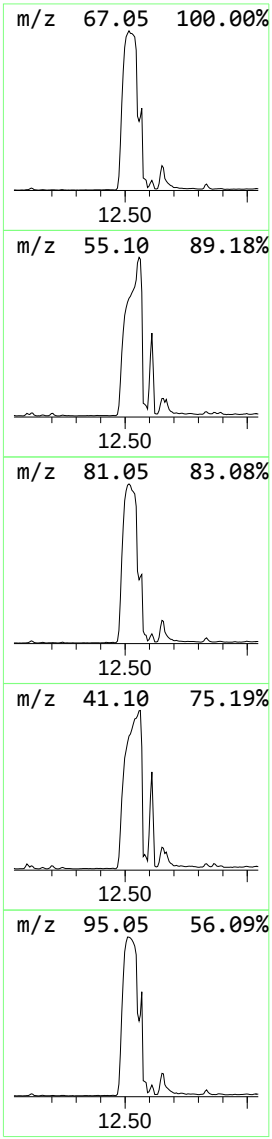
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.545	1370.66 ng	38104600	Phenanthrene-d10	11.416

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, methy...	294	C19H34O2	002566-97-4	99
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	98





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Operator : CG\JU
Sample : N2855-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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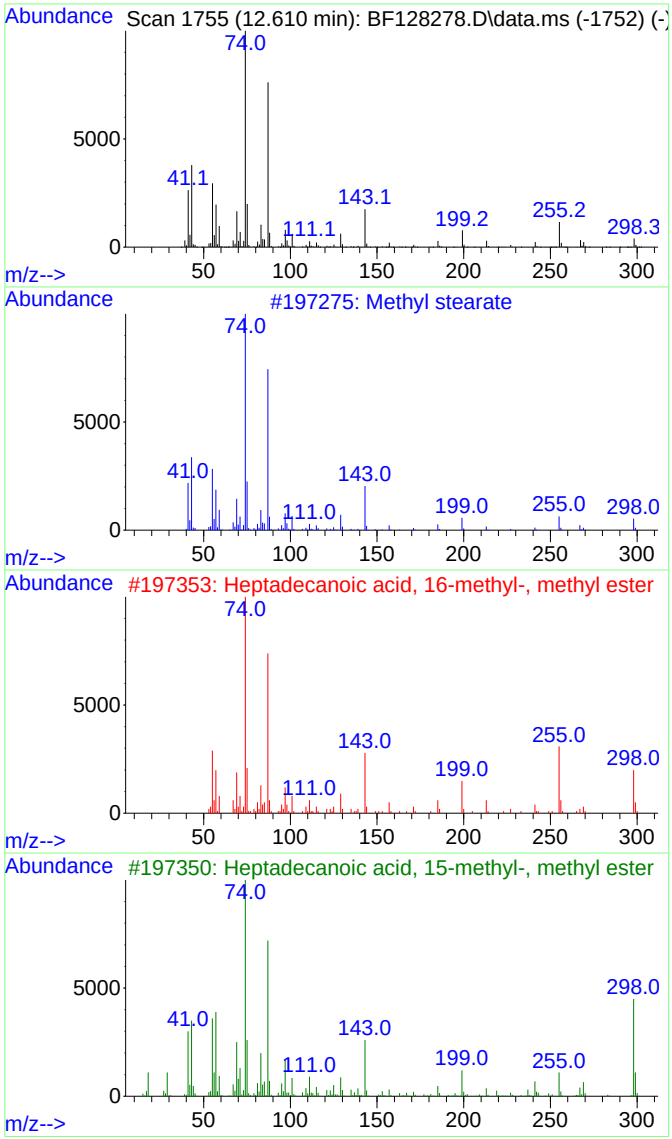
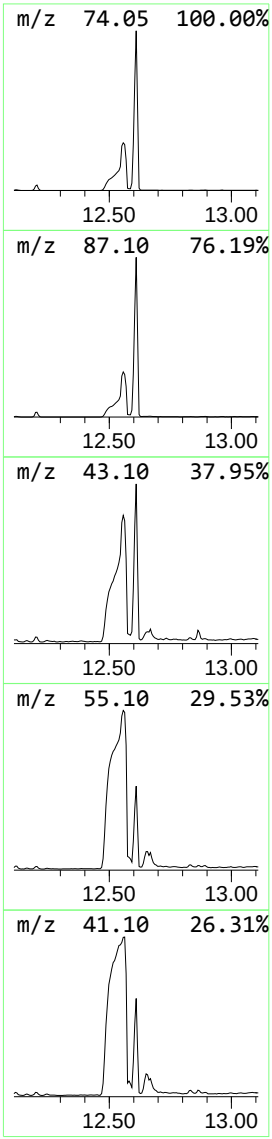
****

Peak Number 4 Methyl stearate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	219.40 ng	6099350	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
3	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	93
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
5	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	90





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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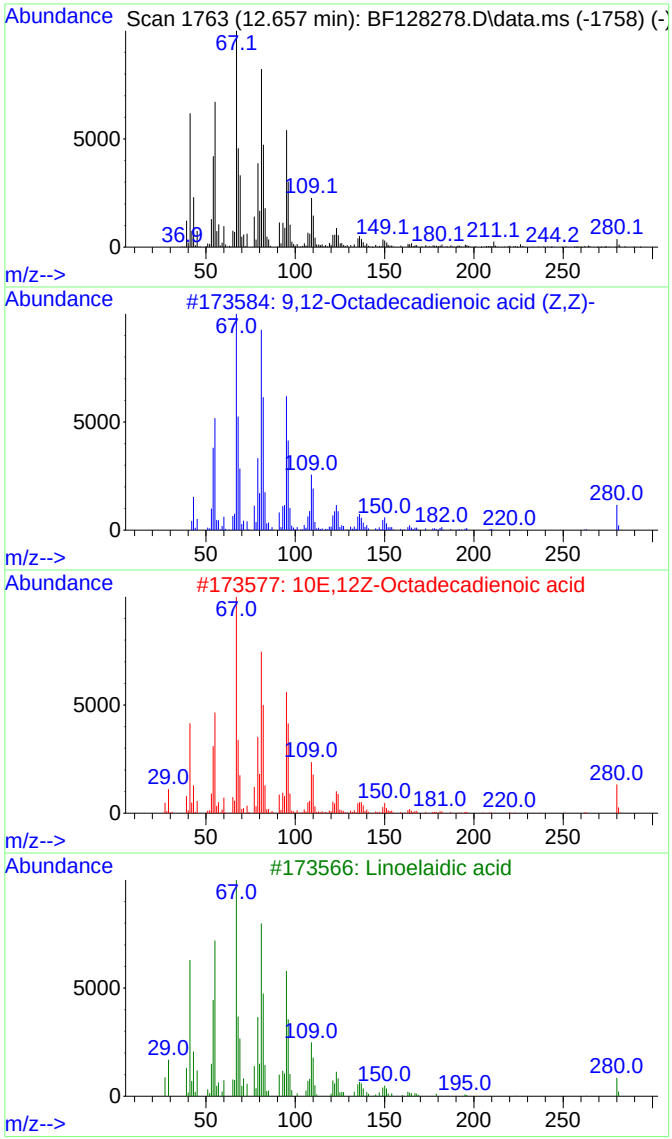
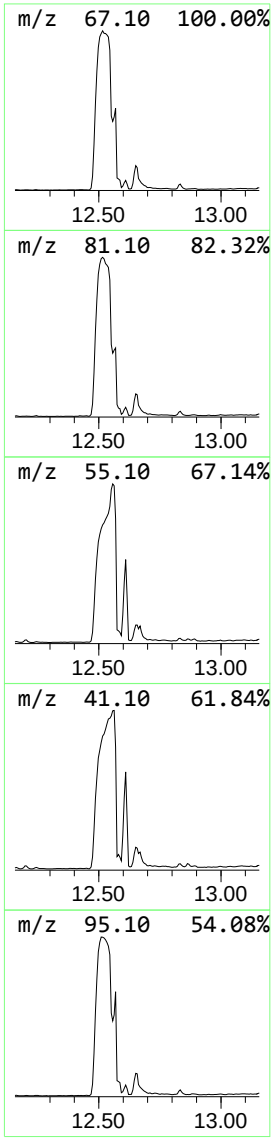
****
Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.657	82.88 ng	2304160	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	98
3	Linoelaidic acid	280	C18H32O2	000506-21-8	98
4	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	97
5	8-Dodecen-1-ol, (Z)-	184	C12H24O	040642-40-8	89





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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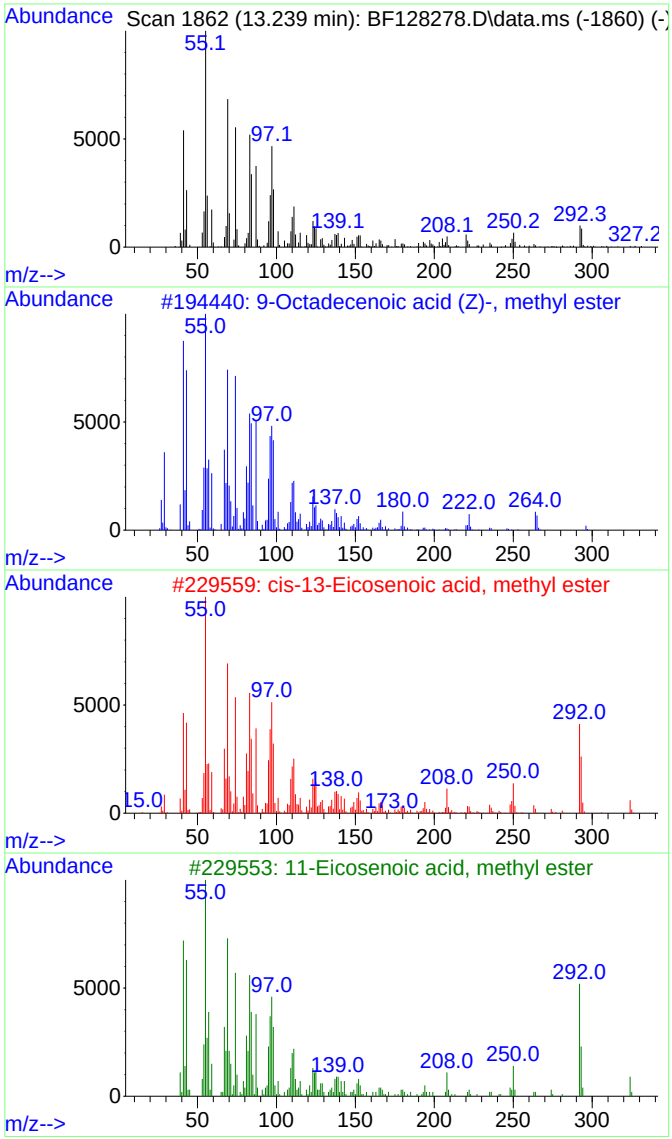
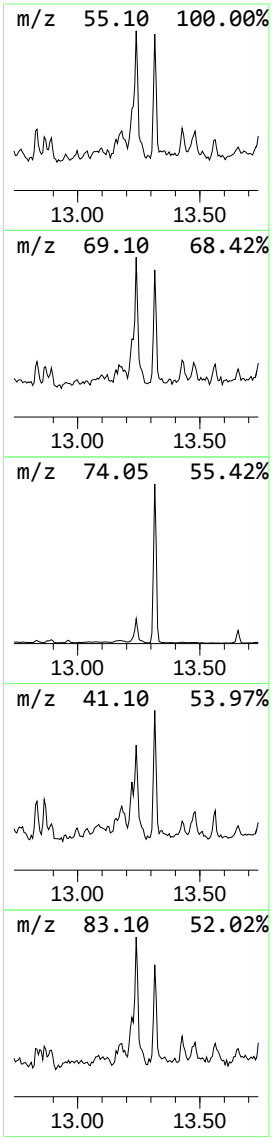
****

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.239	32.96 ng	633523	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	91
3	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	86
4	Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	78
5	Methyl (Z)-10-pentadecenoate	254	C16H30O2	1000426-92-2	53





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TIC Library : C:\Database\NIST20.L
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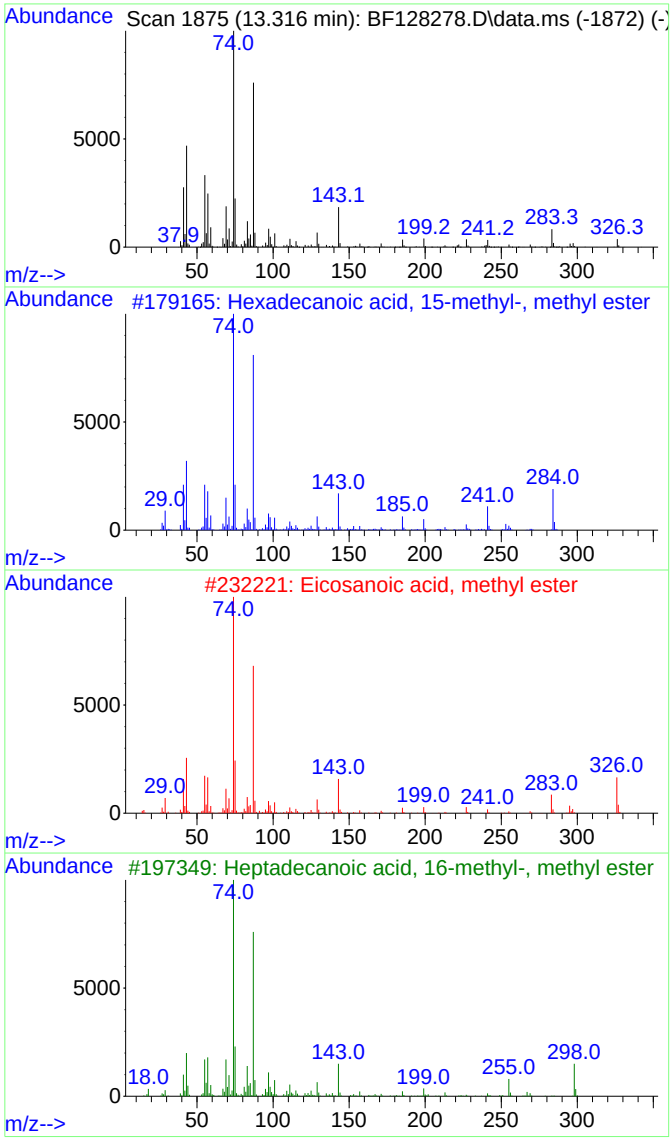
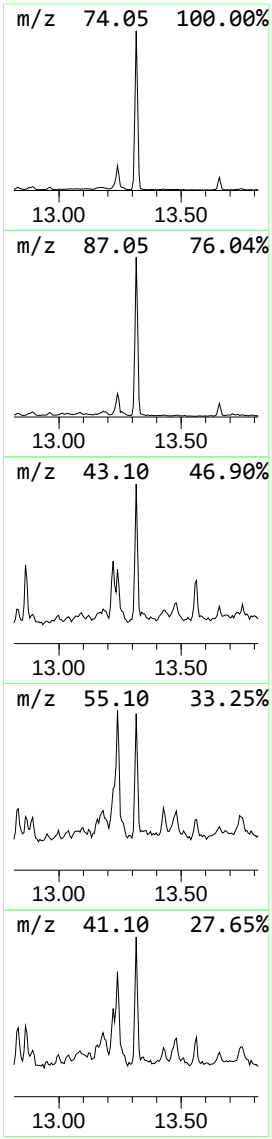
****
Peak Number 7 Hexadecanoic acid, 15-methy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.316	37.43 ng	719597	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	97
2	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	97
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
4	Methyl 18-methylnonadecanoate	326	C21H42O2	1000424-52-4	94
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	93





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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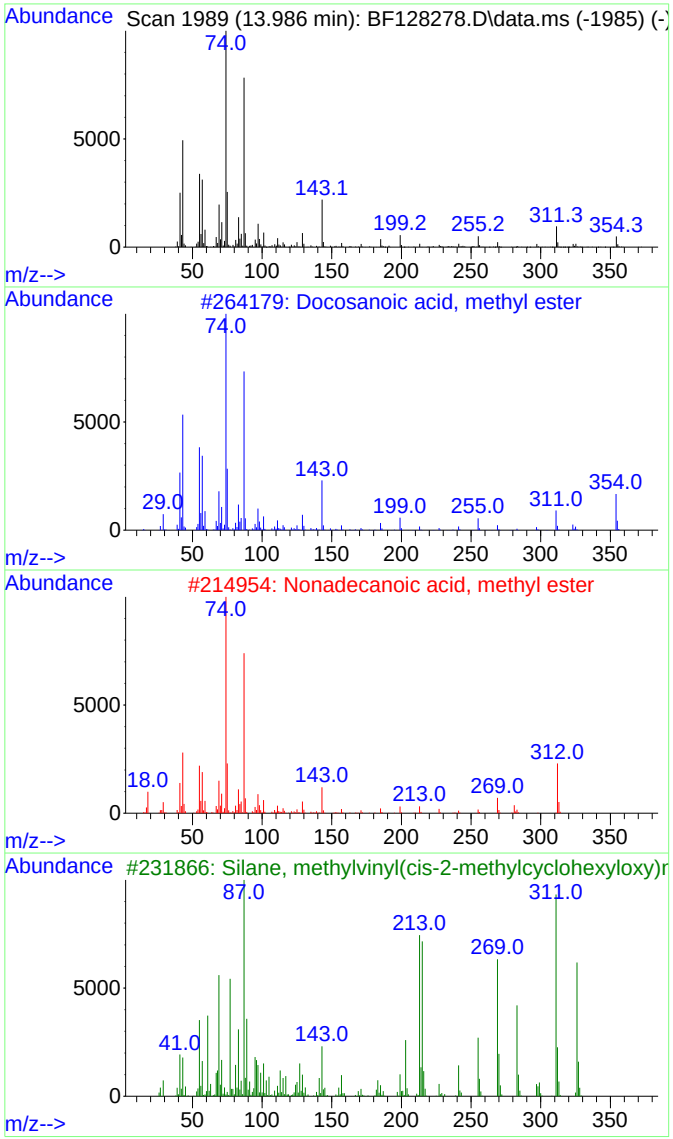
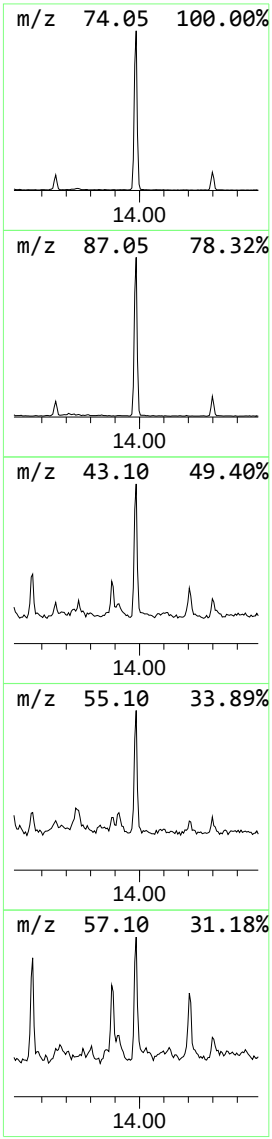
****

Peak Number 8 Docosanoic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.986	36.51 ng	701914	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	99
2	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	97
3	Silane, methylvinyl(cis-2-methyl...	326	C19H38O2Si	1000421-05-3	94
4	Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	91
5	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051622\
Data File : BF128278.D
Acq On : 16 May 2022 20:15
Operator : CG\JU
Sample : N2855-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-051322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050922.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...	11.810	388.9	ng	10813000	4	11.416	556002	20.0
n-Hexadecanoic ...	11.957	21.0	ng	583914	4	11.416	556002	20.0
9,12-Octadecadi...	12.545	1370.7	ng	38104600	4	11.416	556002	20.0
Methyl stearate	12.610	219.4	ng	6099350	4	11.416	556002	20.0
9,12-Octadecadi...	12.657	82.9	ng	2304160	4	11.416	556002	20.0
9-Octadecenoic ...	13.239	33.0	ng	633523	5	14.069	384476	20.0
Hexadecanoic ac...	13.316	37.4	ng	719597	5	14.069	384476	20.0
Docosanoic acid...	13.986	36.5	ng	701914	5	14.069	384476	20.0