LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF011818\
Data File : BF102197.D
Acq On : 18 Jan 2018 17:52
Operator : SJ/JU
Sample : J1010-06 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-011718

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:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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	5.322	545	550	553	rBV	2189198	1967360	10.54%	3.345%
2	6.351	720	725	735	rVB	2232774	2055050	11.01%	3.494%
3	6.487	743	748	751	rBV	2296864	2073117	11.11%	3.525%
4	6.716	784	787	791	rBV	1148103	992120	5.32%	1.687%
5	6.875	810	814	817	rBV	1835012	1575563	8.44%	2.679%
6	7.281	878	883	886	rBV	1439911	1247226	6.68%	2.120%
7	7.998	1000	1005	1009	rBV	1494907	1381994	7.41%	2.350%
8	9.075	1184	1188	1192	rBV	2362934	2160817	11.58%	3.674%
9	9.475	1251	1256	1259	rBV	256074	257571	1.38%	0.438%
10	9.751	1300	1303	1307	rVB	1444582	1303649	6.99%	2.216%
11	10.539	1431	1437	1440	rBV	1259593	1095170	5.87%	1.862%
12	10.657	1454	1457	1462	rBV	174276	195043	1.05%	0.332%
13	11.233	1552	1555	1558	rBV	1285516	1103837	5.92%	1.877%
14	11.645	1619	1625	1628	rBV	6172363	6669907	35.75%	11.340%
15	12.345	1735	1744	1746	rBV	7696819	18657123	100.00%	31.719%
16	12.368	1746	1748	1752	rVV2	7810766	8273412	44.34%	14.066%
17	12.433	1755	1759	1764	rVB	3656185	3376941	18.10%	5.741%
18	12.674	1792	1800	1802	rBV3	123495	199640	1.07%	0.339%
19	12.821	1819	1825	1829	rBV	1702636	1556093	8.34%	2.646%
20	13.068	1861	1867	1875	rVB2	263728	379221	2.03%	0.645%
21	13.145	1877	1880	1883	rBV	362501	319700	1.71%	0.544%
22	13.815	1990	1994	1998	rBV	313125	287328	1.54%	0.488%
23	13.868	1998	2003	2006	rBV	949045	904534	4.85%	1.538%
24	15.286	2239	2244	2247	rBV	650940	787533	4.22%	1.339%

Sum of corrected areas: 58819949

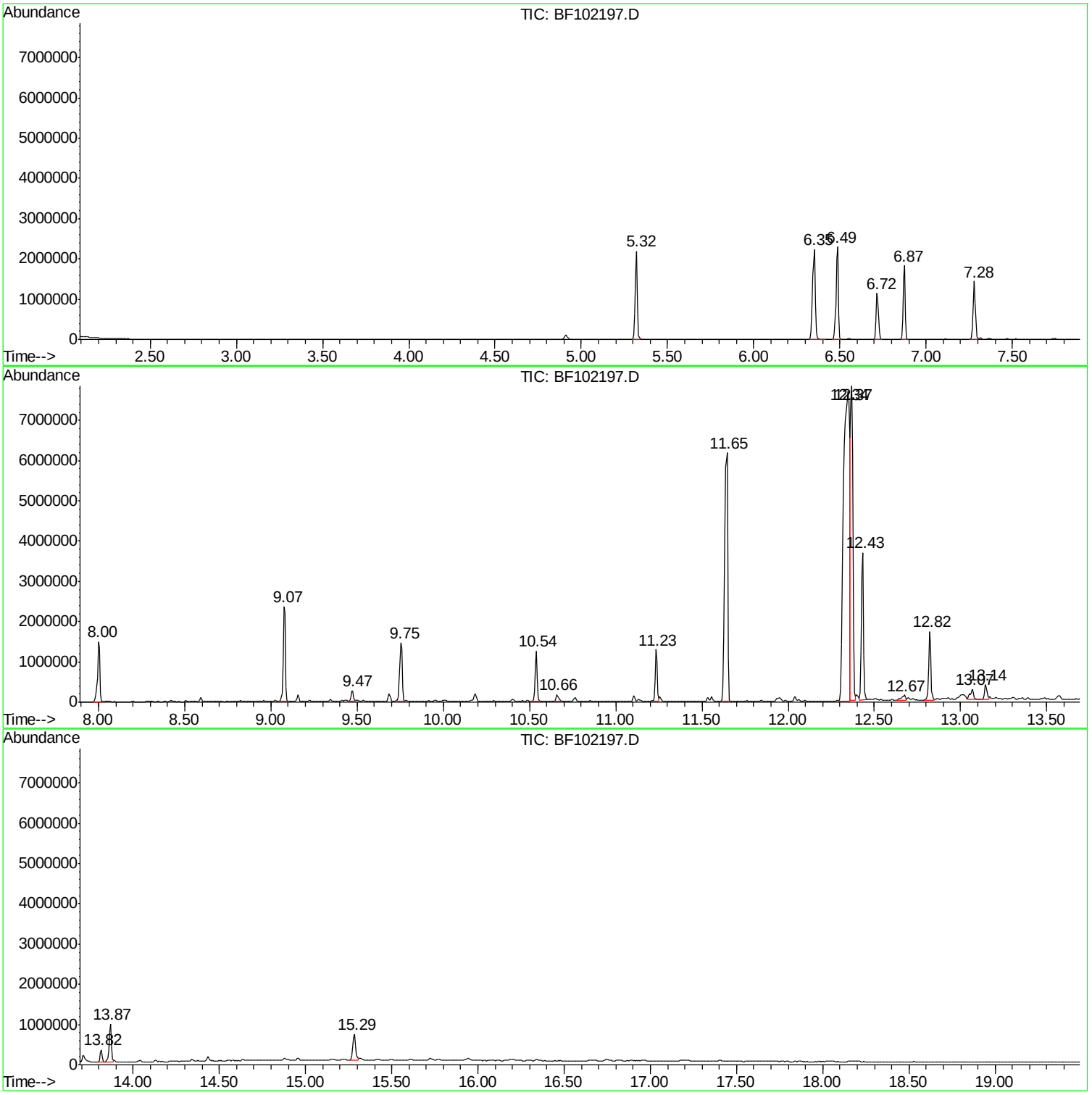
LSC Report - Integrated Chromatogram

Data Path : U:\HPCHEM1\BNA F\DATA\BF011818\
Data File : BF102197.D
Acq On : 18 Jan 2018 17:52
Operator : SJ/JU
Sample : J1010-06 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-011718

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA F\DATA\BF011818\
Data File : BF102197.D
Acq On : 18 Jan 2018 17:52
Operator : SJ/JU
Sample : J1010-06 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-011718

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

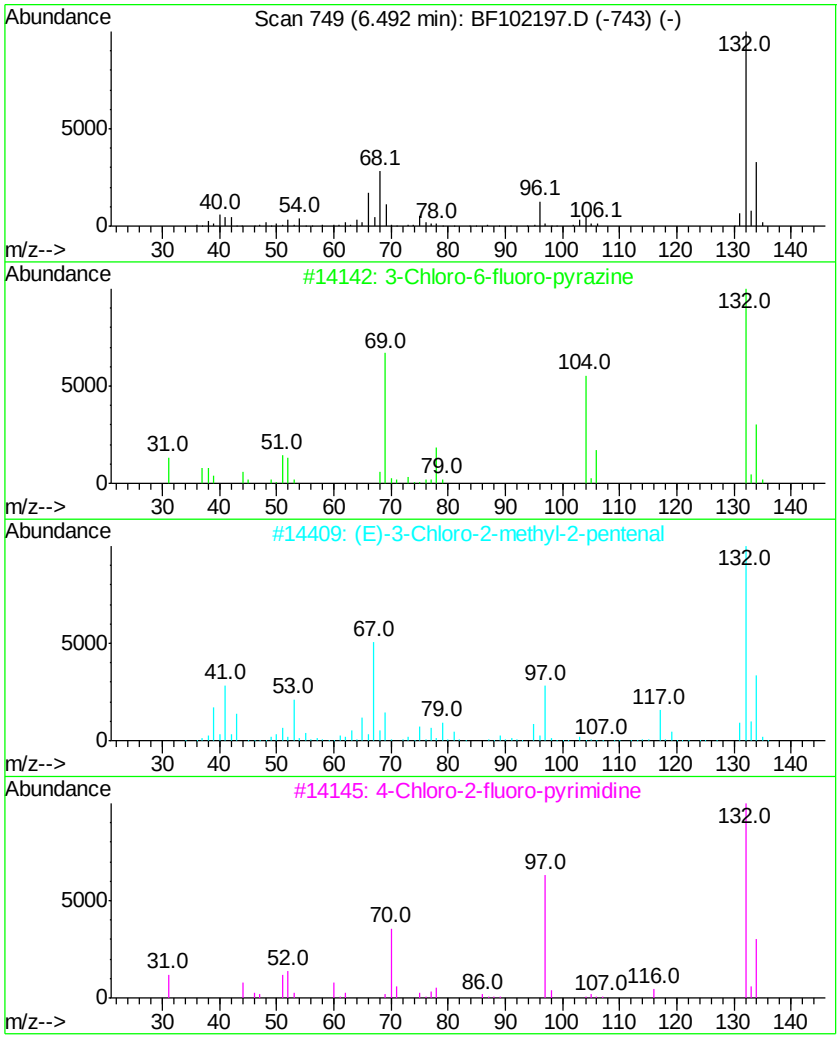
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

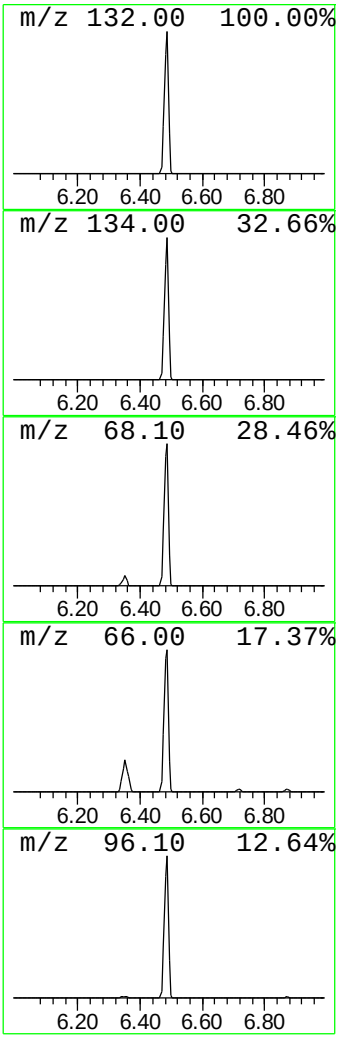
****

Peak Number 1 unknown6.49 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	41.79 ng	2073120	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF011818\
Data File : BF102197.D
Acq On : 18 Jan 2018 17:52
Operator : SJ/JU
Sample : J1010-06 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-011718

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

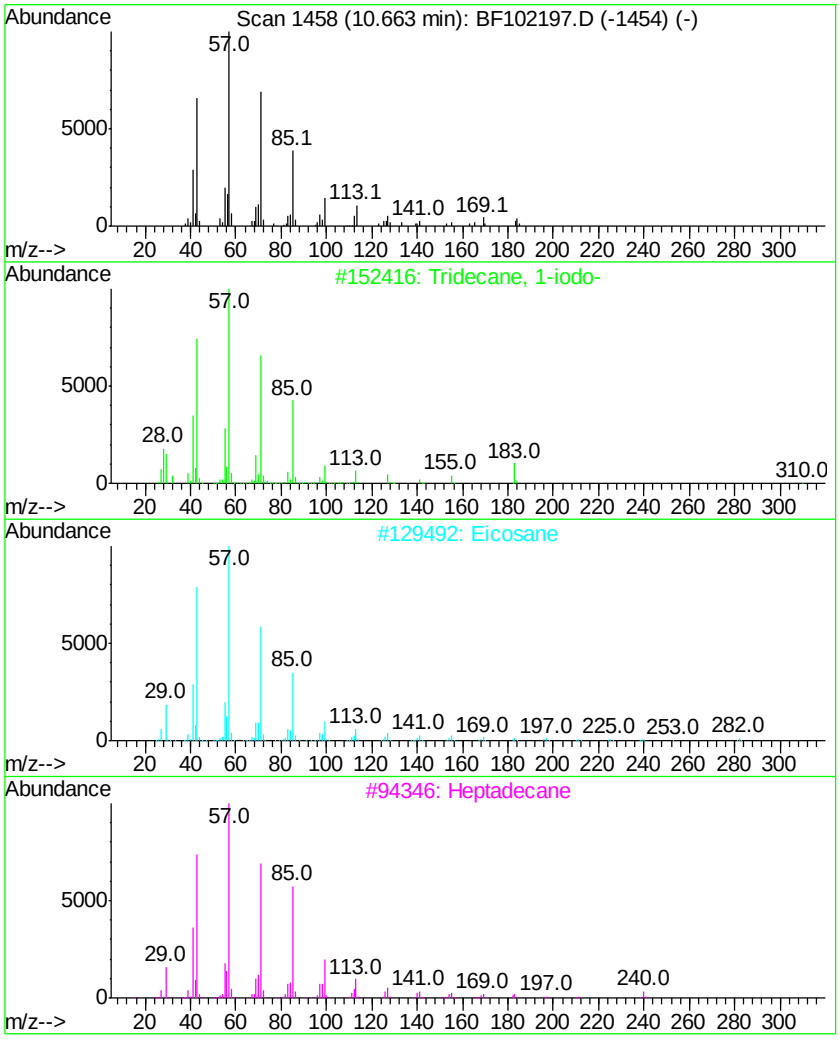
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

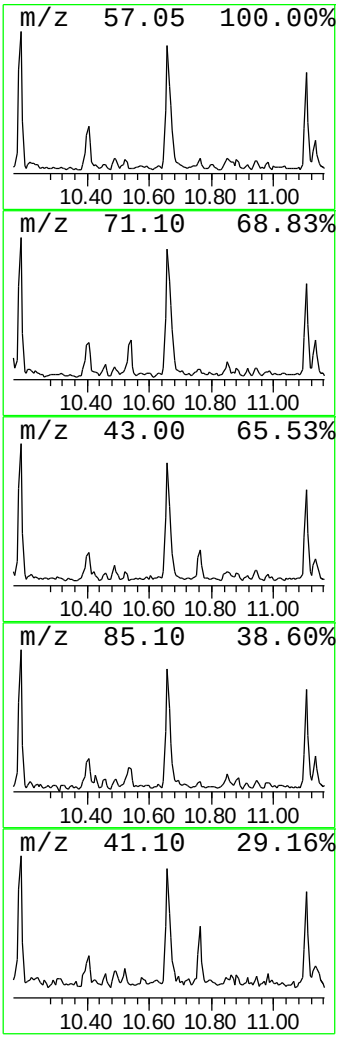
****

Peak Number 3 Tridecane, 1-iodo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	3.53 ng	195043	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
2	Eicosane	282	C20H42	000112-95-8	87
3	Heptadecane	240	C17H36	000629-78-7	87
4	Hexadecane	226	C16H34	000544-76-3	87
5	Octadecane	254	C18H38	000593-45-3	86





Data Path : U:\HPCHEM1\BNA F\DATA\BF011818\
Data File : BF102197.D
Acq On : 18 Jan 2018 17:52
Operator : SJ/JU
Sample : J1010-06 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-011718

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

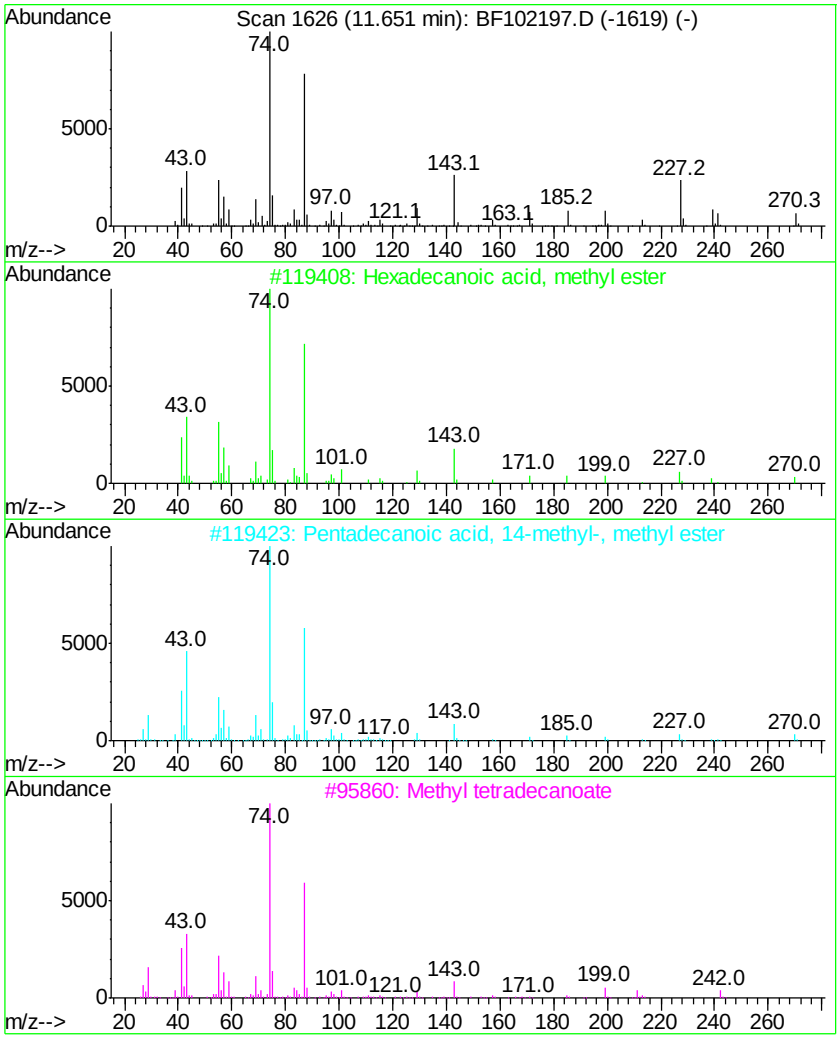
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

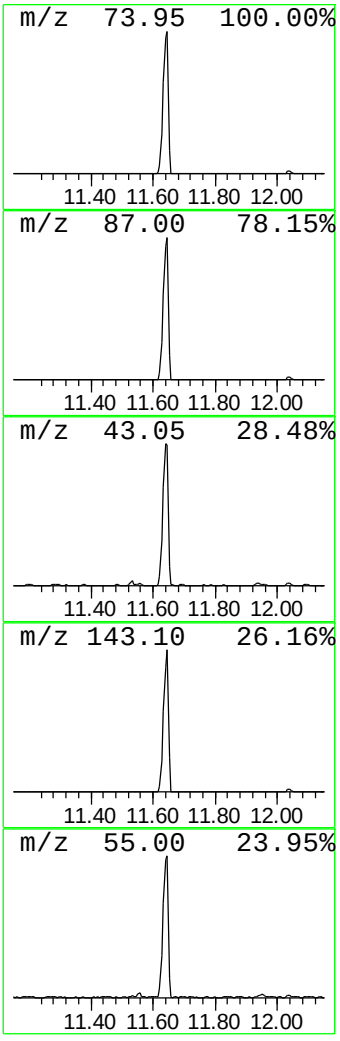
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	120.85 ng	6669910	Phenanthrene-d10	11.23

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	92
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87





Data Path : U:\HPCHEM1\BNA F\DATA\BF011818\
Data File : BF102197.D
Acq On : 18 Jan 2018 17:52
Operator : SJ/JU
Sample : J1010-06 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-011718

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

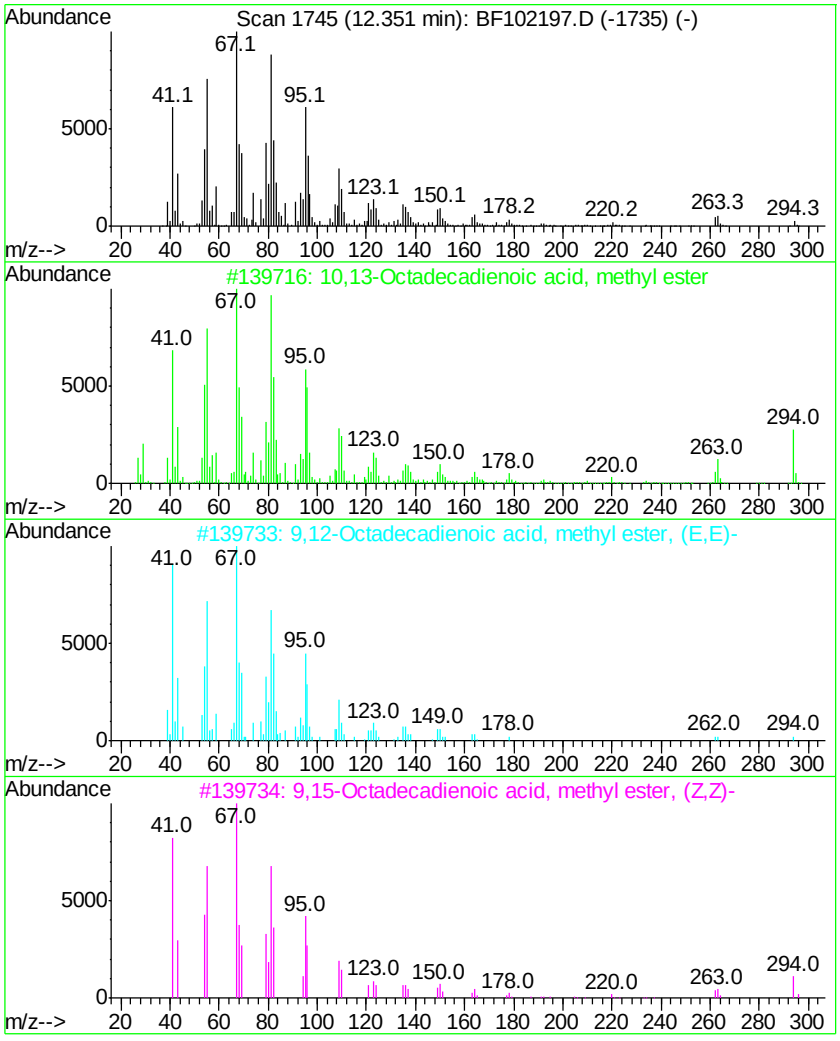
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

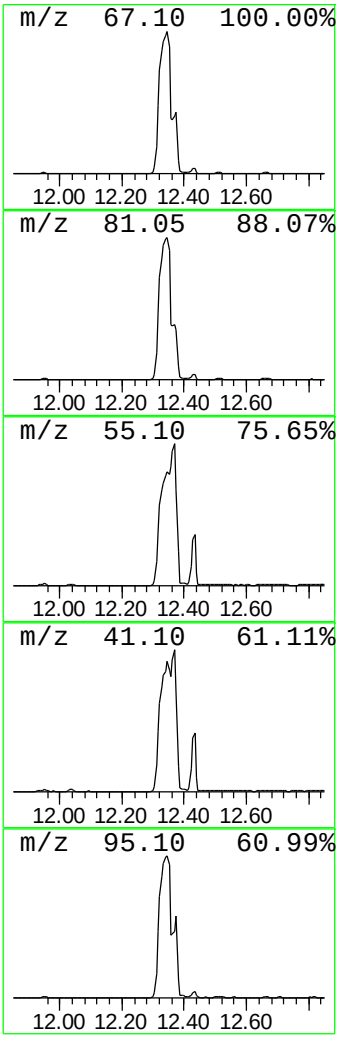
****

Peak Number 5 10,13-Octadecadienoic acid,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.35	338.04 ng	18657100	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99





Data Path : U:\HPCHEM1\BNA F\DATA\BF011818\
Data File : BF102197.D
Acq On : 18 Jan 2018 17:52
Operator : SJ/JU
Sample : J1010-06 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-011718

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

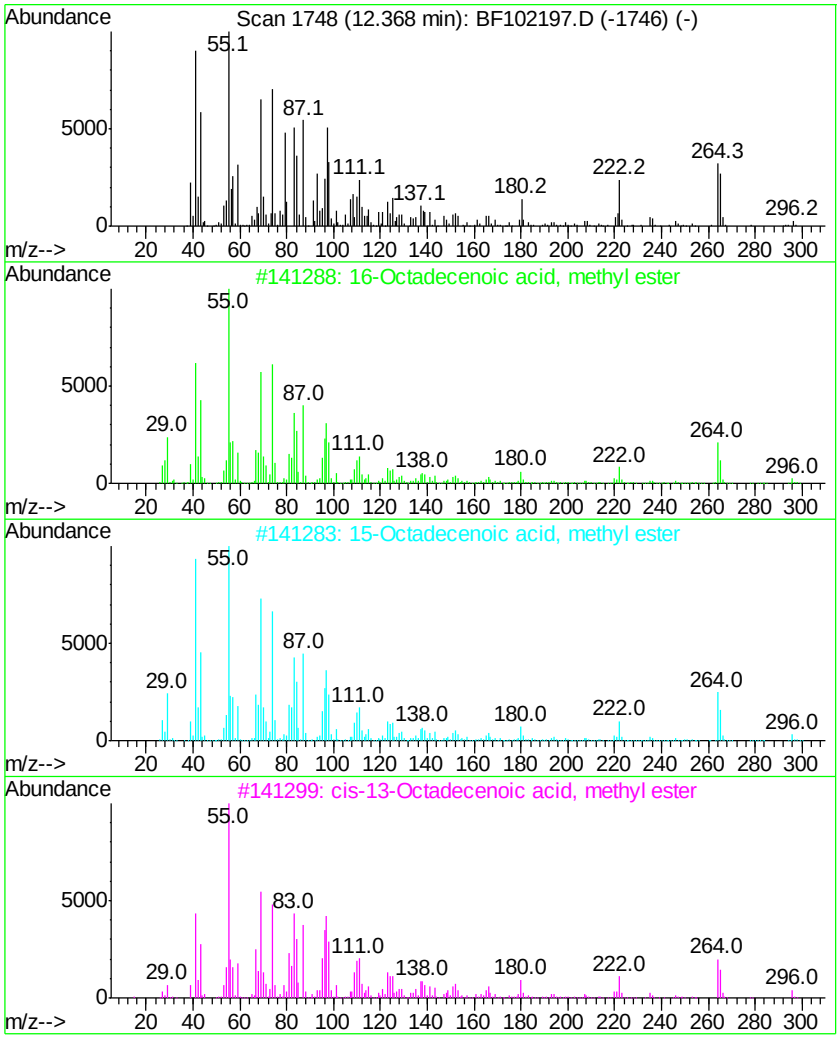
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

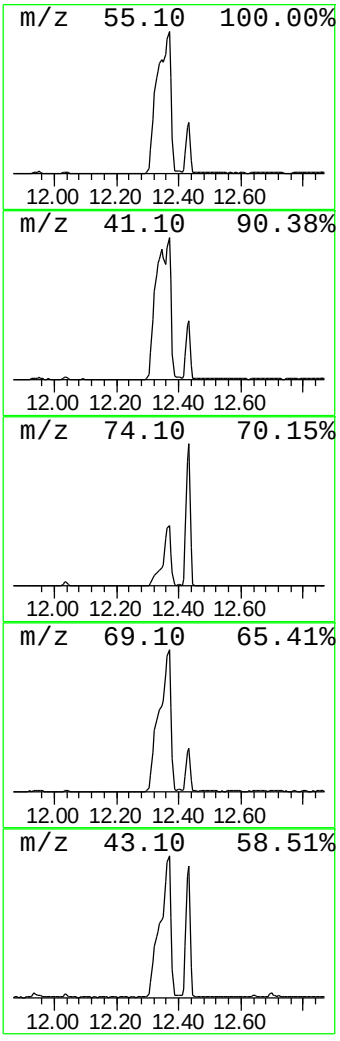
****

Peak Number 6 16-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.37	149.90 ng	8273410	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	90
2	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	89
3	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	83
4	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	80
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	80





Data Path : U:\HPCHEM1\BNA F\DATA\BF011818\
Data File : BF102197.D
Acq On : 18 Jan 2018 17:52
Operator : SJ/JU
Sample : J1010-06 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-011718

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

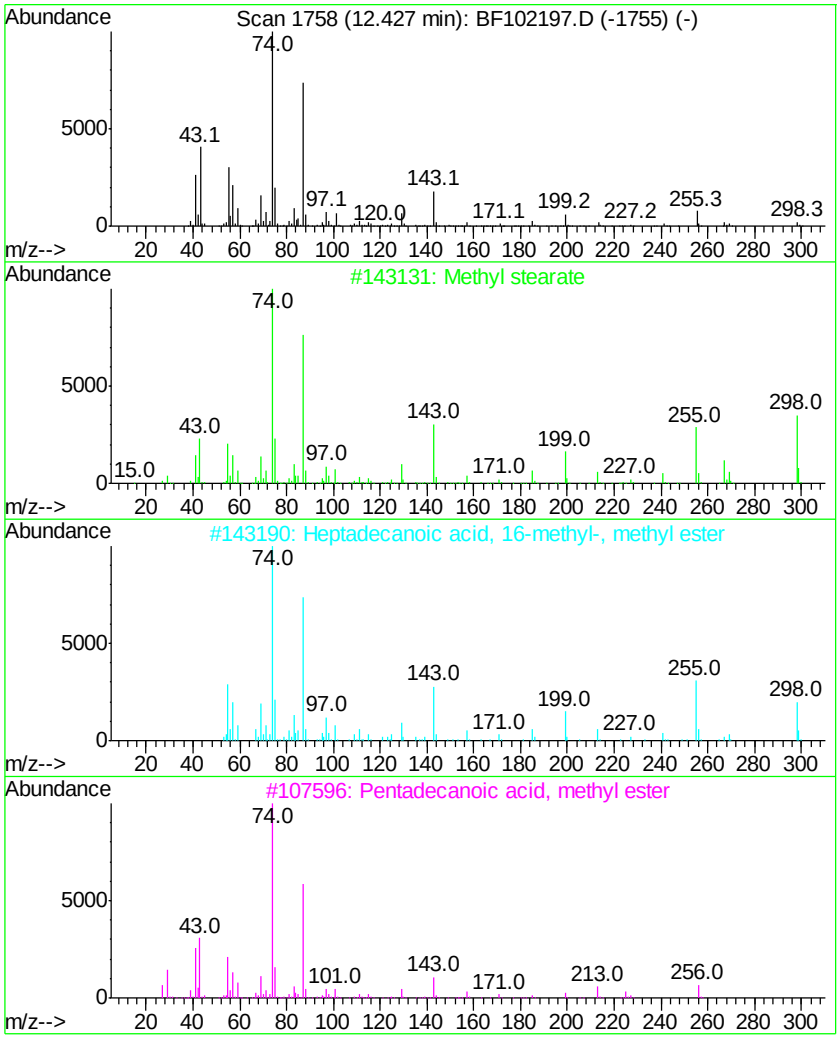
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

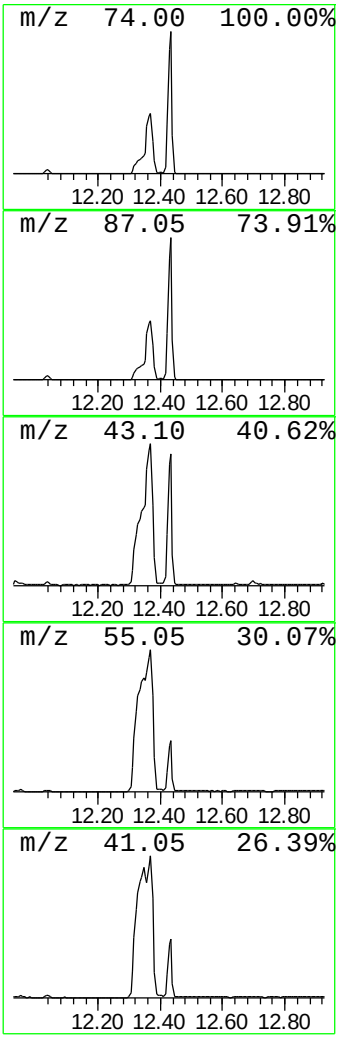
****

Peak Number 7 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	61.19 ng	3376940	Phenanthrene-d10	11.23

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	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	86
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	86





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Data File : BF102197.D
Acq On : 18 Jan 2018 17:52
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Sample : J1010-06 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-011718

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

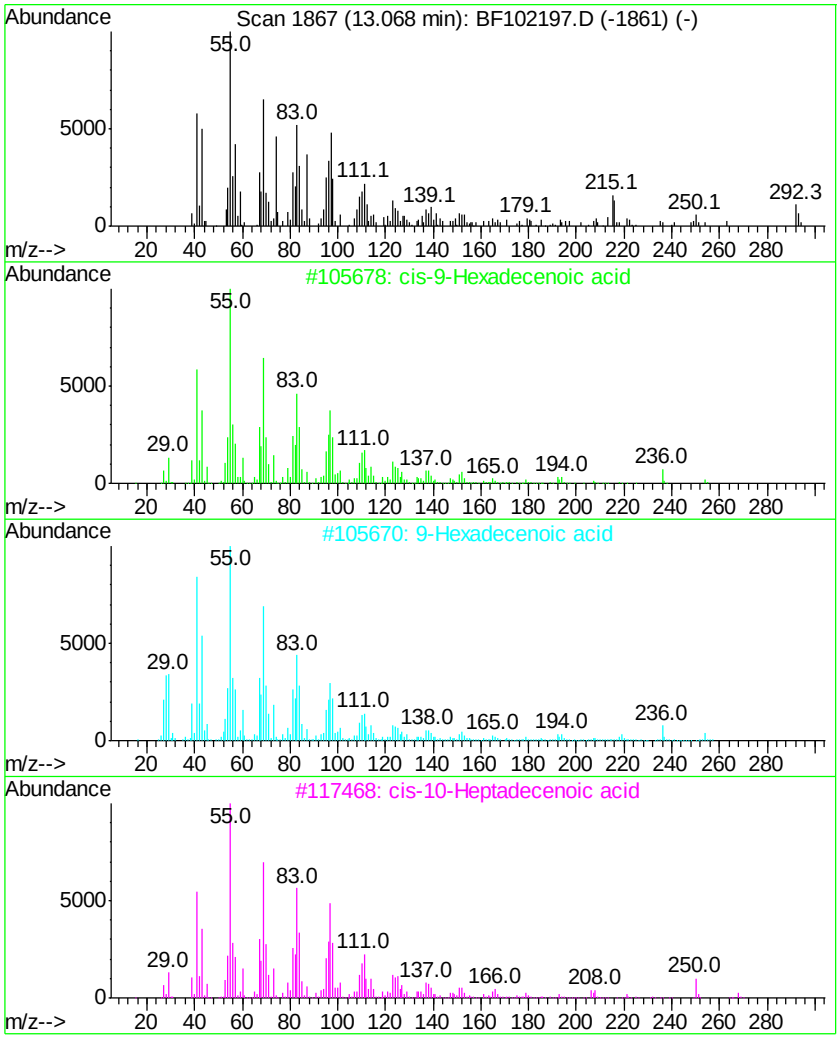
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

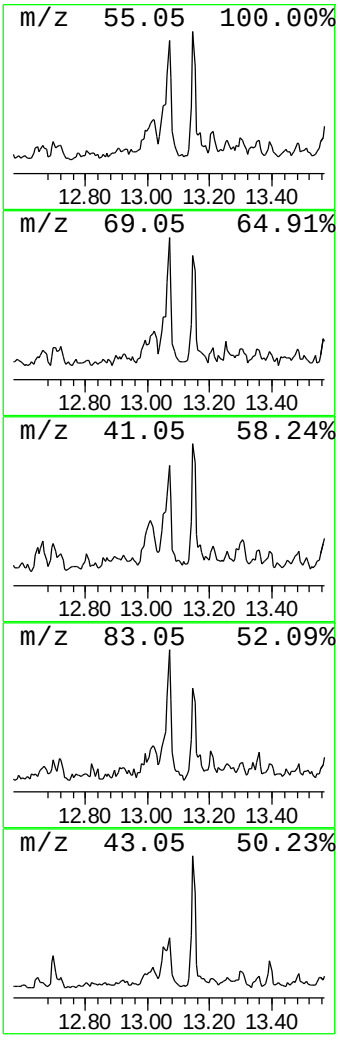
****

Peak Number 9 cis-9-Hexadecenoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.07	8.38 ng	379221	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	76
2	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	72
3	cis-10-Heptadecenoic acid	268	C17H32O2	029743-97-3	72
4	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	72
5	cis-Vaccenic acid	282	C18H34O2	000506-17-2	64





Data Path : U:\HPCHEM1\BNA F\DATA\BF011818\
Data File : BF102197.D
Acq On : 18 Jan 2018 17:52
Operator : SJ/JU
Sample : J1010-06 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-011718

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

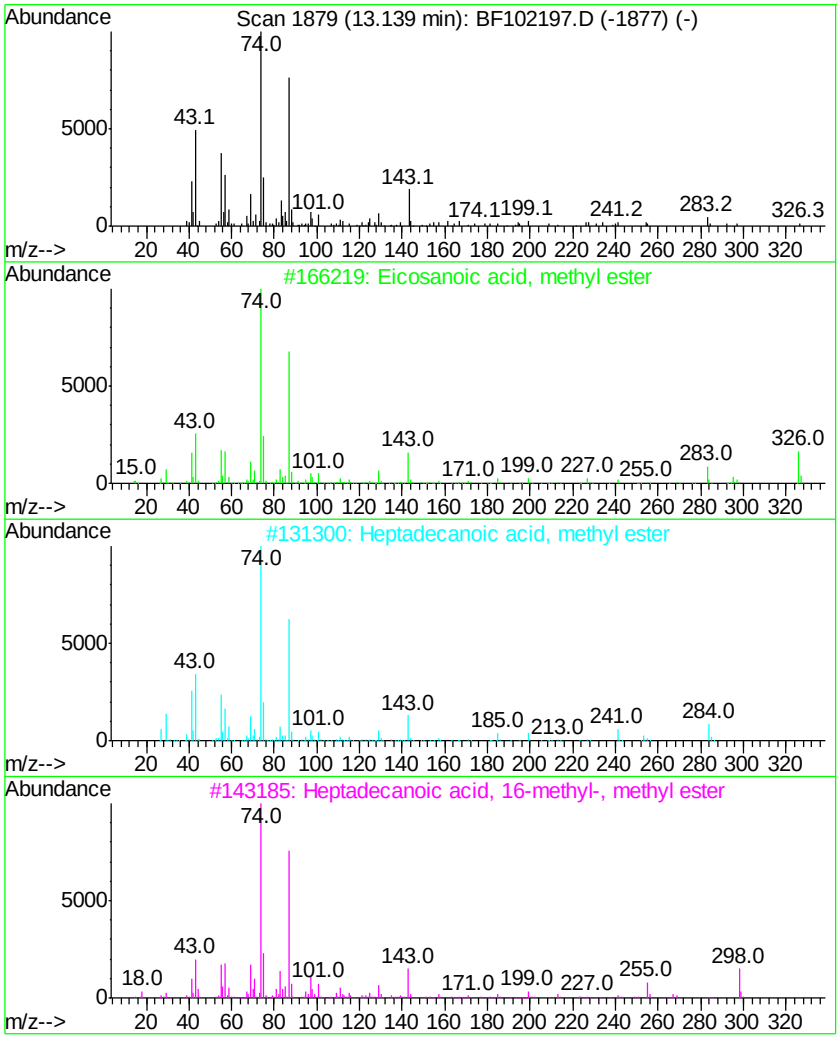
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

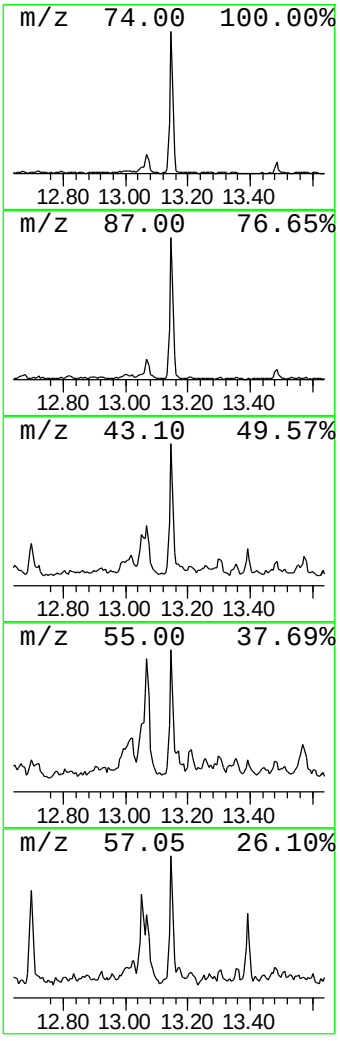
****

Peak Number 10 Eicosanoic acid, methyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.14	7.07 ng	319700	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	97
2	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
4	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	90
5	Methyl stearate	298	C19H38O2	000112-61-8	90





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF011818\
Data File : BF102197.D
Acq On : 18 Jan 2018 17:52
Operator : SJ/JU
Sample : J1010-06 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-011718

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

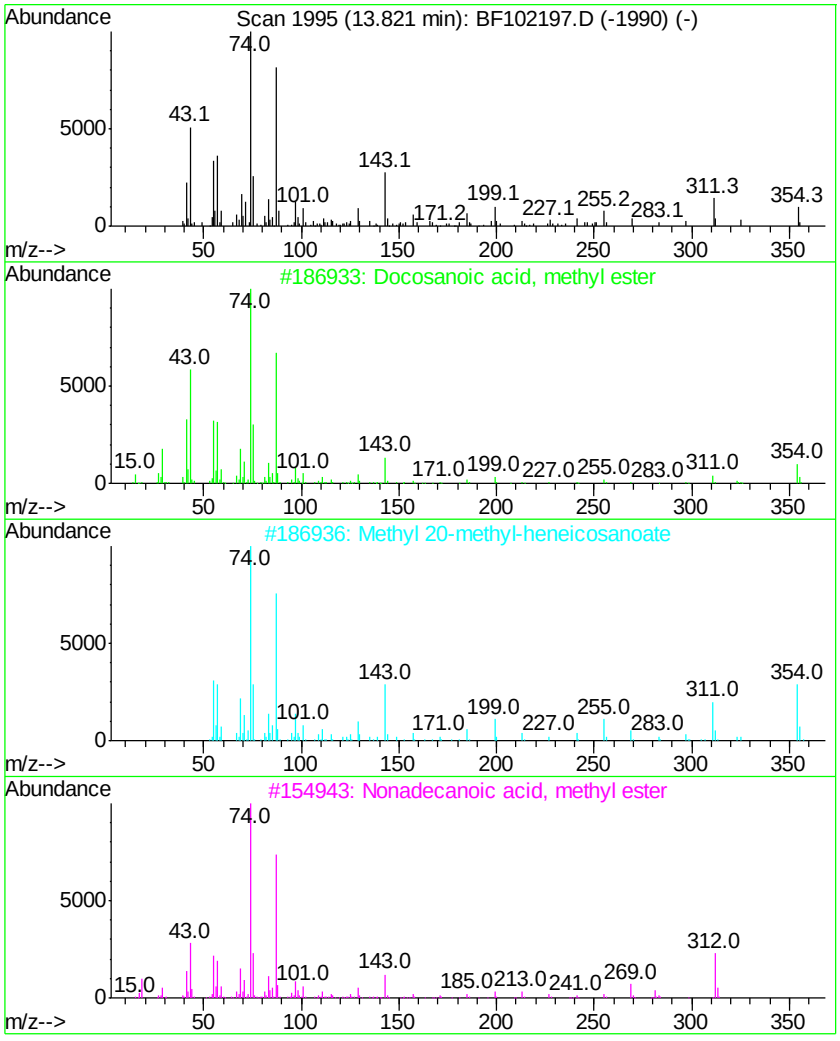
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

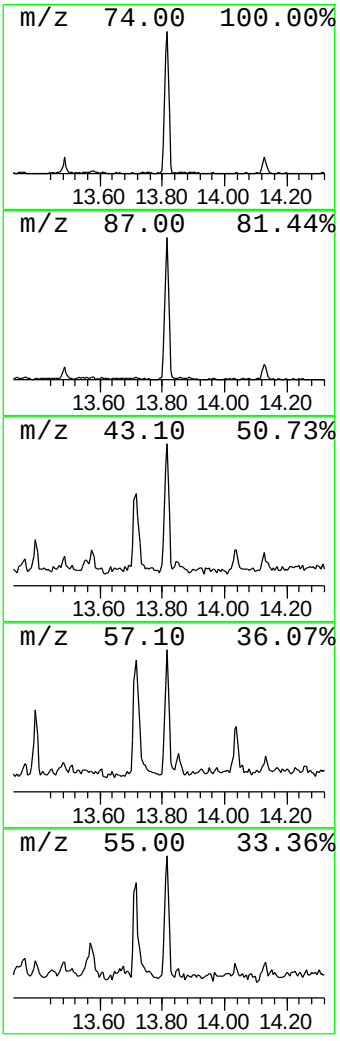
****

Peak Number 11 Docosanoic acid, methyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	6.35 ng	287328	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	99
2	Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	95
3	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	91
4	Methyl stearate	298	C19H38O2	000112-61-8	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80





Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_F\DATA\BF011818\
Data File : BF102197.D
Acq On : 18 Jan 2018 17:52
Operator : SJ/JU
Sample : J1010-06 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-03-011718

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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
unknown6.49	6.49	41.8	ng	2073120	1	6.72	992120	20.0
Tridecane, 1-iodo-	10.66	3.5	ng	195043	4	11.23	1103840	20.0
Hexadecanoic acid...	11.65	120.8	ng	6669910	4	11.23	1103840	20.0
10,13-Octadecadie...	12.35	338.0	ng	18657100	4	11.23	1103840	20.0
16-Octadecenoic a...	12.37	149.9	ng	8273410	4	11.23	1103840	20.0
Methyl stearate	12.43	61.2	ng	3376940	4	11.23	1103840	20.0
cis-9-Hexadecenoi...	13.07	8.4	ng	379221	5	13.87	904534	20.0
Eicosanoic acid, ...	13.14	7.1	ng	319700	5	13.87	904534	20.0
Docosanoic acid, ...	13.82	6.3	ng	287328	5	13.87	904534	20.0