LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022118\
Data File : BF103133.D
Acq On : 21 Feb 2018 13:51
Operator : SJ/JU
Sample : J1391-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-022018-A

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-BF020318.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	2.134	3	8	20	rVB	943085	1218552	22.89%	2.821%
2	5.110	511	514	522	rVB	127460	161677	3.04%	0.374%
3	5.498	576	580	591	rBV	3303336	3650081	68.56%	8.449%
4	6.510	747	752	755	rBV	3173880	3413186	64.12%	7.900%
5	6.651	771	776	779	rBV	3622373	3494217	65.64%	8.088%
6	6.875	811	814	818	rBV	1180777	977757	18.37%	2.263%
7	7.034	837	841	844	rBV	2843399	2470122	46.40%	5.717%
8	7.439	906	910	913	rBV	2263610	2267774	42.60%	5.249%
9	7.522	921	924	935	rVB	41262	75056	1.41%	0.174%
10	8.157	1029	1032	1038	rBV	1311099	1235789	23.21%	2.860%
11	9.233	1211	1215	1224	rBV	3301684	2968939	55.77%	6.872%
12	9.622	1278	1281	1289	rVB	295674	286786	5.39%	0.664%
13	9.833	1313	1317	1321	rBV	115044	92785	1.74%	0.215%
14	9.916	1327	1331	1339	rVB	1335596	1215373	22.83%	2.813%
15	10.333	1399	1402	1405	rVB	172915	130336	2.45%	0.302%
16	10.551	1433	1439	1442	rBV	55501	70714	1.33%	0.164%
17	10.704	1461	1465	1476	rBV	1726831	1694147	31.82%	3.921%
18	10.804	1479	1482	1488	rBV	189848	206338	3.88%	0.478%
19	11.251	1556	1558	1561	rBV	117107	100101	1.88%	0.232%
20	11.280	1561	1563	1570	rVB3	48875	58102	1.09%	0.134%
21	11.404	1580	1584	1593	rBV	1100491	1029017	19.33%	2.382%
22	11.680	1628	1631	1634	rBV	69662	61928	1.16%	0.143%
23	11.786	1645	1649	1652	rBV	2356916	1989311	37.37%	4.605%
24	11.922	1668	1672	1677	rBV3	111215	146715	2.76%	0.340%
25	12.474	1762	1766	1768	rBV	4784241	5323534	100.00%	12.322%
26	12.498	1768	1770	1776	rVV2	3818176	3579396	67.24%	8.285%
27	12.574	1780	1783	1787	rVB	1065754	854995	16.06%	1.979%
28	12.986	1849	1853	1857	rBV	2189241	2111496	39.66%	4.887%
29	13.298	1904	1906	1909	rBV	83822	75051	1.41%	0.174%
30	13.868	2000	2003	2007	rBV	501320	522438	9.81%	1.209%
31	13.968	2018	2020	2024	rBV	102306	102223	1.92%	0.237%
32	14.051	2030	2034	2037	rBV	865374	853546	16.03%	1.976%
33	15.545	2284	2288	2294	rBV	576341	765611	14.38%	1.772%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022118\
Data File : BF103133.D
Acq On : 21 Feb 2018 13:51
Operator : SJ/JU
Sample : J1391-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-022018-A

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-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 43203093

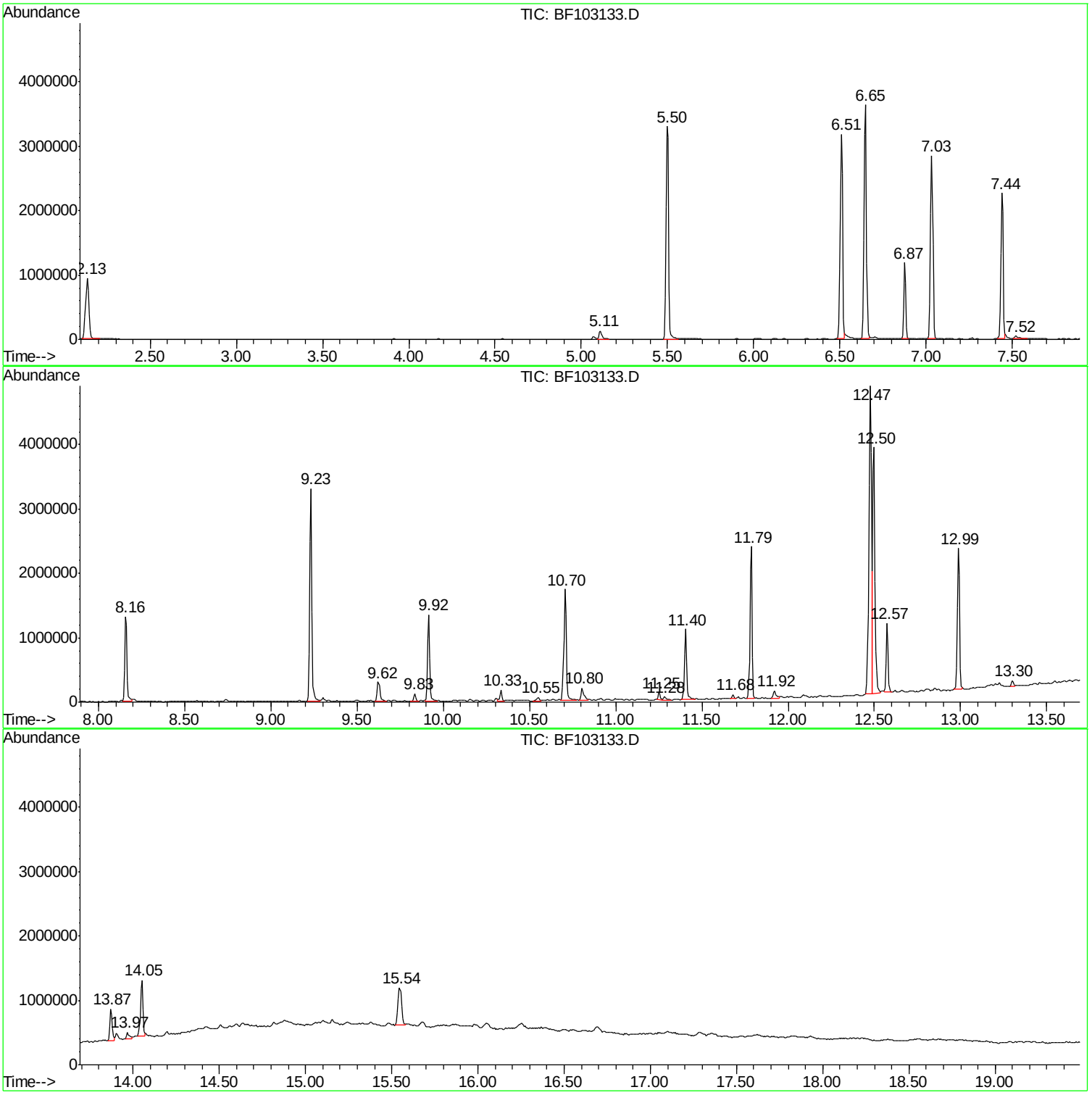
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022118\
Data File : BF103133.D
Acq On : 21 Feb 2018 13:51
Operator : SJ/JU
Sample : J1391-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-022018-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022118\
Data File : BF103133.D
Acq On : 21 Feb 2018 13:51
Operator : SJ/JU
Sample : J1391-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-022018-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

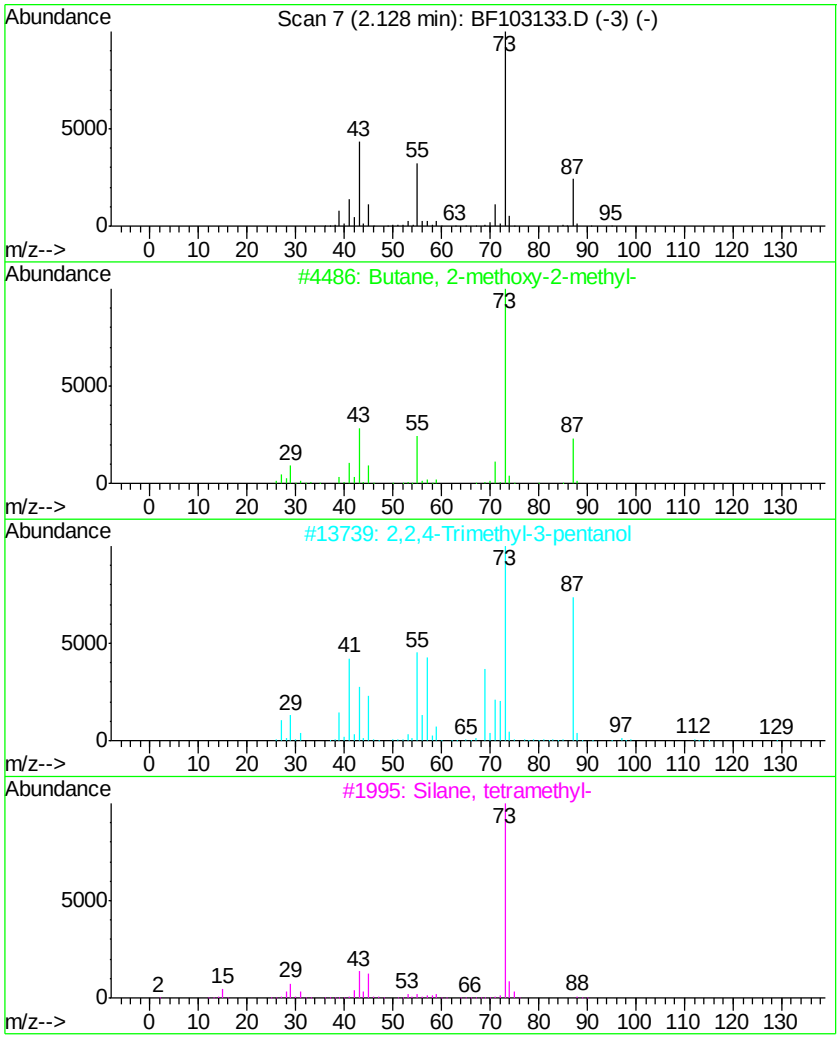
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

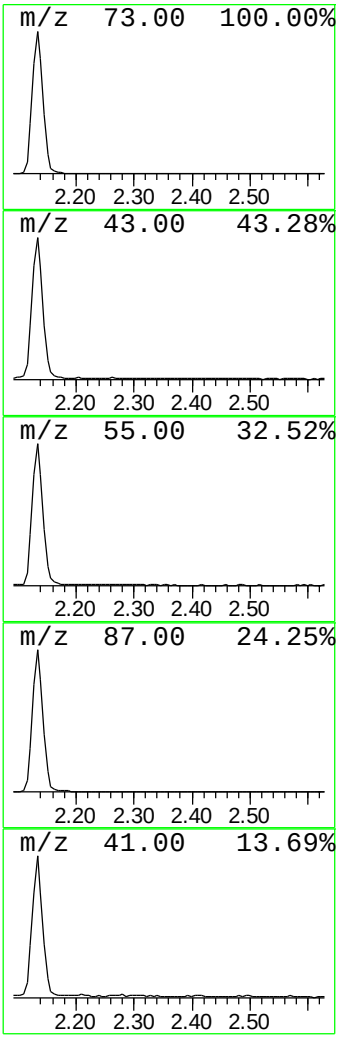
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	24.93 ng	1218550	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022118\
Data File : BF103133.D
Acq On : 21 Feb 2018 13:51
Operator : SJ/JU
Sample : J1391-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-022018-A

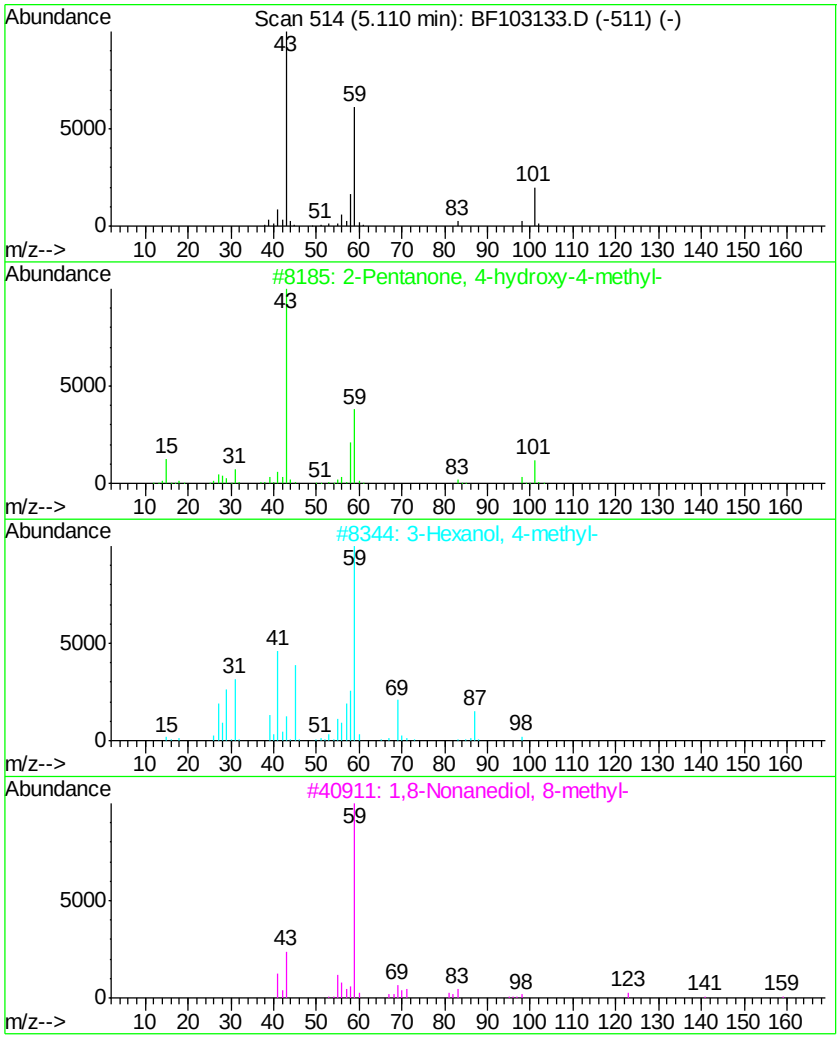
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

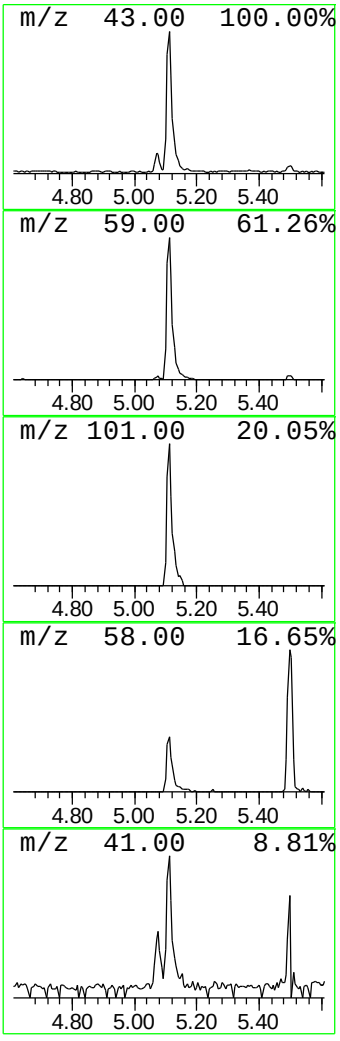
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	3.31 ng	161677	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4	Acetone	58	C3H6O	000067-64-1	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022118\
Data File : BF103133.D
Acq On : 21 Feb 2018 13:51
Operator : SJ/JU
Sample : J1391-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-022018-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

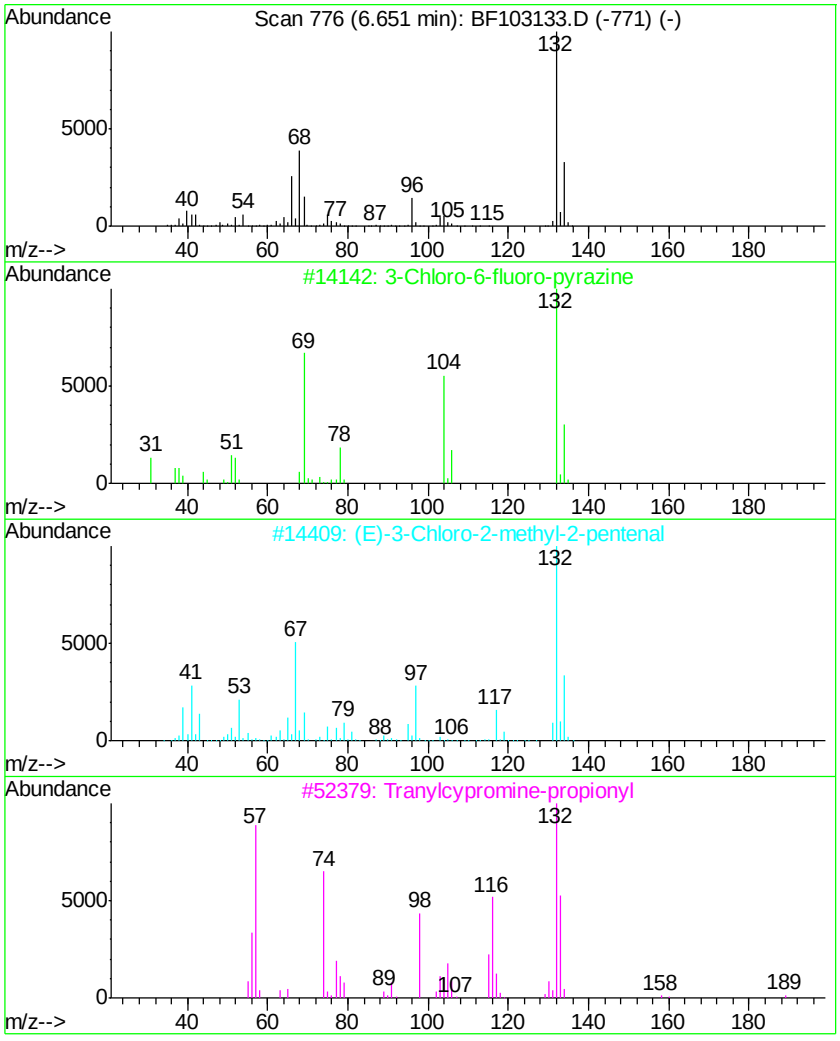
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

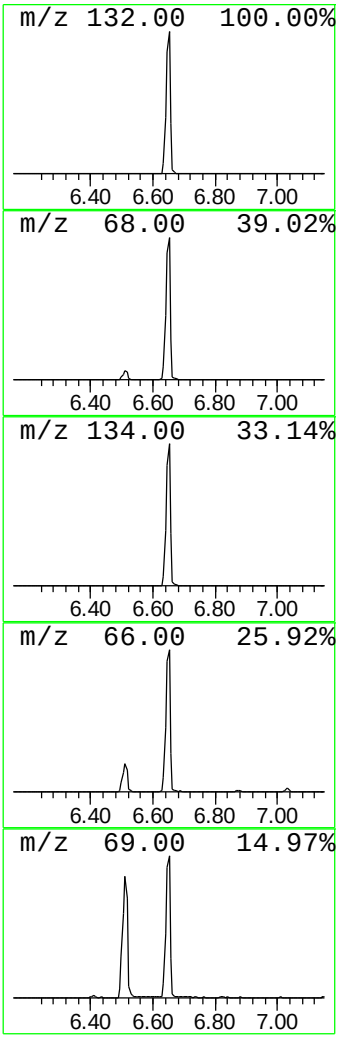
****

Peak Number 3 unknown6.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	71.47 ng	3494220	1,4-Dichlorobenzene-d4	6.87

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	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022118\
Data File : BF103133.D
Acq On : 21 Feb 2018 13:51
Operator : SJ/JU
Sample : J1391-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-022018-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

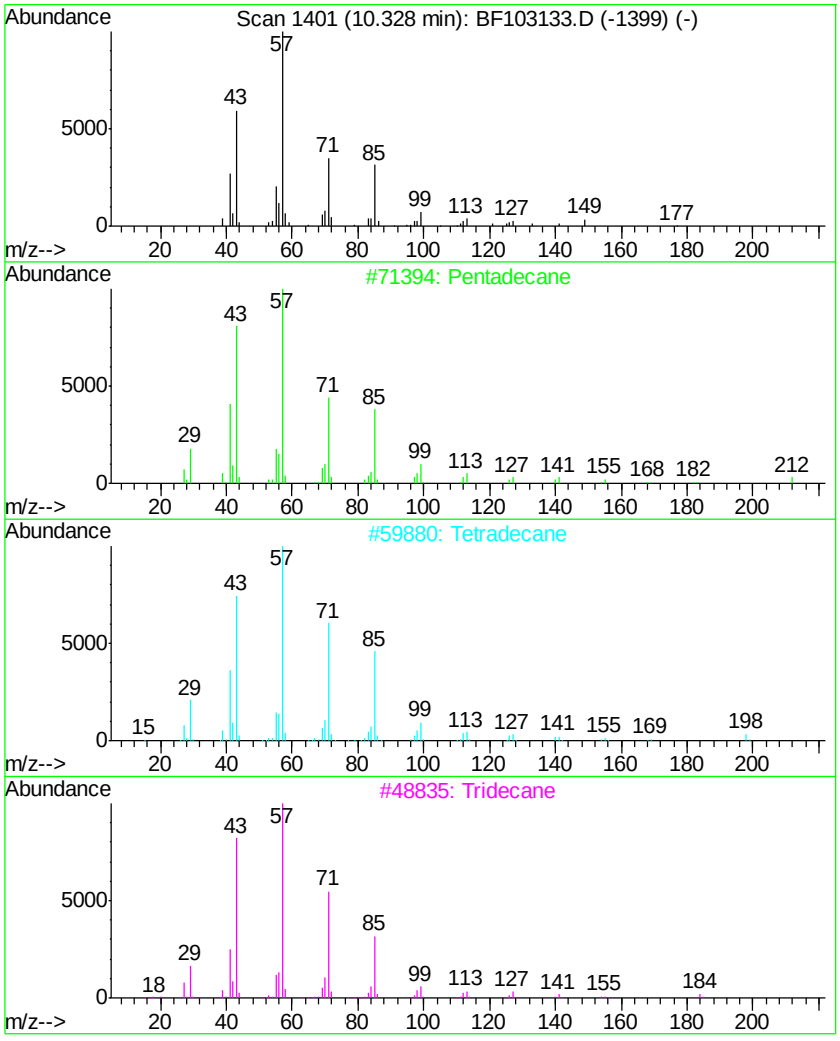
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

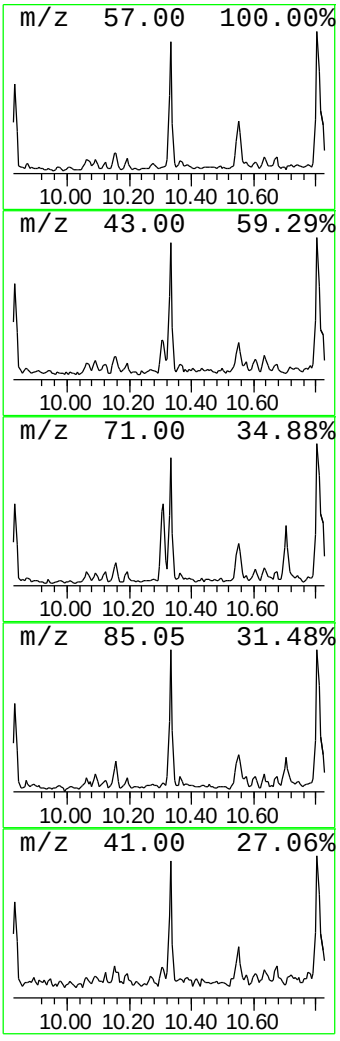
****

Peak Number 5 Pentadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	2.14 ng	130336	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Tetradecane	198	C14H30	000629-59-4	86
3	Tridecane	184	C13H28	000629-50-5	83
4	Heptadecane	240	C17H36	000629-78-7	83
5	Eicosane	282	C20H42	000112-95-8	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022118\
Data File : BF103133.D
Acq On : 21 Feb 2018 13:51
Operator : SJ/JU
Sample : J1391-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-022018-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

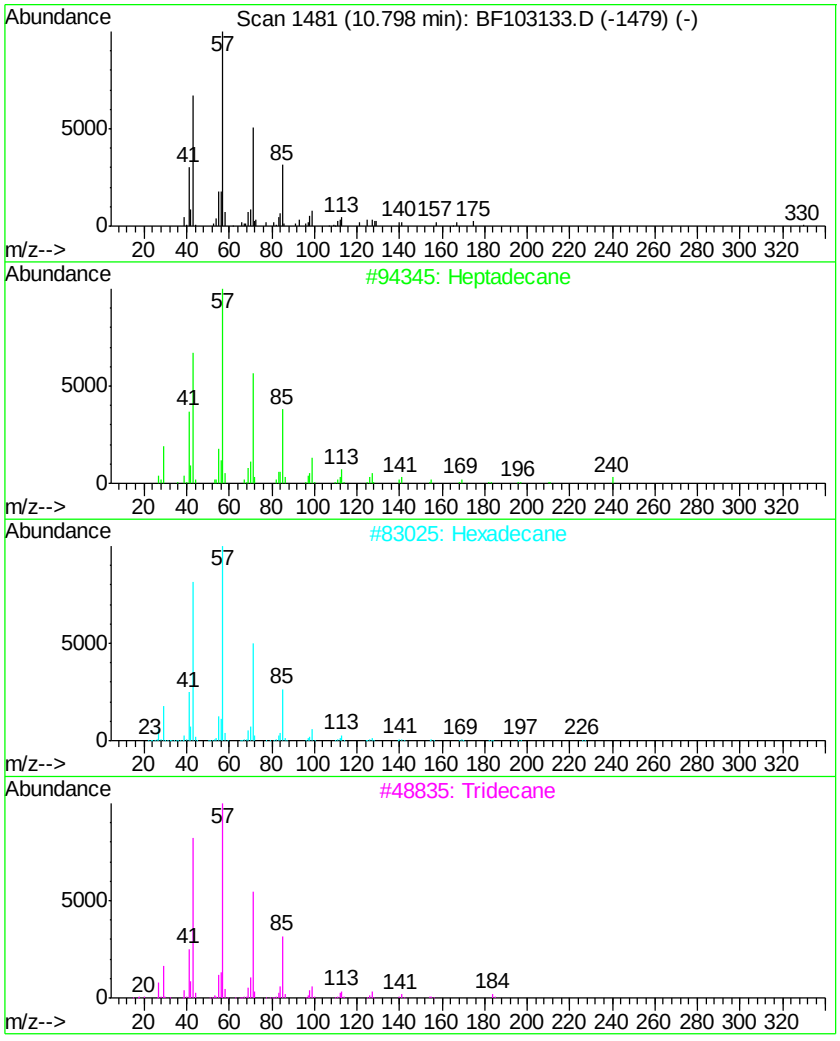
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

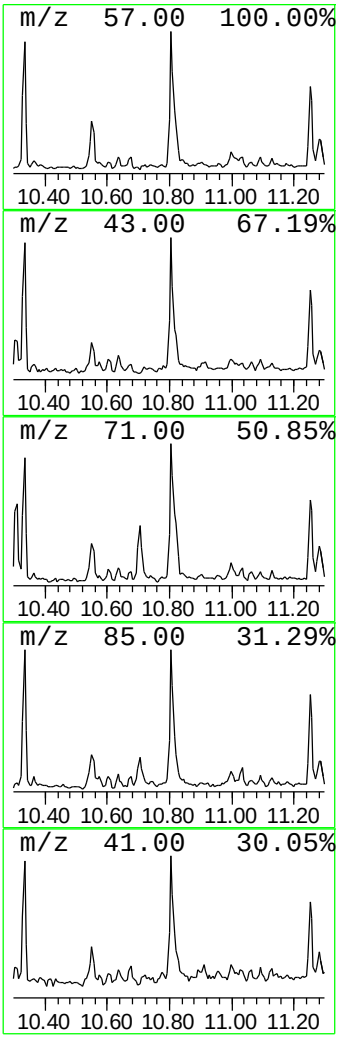
****

Peak Number 6 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	4.01 ng	206338	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Hexadecane	226	C16H34	000544-76-3	86
3	Tridecane	184	C13H28	000629-50-5	86
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022118\
Data File : BF103133.D
Acq On : 21 Feb 2018 13:51
Operator : SJ/JU
Sample : J1391-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-022018-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

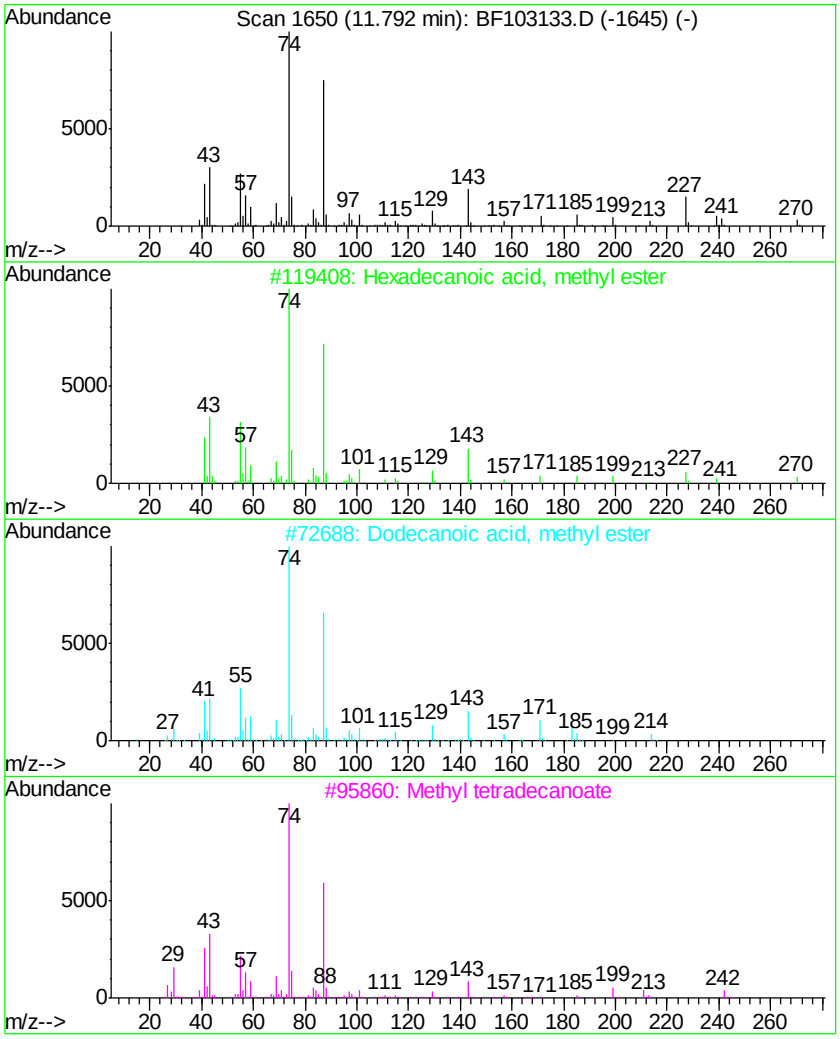
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

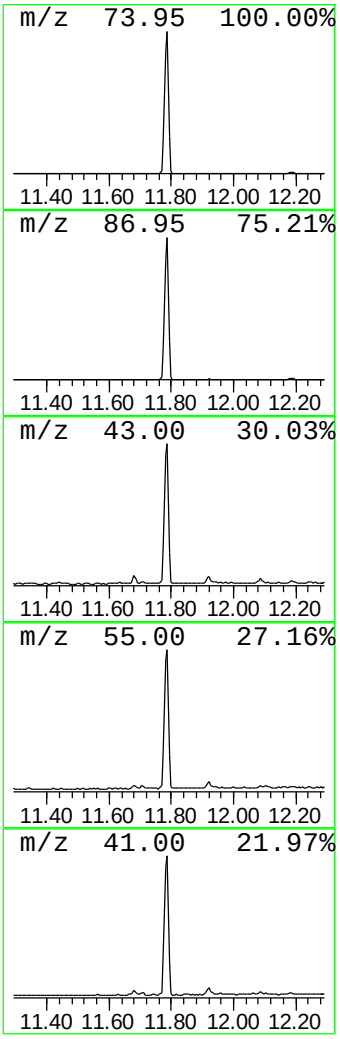
****

Peak Number 7 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	38.66 ng	1989310	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	91
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
4	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022118\
Data File : BF103133.D
Acq On : 21 Feb 2018 13:51
Operator : SJ/JU
Sample : J1391-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-022018-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

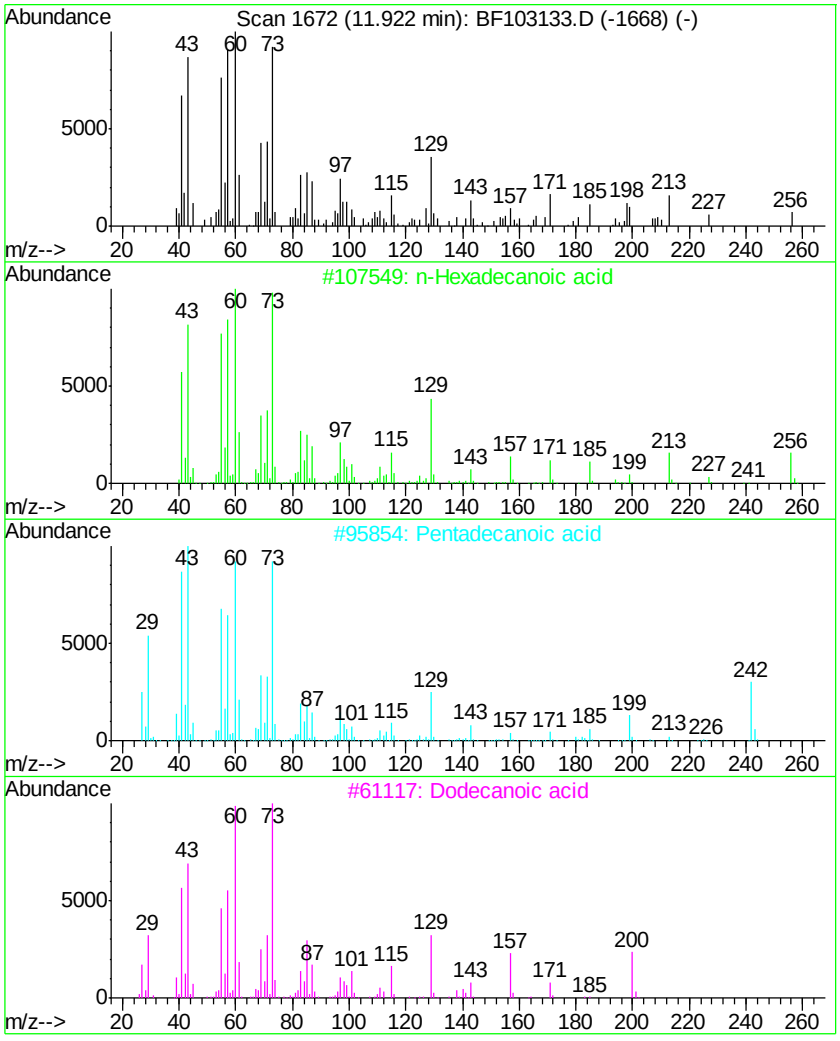
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

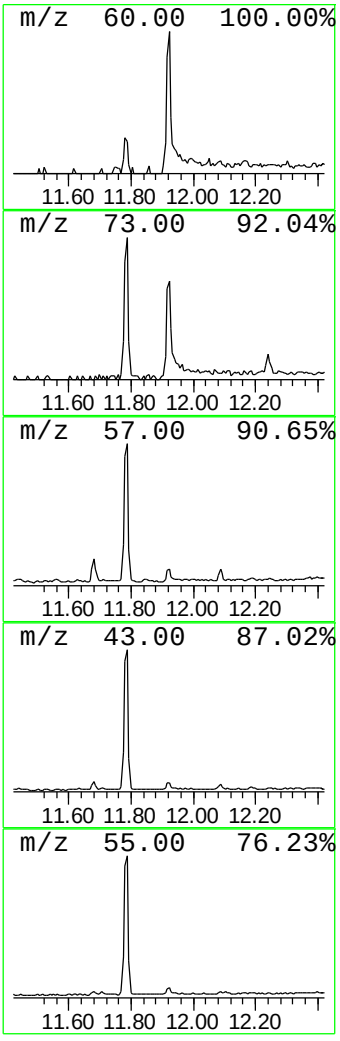
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	2.85 ng	146715	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Dodecanoic acid	200	C12H24O2	000143-07-7	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022118\
Data File : BF103133.D
Acq On : 21 Feb 2018 13:51
Operator : SJ/JU
Sample : J1391-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-022018-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

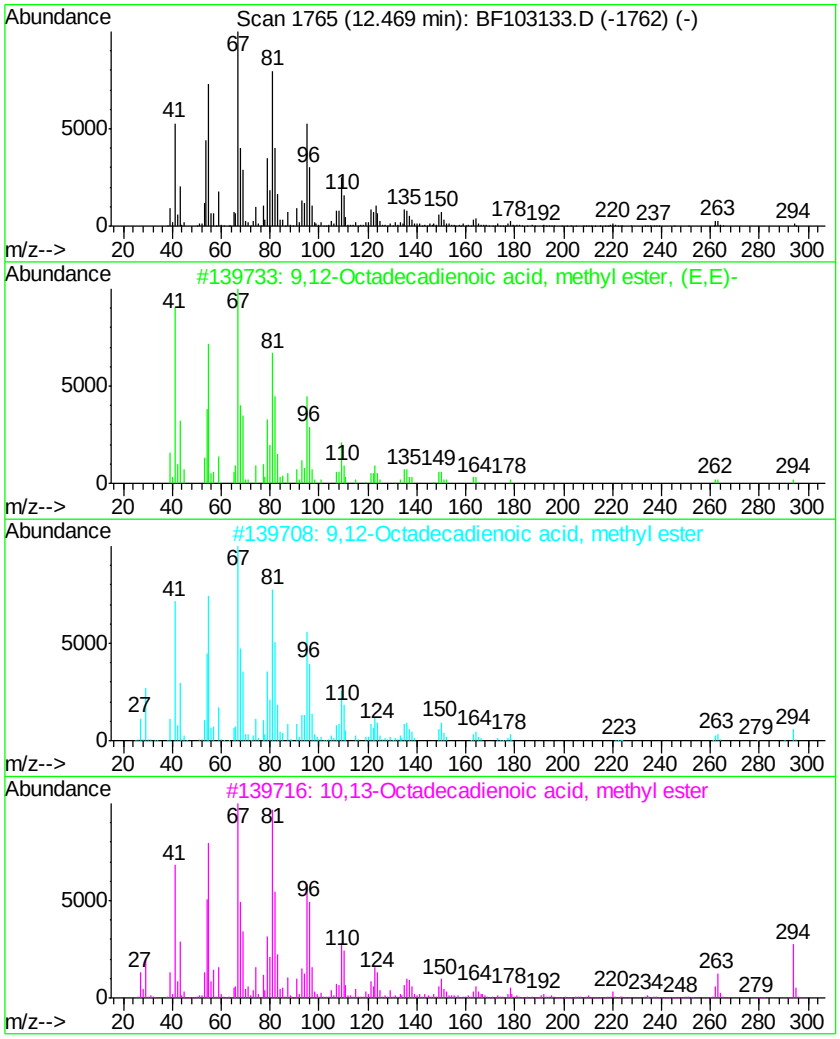
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

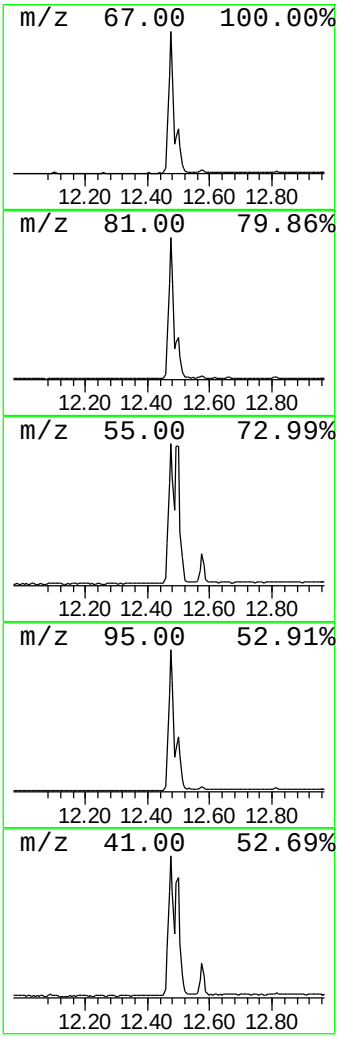
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	103.47 ng	5323530	Phenanthrene-d10	11.40

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





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022118\
Data File : BF103133.D
Acq On : 21 Feb 2018 13:51
Operator : SJ/JU
Sample : J1391-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-022018-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

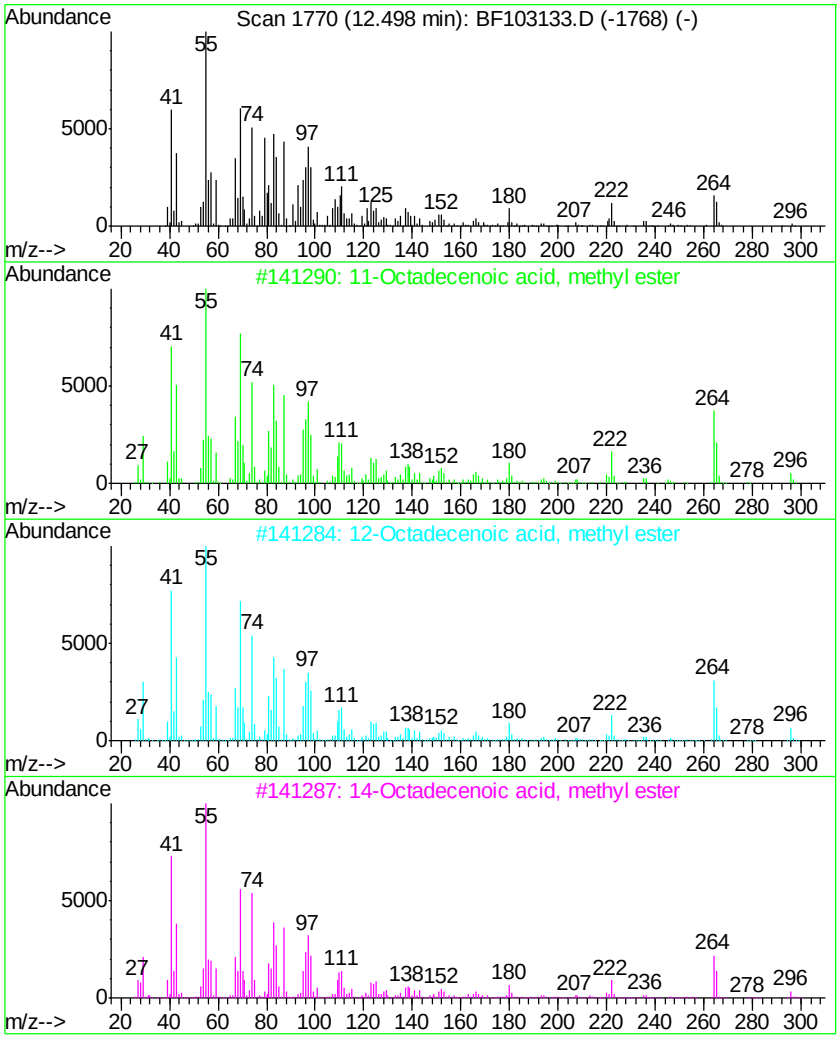
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

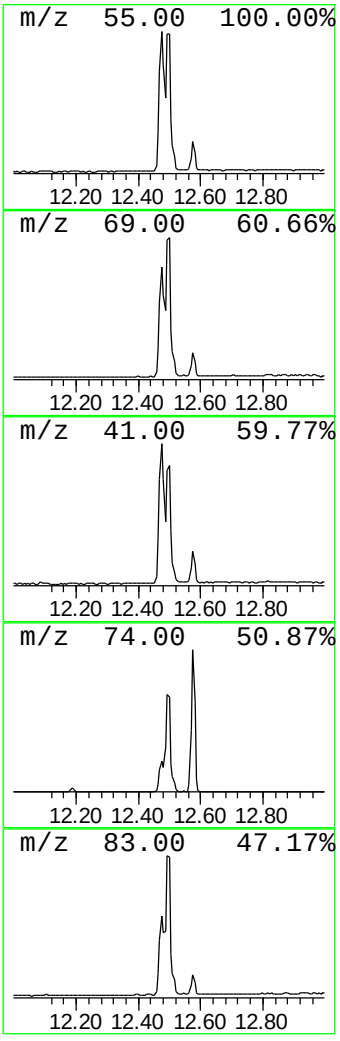
****

Peak Number 10 11-Octadecenoic acid, methy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	69.57 ng	3579400	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99





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Data File : BF103133.D
Acq On : 21 Feb 2018 13:51
Operator : SJ/JU
Sample : J1391-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-022018-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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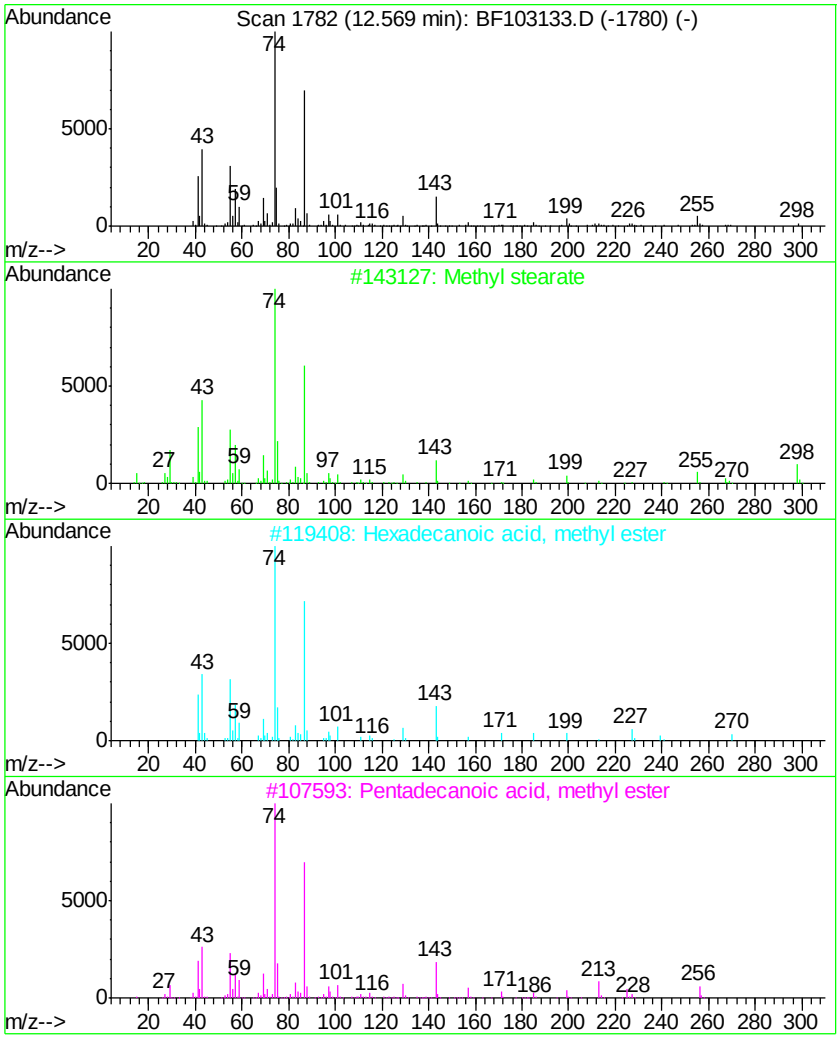
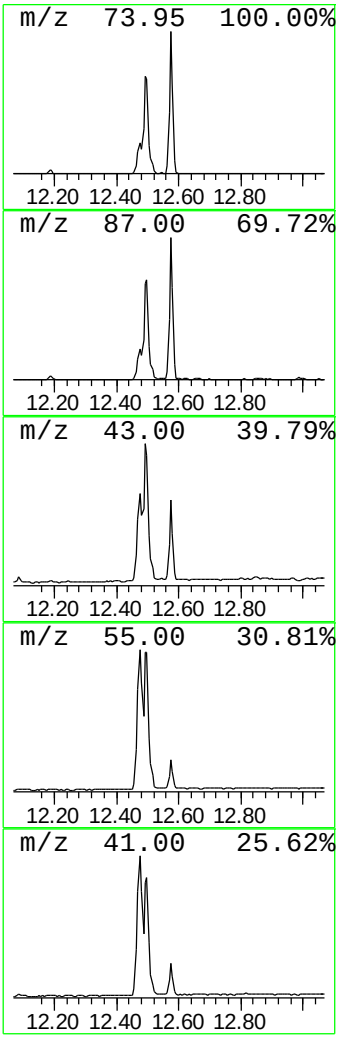
Peak Number 11 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	16.62 ng	854995	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	94
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	94
4	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	92
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022118\
Data File : BF103133.D
Acq On : 21 Feb 2018 13:51
Operator : SJ/JU
Sample : J1391-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-022018-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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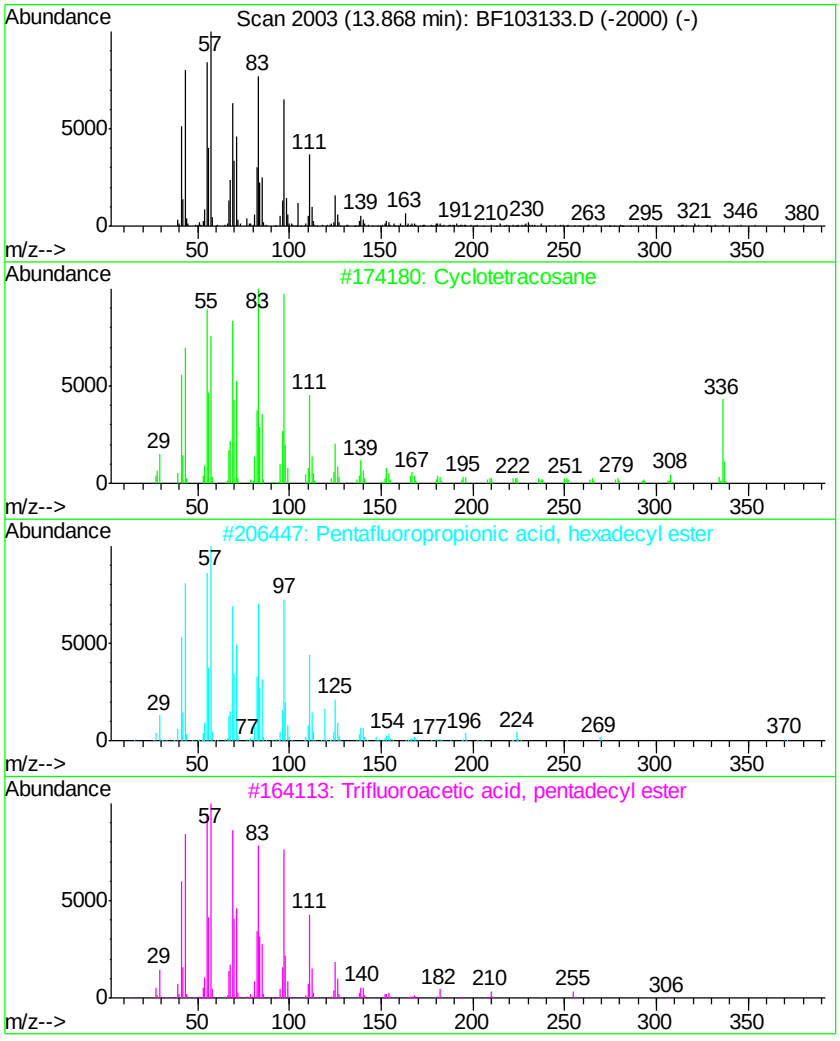
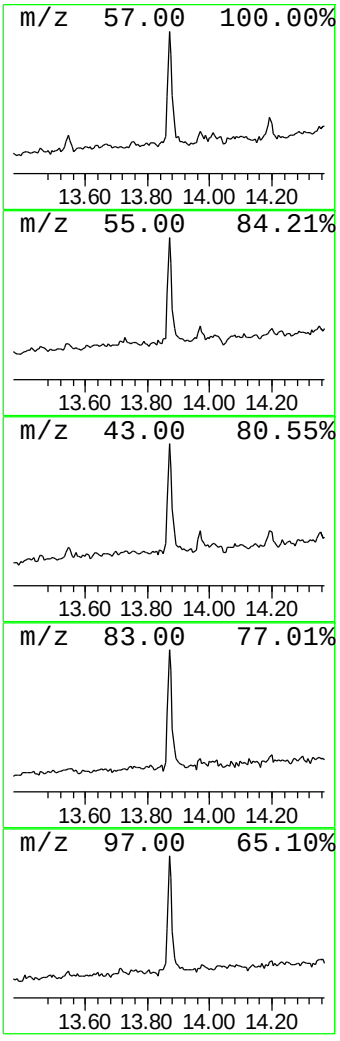
Peak Number 12 Cyclotetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	12.24 ng	522438	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	95
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Octacosanol	410	C28H58O	000557-61-9	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022118\
Data File : BF103133.D
Acq On : 21 Feb 2018 13:51
Operator : SJ/JU
Sample : J1391-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-05-022018-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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...	2.13	24.9	ng	1218550	1	6.87	977757	20.0
2-Pentanone, 4-hy...	5.11	3.3	ng	161677	1	6.87	977757	20.0
unknown6.65	6.65	71.5	ng	3494220	1	6.87	977757	20.0
Pentadecane	10.33	2.1	ng	130336	3	9.92	1215370	20.0
Heptadecane	10.80	4.0	ng	206338	4	11.40	1029020	20.0
Hexadecanoic acid...	11.79	38.7	ng	1989310	4	11.40	1029020	20.0
n-Hexadecanoic acid	11.92	2.9	ng	146715	4	11.40	1029020	20.0
9,12-Octadecadien...	12.47	103.5	ng	5323530	4	11.40	1029020	20.0
11-Octadecenoic a...	12.50	69.6	ng	3579400	4	11.40	1029020	20.0
Methyl stearate	12.57	16.6	ng	854995	4	11.40	1029020	20.0
Cyclotetracosane	13.87	12.2	ng	522438	5	14.05	853546	20.0