LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112210.D
Acq On : 24 Jan 2019 15:51
Operator : JU/SJ
Sample : K1016-05 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-RO-2-012319

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-BF011619.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	5.481	573	577	591	rBV	1645512	1551949	1.44%	0.641%
2	6.493	745	749	764	rBV	1776674	1731343	1.61%	0.715%
3	6.628	768	772	778	rVV	1968563	1779007	1.66%	0.735%
4	6.851	806	810	817	rBV	1440047	1167220	1.09%	0.482%
5	7.010	833	837	840	rBV	1485055	1380989	1.29%	0.570%
6	8.134	1022	1028	1034	rBV	1776670	1773410	1.65%	0.732%
7	9.204	1207	1210	1214	rBV	2340266	2081257	1.94%	0.859%
8	9.892	1323	1327	1330	rVV	1825071	1685045	1.57%	0.696%
9	9.928	1330	1333	1337	rVB	2528429	2020295	1.88%	0.834%
10	10.680	1457	1461	1466	rVB	1243215	1114596	1.04%	0.460%
11	10.898	1494	1498	1501	rBV	6281594	5128887	4.77%	2.118%
12	11.375	1576	1579	1582	rBV	1639356	1544243	1.44%	0.638%
13	11.692	1626	1633	1637	rBV	7830331	7987191	7.43%	3.298%
14	11.810	1642	1653	1655	rVV	17067866	44756747	41.65%	18.480%
15	11.945	1667	1676	1682	rBV2	1571080	2938104	2.73%	1.213%
16	12.086	1698	1700	1705	rVB	1728358	1570301	1.46%	0.648%
17	12.169	1711	1714	1720	rBV	1977745	2073422	1.93%	0.856%
18	12.539	1757	1777	1779	rBV2	21442643	107469137	100.00%	44.374%
19	12.610	1785	1789	1791	rVB2	15611737	22945460	21.35%	9.474%
20	12.639	1791	1794	1795	rVV	4316460	3840317	3.57%	1.586%
21	12.657	1795	1797	1802	rVV2	5677128	6540125	6.09%	2.700%
22	12.804	1819	1822	1826	rVB2	1586673	1365335	1.27%	0.564%
23	12.863	1826	1832	1839	rVB4	851538	1719632	1.60%	0.710%
24	12.980	1849	1852	1855	rBV	2028653	1613116	1.50%	0.666%
25	13.210	1885	1891	1898	rVB	4317004	5581831	5.19%	2.305%
26	13.286	1900	1904	1906	rVV	3243986	2897523	2.70%	1.196%
27	13.951	2013	2017	2022	rVB	2708589	2317622	2.16%	0.957%
28	14.027	2025	2030	2033	rVV2	1753664	2070421	1.93%	0.855%
29	15.498	2276	2280	2289	rVB2	1174445	1547329	1.44%	0.639%

Sum of corrected areas: 242191854

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
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Acq On : 24 Jan 2019 15:51
Operator : JU/SJ
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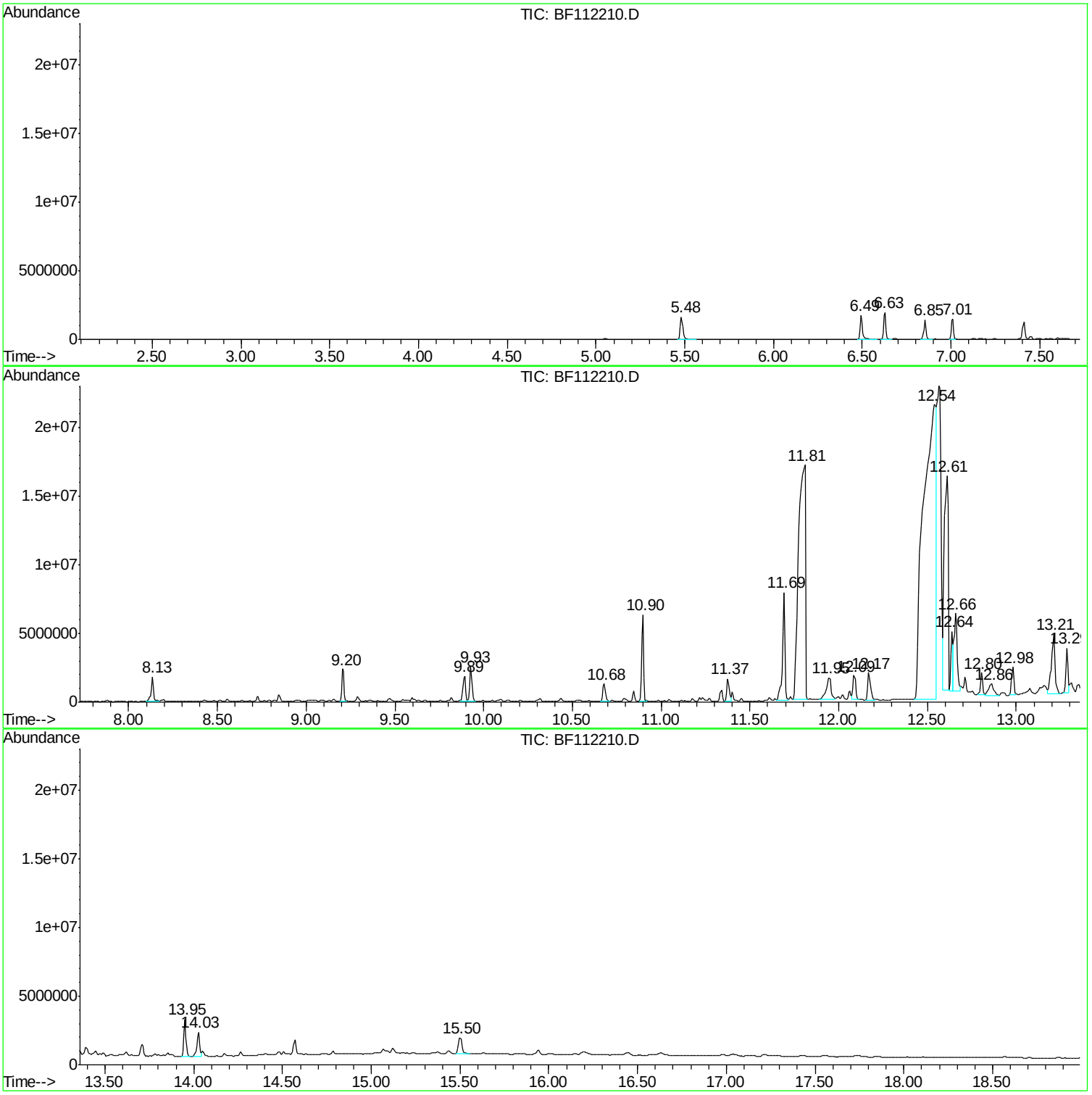
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-RO-2-012319

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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

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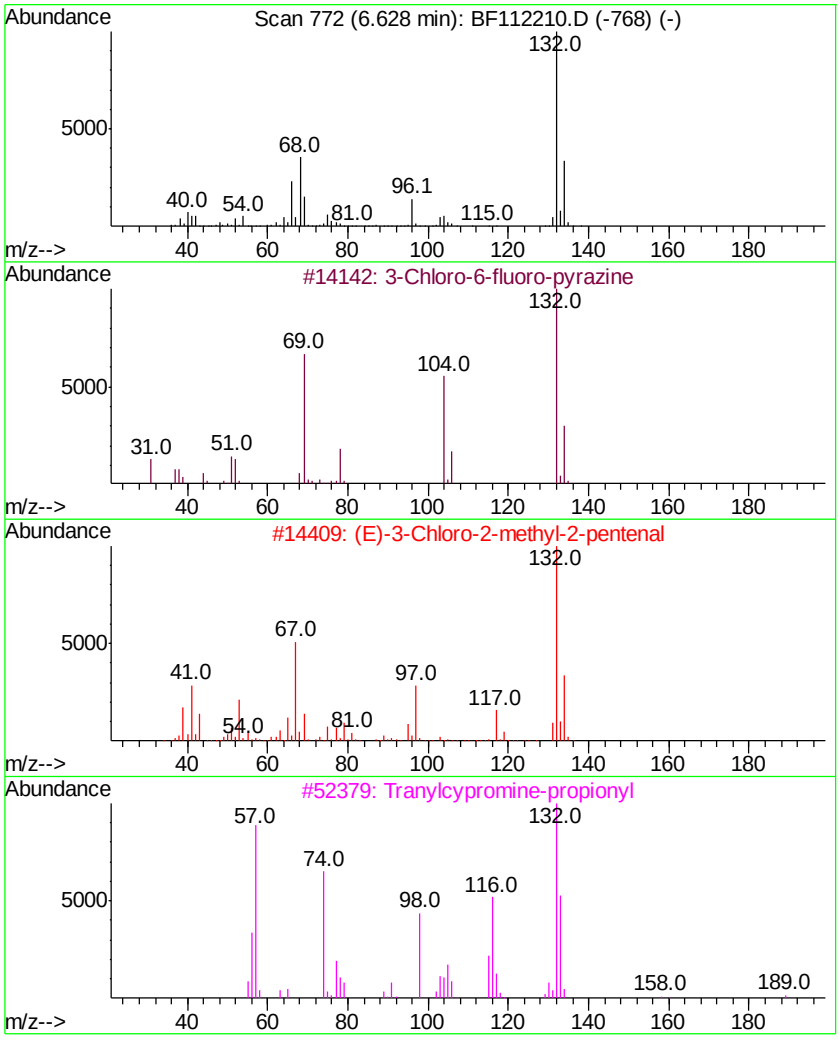
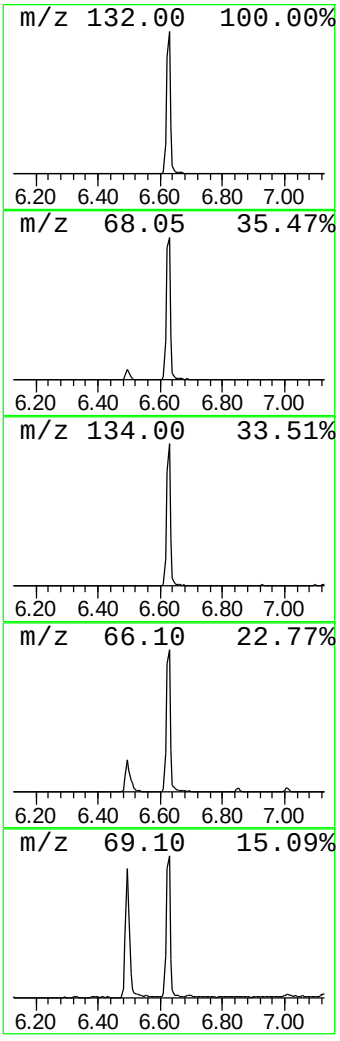
****

Peak Number 1 unknown6.63 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	30.48 ng	1779010	1,4-Dichlorobenzene-d4	6.85

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	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	16
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Misc :
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Instrument : BNA_F
ClientSampleId : TR-05-RO-2-012319

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
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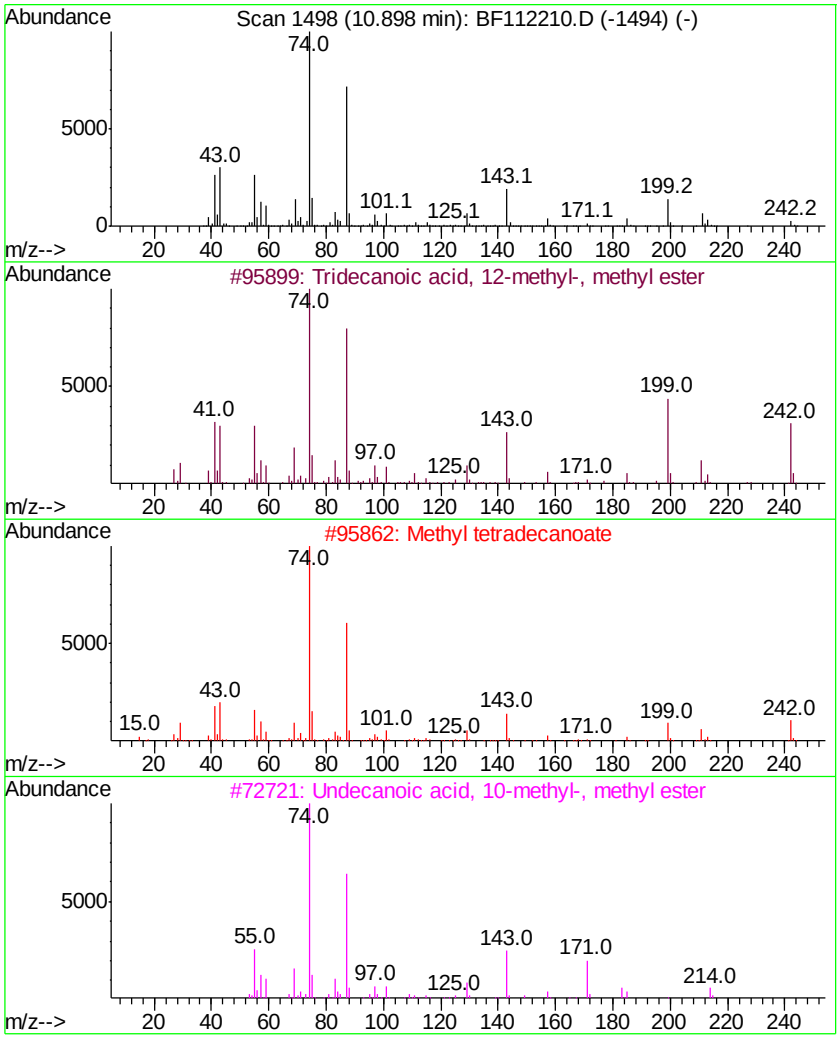
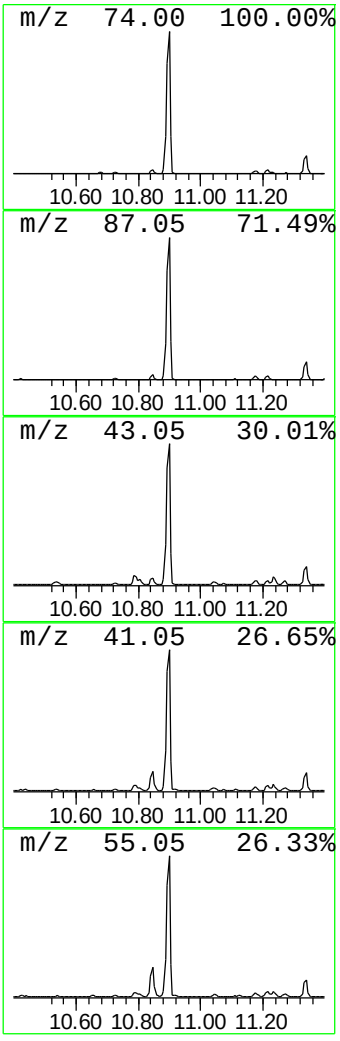
Peak Number 3 Tridecanoic acid, 12-methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	66.43 ng	5128890	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	94
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
3	Undecanoic acid, 10-methyl-, met...	214	C13H26O2	005129-56-6	86
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	80
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	80





Library Search Compound Report

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Operator : JU/SJ
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-RO-2-012319

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
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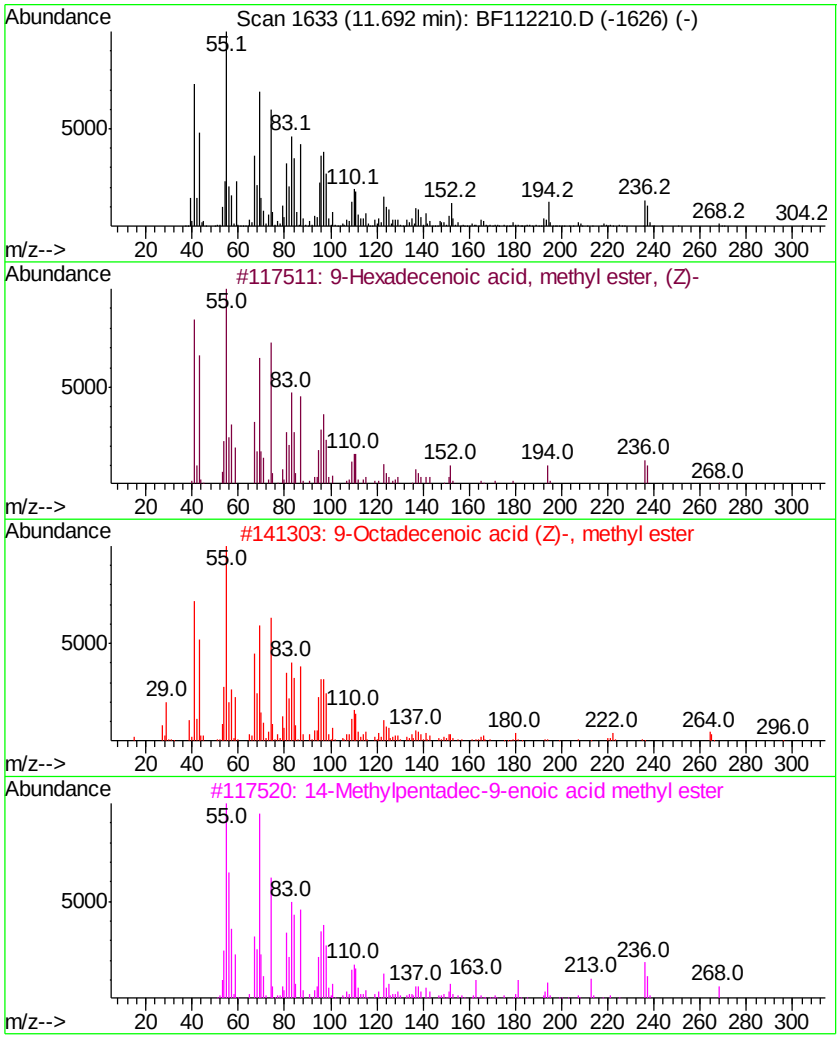
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

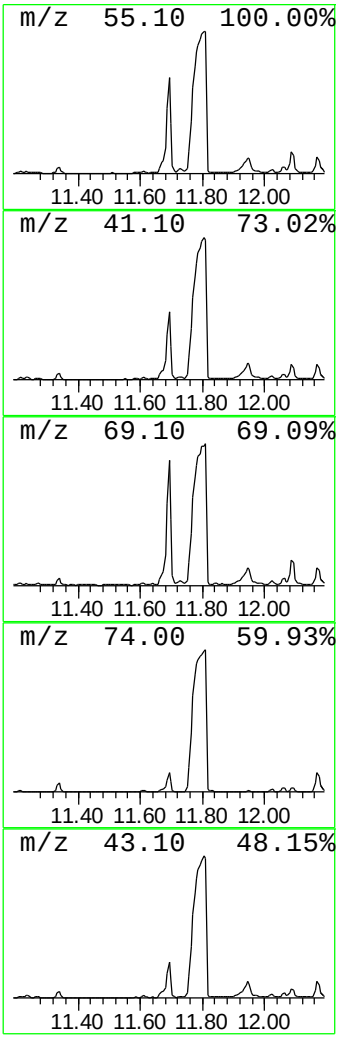
****

Peak Number 4 9-Hexadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	103.45 ng	7987190	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	99
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
3	14-Methylpentadec-9-enoic acid m...	268	C17H32O2	1000365-89-7	91
4	Methyl hexadec-9-enoate	268	C17H32O2	010030-74-7	91
5	11-Hexadecenoic acid, methyl ester	268	C17H32O2	055000-42-5	91





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Data File : BF112210.D
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Operator : JU/SJ
Sample : K1016-05 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-RO-2-012319

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

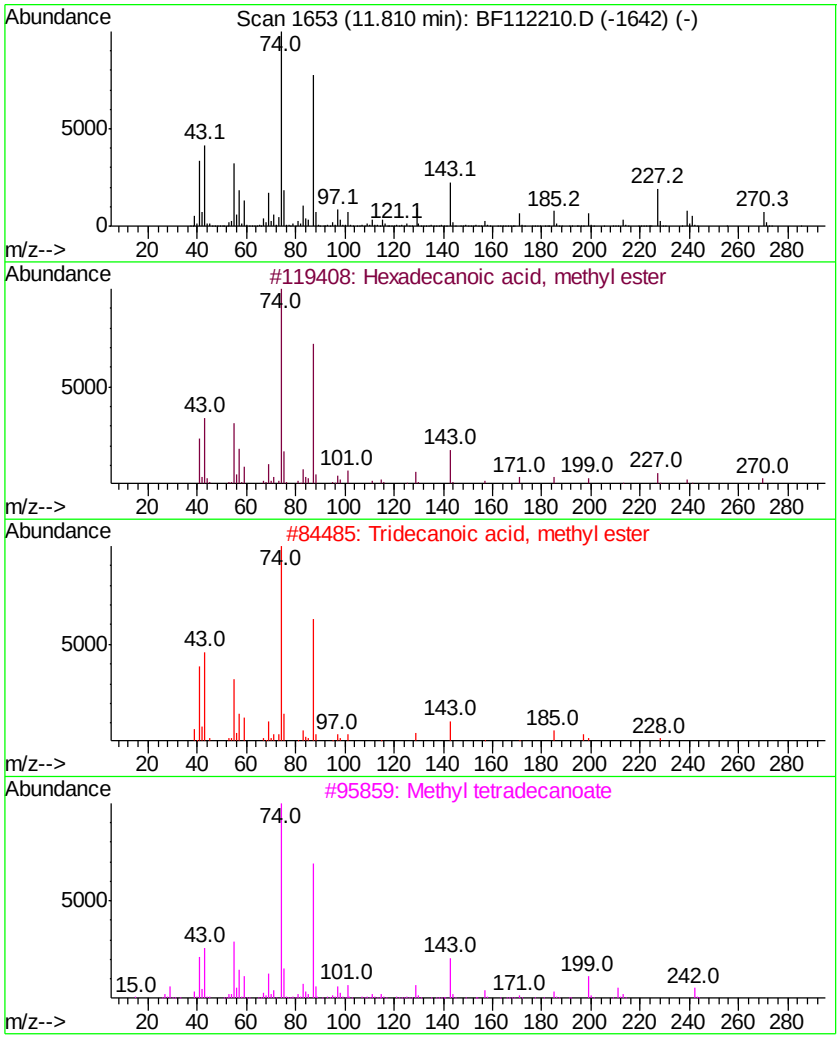
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

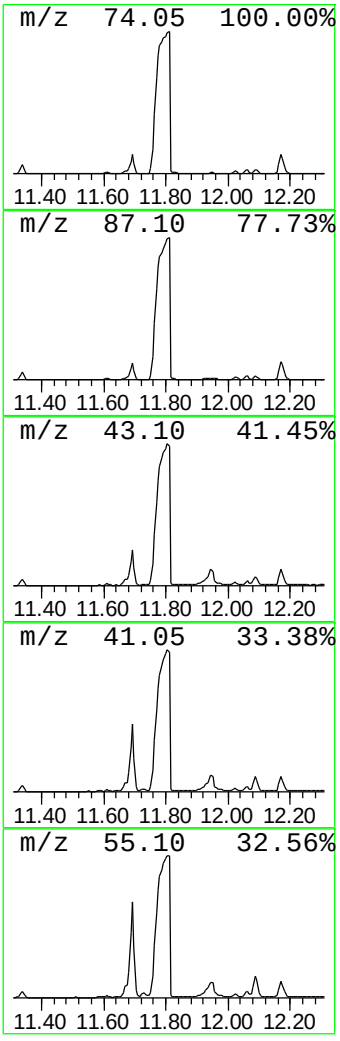
****

Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	579.66 ng	44756700	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	96
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	81
4	Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	81
5	Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	74





Library Search Compound Report

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Operator : JU/SJ
Sample : K1016-05 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-RO-2-012319

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

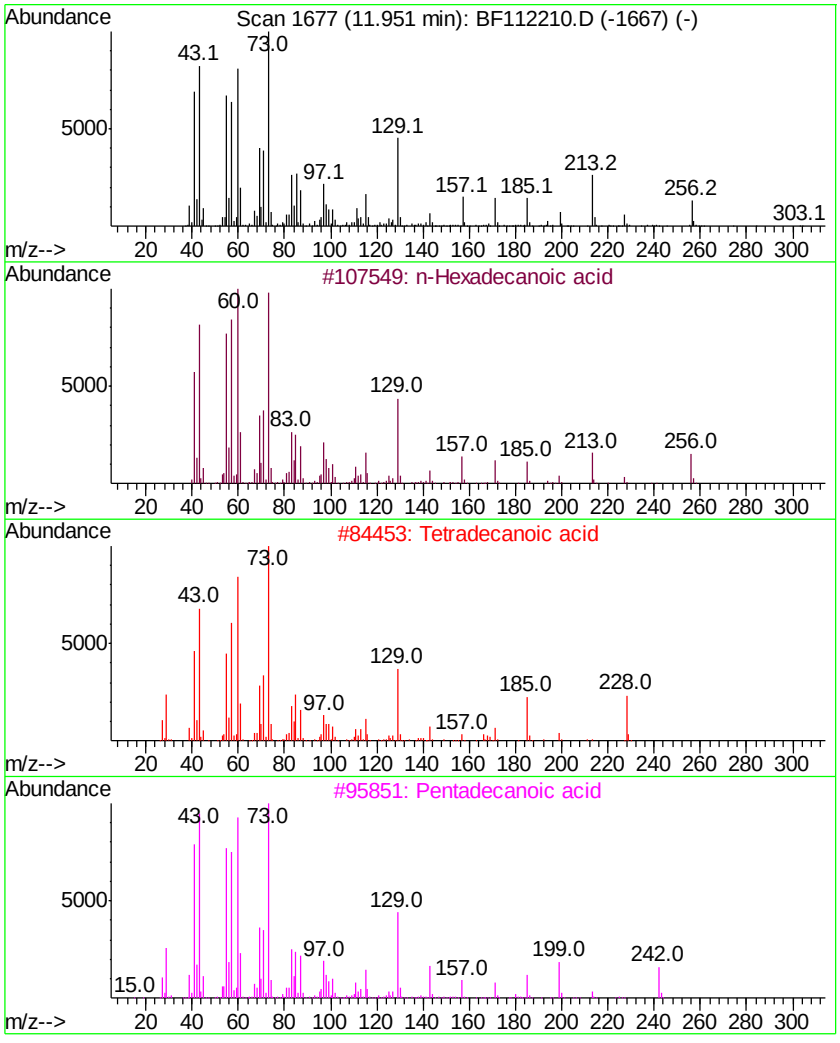
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

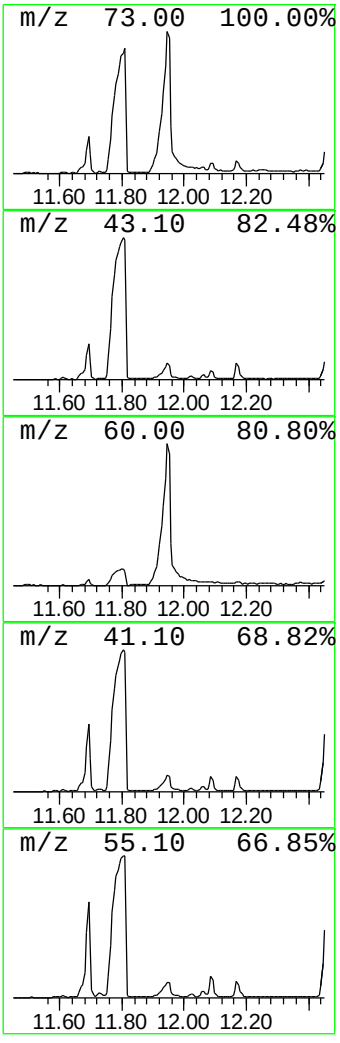
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	38.05 ng	2938100	Phenanthrene-d10	11.37

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Misc :
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Instrument : BNA_F
ClientSampleId : TR-05-RO-2-012319

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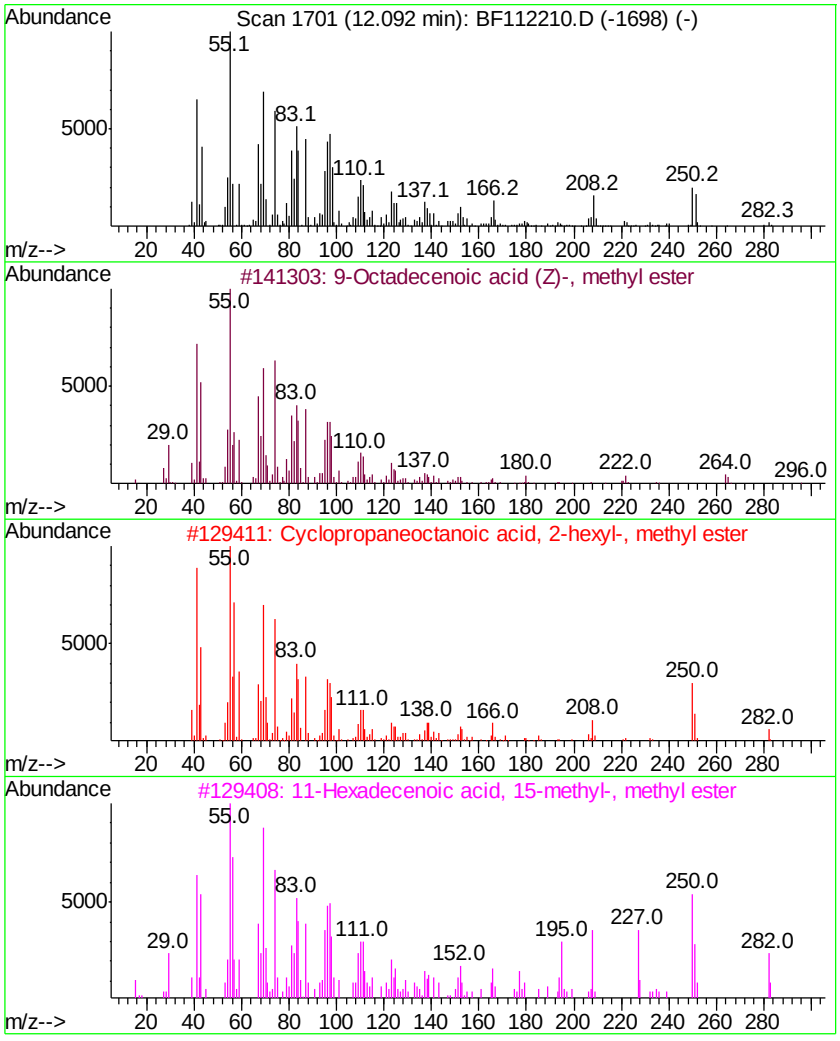
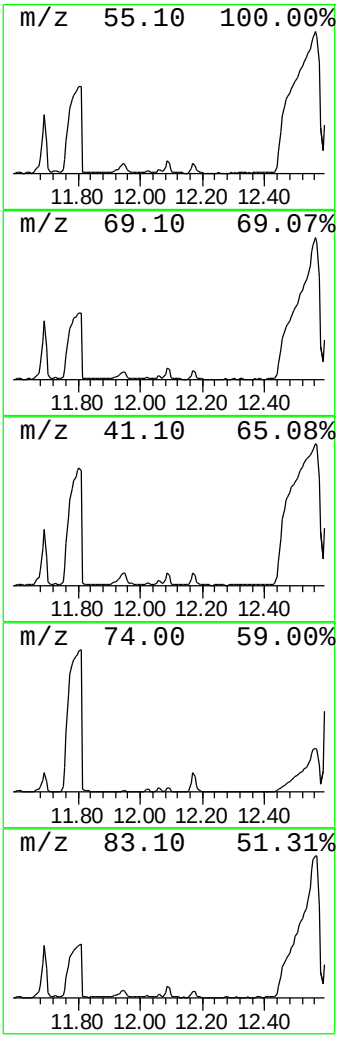
Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.09	20.34 ng	1570300	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
2	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	93
3	11-Hexadecenoic acid, 15-methyl-...	282	C18H34O2	055044-54-7	91
4	cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	91
5	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	87





Library Search Compound Report

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ClientSampleId : TR-05-RO-2-012319

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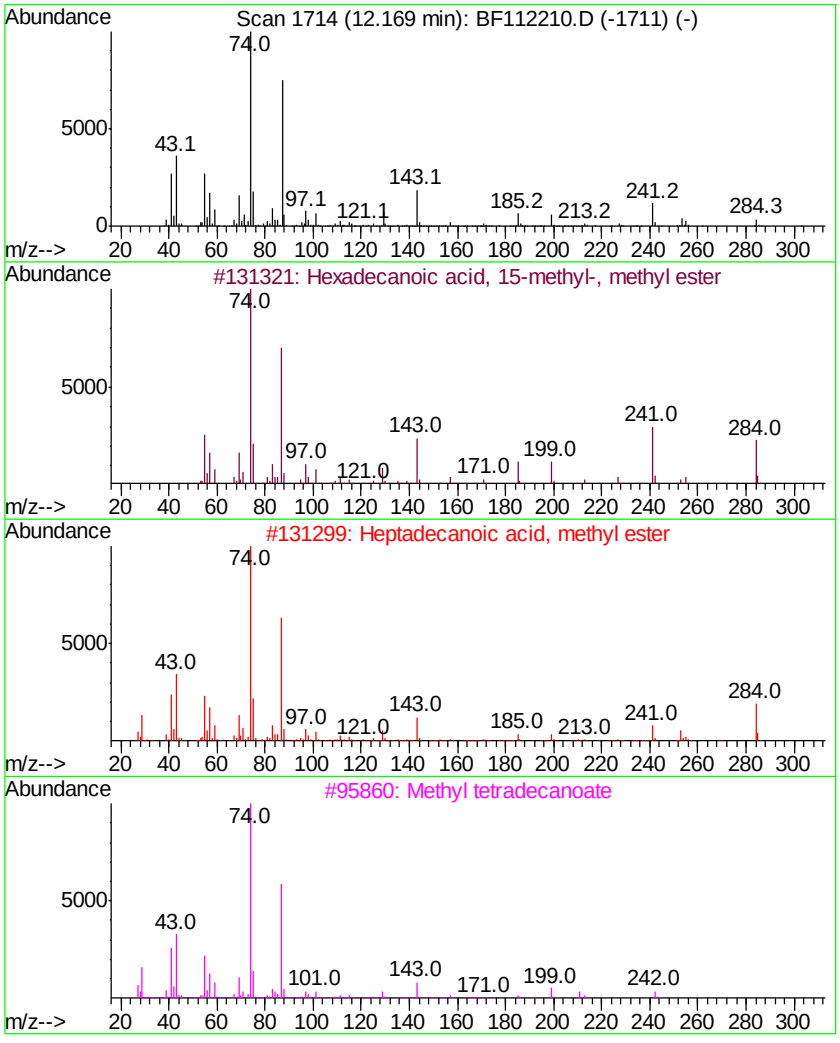
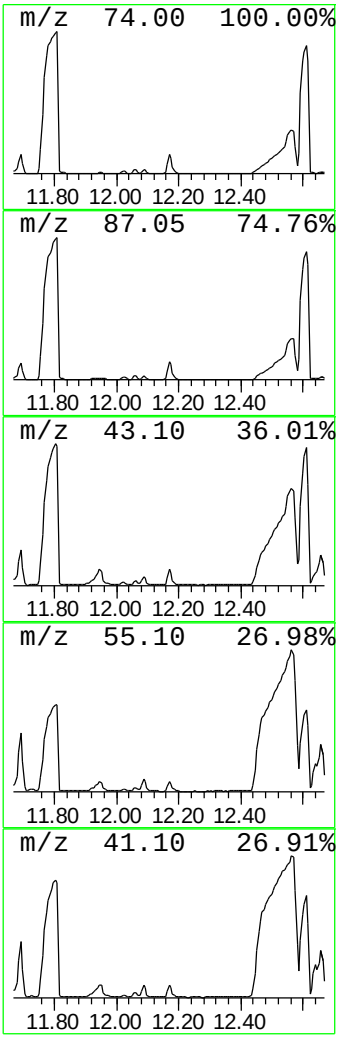
Peak Number 8 Hexadecanoic acid, 15-methy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	26.85 ng	2073420	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	97
2	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	96
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	87





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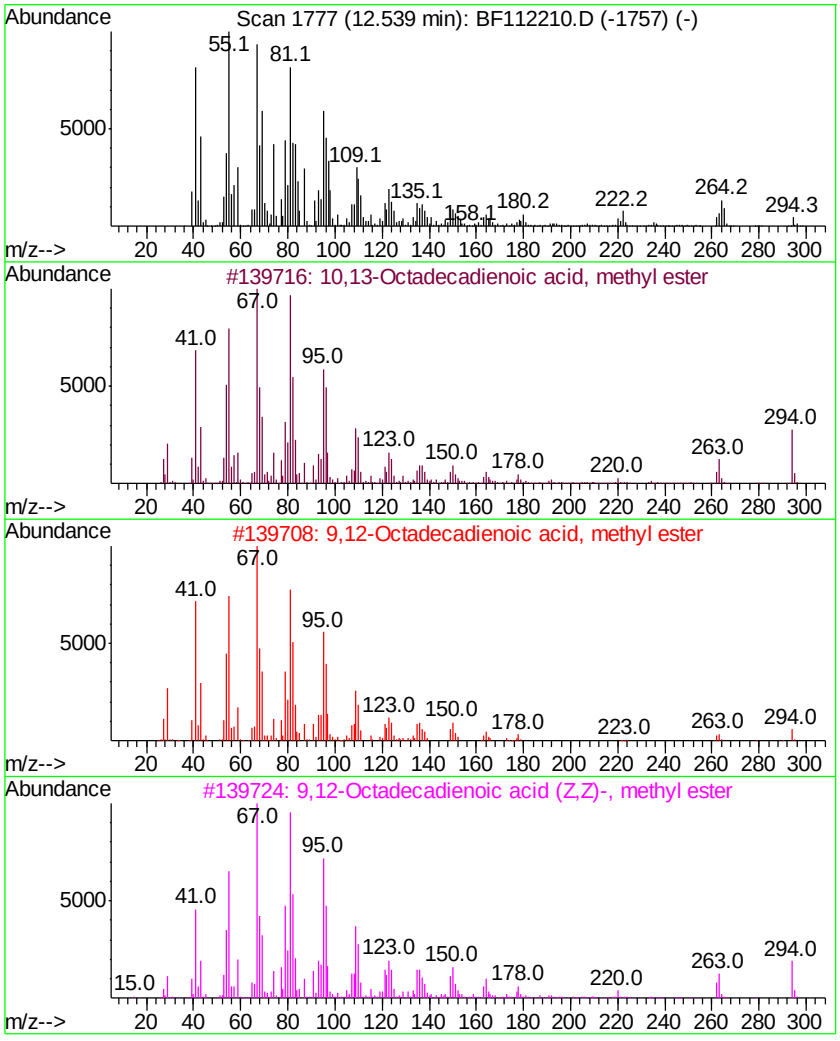
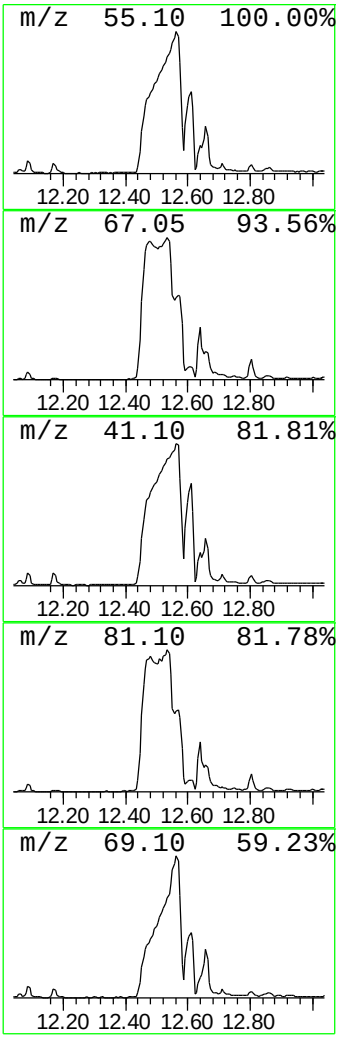
Peak Number 9 10,13-Octadecadienoic acid,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	1391.87 ng	107469000	Phenanthrene-d10	11.37

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	002462-85-3	98
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	95
5	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	95





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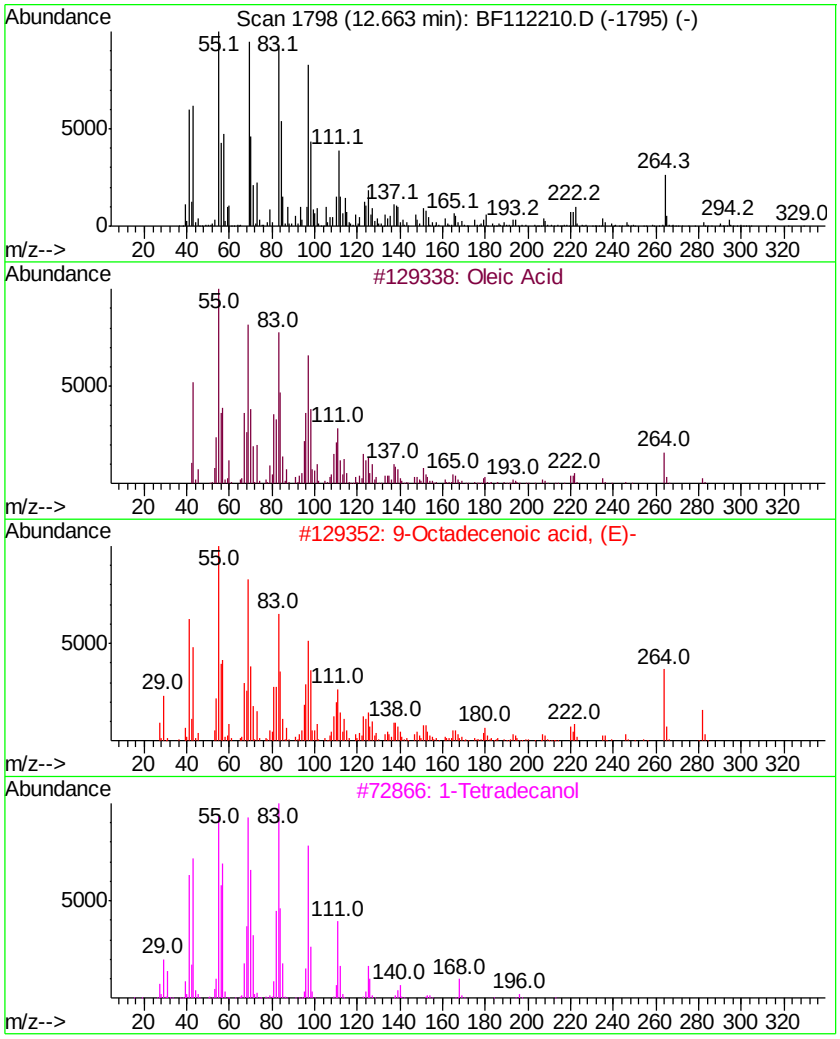
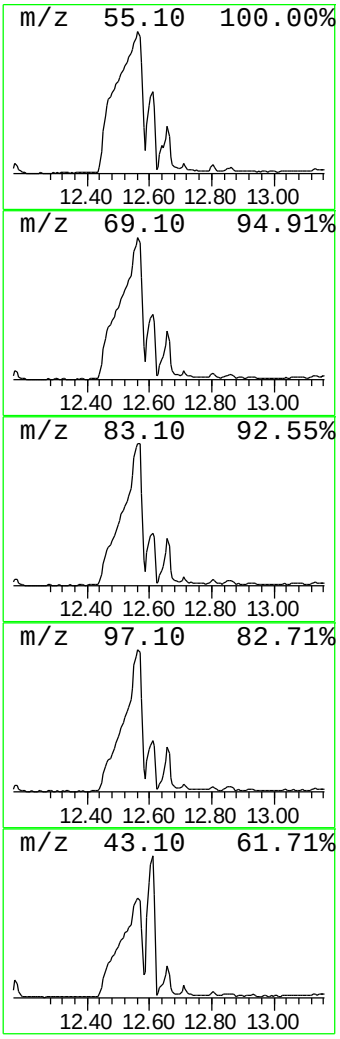
****

Peak Number 10 Oleic Acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	84.70 ng	6540130	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	91
2	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	87
3	1-Tetradecanol	214	C14H30O	000112-72-1	83
4	Acetic acid, trifluoro-, nonyl e...	240	C11H19F3O2	030767-14-7	72
5	n-Pentadecanol	228	C15H32O	000629-76-5	68





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112210.D
Acq On : 24 Jan 2019 15:51
Operator : JU/SJ
Sample : K1016-05 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-RO-2-012319

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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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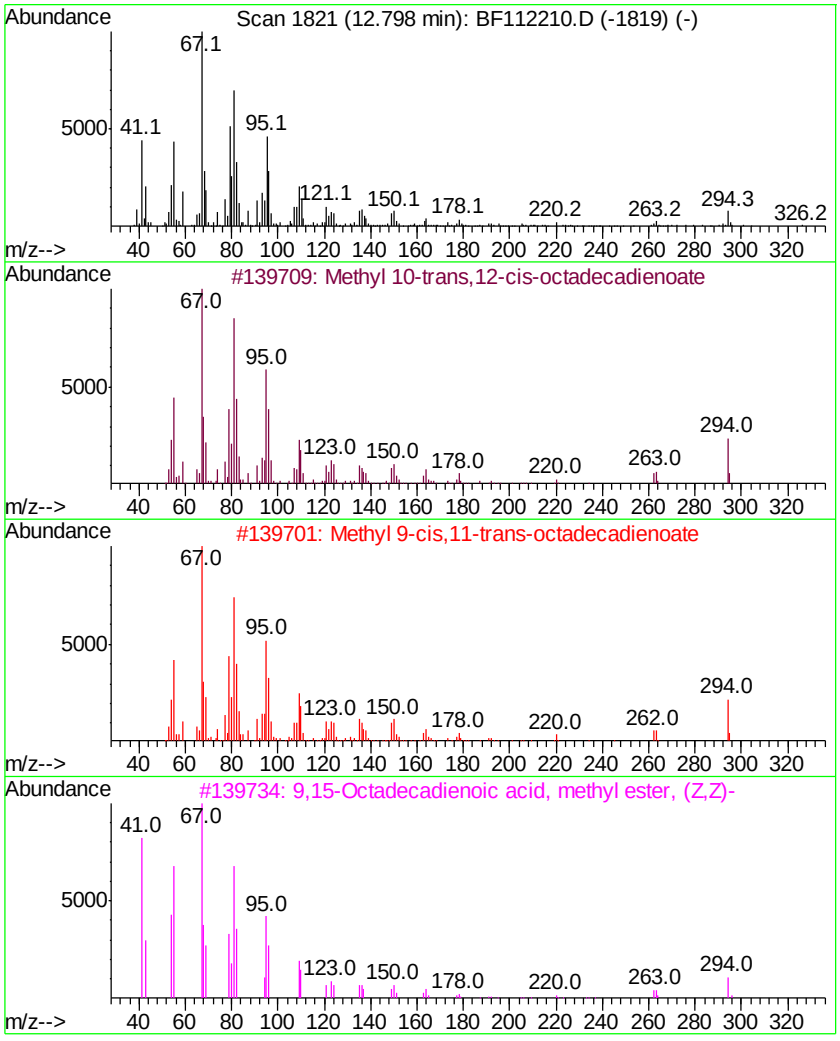
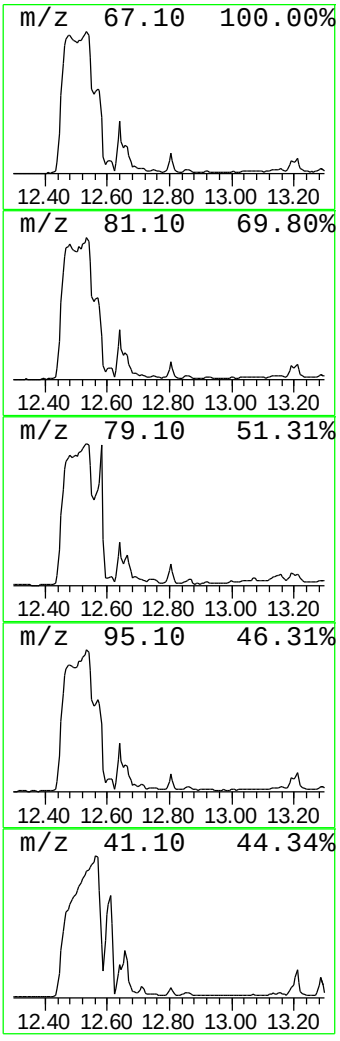
Peak Number 11 Methyl 10-trans,12-cis-octa... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	13.19 ng	1365340	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99
2	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	98
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	95
4	7,10-Octadecadienoic acid, methy...	294	C19H34O2	056554-24-6	93
5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	91





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Operator : JU/SJ
Sample : K1016-05 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-RO-2-012319

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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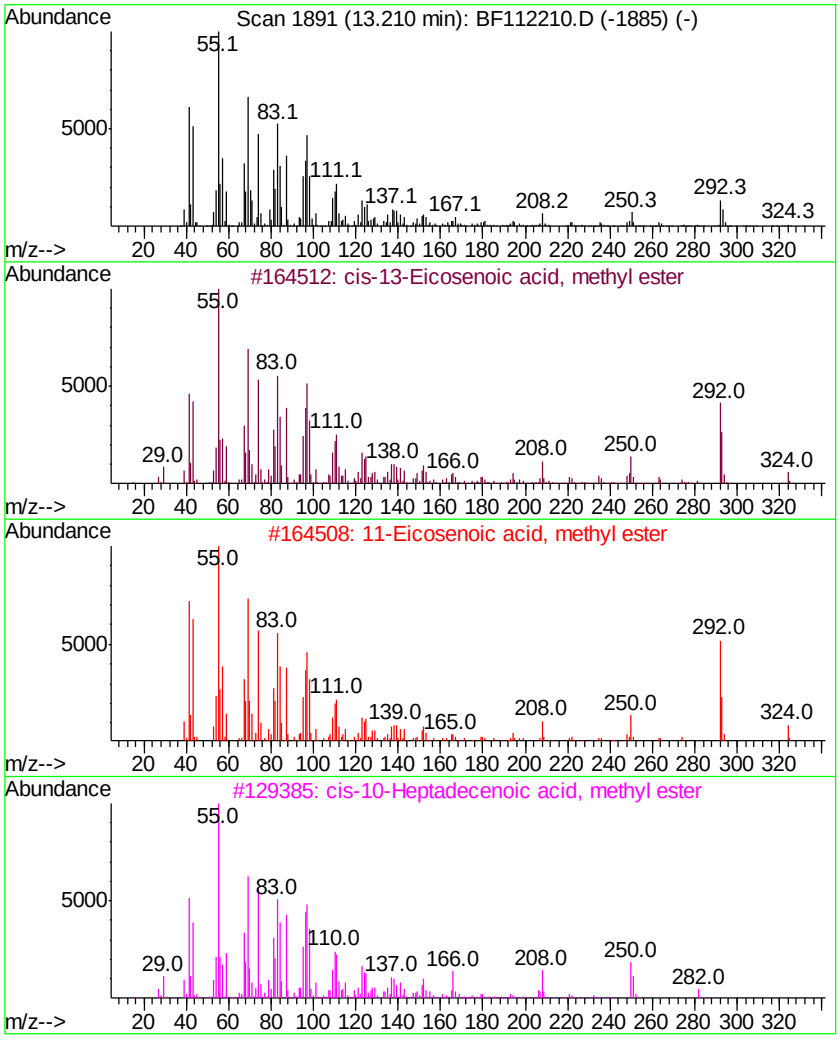
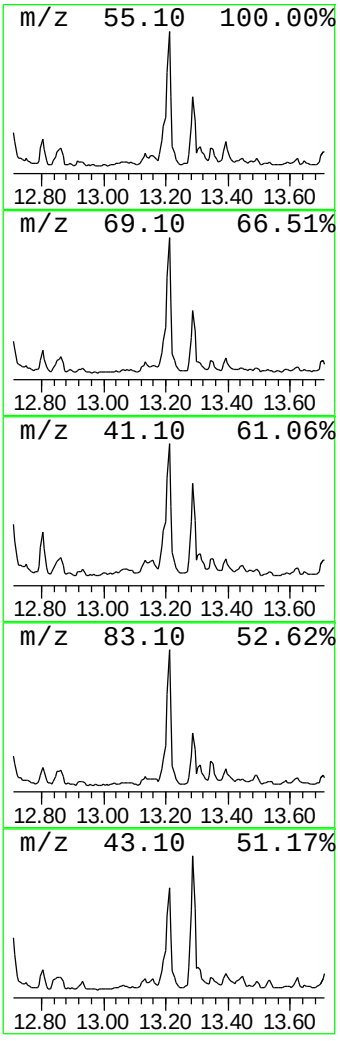
Peak Number 12 cis-13-Eicosenoic acid, met... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	53.92 ng	5581830	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-52-1	99
2	11-Eicosenoic acid, methyl ester	324	C21H40O2	003946-08-5	99
3	cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	91
4	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
5	cis-11-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-63-8	91





Library Search Compound Report

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Data File : BF112210.D
Acq On : 24 Jan 2019 15:51
Operator : JU/SJ
Sample : K1016-05 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-RO-2-012319

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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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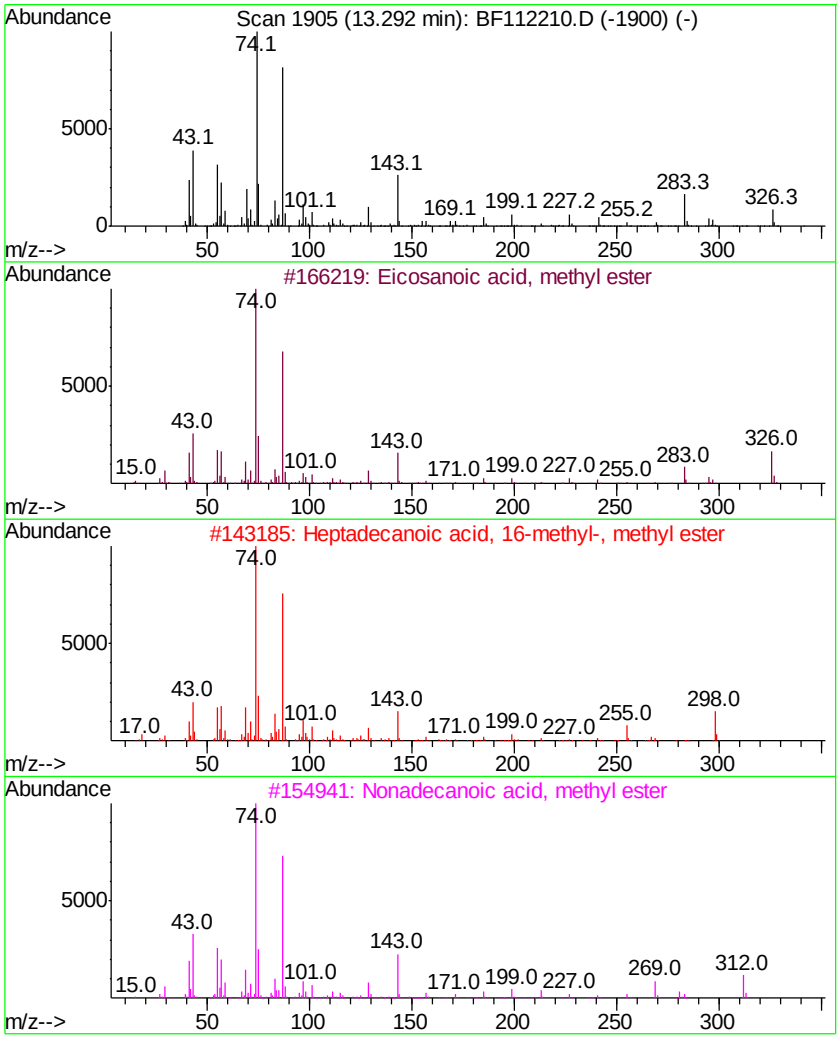
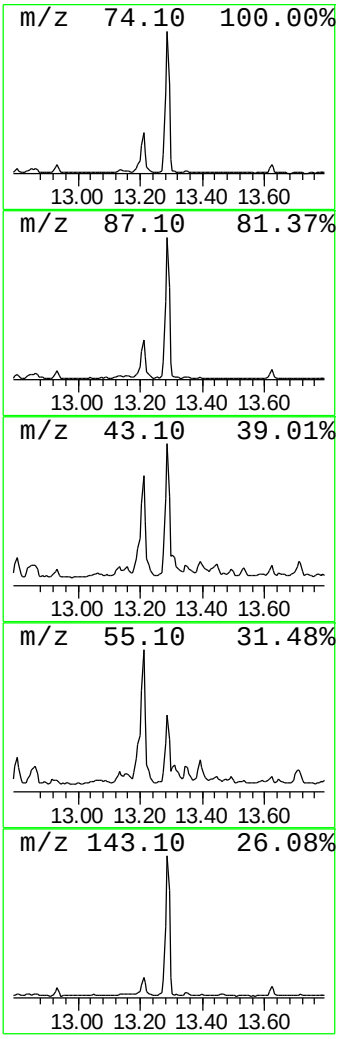
Peak Number 13 Eicosanoic acid, methyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.29	27.99 ng	2897520	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	99
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
3	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	90
4	Methyl stearate	298	C19H38O2	000112-61-8	90
5	Methyl 18-methylnonadecanoate	326	C21H42O2	1000352-20-6	89





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Data File : BF112210.D
Acq On : 24 Jan 2019 15:51
Operator : JU/SJ
Sample : K1016-05 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-RO-2-012319

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

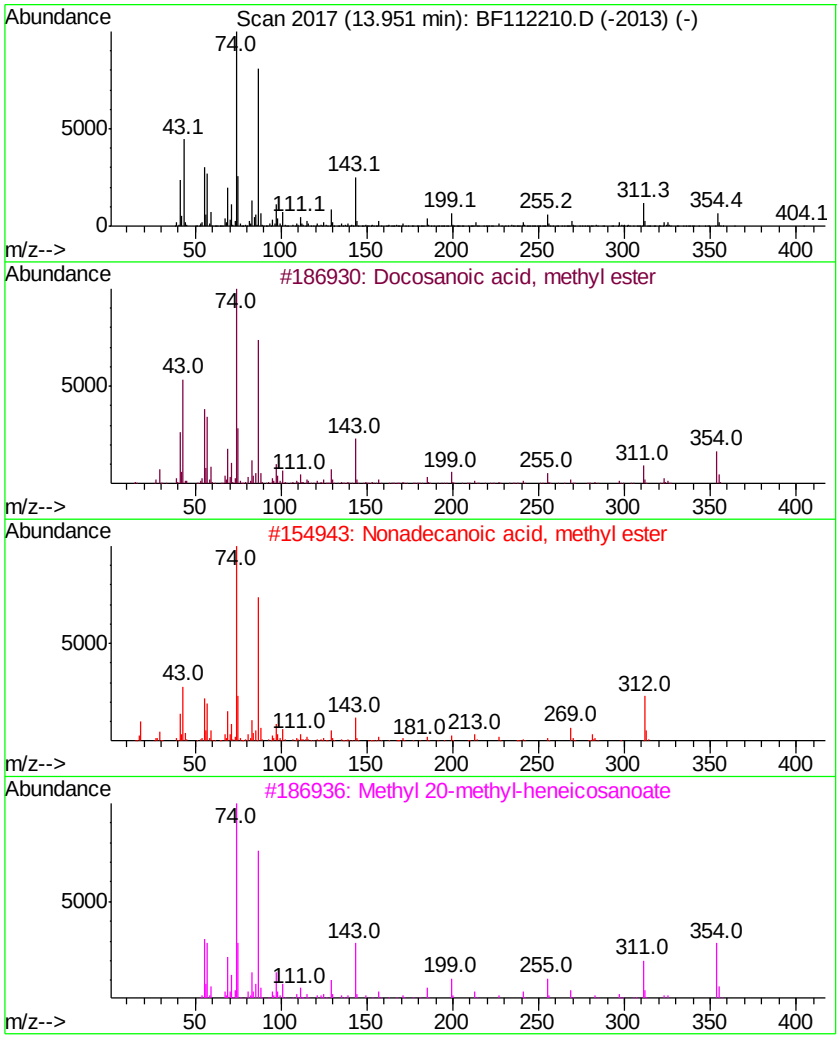
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

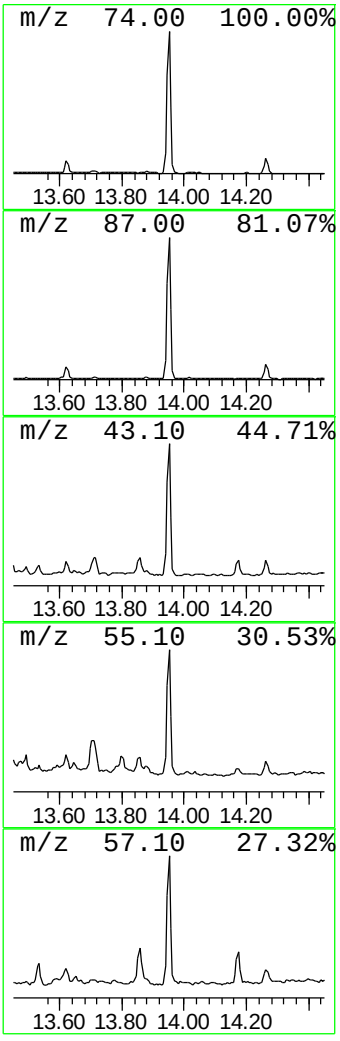
****

Peak Number 14 Docosanoic acid, methyl ester Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	22.39 ng	2317620	Chrysene-d12	14.03

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	94
3	Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	91
4	Methyl 18-methylnonadecanoate	326	C21H42O2	1000352-20-6	90
5	Methyl stearate	298	C19H38O2	000112-61-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012419\
Data File : BF112210.D
Acq On : 24 Jan 2019 15:51
Operator : JU/SJ
Sample : K1016-05 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-RO-2-012319

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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
unknown6.63	6.63	30.5	ng	1779010	1	6.85	1167220	20.0
Tridecanoic acid,...	10.90	66.4	ng	5128890	4	11.37	1544240	20.0
9-Hexadecenoic ac...	11.69	103.5	ng	7987190	4	11.37	1544240	20.0
Hexadecanoic acid...	11.81	579.7	ng	44756700	4	11.37	1544240	20.0
n-Hexadecanoic acid	11.95	38.0	ng	2938100	4	11.37	1544240	20.0
9-Octadecenoic ac...	12.09	20.3	ng	1570300	4	11.37	1544240	20.0
Hexadecanoic acid...	12.17	26.9	ng	2073420	4	11.37	1544240	20.0
10,13-Octadecadie...	12.54	1391.9	ng	107469000	4	11.37	1544240	20.0
Oleic Acid	12.66	84.7	ng	6540130	4	11.37	1544240	20.0
Methyl 10-trans,1...	12.80	13.2	ng	1365340	5	14.03	2070420	20.0
cis-13-Eicosenoic...	13.21	53.9	ng	5581830	5	14.03	2070420	20.0
Eicosanoic acid, ...	13.29	28.0	ng	2897520	5	14.03	2070420	20.0
Docosanoic acid, ...	13.95	22.4	ng	2317620	5	14.03	2070420	20.0