LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012919\
Data File : BF112298.D
Acq On : 29 Jan 2019 16:38
Operator : JU/SJ
Sample : K1016-11 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-012819

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-BF012519.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	5.469	572	575	591	rBV	431956	525331	1.11%	0.548%
2	6.487	744	748	765	rBV	466615	573596	1.21%	0.599%
3	6.616	766	770	776	rVV	655522	605160	1.28%	0.631%
4	6.839	804	808	816	rBV	1002250	864486	1.83%	0.902%
5	6.992	831	834	842	rBV	568276	506341	1.07%	0.528%
6	8.122	1020	1026	1029	rBV	1196855	1190229	2.52%	1.242%
7	9.192	1204	1208	1213	rBV	858772	693408	1.47%	0.724%
8	9.875	1320	1324	1327	rBV	1252953	1045870	2.22%	1.091%
9	10.874	1491	1494	1497	rBV	890167	694830	1.47%	0.725%
10	11.363	1573	1577	1579	rBV	1077778	1010913	2.14%	1.055%
11	11.669	1623	1629	1634	rBV	1138650	1113664	2.36%	1.162%
12	11.763	1638	1645	1648	rBV2	13265962	17970012	38.06%	18.751%
13	12.474	1752	1766	1768	rBV3	15076336	47214369	100.00%	49.266%
14	12.527	1773	1775	1776	rVV	1778597	1333664	2.82%	1.392%
15	12.557	1776	1780	1782	rVB	10667929	9743611	20.64%	10.167%
16	12.580	1782	1784	1786	rBV	861855	812140	1.72%	0.847%
17	12.774	1813	1817	1820	rBV	754443	721422	1.53%	0.753%
18	12.816	1820	1824	1831	rVB	598212	1079627	2.29%	1.127%
19	12.945	1843	1846	1849	rBV	781087	724360	1.53%	0.756%
20	13.139	1873	1879	1881	rBV4	384385	594461	1.26%	0.620%
21	13.186	1881	1887	1893	rVB2	1101621	1460363	3.09%	1.524%
22	13.263	1897	1900	1902	rBV	1213228	980029	2.08%	1.023%
23	13.686	1968	1972	1976	rBV2	451384	615167	1.30%	0.642%
24	13.927	2010	2013	2018	rVB	1123579	974042	2.06%	1.016%
25	14.004	2021	2026	2029	rVV2	1395102	1595478	3.38%	1.665%
26	15.474	2272	2276	2284	rVV	956803	1192224	2.53%	1.244%

Sum of corrected areas: 95834797

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012919\
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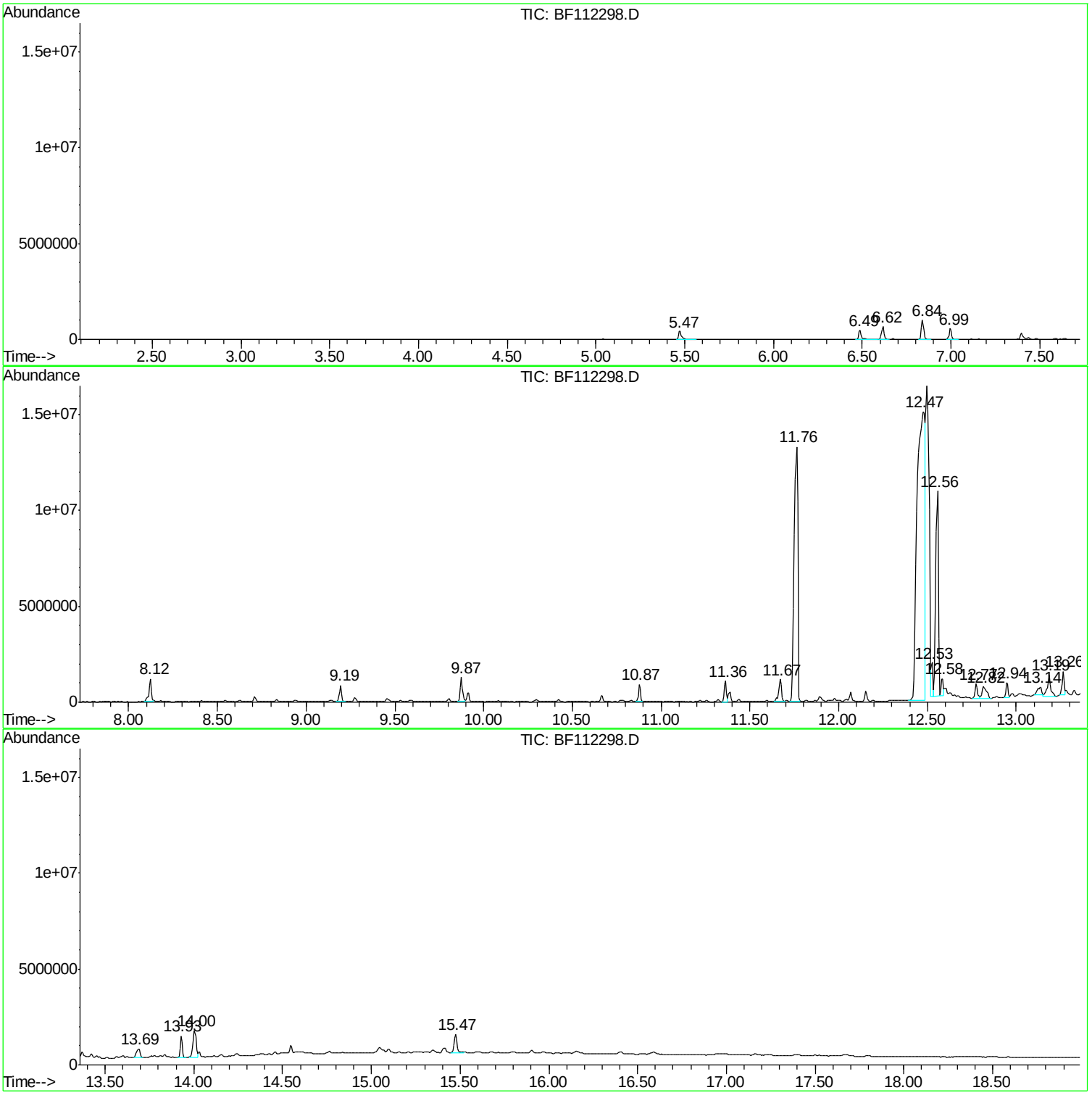
Operator : JU/SJ
Sample : K1016-11 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-012819

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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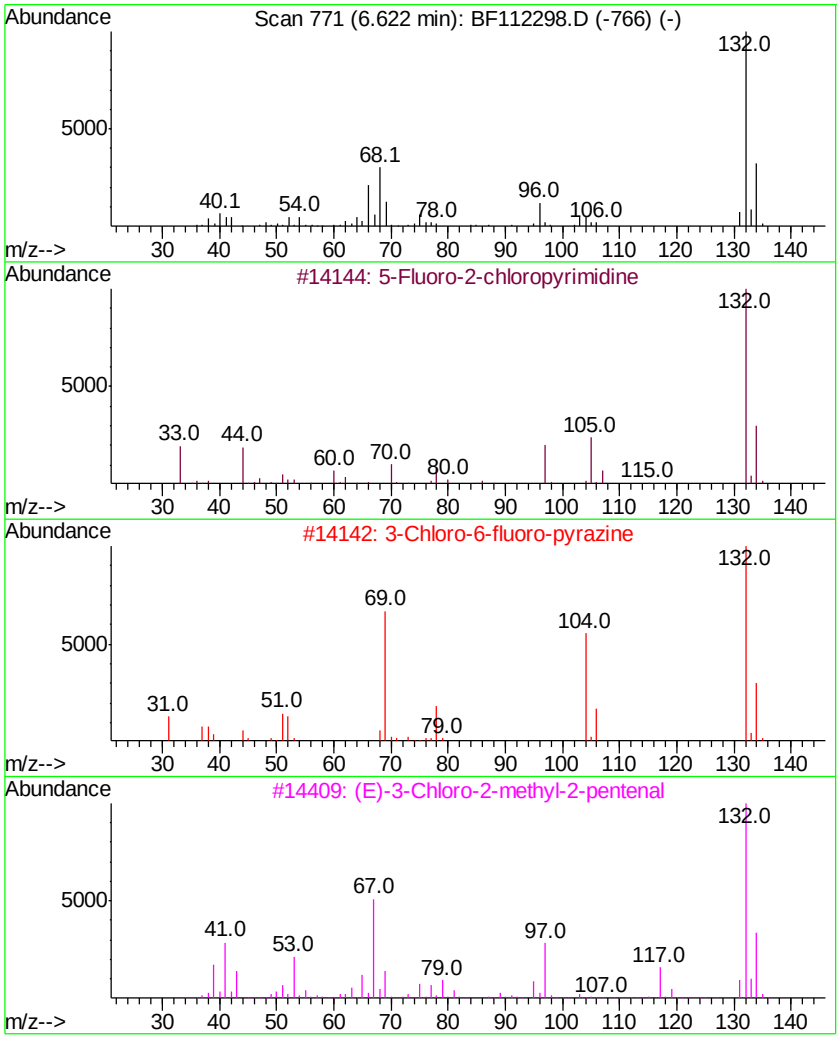
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

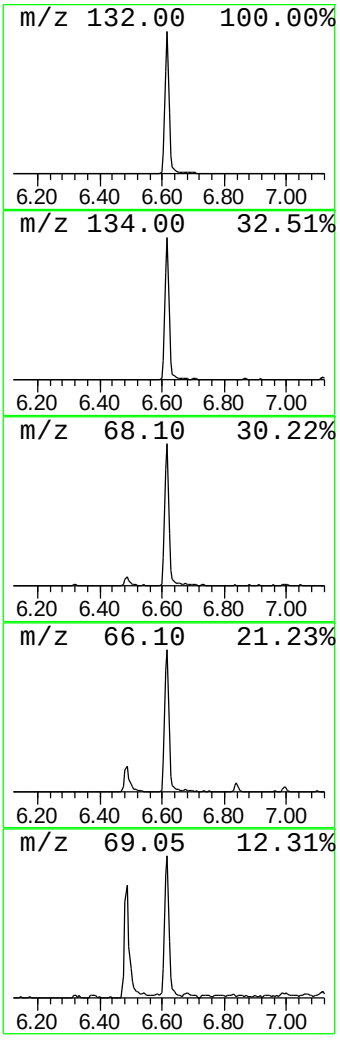
****

Peak Number 1 unknown6.62 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	14.00 ng	605160	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
5	5-Aminoindole	132	C8H8N2	005192-03-0	16





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : TR-05-012819

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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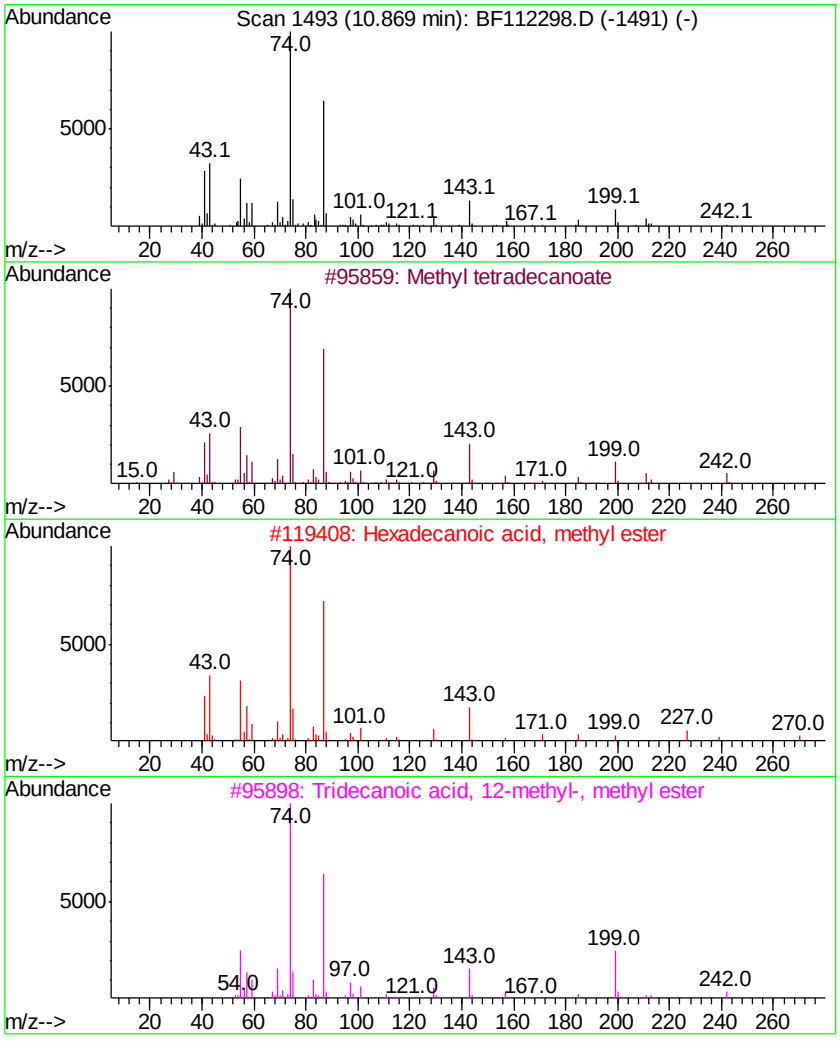
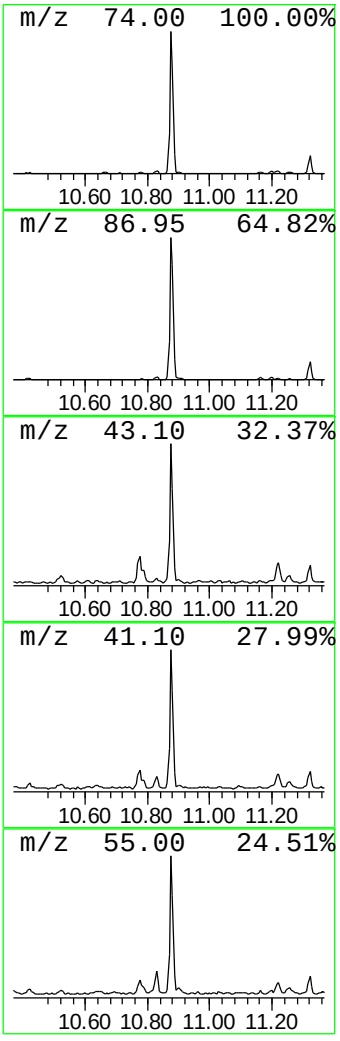
Peak Number 3 Methyl tetradecanoate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.87	13.75 ng	694830	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	87
3	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	86
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	86





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Sample : K1016-11 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-012819

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

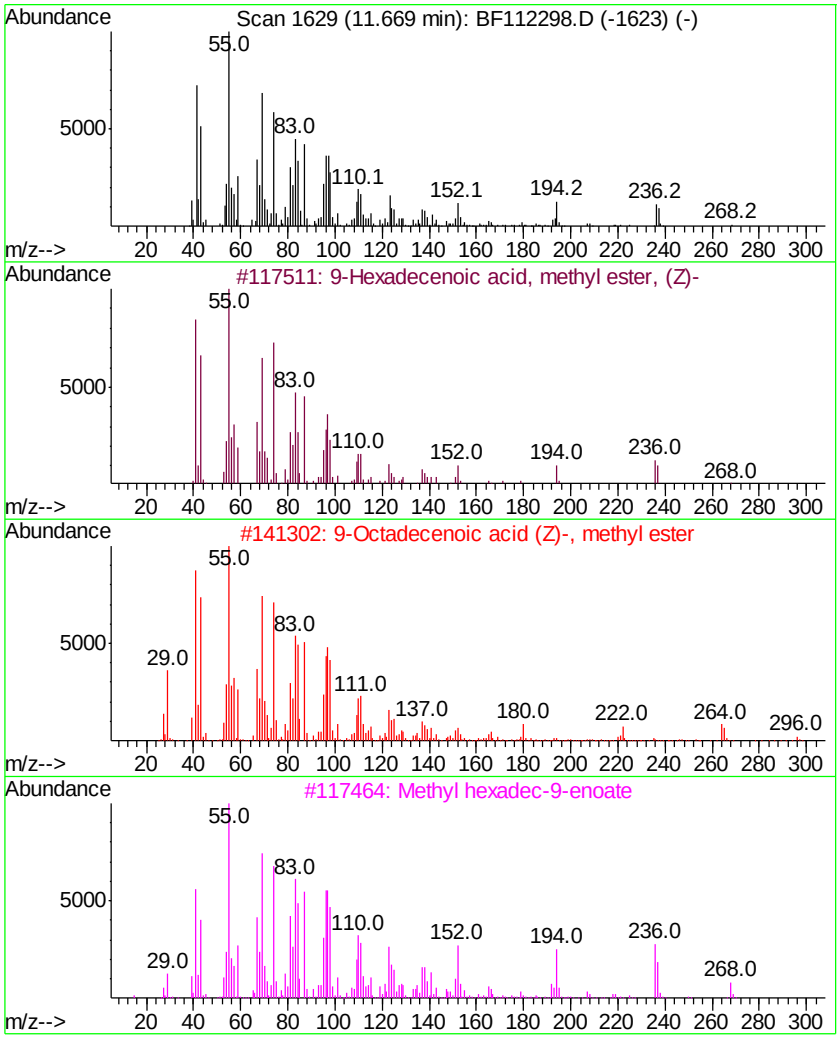
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

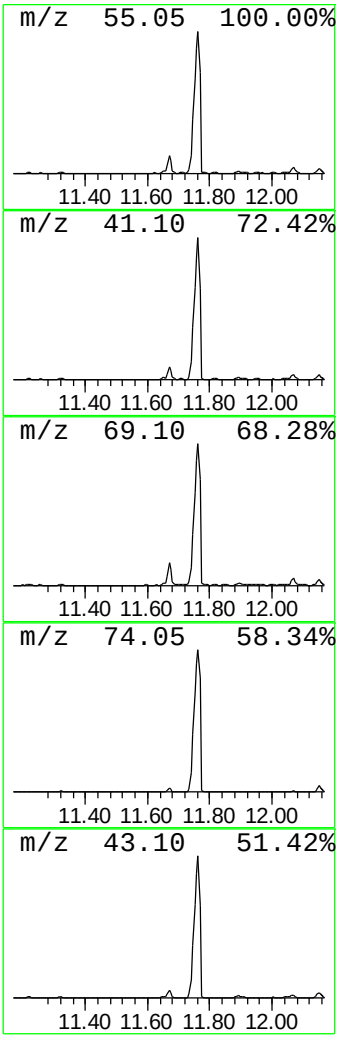
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	22.03 ng	1113660	Phenanthrene-d10	11.36

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	Methyl hexadec-9-enoate	268	C17H32O2	010030-74-7	91
4	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	87
5	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012919\
Data File : BF112298.D
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Operator : JU/SJ
Sample : K1016-11 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-012819

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

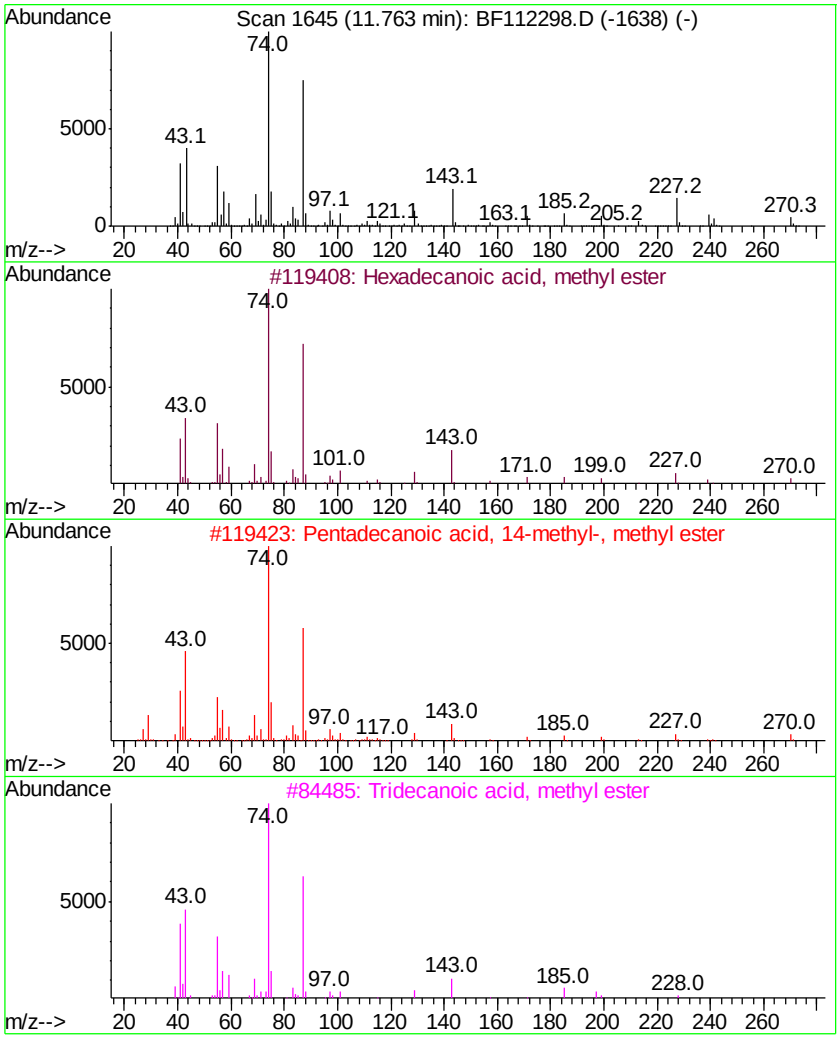
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	355.52 ng	17970000	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	95
4	Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	83
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	81



m/z 74.05 100.00%
m/z 87.10 75.19%
m/z 43.10 39.92%
m/z 41.05 32.16%
m/z 55.10 31.20%

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012919\
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Acq On : 29 Jan 2019 16:38
Operator : JU/SJ
Sample : K1016-11 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-012819

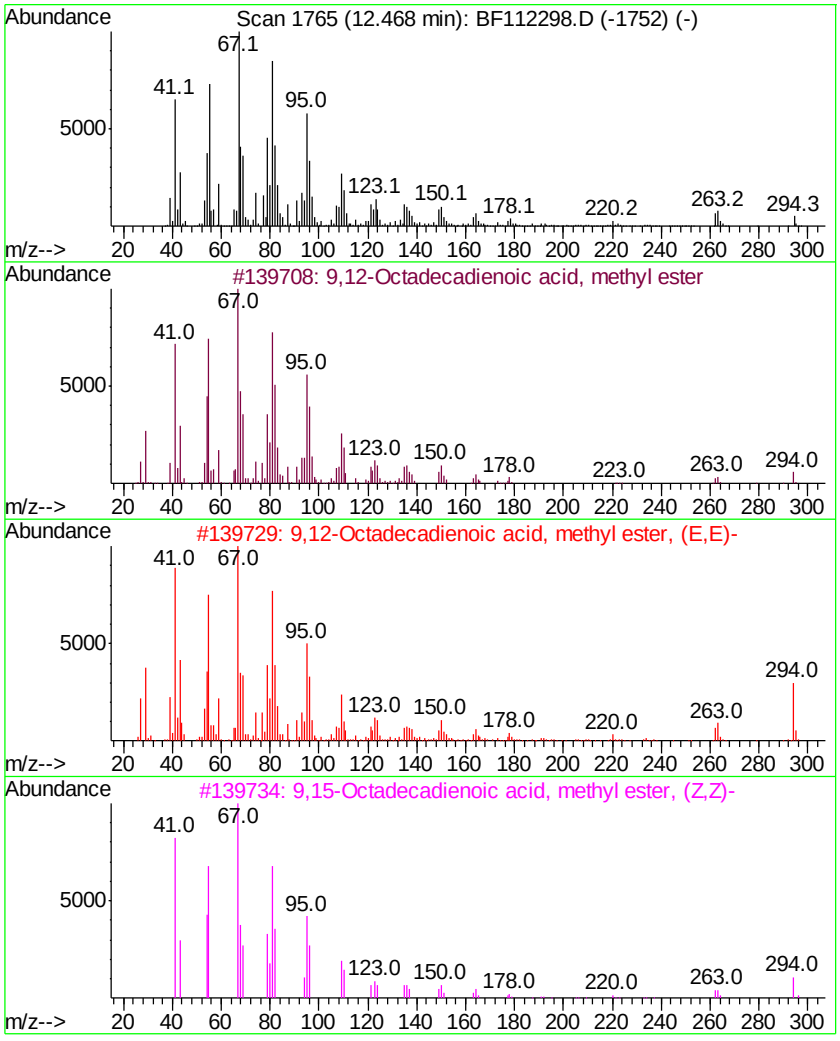
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

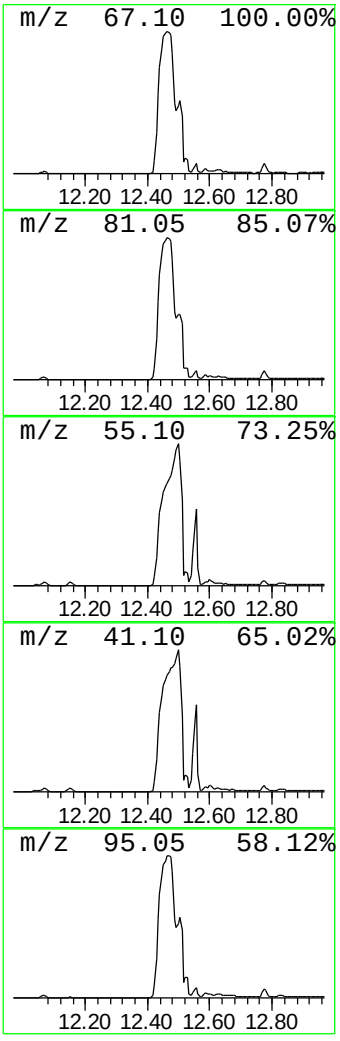
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	934.09 ng	47214400	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	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	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-012819

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

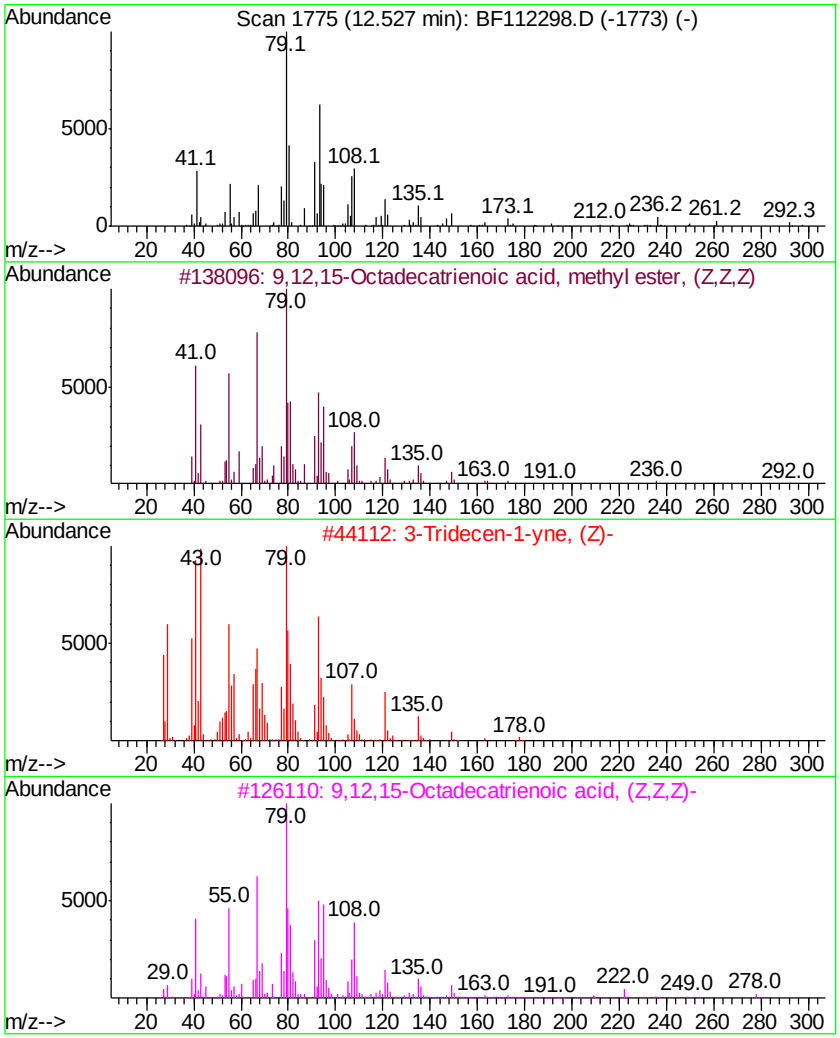
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

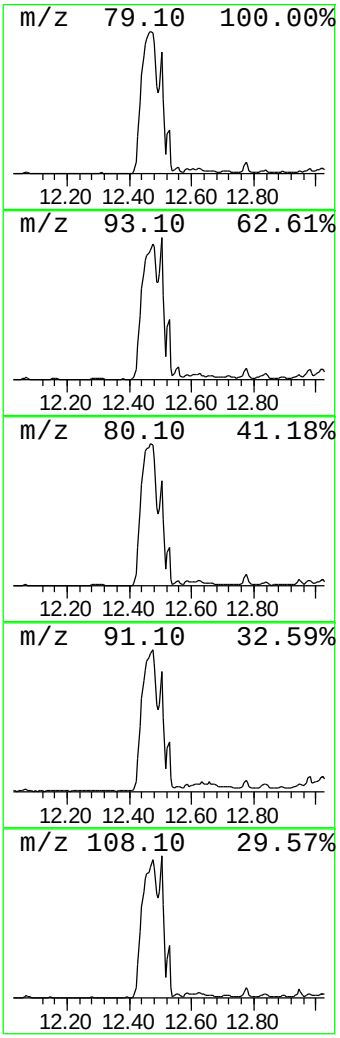
****

Peak Number 7 9,12,15-Octadecatrienoic ac... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.53	26.39 ng	1333660	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	93
2	3-Tridecen-1-yne, (Z)-	178	C13H22	037981-62-7	72
3	9,12,15-Octadecatrienoic acid, (...	278	C18H30O2	000463-40-1	64
4	2-Methylenebicyclo[2.2.1]-heptane	108	C8H12	000497-35-8	58
5	3-6-Nonadien-1-yl-acetate	182	C11H18O2	076649-26-8	50





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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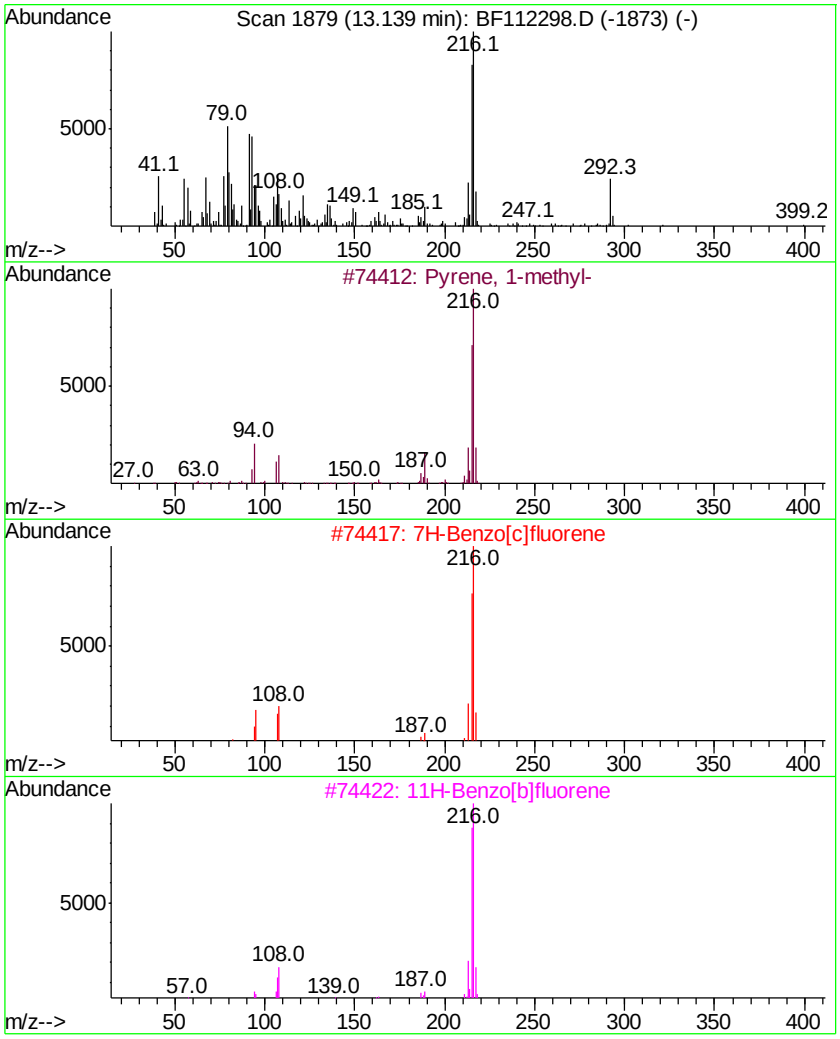
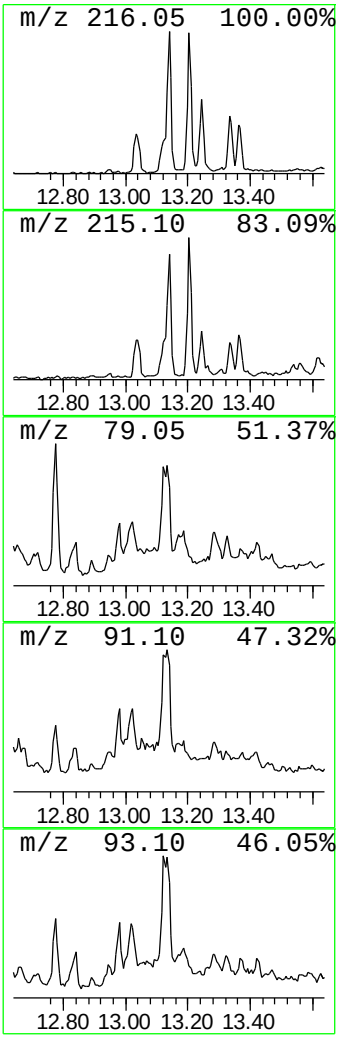
****

Peak Number 8 Pyrene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.14	7.45 ng	594461	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	86
2	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	64
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	64
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	64
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	46





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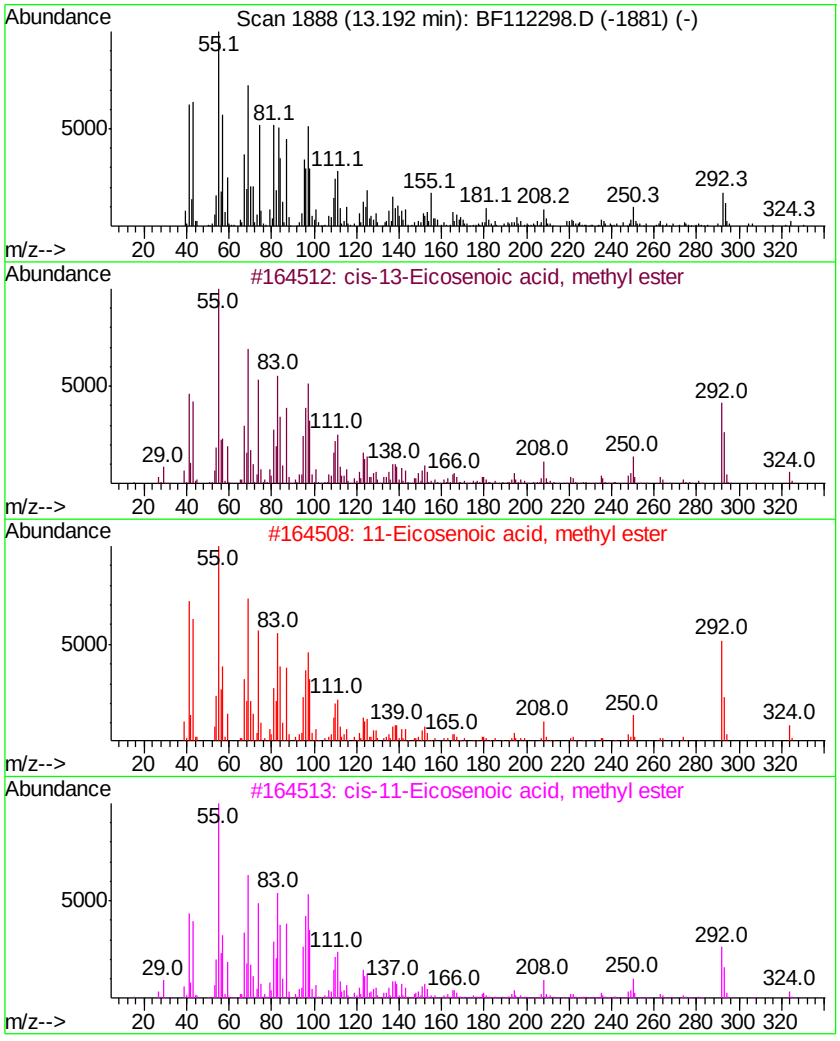
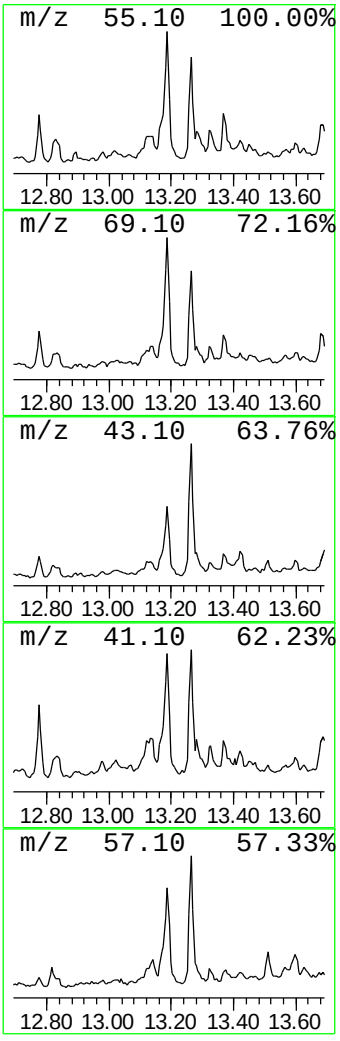
****

Peak Number 9 cis-13-Eicosenoic acid, met... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	18.31 ng	1460360	Chrysene-d12	14.00

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-11-Eicosenoic acid, methyl e...	324	C21H40O2	1000333-63-8	99
4	Methyl 9-eicosenoate	324	C21H40O2	1000336-50-5	90
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	89





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

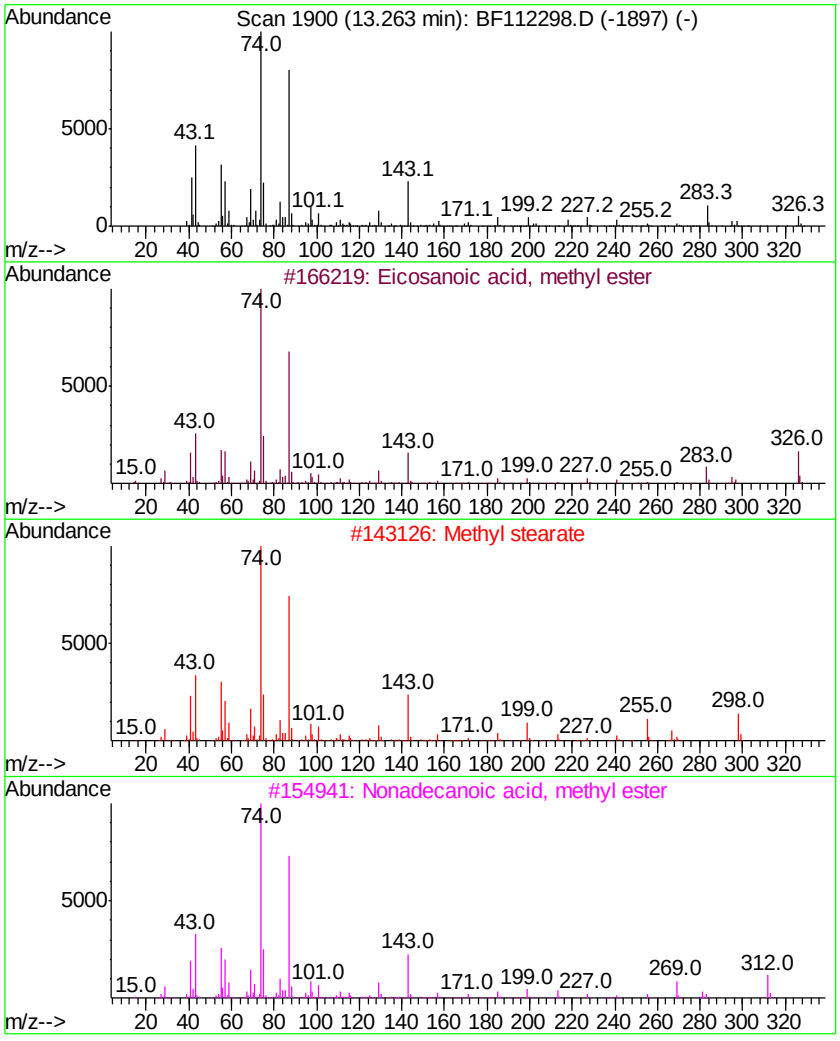
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

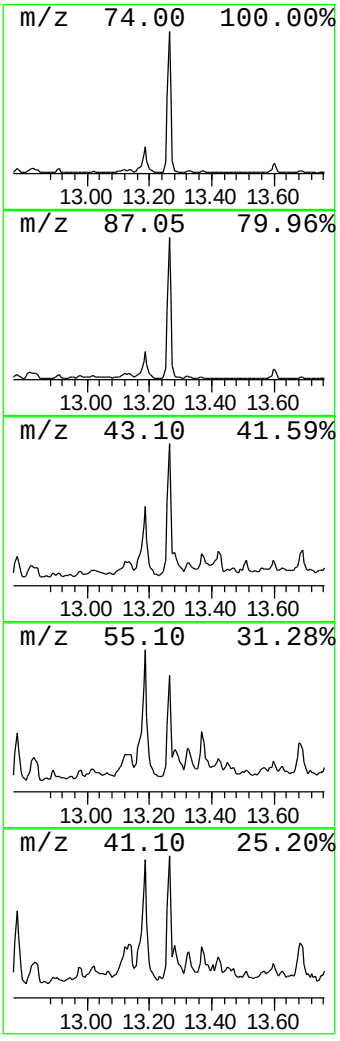
****

Peak Number 10 Eicosanoic acid, methyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	12.29 ng	980029	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	98
2	Methyl stearate	298	C19H38O2	000112-61-8	90
3	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	90
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	87
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	86





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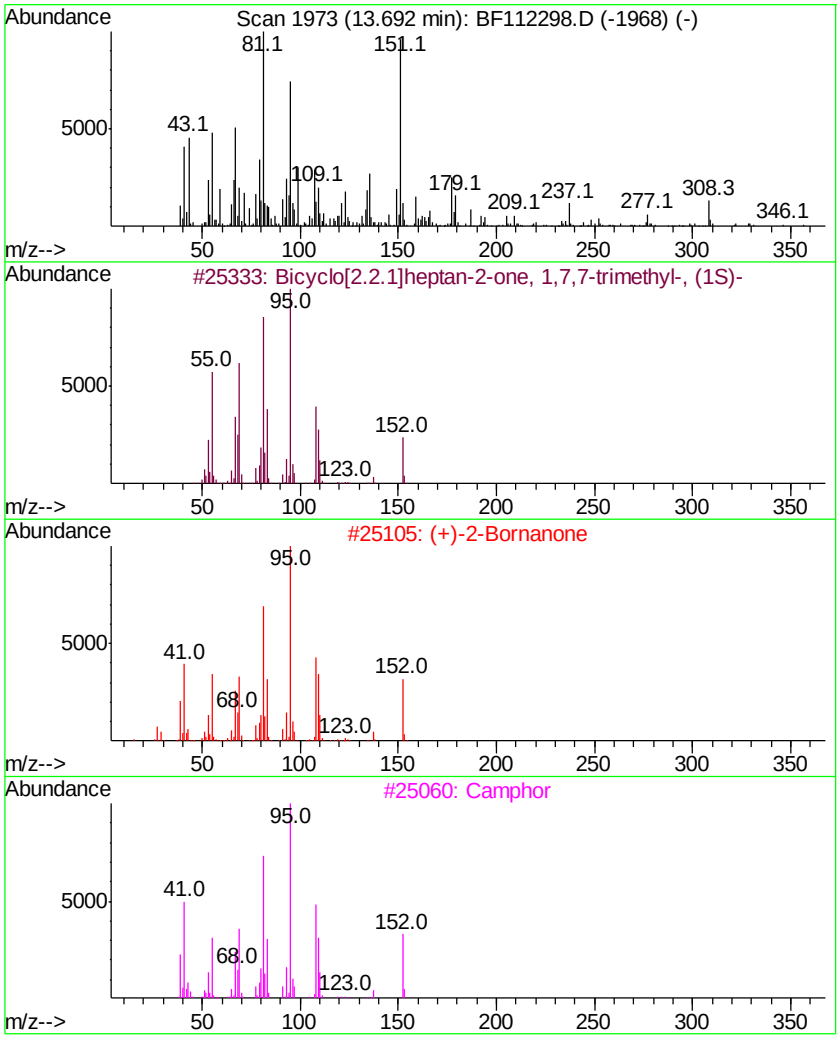
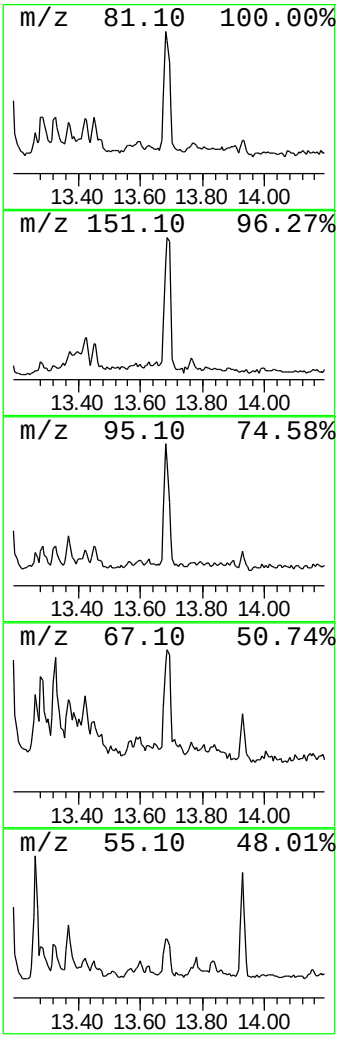
****

Peak Number 11 unknown13.69 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	7.71 ng	615167	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	45
2	(+)-2-Bornanone	152	C10H16O	000464-49-3	43
3	Camphor	152	C10H16O	000076-22-2	43
4	1,4 Benzodioxan-6-amine	151	C8H9NO2	022013-33-8	38
5	2,6-Dimethylbenzoquinone-4-oxime	151	C8H9NO2	004965-29-1	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012919\
Data File : BF112298.D
Acq On : 29 Jan 2019 16:38
Operator : JU/SJ
Sample : K1016-11 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-012819

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

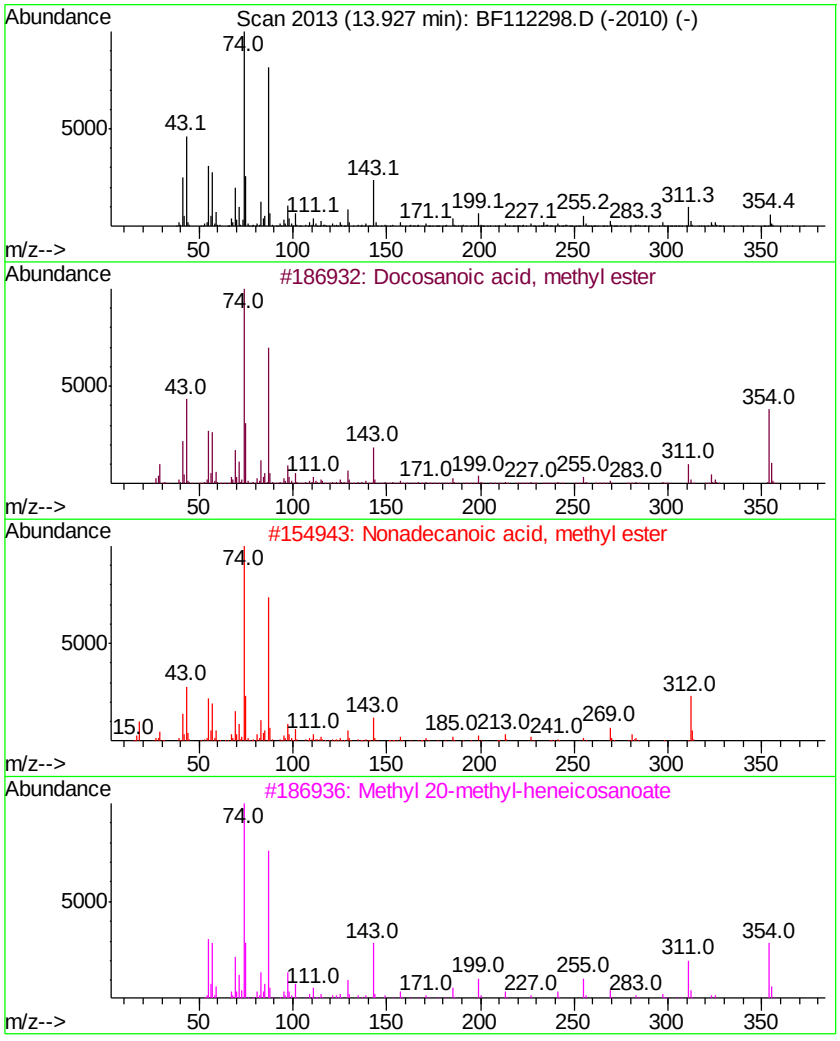
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

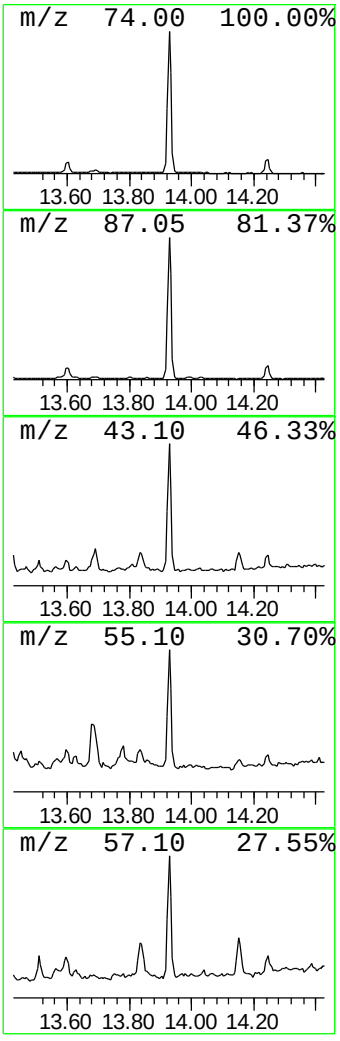
****

Peak Number 12 Docosanoic acid, methyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	12.21 ng	974042	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	98
2	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	93
3	Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	90
4	Methyl stearate	298	C19H38O2	000112-61-8	87
5	Methyl 18-methylnonadecanoate	326	C21H42O2	1000352-20-6	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012919\
Data File : BF112298.D
Acq On : 29 Jan 2019 16:38
Operator : JU/SJ
Sample : K1016-11 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-05-012819

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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
unknown6.62	6.62	14.0	ng	605160	1	6.84	864486	20.0
Methyl tetradecan...	10.87	13.8	ng	694830	4	11.36	1010910	20.0
9-Hexadecenoic ac...	11.67	22.0	ng	1113660	4	11.36	1010910	20.0
Hexadecanoic acid...	11.76	355.5	ng	17970000	4	11.36	1010910	20.0
9,12-Octadecadien...	12.47	934.1	ng	47214400	4	11.36	1010910	20.0
9,12,15-Octadecat...	12.53	26.4	ng	1333660	4	11.36	1010910	20.0
Pyrene, 1-methyl-	13.14	7.5	ng	594461	5	14.00	1595480	20.0
cis-13-Eicosenoic...	13.19	18.3	ng	1460360	5	14.00	1595480	20.0
Eicosanoic acid, ...	13.26	12.3	ng	980029	5	14.00	1595480	20.0
unknown13.69	13.69	7.7	ng	615167	5	14.00	1595480	20.0
Docosanoic acid, ...	13.93	12.2	ng	974042	5	14.00	1595480	20.0