LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
Data File : BF113428.D
Acq On : 29 Mar 2019 22:18
Operator : JU/SJ
Sample : K1685-13 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-032819-C

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-BF032519.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	5.310	545	548	571	rBV	1116066	1295617	23.56%	4.454%
2	6.346	720	724	739	rBV	1365314	1395677	25.38%	4.798%
3	6.475	742	746	757	rVV	1452833	1414818	25.73%	4.863%
4	6.698	781	784	795	rBV	814126	749861	13.64%	2.578%
5	6.857	807	811	824	rVB	1252396	1074141	19.53%	3.692%
6	7.263	876	880	900	rBV	826337	867040	15.77%	2.980%
7	7.981	999	1002	1013	rBV	946416	964356	17.54%	3.315%
8	9.057	1181	1185	1196	rBV	1716369	1596098	29.03%	5.486%
9	9.451	1248	1252	1257	rBV2	79577	111952	2.04%	0.385%
10	9.734	1296	1300	1315	rVB	1177469	1176837	21.40%	4.045%
11	10.516	1429	1433	1445	rBV	981863	1024760	18.64%	3.523%
12	10.657	1451	1457	1462	rVB3	65474	95933	1.74%	0.330%
13	11.210	1547	1551	1554	rBV	1288760	1174407	21.36%	4.037%
14	11.610	1615	1619	1623	rBV	1599038	1301326	23.66%	4.473%
15	11.745	1639	1642	1651	rBV2	262473	313814	5.71%	1.079%
16	11.916	1665	1671	1678	rBV5	34913	68242	1.24%	0.235%
17	12.298	1731	1736	1738	rBV	4890067	5498958	100.00%	18.902%
18	12.316	1738	1739	1745	rVB2	3695195	2728080	49.61%	9.378%
19	12.398	1750	1753	1755	rBV	743098	615195	11.19%	2.115%
20	12.416	1755	1756	1761	rVB	131719	118967	2.16%	0.409%
21	12.527	1772	1775	1780	rBV	105453	139226	2.53%	0.479%
22	12.645	1791	1795	1798	rVB	147785	135404	2.46%	0.465%
23	12.786	1815	1819	1829	rVB	1734411	1630928	29.66%	5.606%
24	13.039	1857	1862	1865	rBV2	66636	103730	1.89%	0.357%
25	13.780	1986	1988	1993	rVB2	60100	60507	1.10%	0.208%
26	13.839	1994	1998	2006	rVB	1272522	1287569	23.41%	4.426%
27	14.010	2024	2027	2032	rVB	89154	75416	1.37%	0.259%
28	14.310	2076	2078	2082	rVB	116467	96866	1.76%	0.333%
29	14.604	2126	2128	2131	rVB	146959	117967	2.15%	0.406%
30	14.674	2137	2140	2143	rVB	204422	185986	3.38%	0.639%
31	14.916	2178	2181	2186	rVB	195259	217986	3.96%	0.749%
32	15.245	2232	2237	2245	rVB	868808	1276199	23.21%	4.387%
33	15.663	2305	2308	2313	rVB	145893	177774	3.23%	0.611%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
Data File : BF113428.D
Acq On : 29 Mar 2019 22:18
Operator : JU/SJ
Sample : K1685-13 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-06-032819-C

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-BF032519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

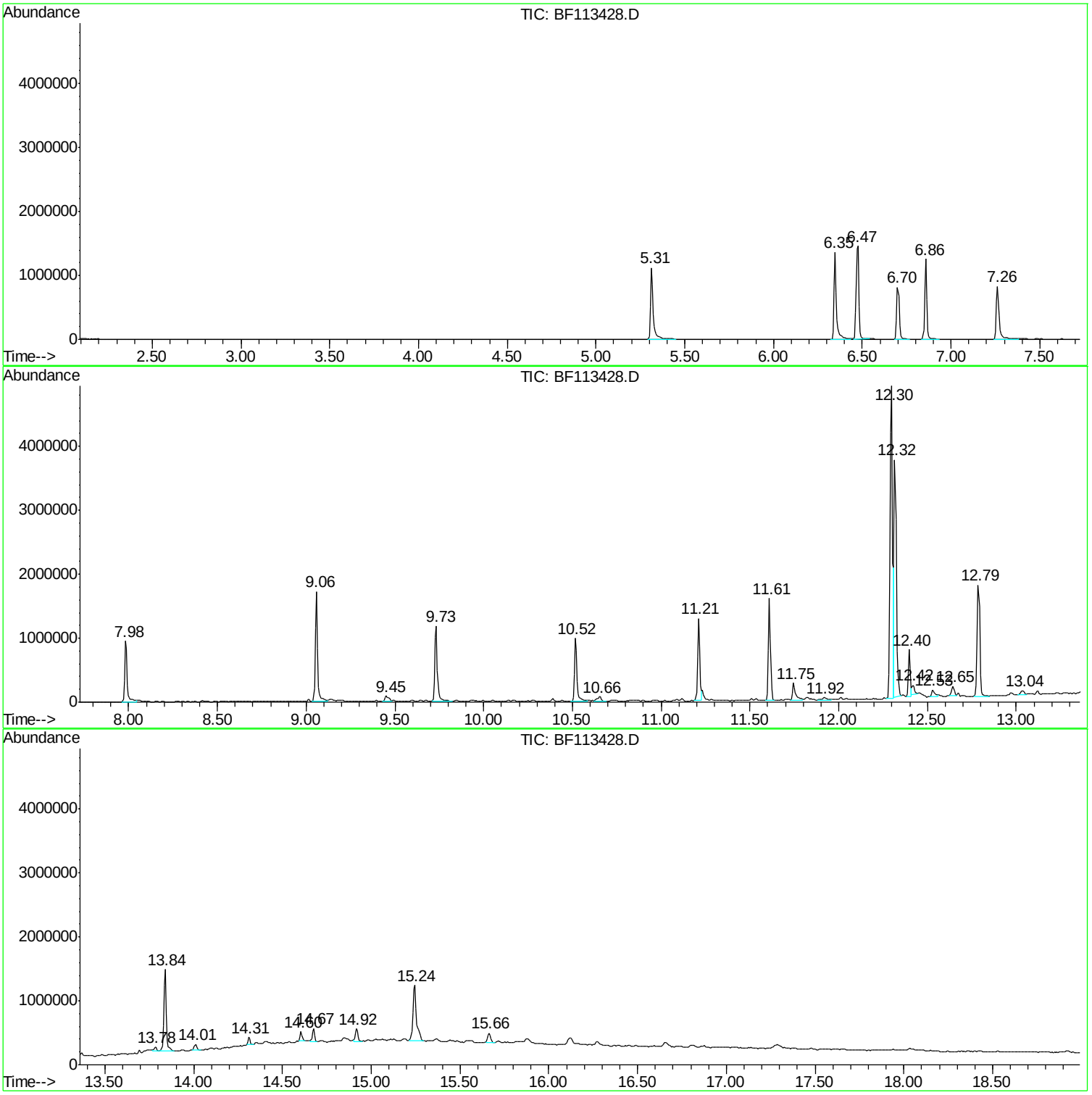
Sum of corrected areas: 29091637

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
Data File : BF113428.D
Acq On : 29 Mar 2019 22:18
Operator : JU/SJ
Sample : K1685-13 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-06-032819-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
Data File : BF113428.D
Acq On : 29 Mar 2019 22:18
Operator : JU/SJ
Sample : K1685-13 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-032819-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.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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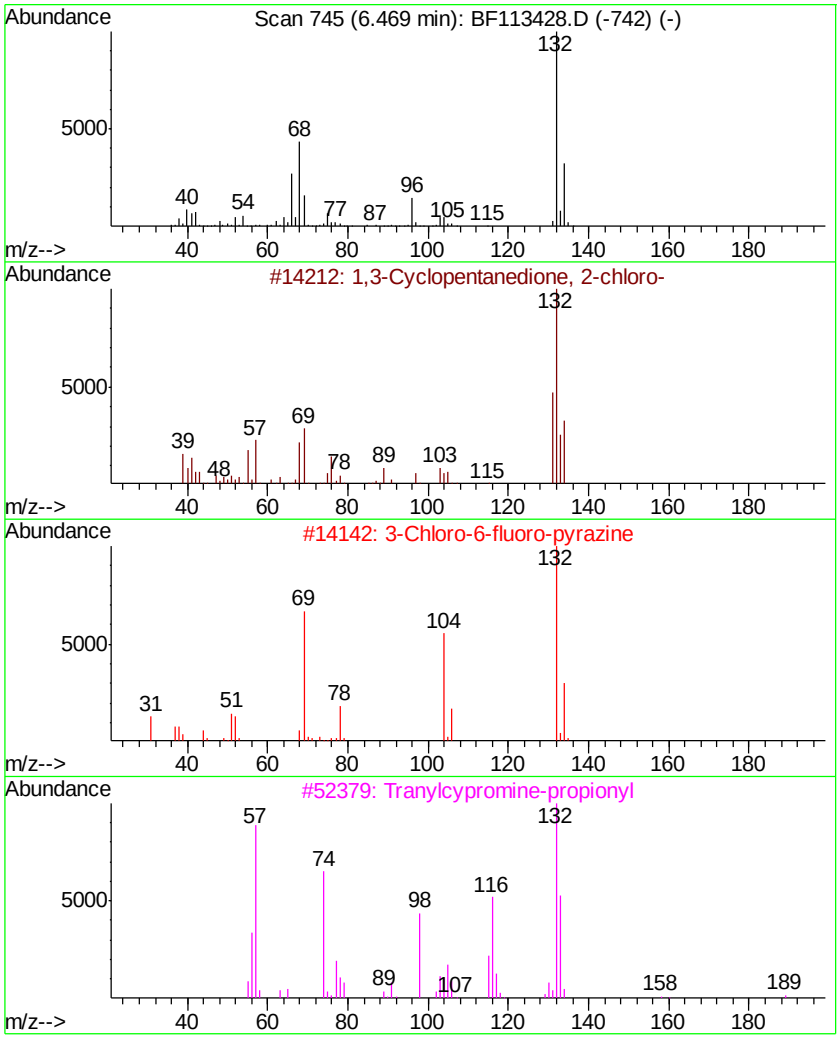
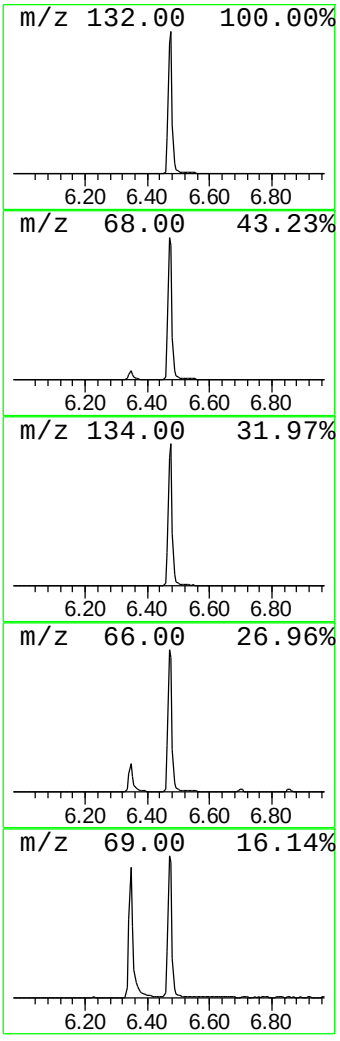
Peak Number 1 unknown6.47 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	37.74 ng	1414820	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	43
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
Data File : BF113428.D
Acq On : 29 Mar 2019 22:18
Operator : JU/SJ
Sample : K1685-13 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-032819-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

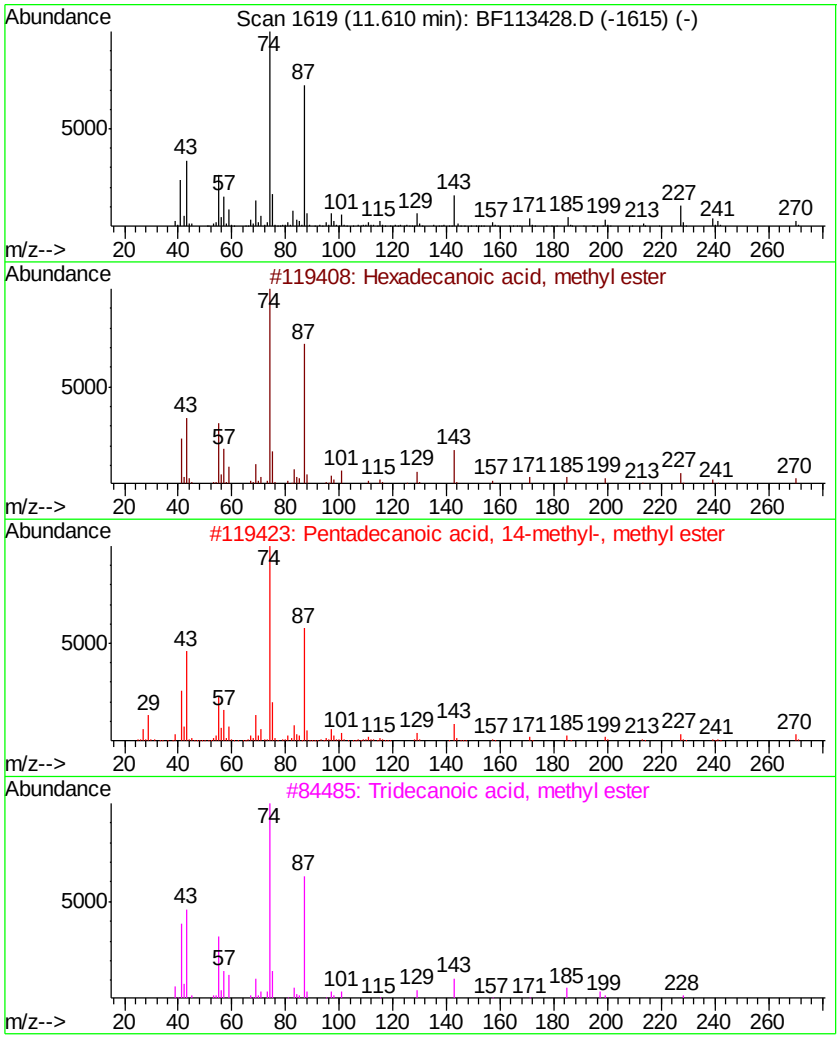
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

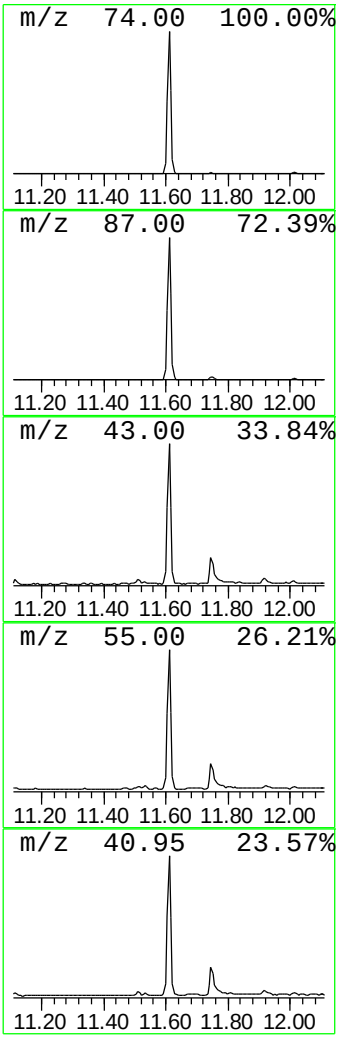
****

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.61	22.16 ng	1301330	Phenanthrene-d10	11.21

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	97
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
Data File : BF113428.D
Acq On : 29 Mar 2019 22:18
Operator : JU/SJ
Sample : K1685-13 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-032819-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

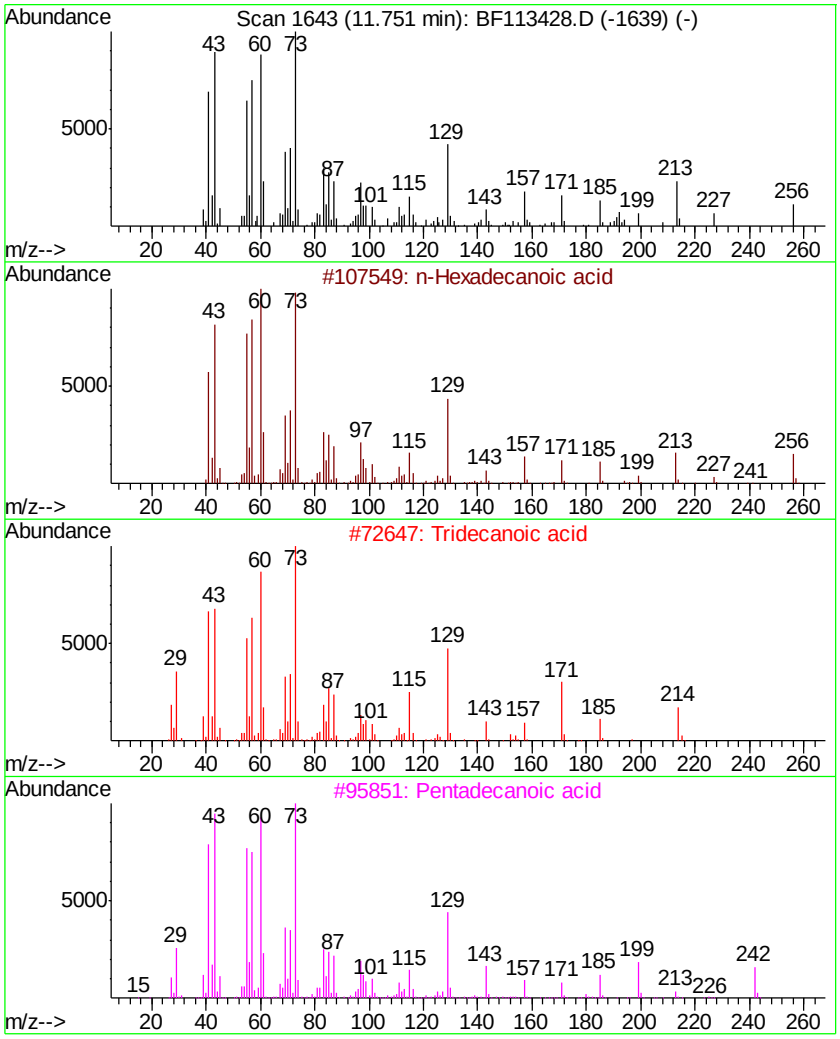
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

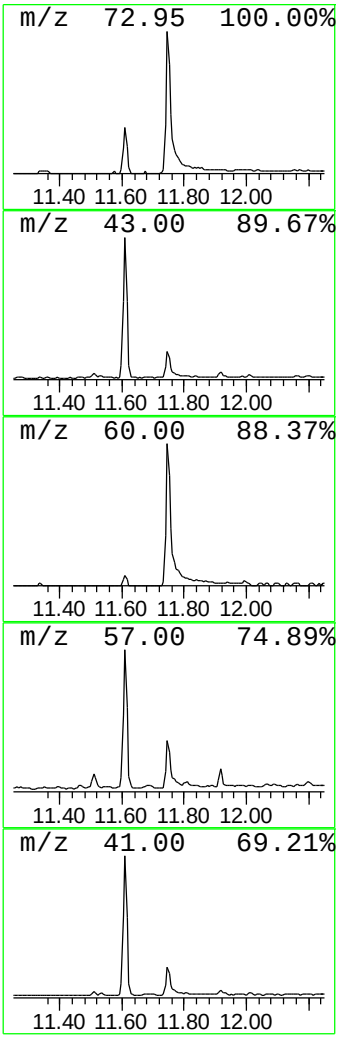
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	5.34 ng	313814	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	15





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
Data File : BF113428.D
Acq On : 29 Mar 2019 22:18
Operator : JU/SJ
Sample : K1685-13 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-032819-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

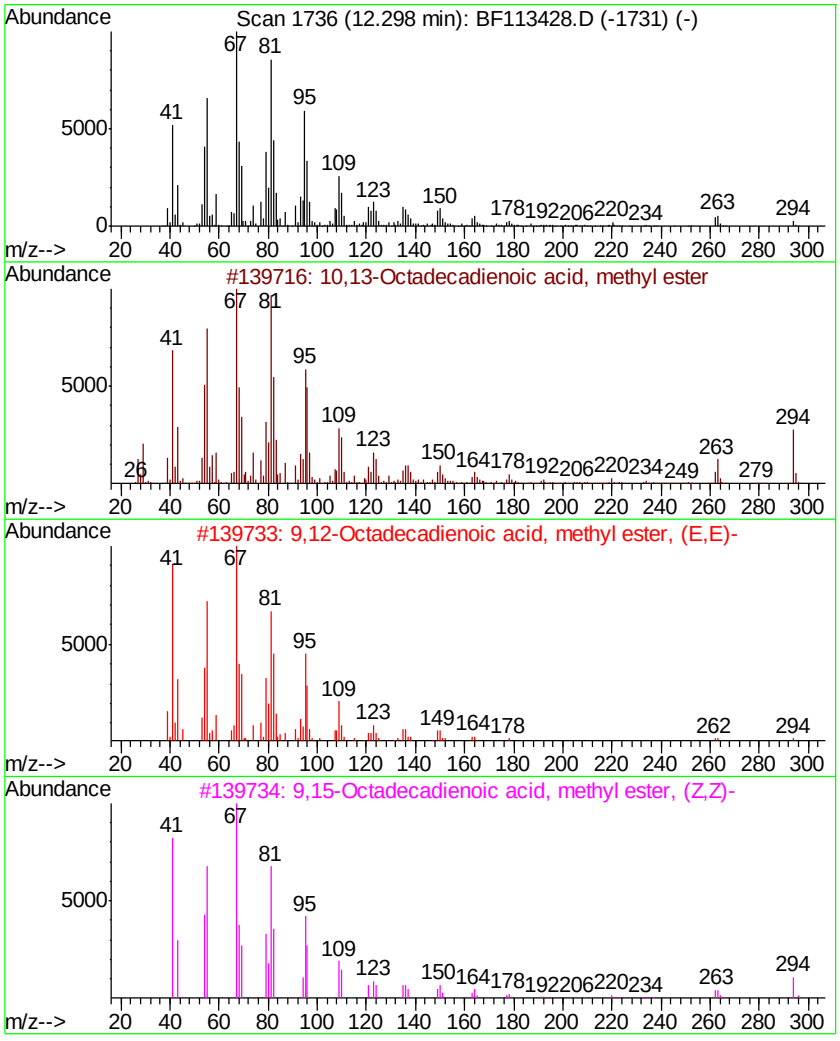
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

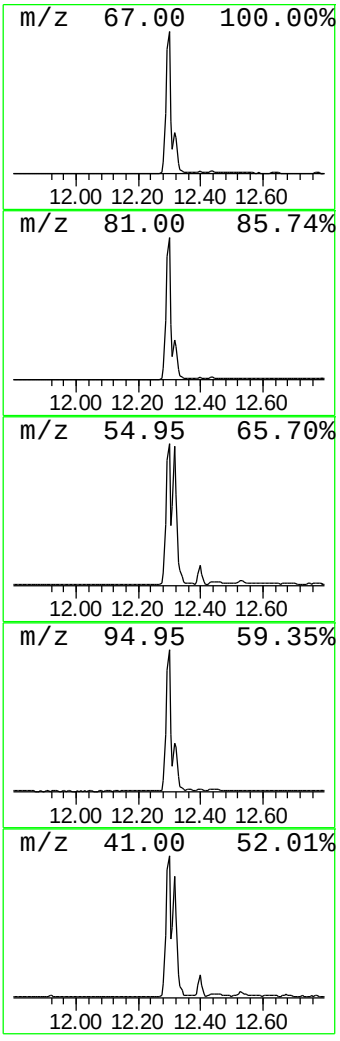
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	93.65 ng	5498960	Phenanthrene-d10	11.21

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	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
Data File : BF113428.D
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Sample : K1685-13 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-032819-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

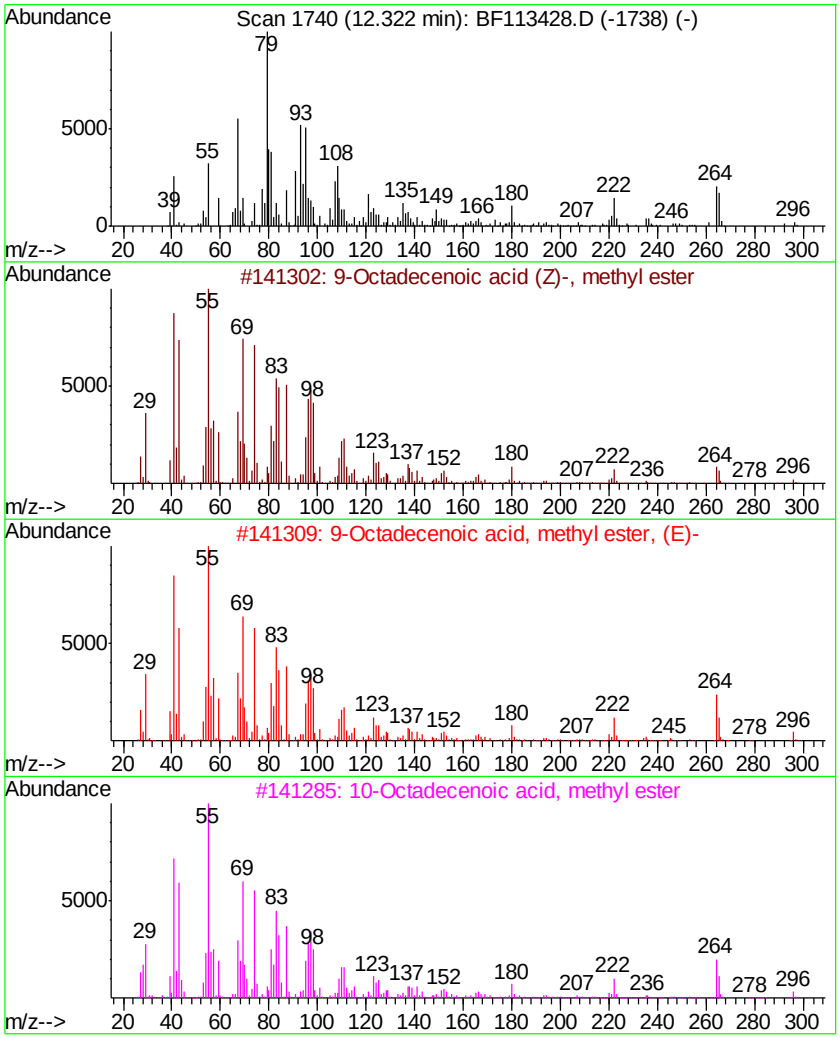
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

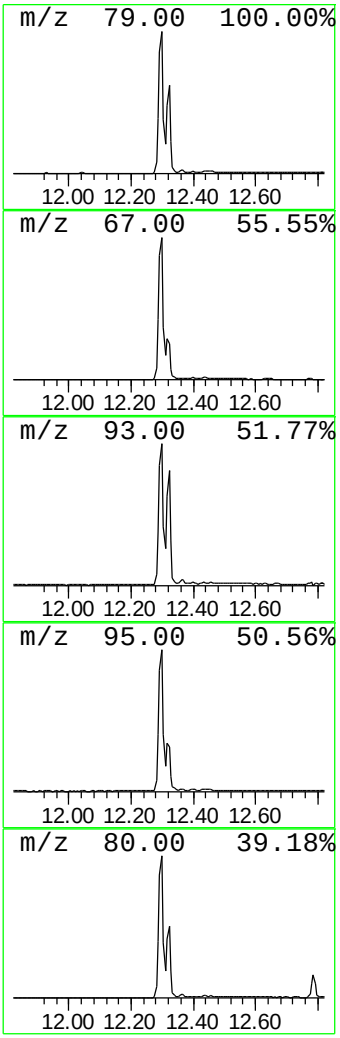
****

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	46.46 ng	2728080	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
5	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	99





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
Data File : BF113428.D
Acq On : 29 Mar 2019 22:18
Operator : JU/SJ
Sample : K1685-13 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-032819-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

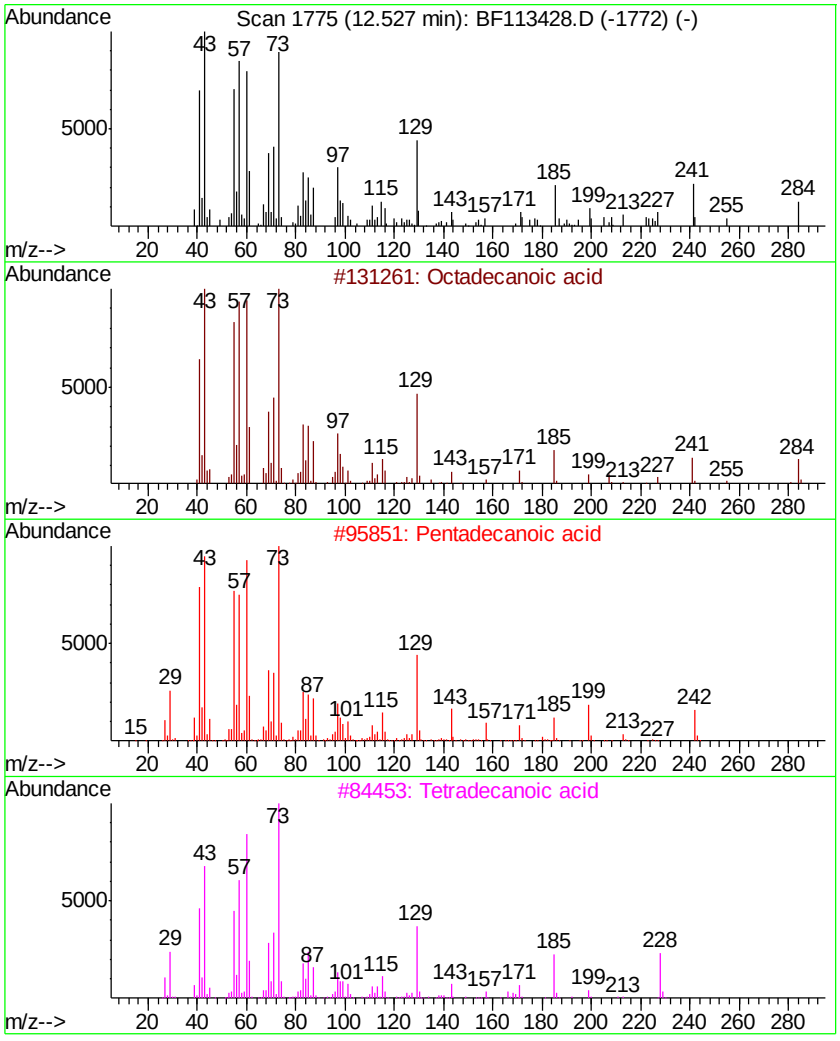
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

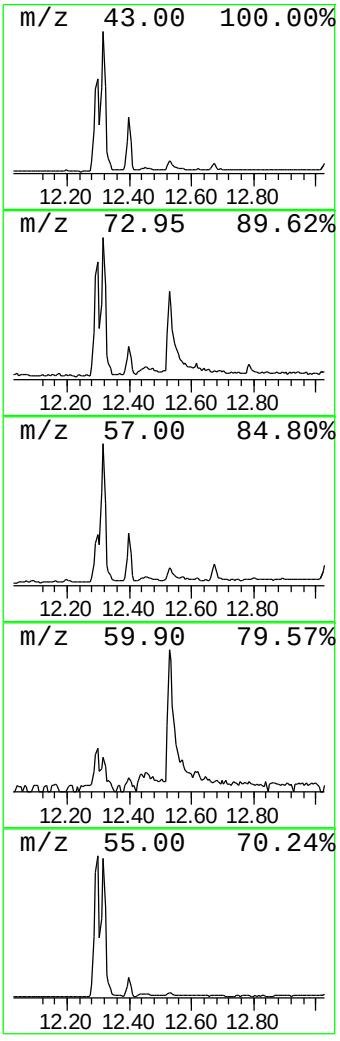
****

Peak Number 7 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.53	2.16 ng	139226	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Tridecanoic acid	214	C13H26O2	000638-53-9	59





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Data File : BF113428.D
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-032819-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

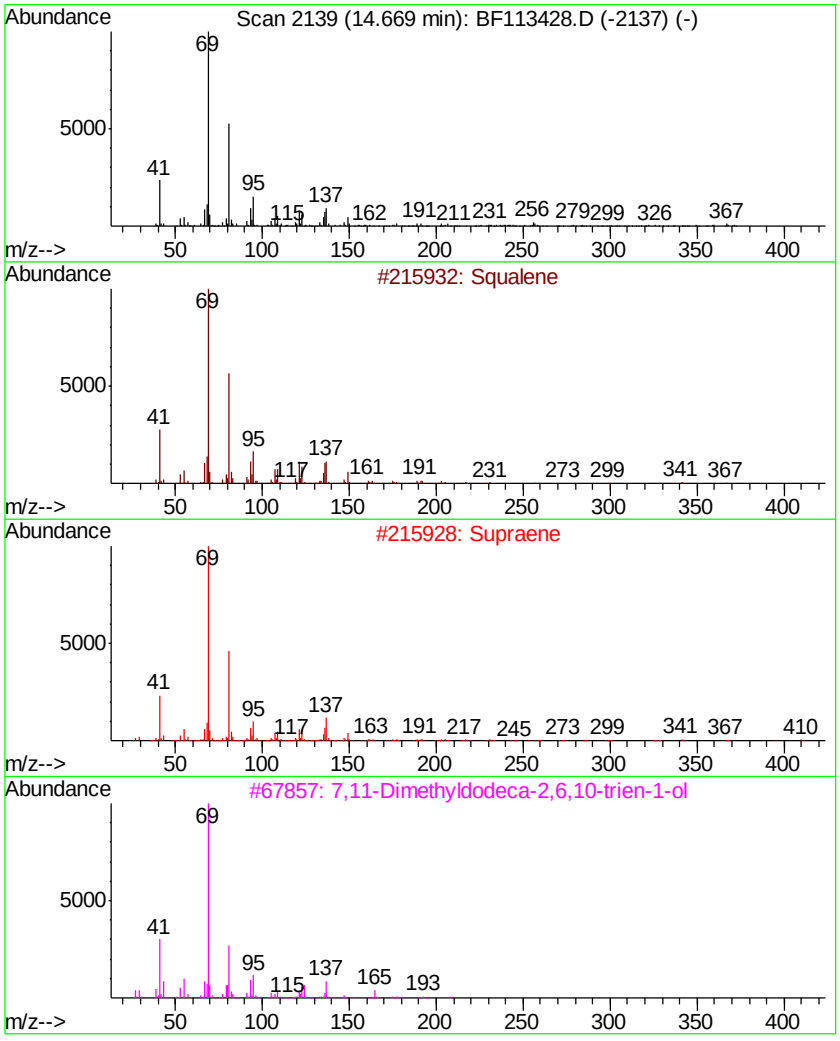
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

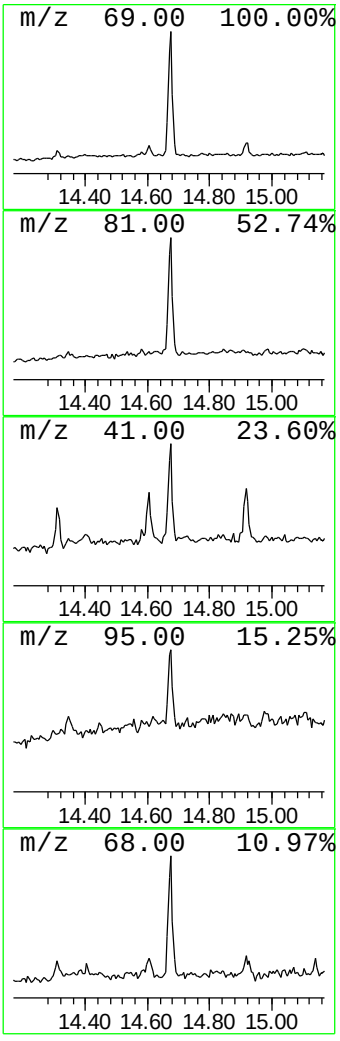
****

Peak Number 8 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	2.91 ng	185986	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	68
4	2,6,10-Dodecatrienoic acid, 3,7,...	250	C16H26O2	004176-79-8	59
5	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	50





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Data File : BF113428.D
Acq On : 29 Mar 2019 22:18
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Sample : K1685-13 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-032819-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

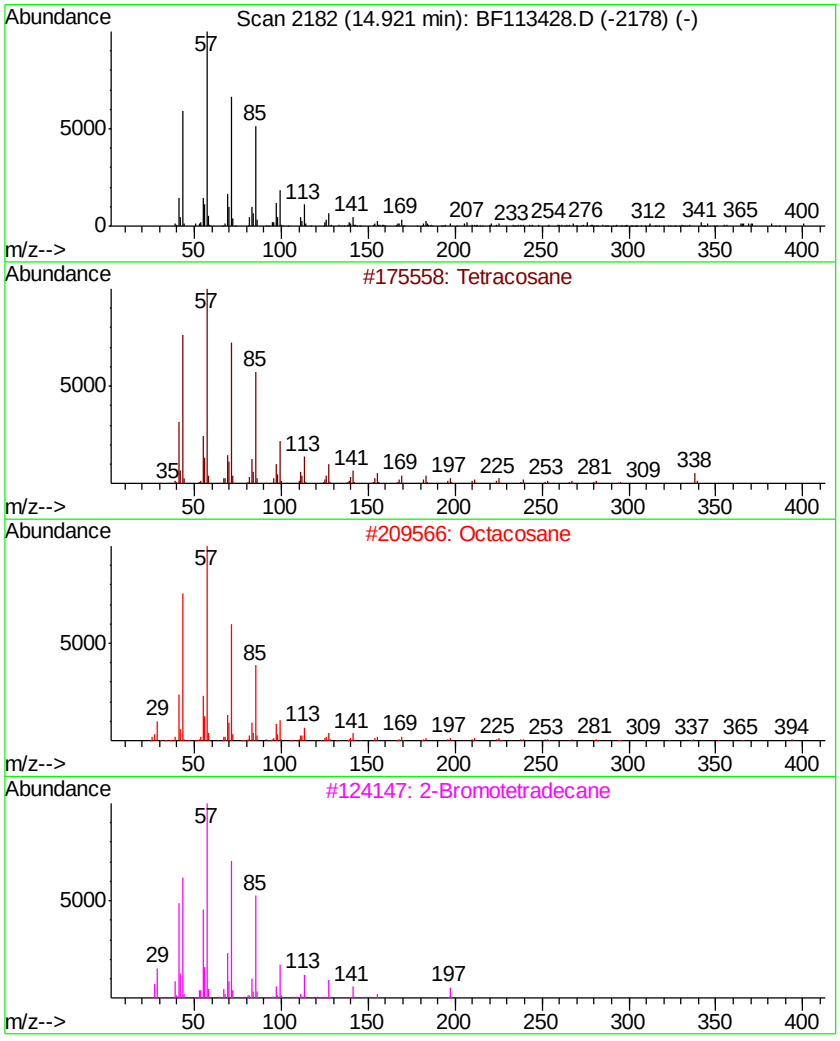
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

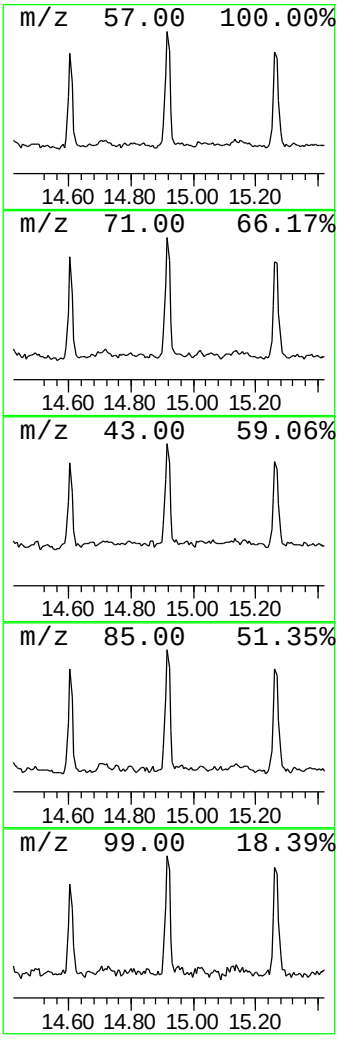
****

Peak Number 9 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	3.42 ng	217986	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	95
2	Octacosane	394	C28H58	000630-02-4	87
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	86
4	Hexacosane	366	C26H54	000630-01-3	86
5	Nonadecane	268	C19H40	000629-92-5	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
Data File : BF113428.D
Acq On : 29 Mar 2019 22:18
Operator : JU/SJ
Sample : K1685-13 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-032819-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.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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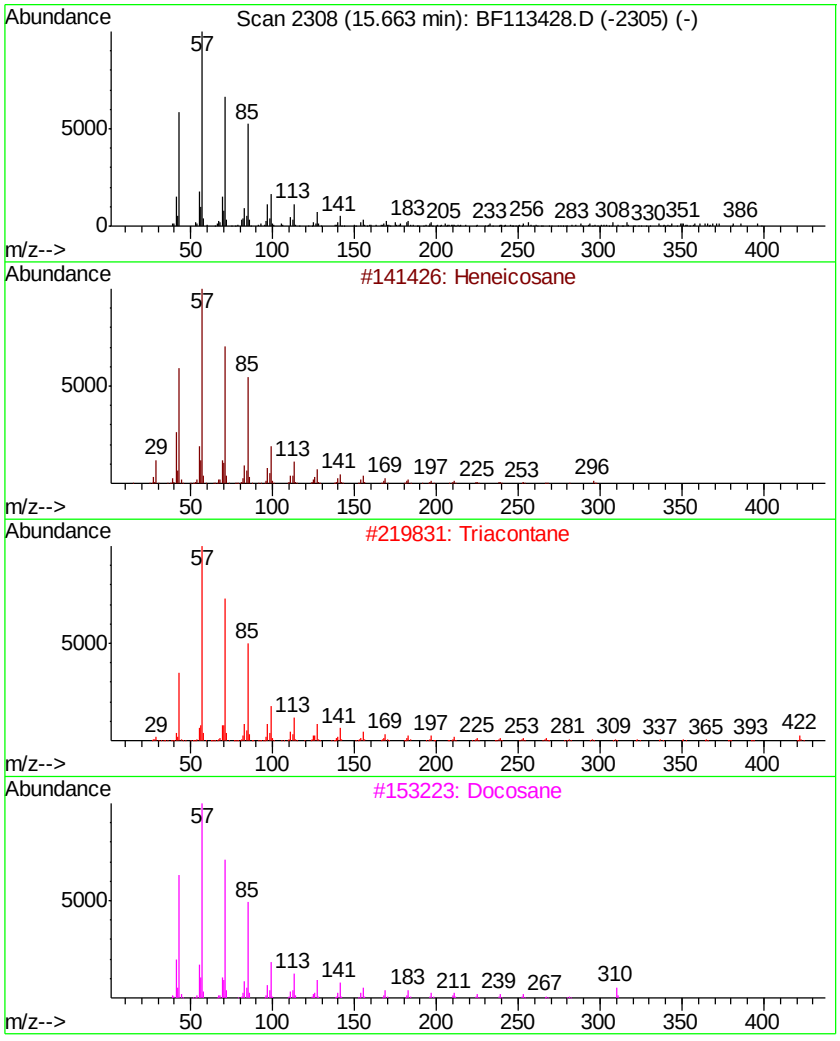
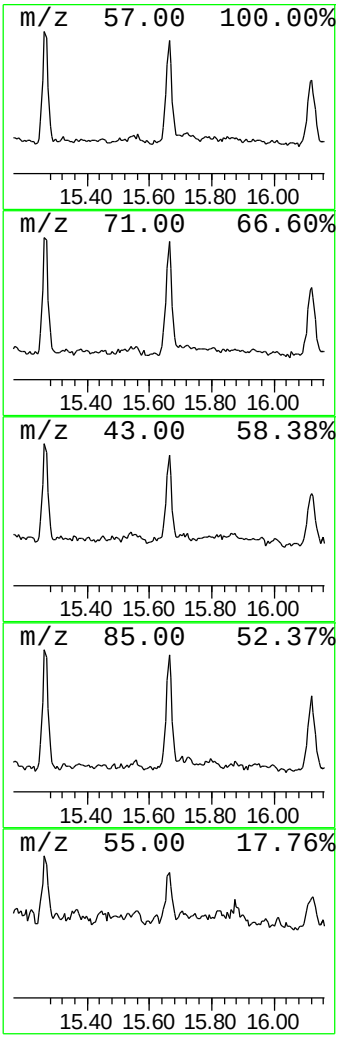
Peak Number 10 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	2.79 ng	177774	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Triacontane	422	C30H62	000638-68-6	86
3	Docosane	310	C22H46	000629-97-0	86
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	83
5	Nonadecane	268	C19H40	000629-92-5	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032919\
Data File : BF113428.D
Acq On : 29 Mar 2019 22:18
Operator : JU/SJ
Sample : K1685-13 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-032819-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.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
unknown6.47	6.47	37.7	ng	1414820	1	6.70	749861	20.0
Hexadecanoic acid...	11.61	22.2	ng	1301330	4	11.21	1174410	20.0
n-Hexadecanoic acid	11.75	5.3	ng	313814	4	11.21	1174410	20.0
10,13-Octadecadie...	12.30	93.7	ng	5498960	4	11.21	1174410	20.0
9-Octadecenoic ac...	12.32	46.5	ng	2728080	4	11.21	1174410	20.0
Octadecanoic acid	12.53	2.2	ng	139226	5	13.84	1287570	20.0
Squalene	14.67	2.9	ng	185986	6	15.24	1276200	20.0
Tetracosane	14.92	3.4	ng	217986	6	15.24	1276200	20.0
Heneicosane	15.66	2.8	ng	177774	6	15.24	1276200	20.0