LSC Area Percent Report

Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_F\DATA\BF062919\
Data File : BF115314.D
Acq On : 29 Jun 2019 11:19
Operator : HP/JU
Sample : K3555-22
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-14

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-BF062119.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	4.425	418	423	429	rVB	102978	121098	2.35%	0.252%
2	5.195	549	554	557	rBV	3749508	3667155	71.16%	7.633%
3	6.237	726	731	734	rBV	3689238	3857884	74.86%	8.030%
4	6.260	734	735	748	rVB	112337	105577	2.05%	0.220%
5	6.366	748	753	756	rBV	4362910	4028192	78.16%	8.385%
6	6.595	789	792	796	rBV	1587310	1327613	25.76%	2.763%
7	6.754	815	819	822	rBV	3858950	3177428	61.66%	6.614%
8	7.160	882	888	891	rBV	2468122	2522512	48.95%	5.251%
9	7.878	1006	1010	1014	rBV	2052055	1751255	33.98%	3.645%
10	8.954	1188	1193	1196	rBV	5210476	4627254	89.79%	9.632%
11	9.348	1256	1260	1269	rVB	534645	430055	8.34%	0.895%
12	9.625	1302	1307	1310	rBV	2371522	2104669	40.84%	4.381%
13	10.407	1434	1440	1443	rBV	2970893	3060788	59.39%	6.371%
14	11.095	1553	1557	1560	rBV	2806399	2289540	44.43%	4.766%
15	11.642	1645	1650	1671	rBV	588254	852425	16.54%	1.774%
16	12.348	1764	1770	1775	rBV7	26529	59984	1.16%	0.125%
17	12.424	1778	1783	1796	rVV	792295	1191433	23.12%	2.480%
18	12.677	1821	1826	1830	rBV	5178573	5153453	100.00%	10.727%
19	13.177	1908	1911	1914	rVB2	76724	73138	1.42%	0.152%
20	13.683	1989	1997	1998	rBV3	105579	211483	4.10%	0.440%
21	13.713	1998	2002	2015	rVB	2711435	2634451	51.12%	5.484%
22	13.913	2032	2036	2040	rBV	76261	75627	1.47%	0.157%
23	14.218	2084	2088	2091	rBV	145796	131355	2.55%	0.273%
24	14.513	2134	2138	2143	rBV	257438	236114	4.58%	0.491%
25	14.577	2145	2149	2153	rBV	136082	121706	2.36%	0.253%
26	14.812	2184	2189	2194	rBV	298213	328642	6.38%	0.684%
27	15.077	2229	2234	2240	rVV	2183801	2500745	48.53%	5.205%
28	15.142	2241	2245	2252	rVB	349022	427020	8.29%	0.889%
29	15.524	2304	2310	2316	rBV	290140	427704	8.30%	0.890%
30	15.959	2378	2384	2390	rBV	192617	338790	6.57%	0.705%
31	16.471	2465	2471	2477	rBV2	66460	132601	2.57%	0.276%
32	17.071	2569	2573	2584	rVB2	38990	74687	1.45%	0.155%

LSC Area Percent Report

Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_F\DATA\BF062919\
Data File : BF115314.D
Acq On : 29 Jun 2019 11:19
Operator : HP/JU
Sample : K3555-22
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-14

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-BF062119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

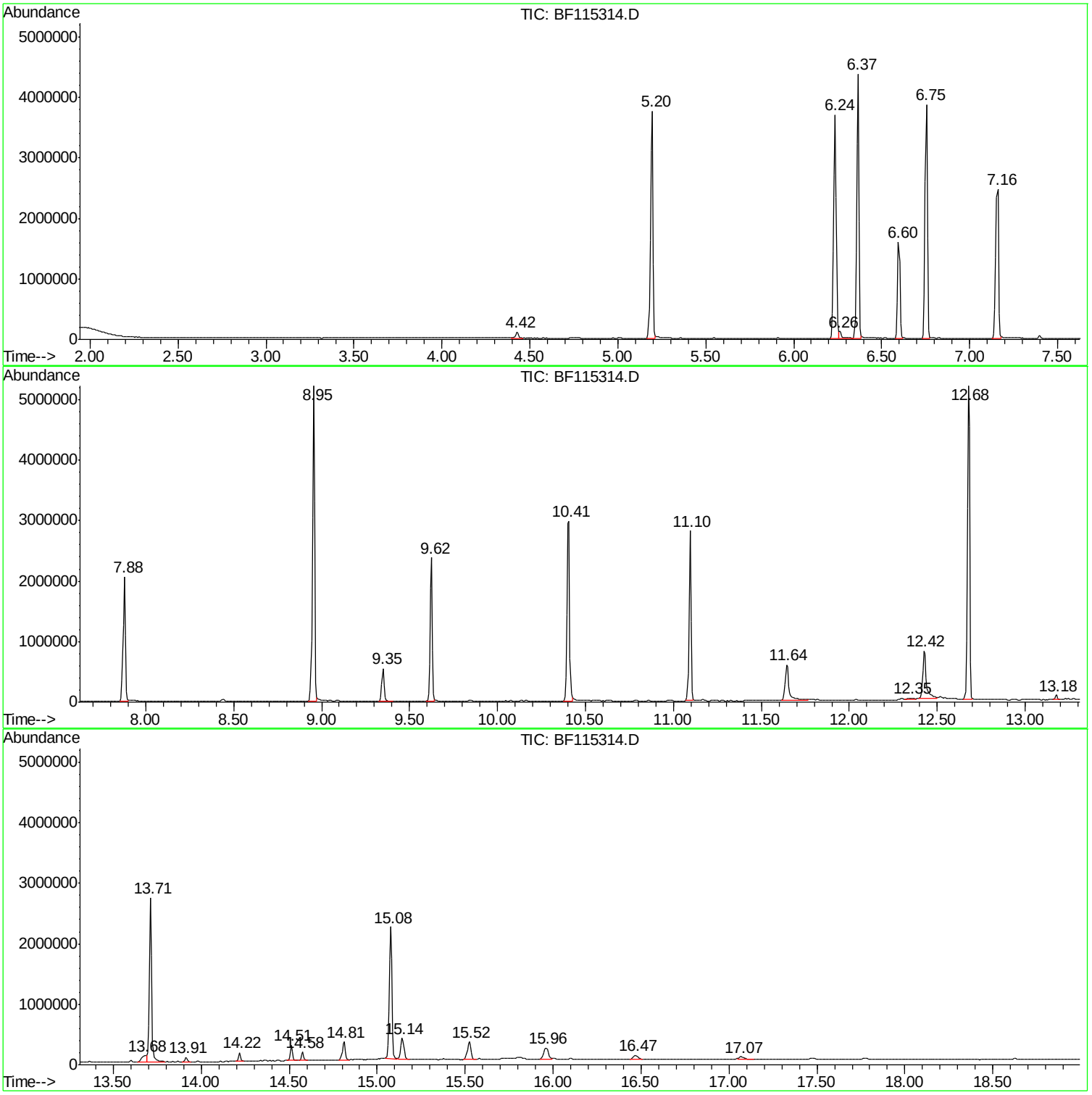
Sum of corrected areas: 48042378

Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_F\DATA\BF062919\
Data File : BF115314.D
Acq On : 29 Jun 2019 11:19
Operator : HP/JU
Sample : K3555-22
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062119.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

Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_F\DATA\BF062919\
Data File : BF115314.D
Acq On : 29 Jun 2019 11:19
Operator : HP/JU
Sample : K3555-22
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062119.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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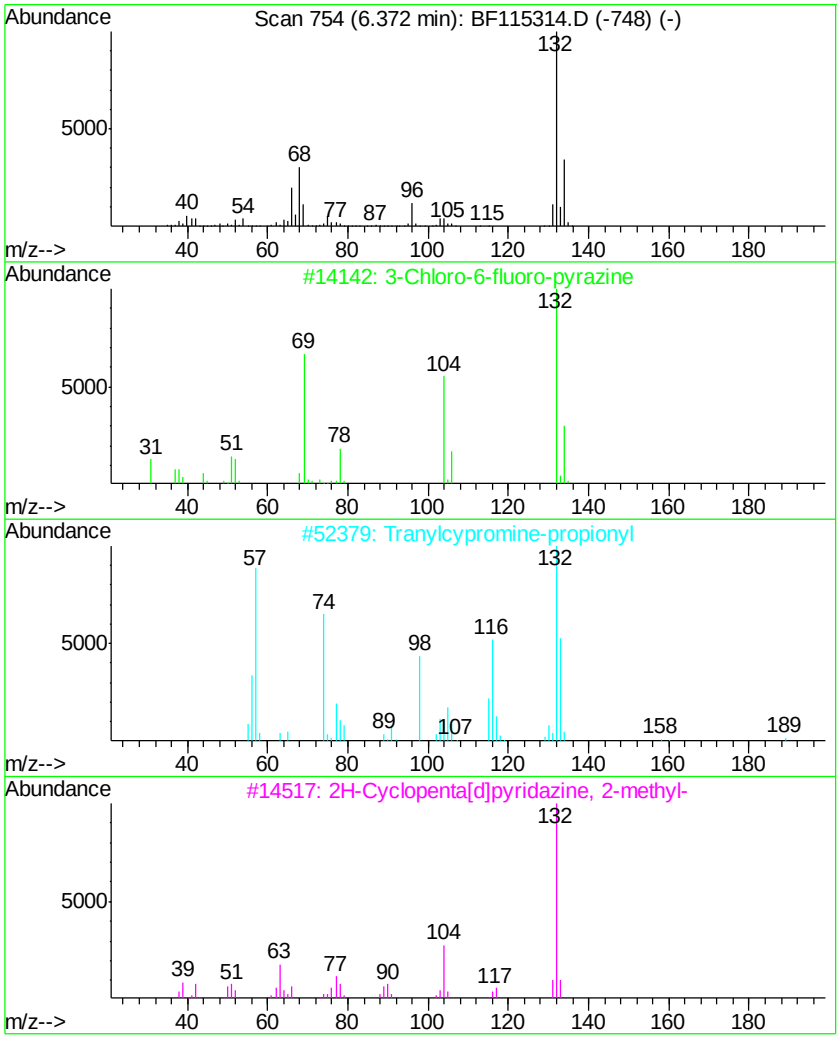
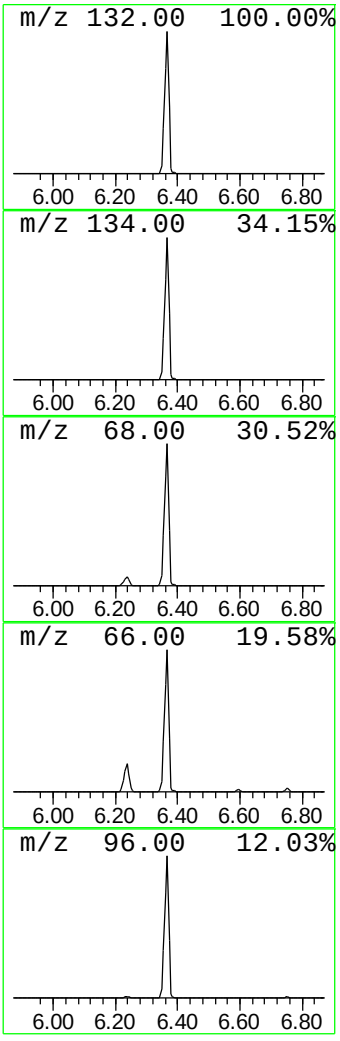
Peak Number 1 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	60.68 ng	4028190	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9





Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_F\DATA\BF062919\
Data File : BF115314.D
Acq On : 29 Jun 2019 11:19
Operator : HP/JU
Sample : K3555-22
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062119.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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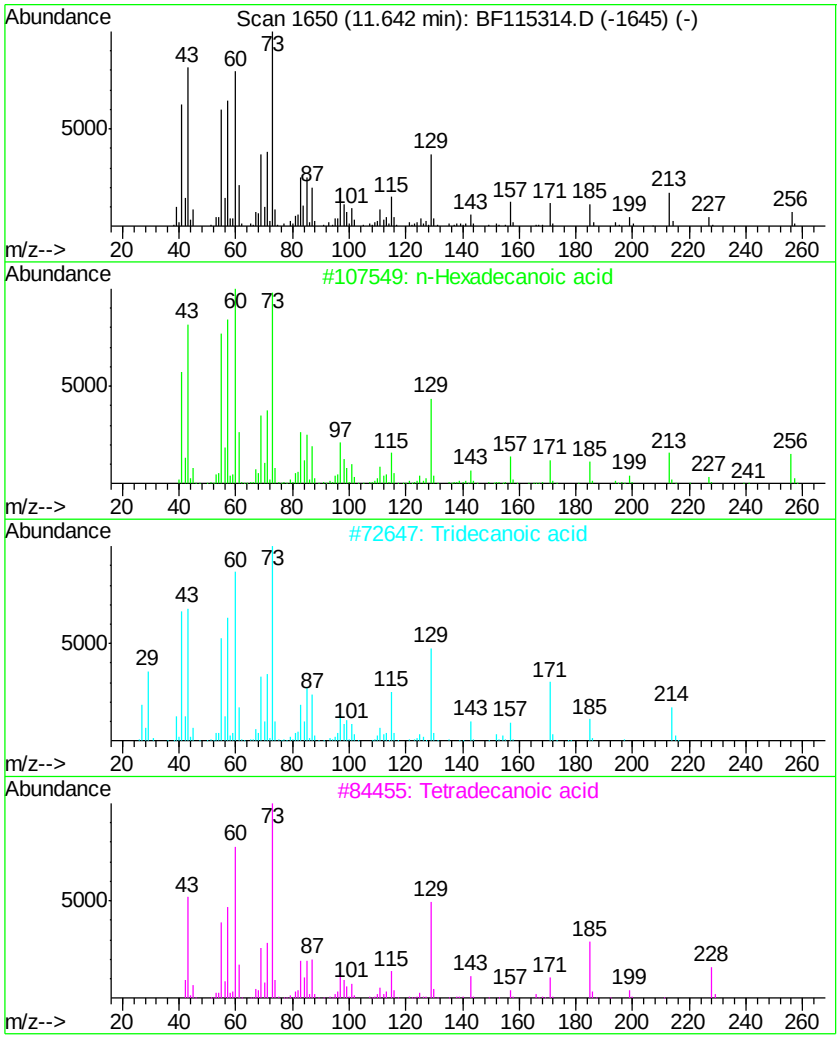
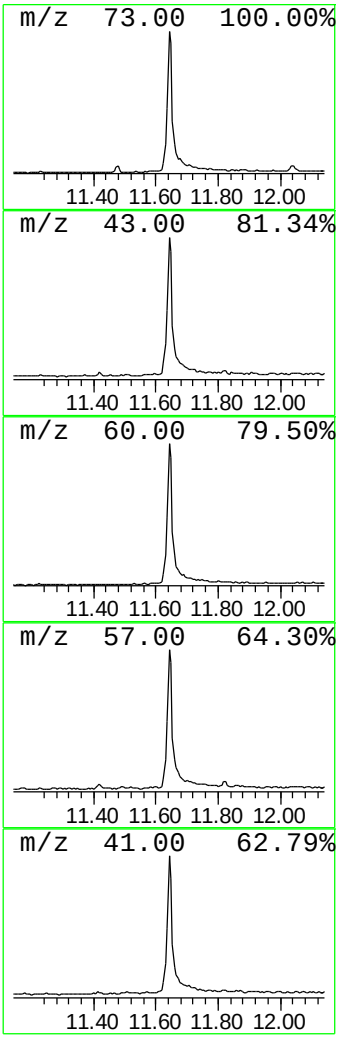
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.64	7.45 ng	852425	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_F\DATA\BF062919\
Data File : BF115314.D
Acq On : 29 Jun 2019 11:19
Operator : HP/JU
Sample : K3555-22
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062119.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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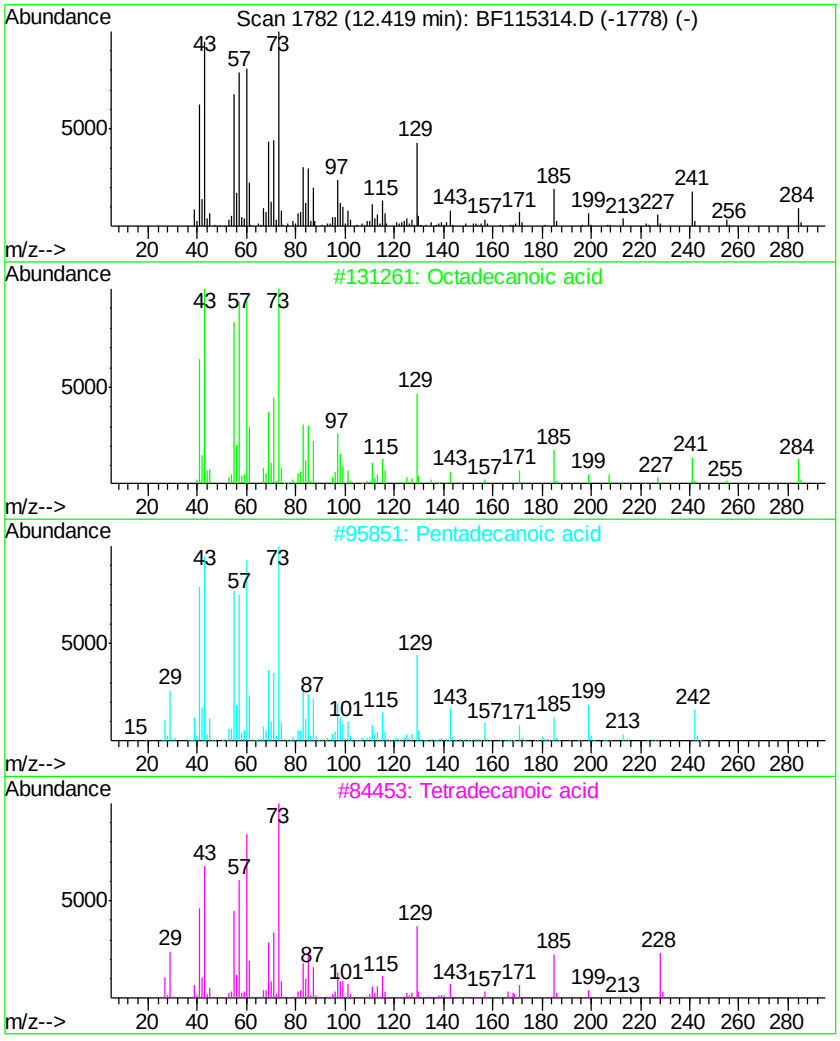
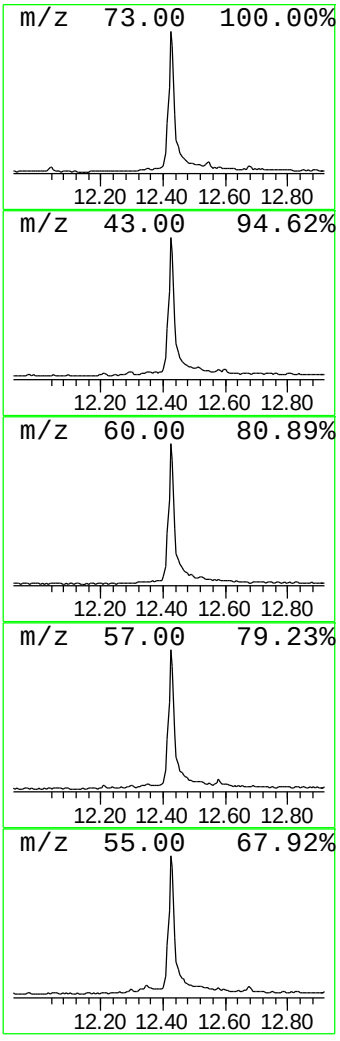
Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	9.05 ng	1191430	Chrysene-d12	13.71

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	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Library Search Compound Report

Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_F\DATA\BF062919\
Data File : BF115314.D
Acq On : 29 Jun 2019 11:19
Operator : HP/JU
Sample : K3555-22
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

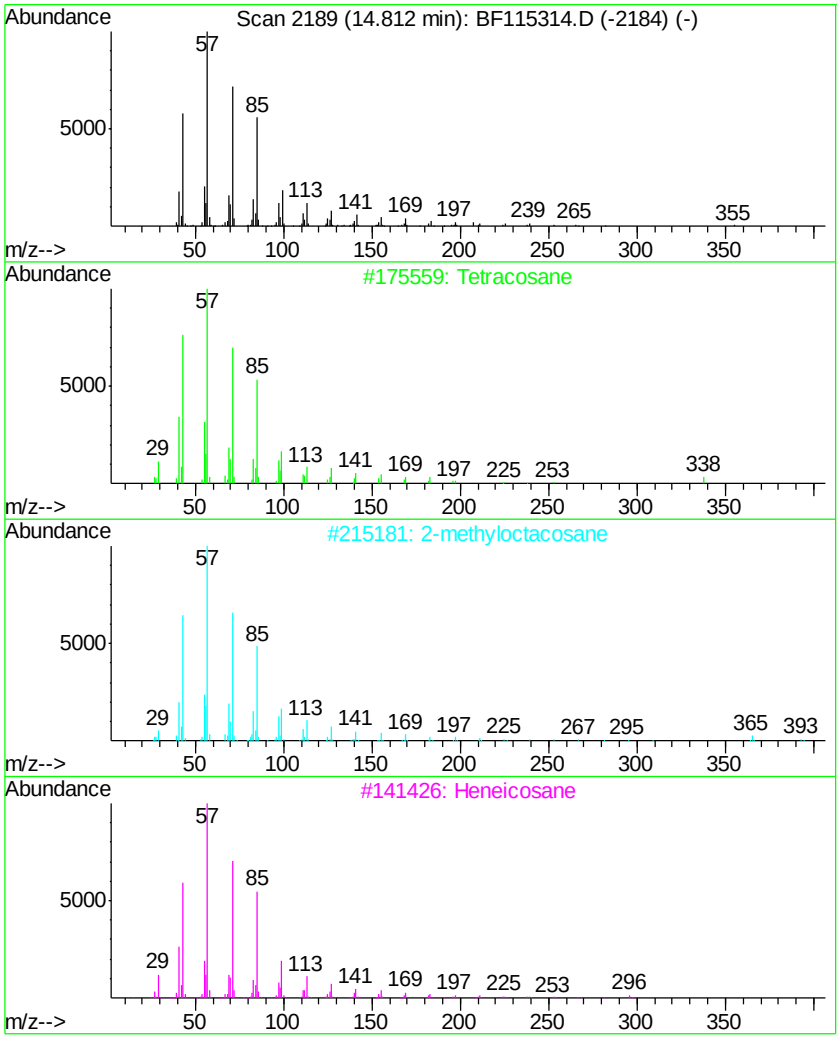
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

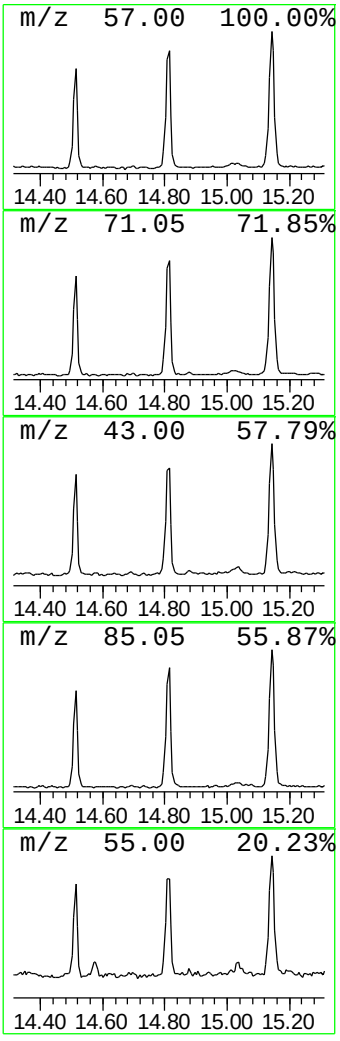
****

Peak Number 5 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	2.63 ng	328642	Perylene-d12	15.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Hexacosane	366	C26H54	000630-01-3	90





Library Search Compound Report

Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_F\DATA\BF062919\
Data File : BF115314.D
Acq On : 29 Jun 2019 11:19
Operator : HP/JU
Sample : K3555-22
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062119.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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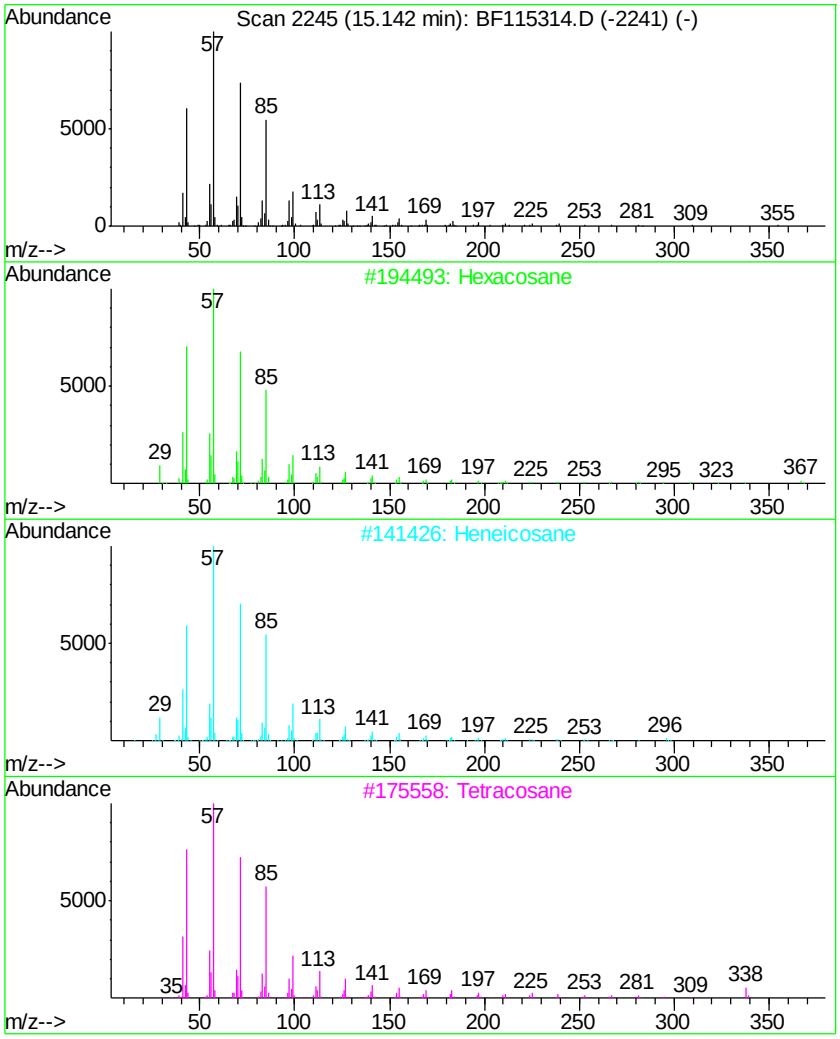
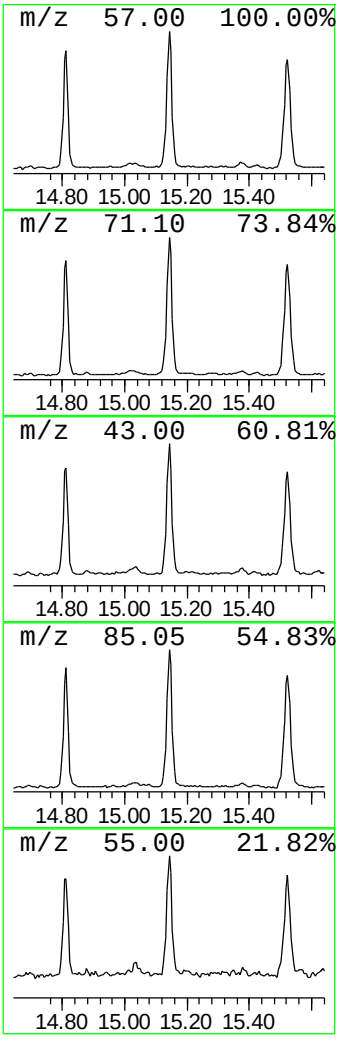
Peak Number 6 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	3.42 ng	427020	Perylene-d12	15.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Docosane	310	C22H46	000629-97-0	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_F\DATA\BF062919\
Data File : BF115314.D
Acq On : 29 Jun 2019 11:19
Operator : HP/JU
Sample : K3555-22
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062119.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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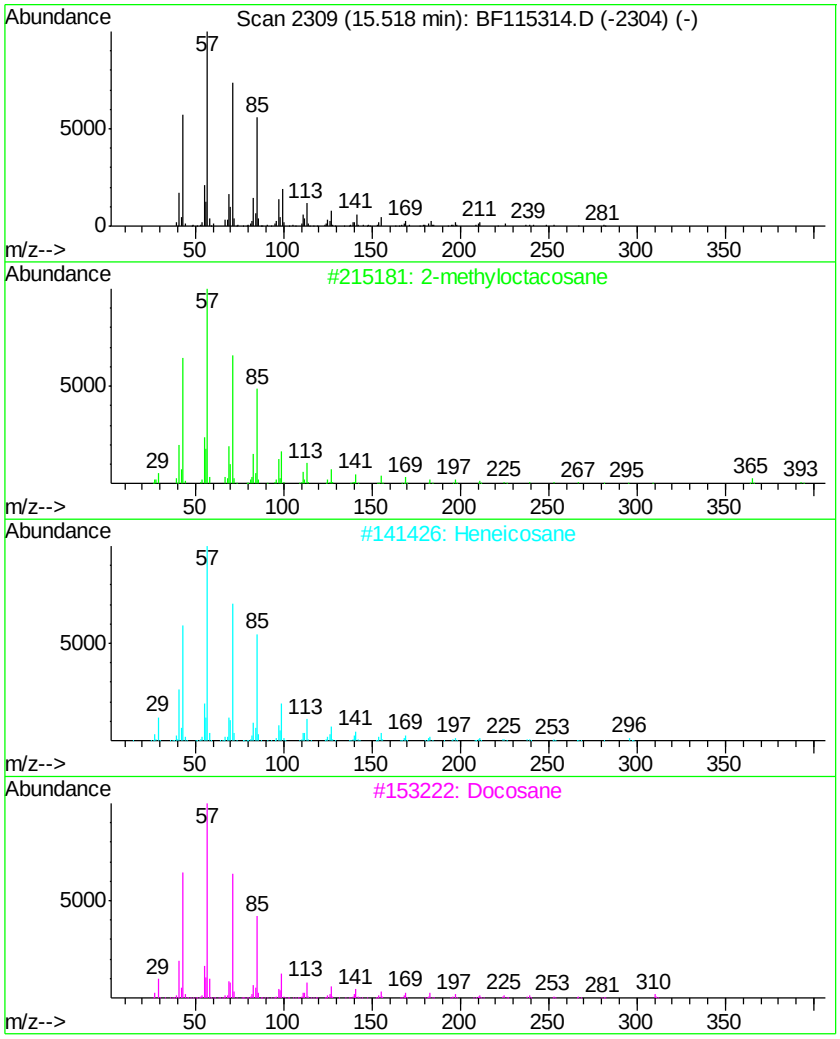
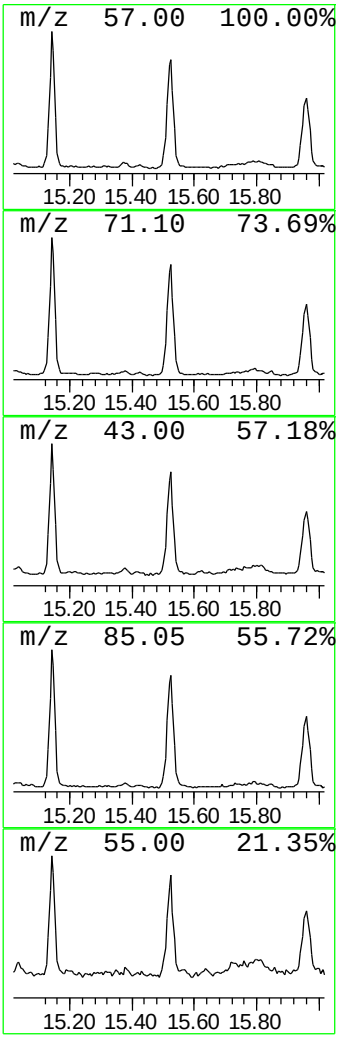
Peak Number 7 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.52	3.42 ng	427704	Perylene-d12	15.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Docosane	310	C22H46	000629-97-0	91
4	Heptadecane	240	C17H36	000629-78-7	91
5	Hexacosane	366	C26H54	000630-01-3	90





Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_F\DATA\BF062919\
Data File : BF115314.D
Acq On : 29 Jun 2019 11:19
Operator : HP/JU
Sample : K3555-22
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062119.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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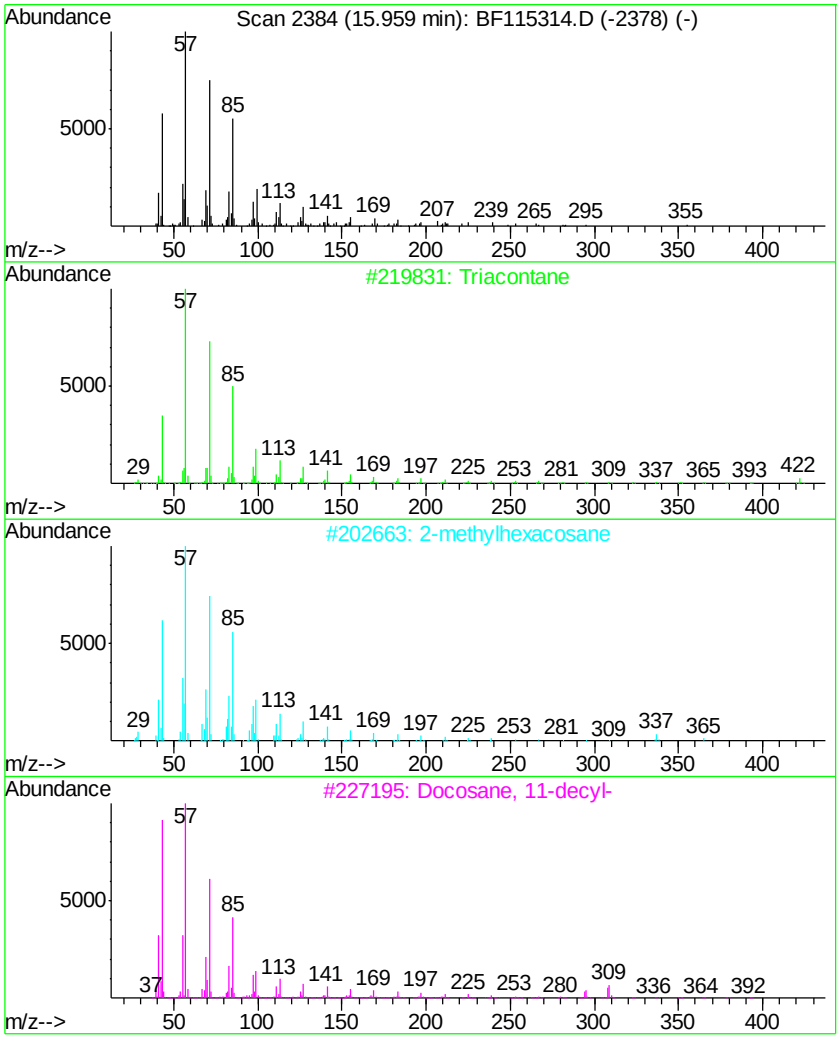
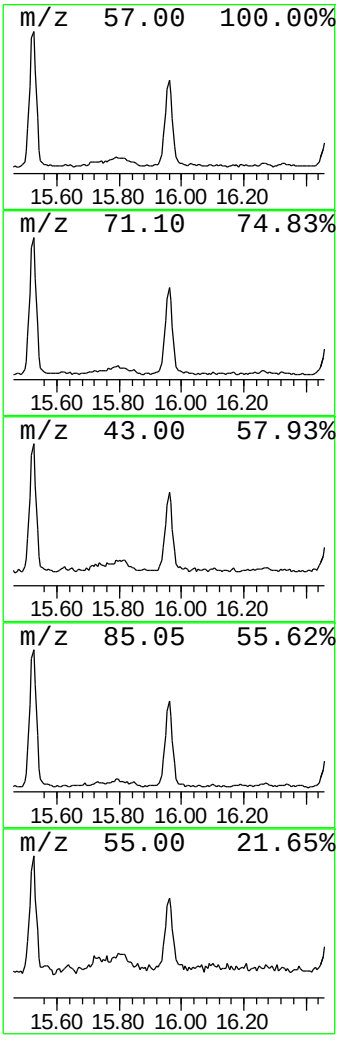
Peak Number 8 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	2.71 ng	338790	Perylene-d12	15.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	2-methylhexacosane	380	C27H56	1000376-72-7	91
3	Docosane, 11-decyl-	451	C32H66	055401-55-3	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heneicosane	296	C21H44	000629-94-7	91





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\TERASTORAGE\SVOASRV\HPCHEM1\BNA_F\DATA\BF062919\
Data File : BF115314.D
Acq On : 29 Jun 2019 11:19
Operator : HP/JU
Sample : K3555-22
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062119.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
unknown6.37	6.37	60.7	ng	4028190	1	6.60	1327610	20.0
n-Hexadecanoic acid	11.64	7.5	ng	852425	4	11.10	2289540	20.0
Octadecanoic acid	12.42	9.1	ng	1191430	5	13.71	2634450	20.0
Tetracosane	14.81	2.6	ng	328642	6	15.08	2500750	20.0
Hexacosane	15.14	3.4	ng	427020	6	15.08	2500750	20.0
2-methyloctacosane	15.52	3.4	ng	427704	6	15.08	2500750	20.0
Triacontane	15.96	2.7	ng	338790	6	15.08	2500750	20.0