LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112960.D
Acq On : 11 Mar 2019 17:47
Operator : JU/SJ
Sample : K1785-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SD2-0.0-0.5

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-BF022719.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	5.334	548	552	563	rBV	2462646	2295620	93.59%	8.073%
2	6.363	722	727	745	rBV	2642724	2452734	100.00%	8.625%
3	6.498	745	750	753	rBV	2607314	2429818	99.07%	8.545%
4	6.728	785	789	796	rBV	1010885	823384	33.57%	2.896%
5	6.887	812	816	819	rBV	1864302	1635525	66.68%	5.752%
6	7.287	880	884	896	rBV	1558336	1435685	58.53%	5.049%
7	8.010	1003	1007	1014	rBV	1024935	1016566	41.45%	3.575%
8	9.086	1186	1190	1205	rBV	2002351	1948515	79.44%	6.852%
9	9.428	1245	1248	1251	rBV2	33562	25880	1.06%	0.091%
10	9.480	1253	1257	1267	rVB	143474	145614	5.94%	0.512%
11	9.763	1301	1305	1317	rBV	1278296	1289965	52.59%	4.536%
12	10.545	1434	1438	1453	rBV	1836828	1879102	76.61%	6.608%
13	11.239	1552	1556	1563	rBV	1561937	1546088	63.04%	5.437%
14	11.292	1563	1565	1573	rVB5	27315	42680	1.74%	0.150%
15	11.616	1617	1620	1623	rBV	82344	73230	2.99%	0.258%
16	11.774	1643	1647	1657	rBV2	508873	620753	25.31%	2.183%
17	12.163	1710	1713	1719	rVB	142472	131084	5.34%	0.461%
18	12.445	1757	1761	1764	rBV	157829	152359	6.21%	0.536%
19	12.557	1777	1780	1791	rBV2	161333	209768	8.55%	0.738%
20	12.669	1793	1799	1803	rVB	144073	156154	6.37%	0.549%
21	12.816	1820	1824	1832	rVB	2460078	2162192	88.15%	7.604%
22	13.298	1904	1906	1911	rVB4	21509	27771	1.13%	0.098%
23	13.721	1974	1978	1986	rBV	398778	573600	23.39%	2.017%
24	13.863	1997	2002	2015	rVB	1732235	1872530	76.34%	6.585%
25	14.045	2029	2033	2038	rBV2	66234	80394	3.28%	0.283%
26	14.251	2065	2068	2071	rBV3	26991	37162	1.52%	0.131%
27	14.310	2076	2078	2081	rVV4	24633	31643	1.29%	0.111%
28	14.345	2081	2084	2090	rVB2	154597	181792	7.41%	0.639%
29	14.639	2131	2134	2138	rBV	131500	132284	5.39%	0.465%
30	14.774	2154	2157	2162	rVB5	31634	35286	1.44%	0.124%
31	14.868	2169	2173	2182	rBV	69320	139527	5.69%	0.491%
32	14.957	2184	2188	2192	rBV	205017	235930	9.62%	0.830%
33	15.145	2218	2220	2224	rBV	28952	34335	1.40%	0.121%
34	15.204	2227	2230	2235	rVB	50200	64890	2.65%	0.228%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112960.D
Acq On : 11 Mar 2019 17:47
Operator : JU/SJ
Sample : K1785-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SD2-0.0-0.5

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-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.268	2235	2241	2245	rBV	1113630	1411003	57.53%	4.962%
36	15.310	2245	2248	2255	rVB	157936	222430	9.07%	0.782%
37	15.715	2312	2317	2322	rBV	241233	341420	13.92%	1.201%
38	15.762	2322	2325	2333	rVV4	60288	135110	5.51%	0.475%
39	16.186	2392	2397	2402	rBV	88266	146091	5.96%	0.514%
40	16.727	2485	2489	2496	rVB2	71884	135720	5.53%	0.477%
41	16.804	2498	2502	2515	rVB2	45264	124794	5.09%	0.439%

Sum of corrected areas: 28436428

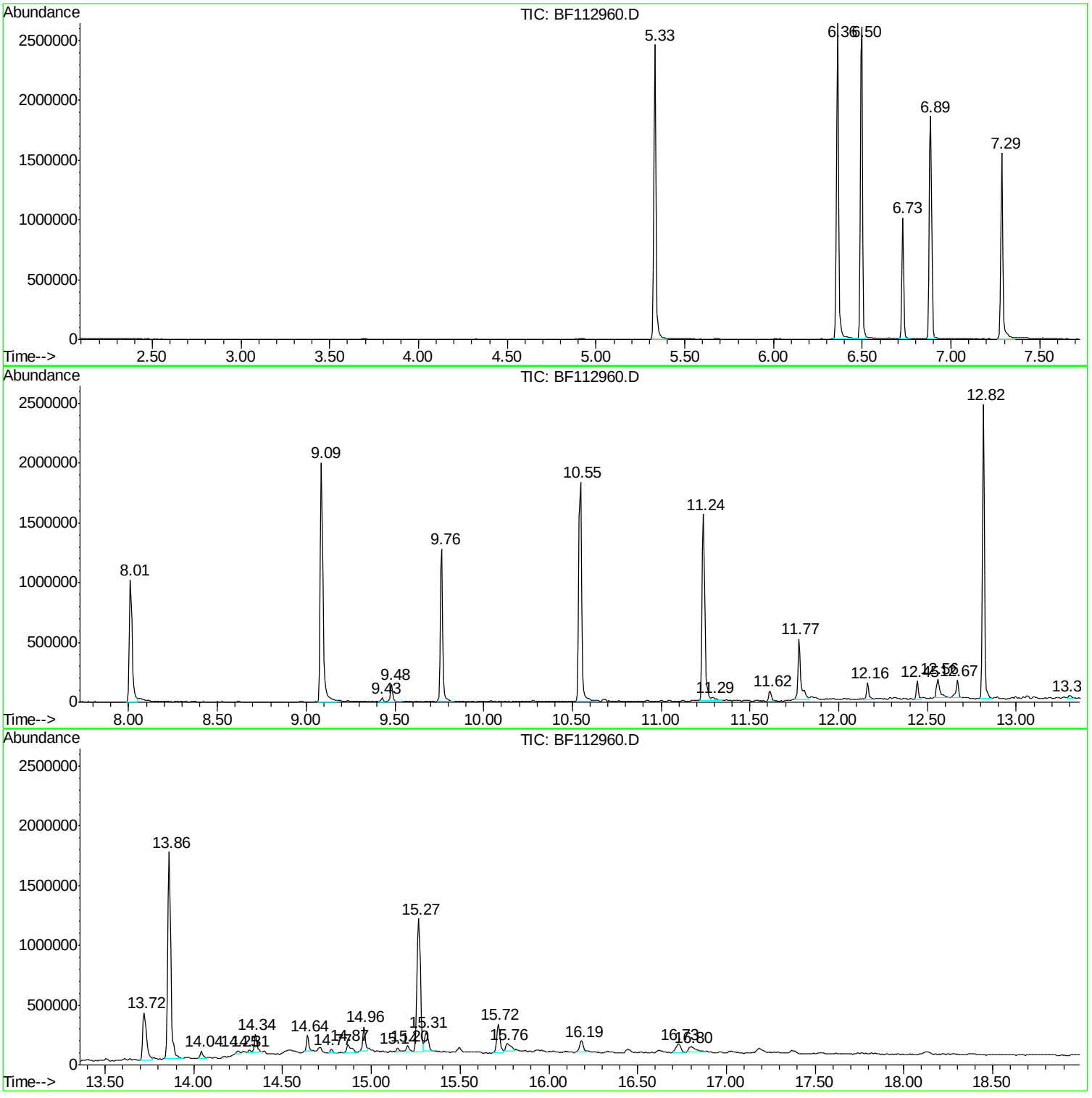
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112960.D
Acq On : 11 Mar 2019 17:47
Operator : JU/SJ
Sample : K1785-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SD2-0.0-0.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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\BF031119\
Data File : BF112960.D
Acq On : 11 Mar 2019 17:47
Operator : JU/SJ
Sample : K1785-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SD2-0.0-0.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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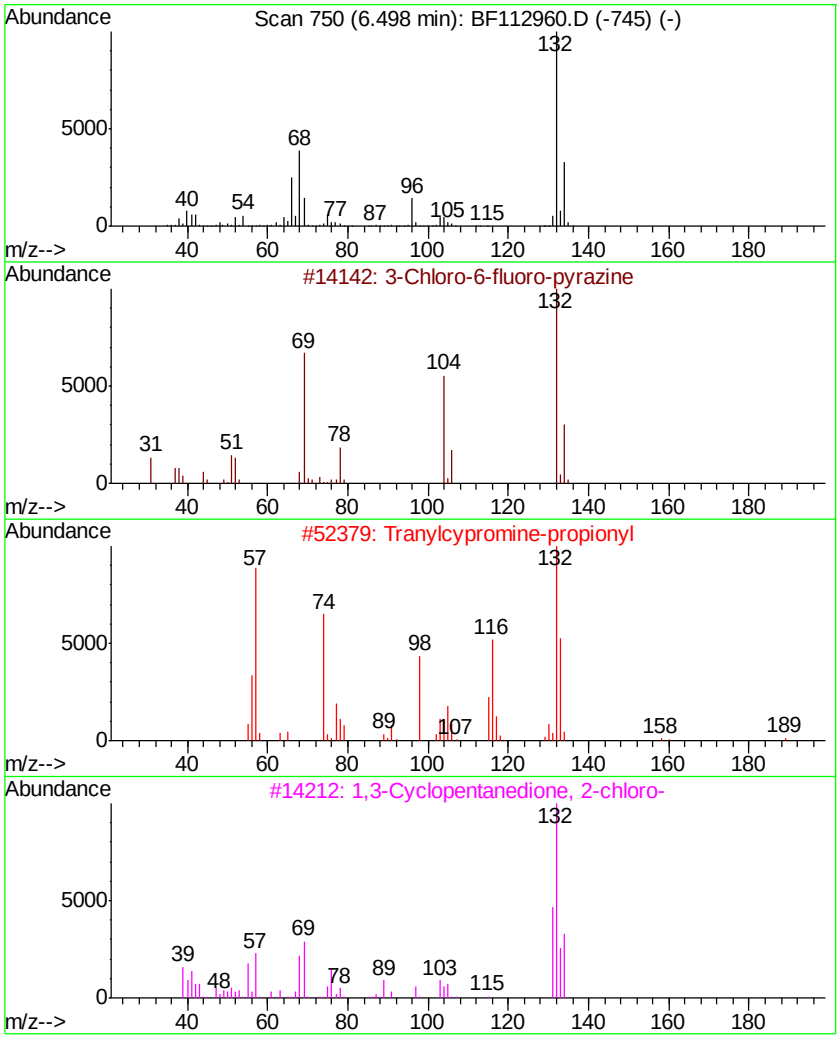
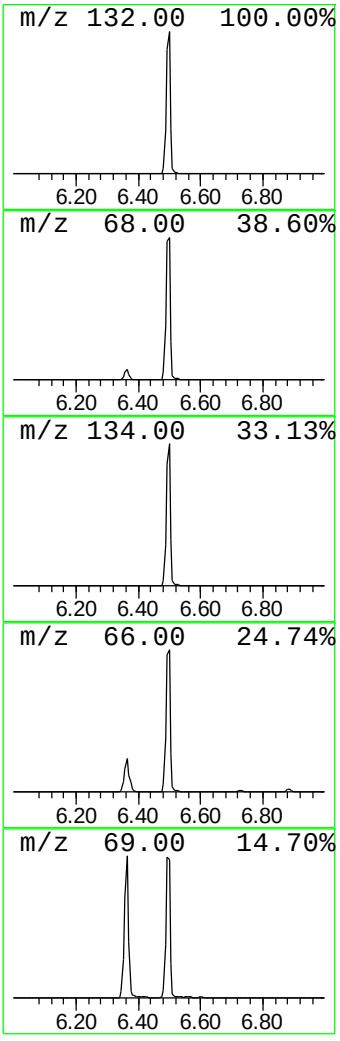
Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	59.02 ng	2429820	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112960.D
Acq On : 11 Mar 2019 17:47
Operator : JU/SJ
Sample : K1785-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SD2-0.0-0.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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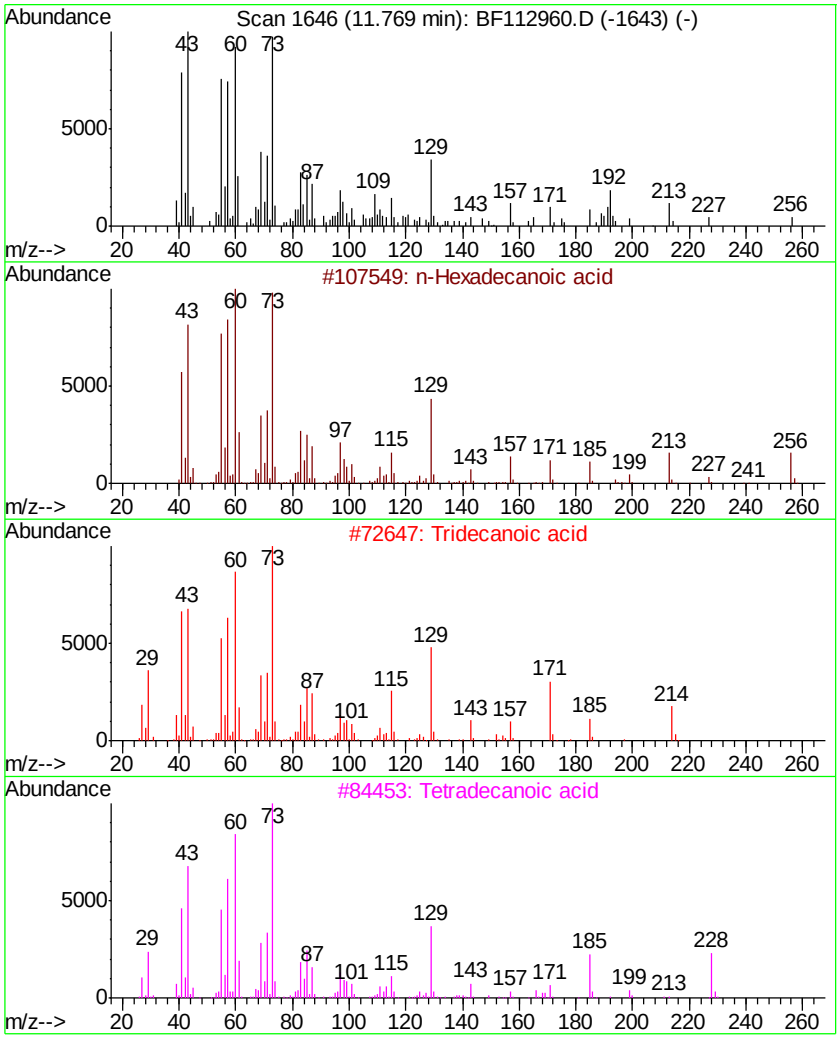
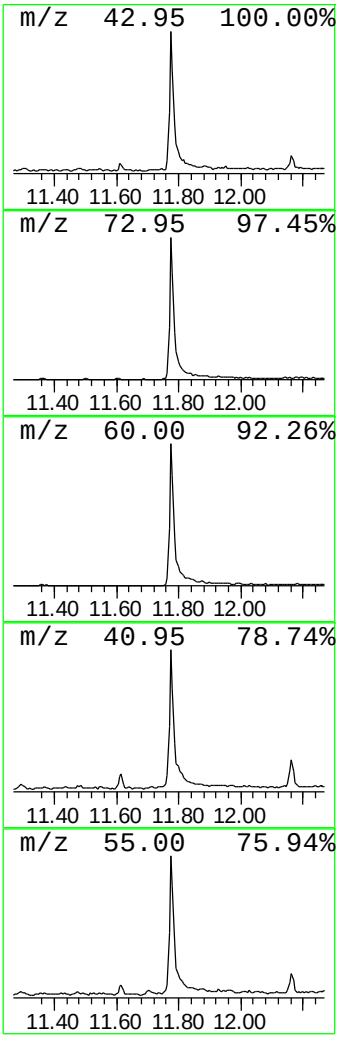
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	8.03 ng	620753	Phenanthrene-d10	11.24

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	96
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112960.D
Acq On : 11 Mar 2019 17:47
Operator : JU/SJ
Sample : K1785-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SD2-0.0-0.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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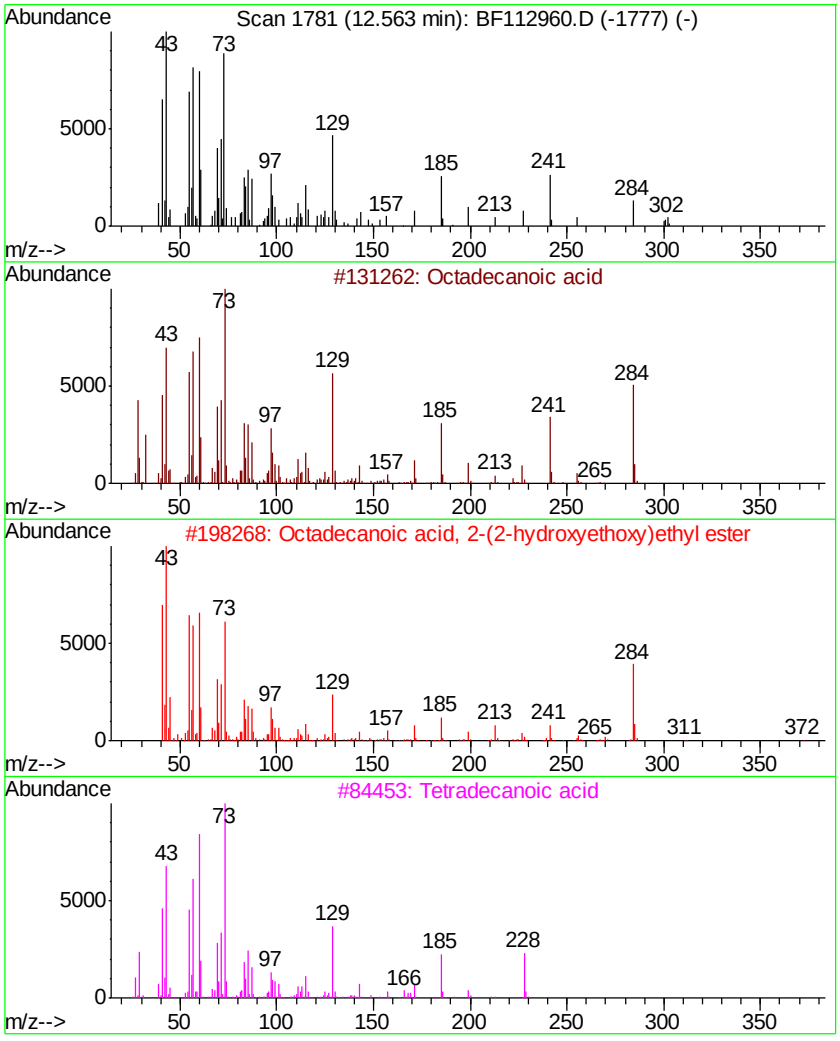
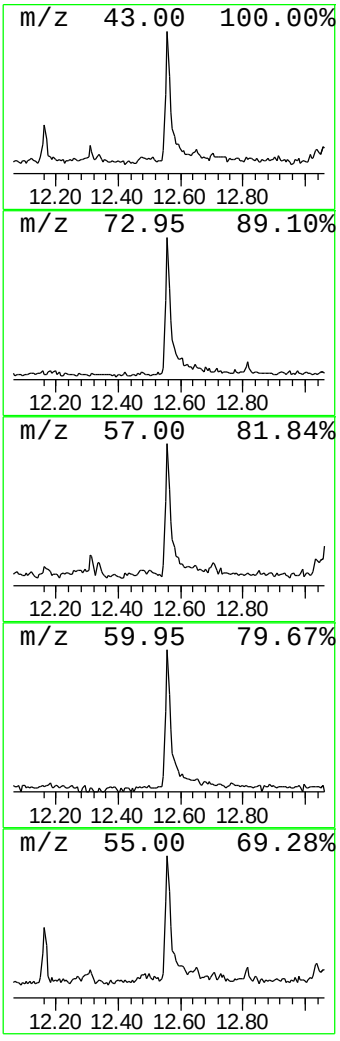
Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	2.24 ng	209768	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112960.D
Acq On : 11 Mar 2019 17:47
Operator : JU/SJ
Sample : K1785-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SD2-0.0-0.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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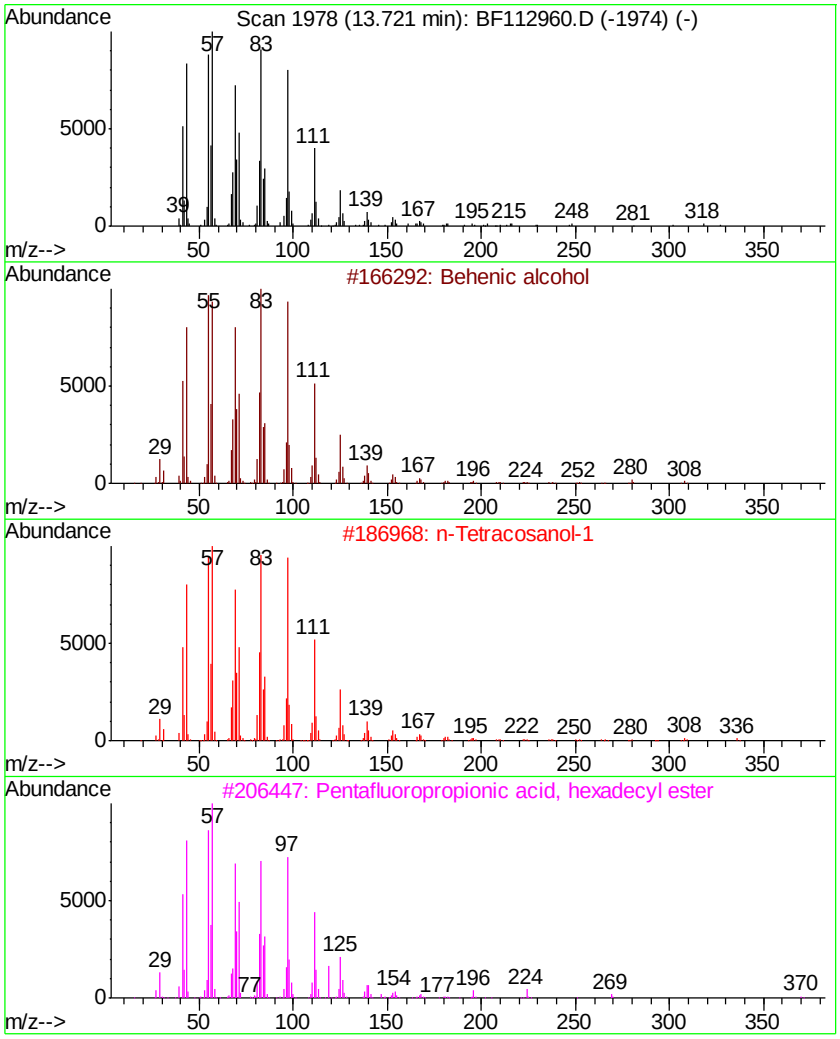
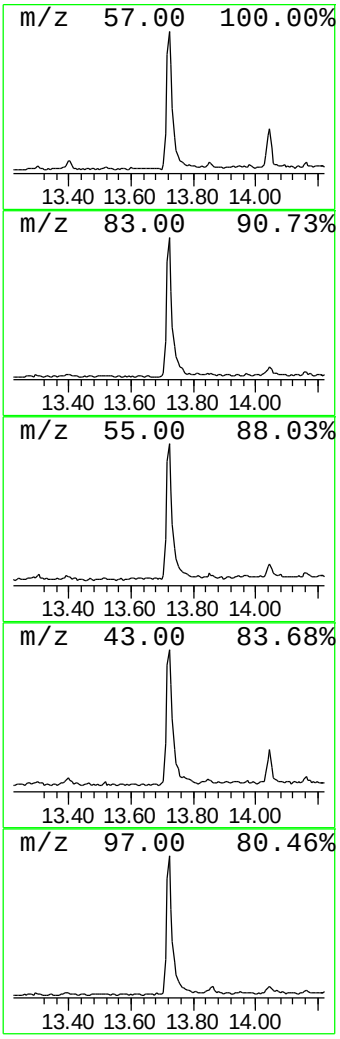
Peak Number 5 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	6.13 ng	573600	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112960.D
Acq On : 11 Mar 2019 17:47
Operator : JU/SJ
Sample : K1785-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SD2-0.0-0.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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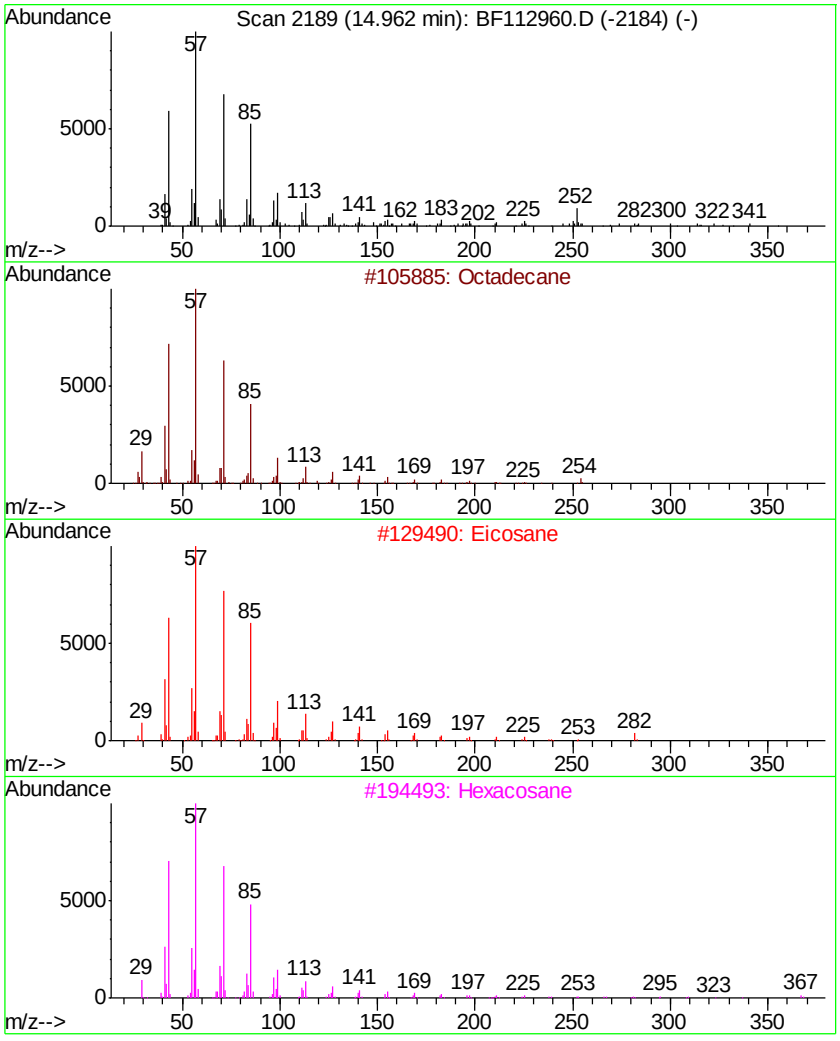
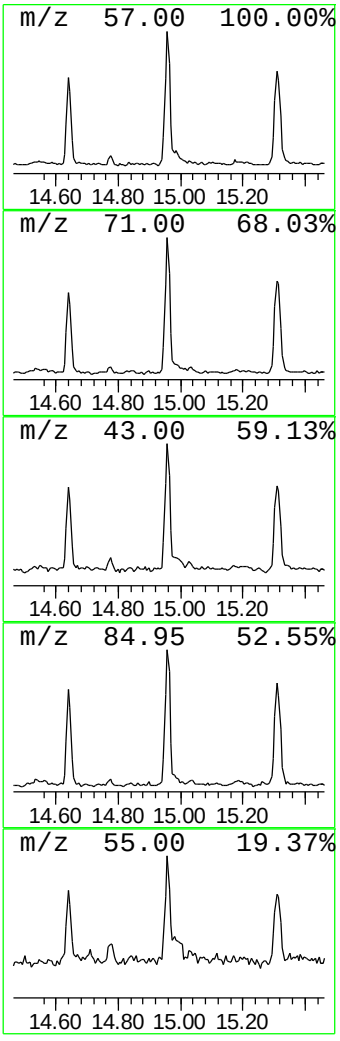
Peak Number 6 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.34 ng	235930	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Eicosane	282	C20H42	000112-95-8	93
3	Hexacosane	366	C26H54	000630-01-3	90
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Heneicosane	296	C21H44	000629-94-7	90





Library Search Compound Report

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Data File : BF112960.D
Acq On : 11 Mar 2019 17:47
Operator : JU/SJ
Sample : K1785-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SD2-0.0-0.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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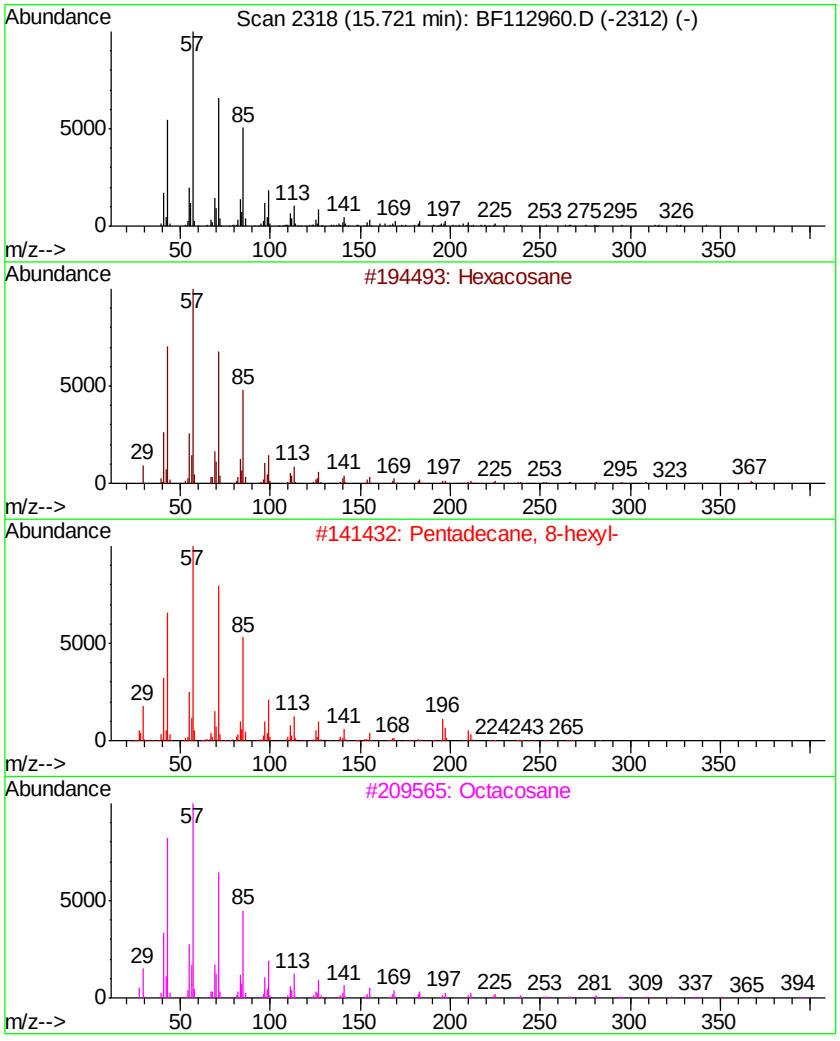
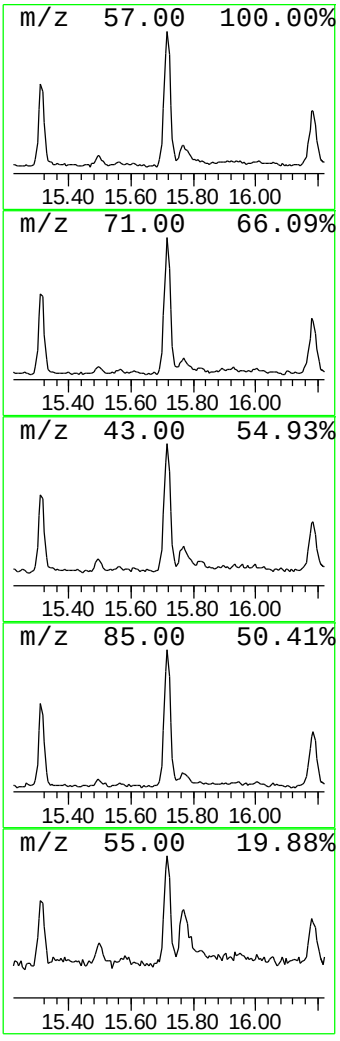
Peak Number 7 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	4.84 ng	341420	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heneicosane	296	C21H44	000629-94-7	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112960.D
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Operator : JU/SJ
Sample : K1785-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SD2-0.0-0.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

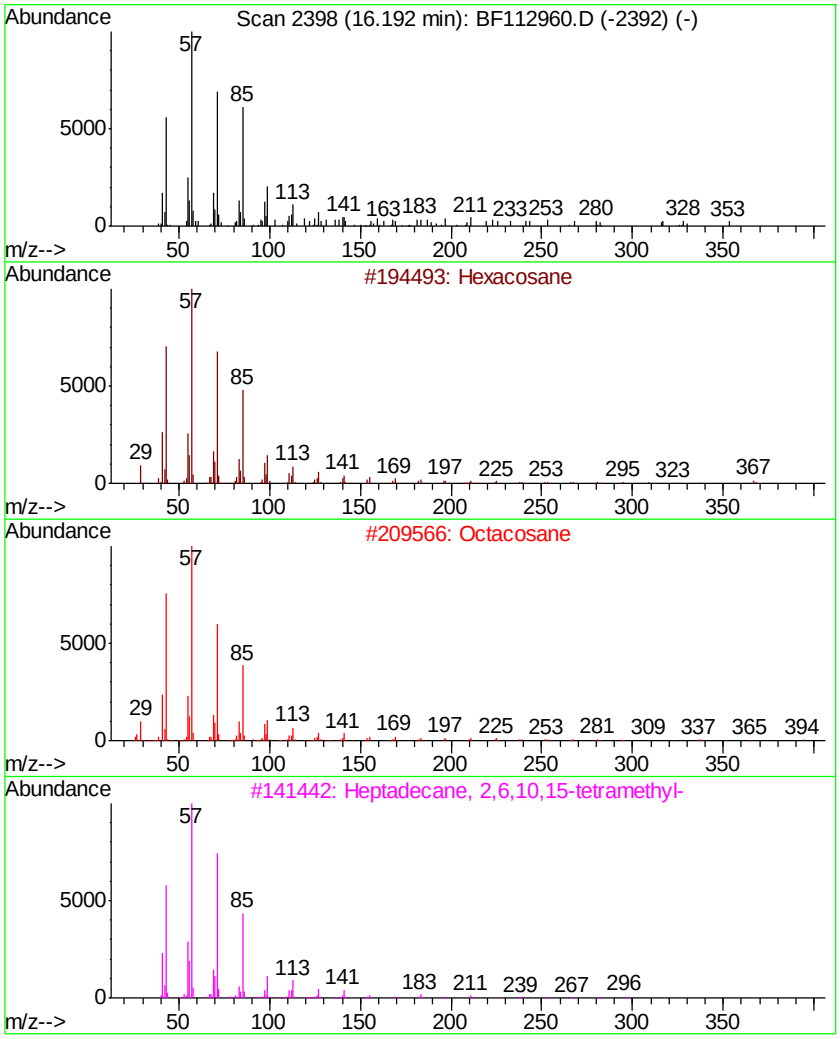
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

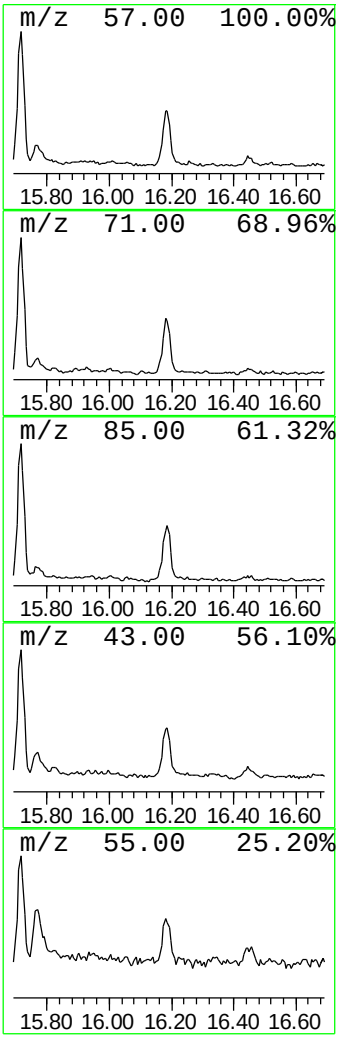
****

Peak Number 8 unknown16.19 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.07 ng	146091	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031119\
Data File : BF112960.D
Acq On : 11 Mar 2019 17:47
Operator : JU/SJ
Sample : K1785-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SD2-0.0-0.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.50	6.50	59.0	ng	2429820	1	6.73	823384	20.0
n-Hexadecanoic acid	11.77	8.0	ng	620753	4	11.24	1546090	20.0
Octadecanoic acid	12.56	2.2	ng	209768	5	13.86	1872530	20.0
Behenic alcohol	13.72	6.1	ng	573600	5	13.86	1872530	20.0
Octadecane	14.96	3.3	ng	235930	6	15.27	1411000	20.0
Hexacosane	15.72	4.8	ng	341420	6	15.27	1411000	20.0
unknown16.19	16.19	2.1	ng	146091	6	15.27	1411000	20.0