LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11(0-2)

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-BF071219.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	2.222	15	23	34	rVB	573369	758634	23.15%	2.246%
2	5.510	577	582	585	rBV	3130495	3001511	91.58%	8.885%
3	6.510	747	752	755	rBV	3089919	3185822	97.20%	9.430%
4	6.651	771	776	779	rBV	3472989	3269121	99.75%	9.677%
5	6.710	783	786	800	rVB	68066	92626	2.83%	0.274%
6	6.881	811	815	819	rBV	1396122	1129985	34.48%	3.345%
7	7.039	837	842	845	rBV	3025153	2695611	82.25%	7.979%
8	7.439	904	910	913	rBV	2164192	2102945	64.16%	6.225%
9	8.163	1028	1033	1036	rBV	1438531	1245938	38.02%	3.688%
10	9.233	1210	1215	1218	rBV	3658104	3277451	100.00%	9.702%
11	9.622	1277	1281	1286	rBV	631206	481445	14.69%	1.425%
12	9.910	1326	1330	1334	rBV	1462627	1373808	41.92%	4.067%
13	10.698	1459	1464	1467	rBV	2068831	1821092	55.56%	5.391%
14	11.392	1579	1582	1585	rBV	1402086	1231410	37.57%	3.645%
15	11.916	1665	1671	1676	rBV	399944	412737	12.59%	1.222%
16	12.604	1786	1788	1790	rBV	65148	51163	1.56%	0.151%
17	12.698	1801	1804	1812	rBV	118717	135487	4.13%	0.401%
18	12.833	1822	1827	1829	rBV	47568	48571	1.48%	0.144%
19	12.974	1847	1851	1854	rBV	2632766	2286137	69.75%	6.767%
20	13.210	1888	1891	1899	rBV3	46446	74453	2.27%	0.220%
21	13.551	1946	1949	1958	rVB6	32374	59922	1.83%	0.177%
22	13.686	1970	1972	1974	rVB	61142	46545	1.42%	0.138%
23	13.892	2002	2007	2017	rBV2	236696	479801	14.64%	1.420%
24	14.027	2024	2030	2037	rVB	1008069	988135	30.15%	2.925%
25	14.315	2076	2079	2081	rVB2	45426	39689	1.21%	0.117%
26	14.498	2107	2110	2112	rBV	84228	81696	2.49%	0.242%
27	14.527	2112	2115	2123	rVB	301404	566975	17.30%	1.678%
28	14.804	2159	2162	2165	rVB	63775	57070	1.74%	0.169%
29	14.945	2183	2186	2190	rBV	130354	126898	3.87%	0.376%
30	15.068	2203	2207	2214	rVB	45270	92343	2.82%	0.273%
31	15.139	2215	2219	2224	rBV	187029	234719	7.16%	0.695%
32	15.198	2225	2229	2244	rVV3	179461	508953	15.53%	1.507%
33	15.492	2274	2279	2283	rBV	742566	931968	28.44%	2.759%
34	15.721	2314	2318	2323	rVB	159454	213351	6.51%	0.632%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11(0-2)

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-BF071219.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.962	2354	2359	2365	rVB	171160	255177	7.79%	0.755%
36	16.068	2371	2377	2383	rBV3	82229	208838	6.37%	0.618%
37	16.756	2490	2494	2508	rVB6	59255	125859	3.84%	0.373%
38	17.056	2543	2545	2552	rVB3	50464	88268	2.69%	0.261%

Sum of corrected areas: 33782154

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
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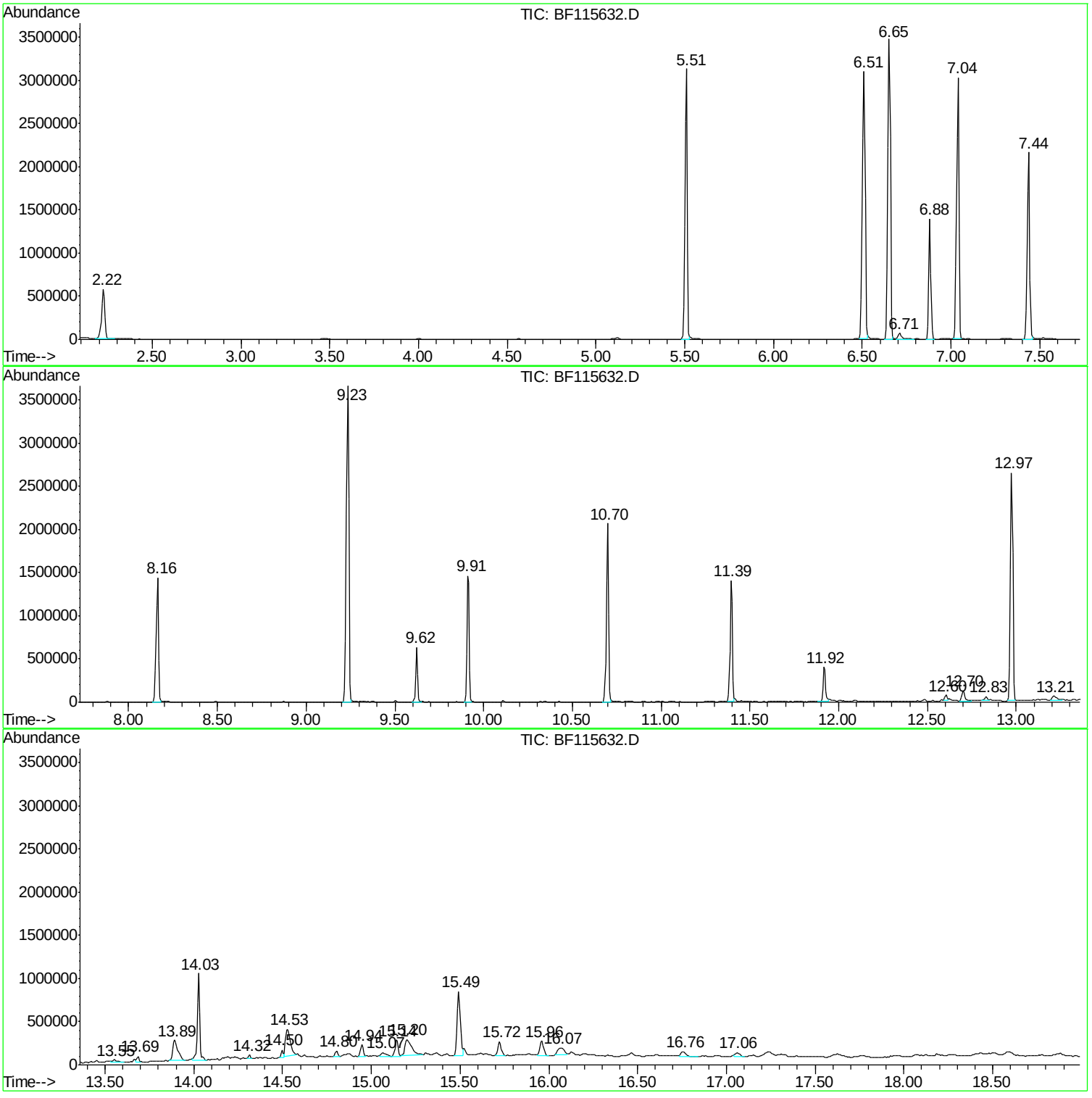
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-11(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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 : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11(0-2)

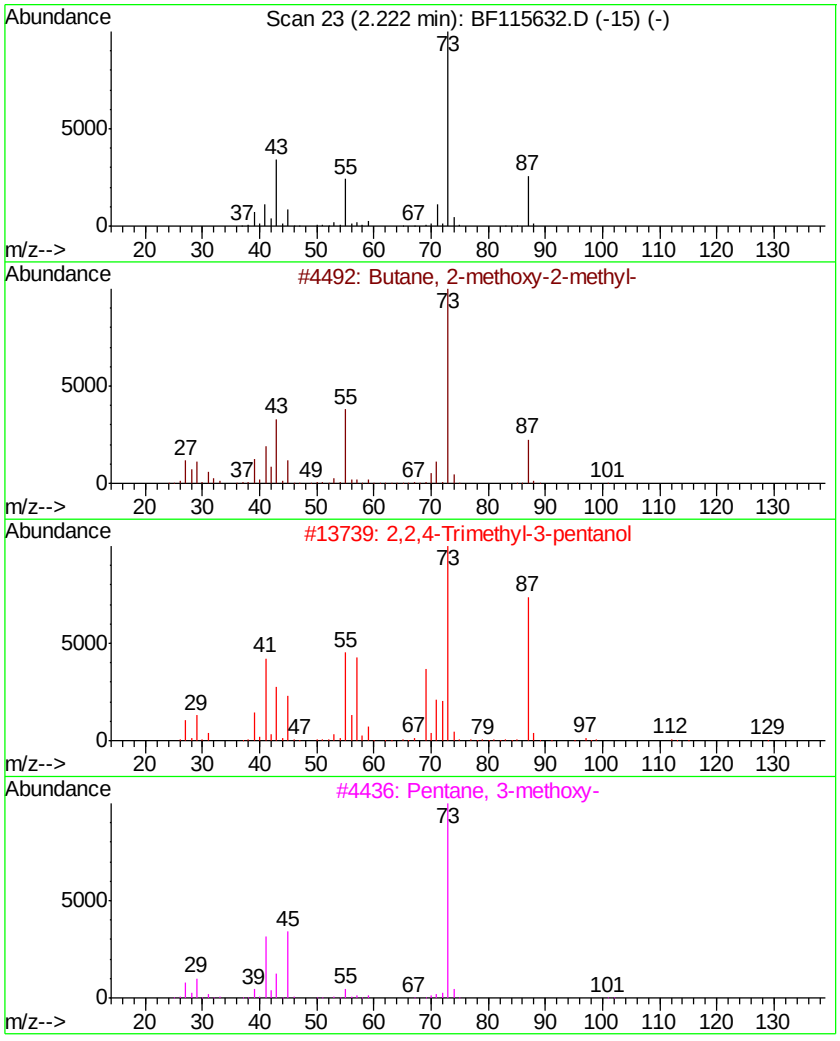
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

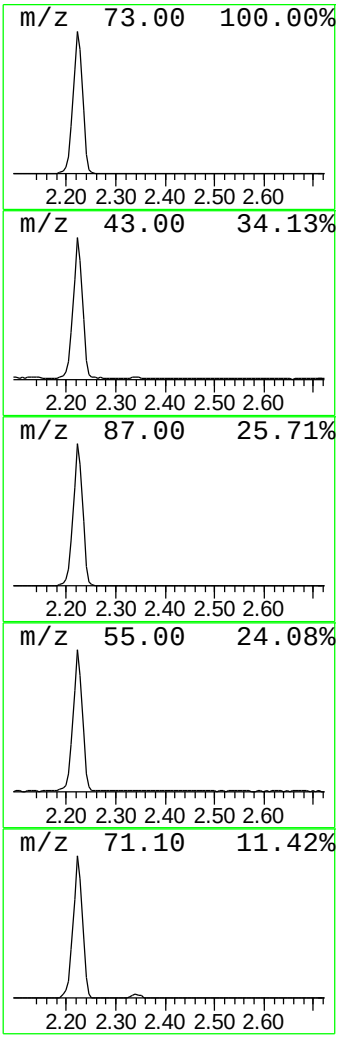
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	13.43 ng	758634	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

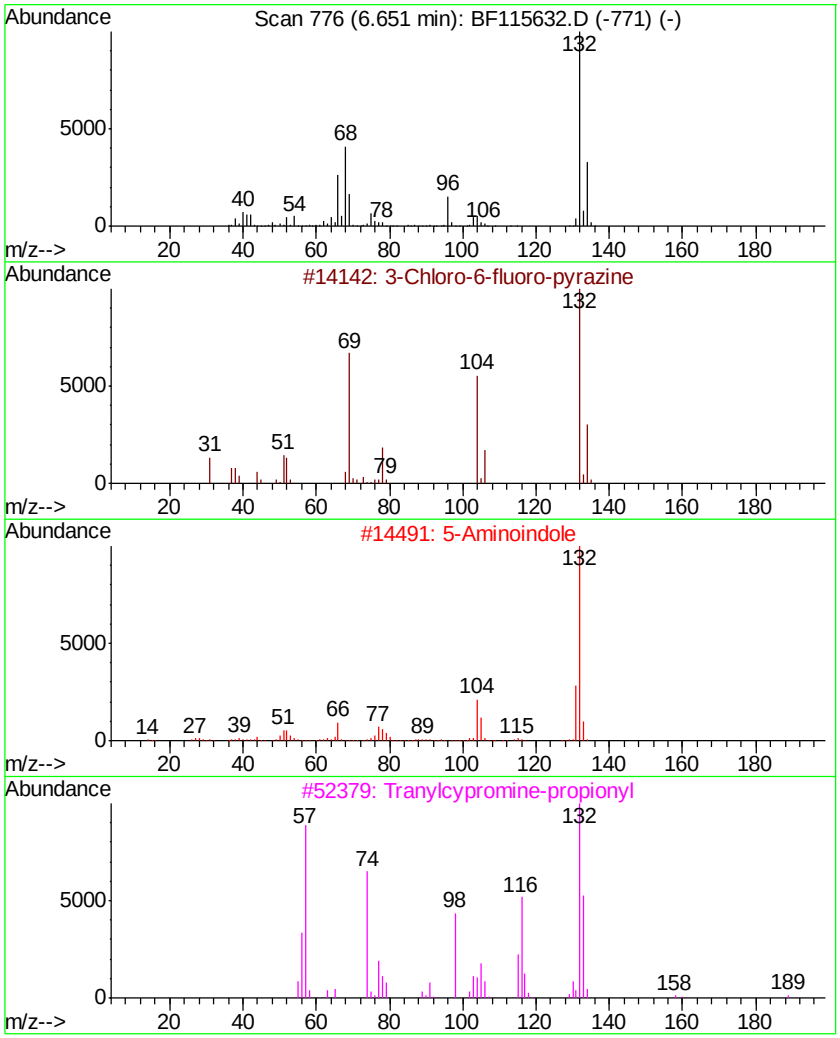
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

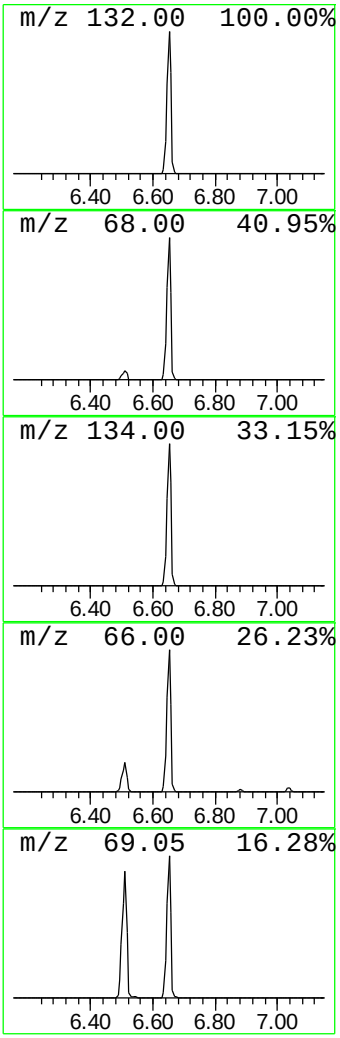
****

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	57.86 ng	3269120	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

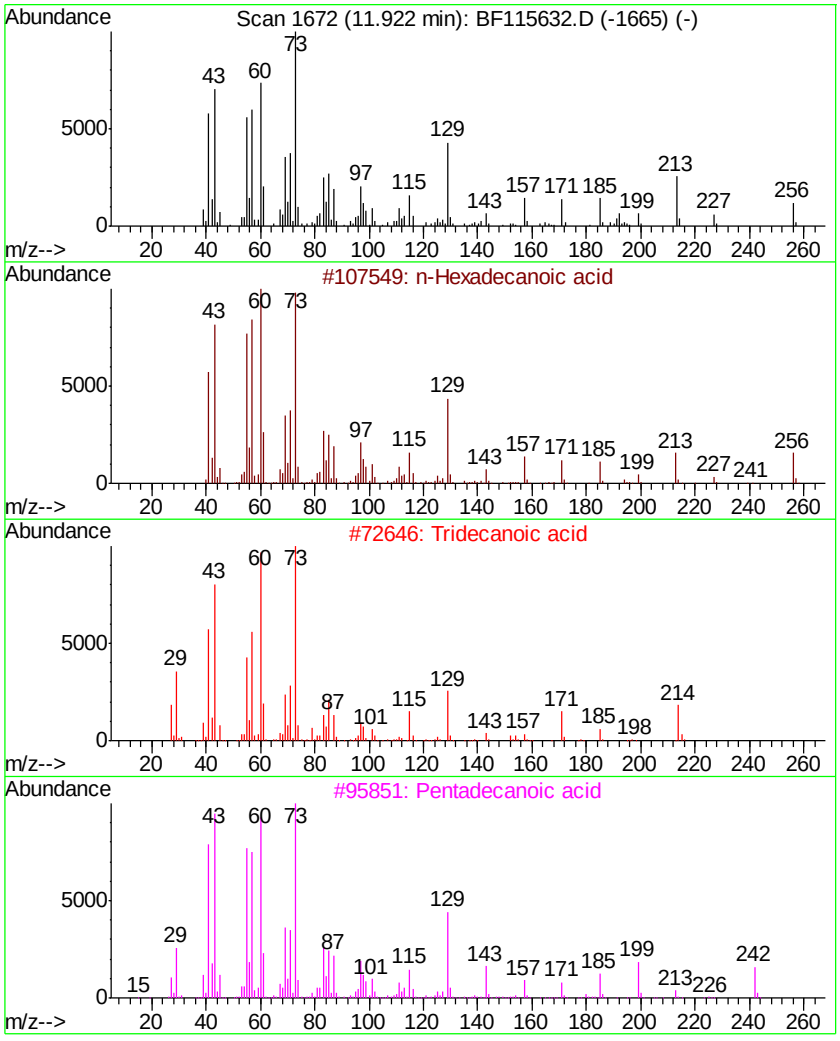
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

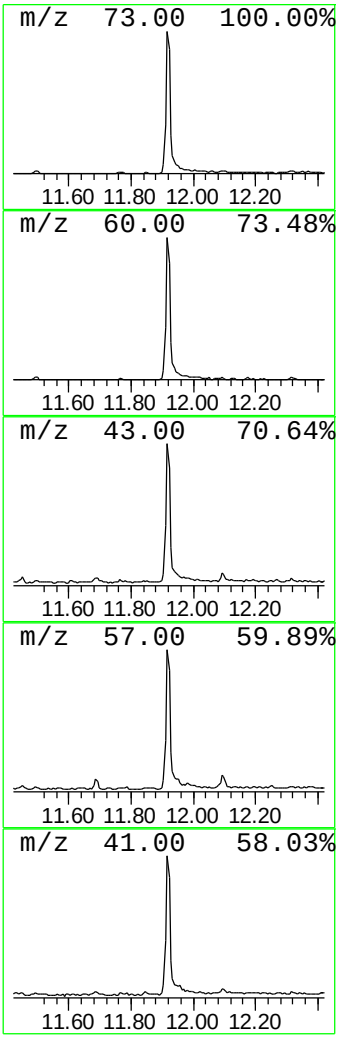
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	6.70 ng	412737	Phenanthrene-d10	11.39

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

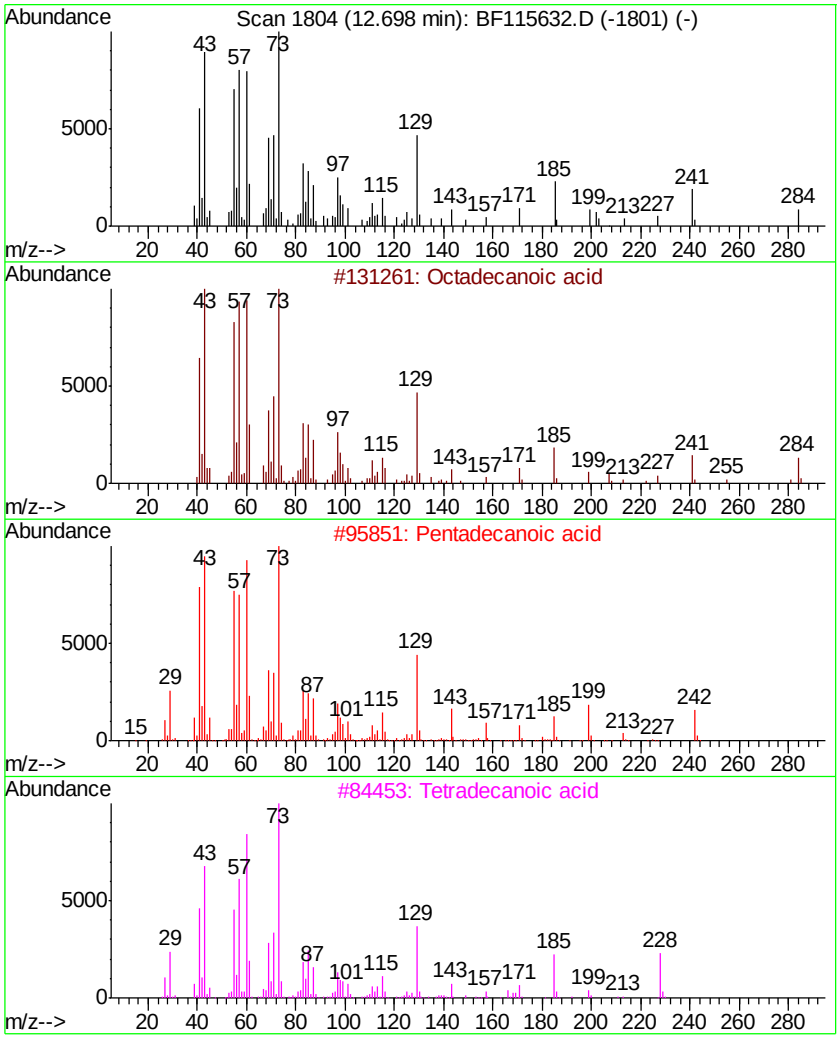
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

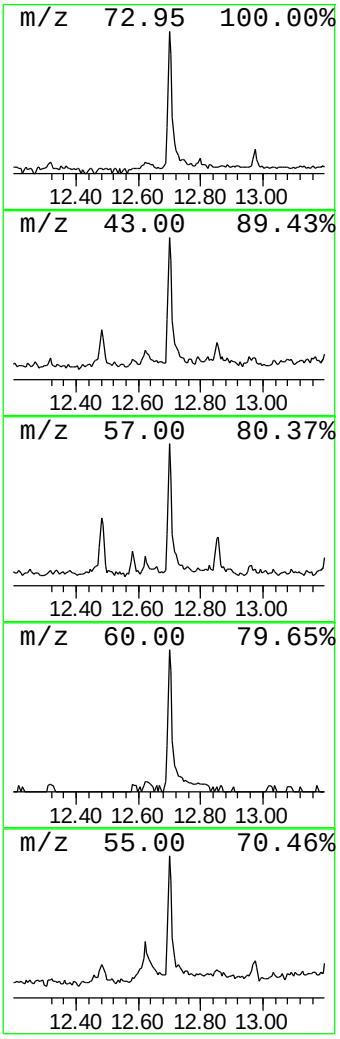
****

Peak Number 5 Octadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	2.20 ng	135487	Phenanthrene-d10	11.39

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	91
4	Undecanoic acid	186	C11H22O2	000112-37-8	83
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

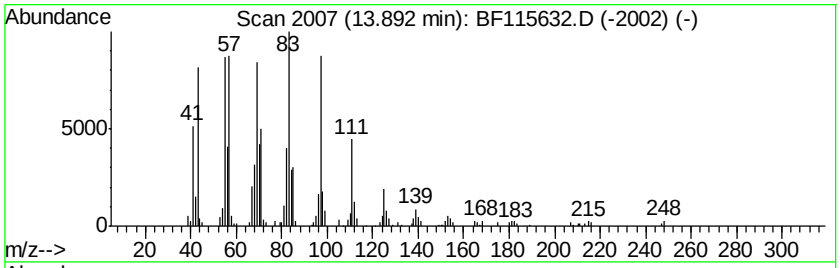
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

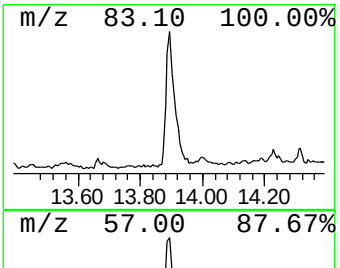
****

Peak Number 6 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	9.71 ng	479801	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

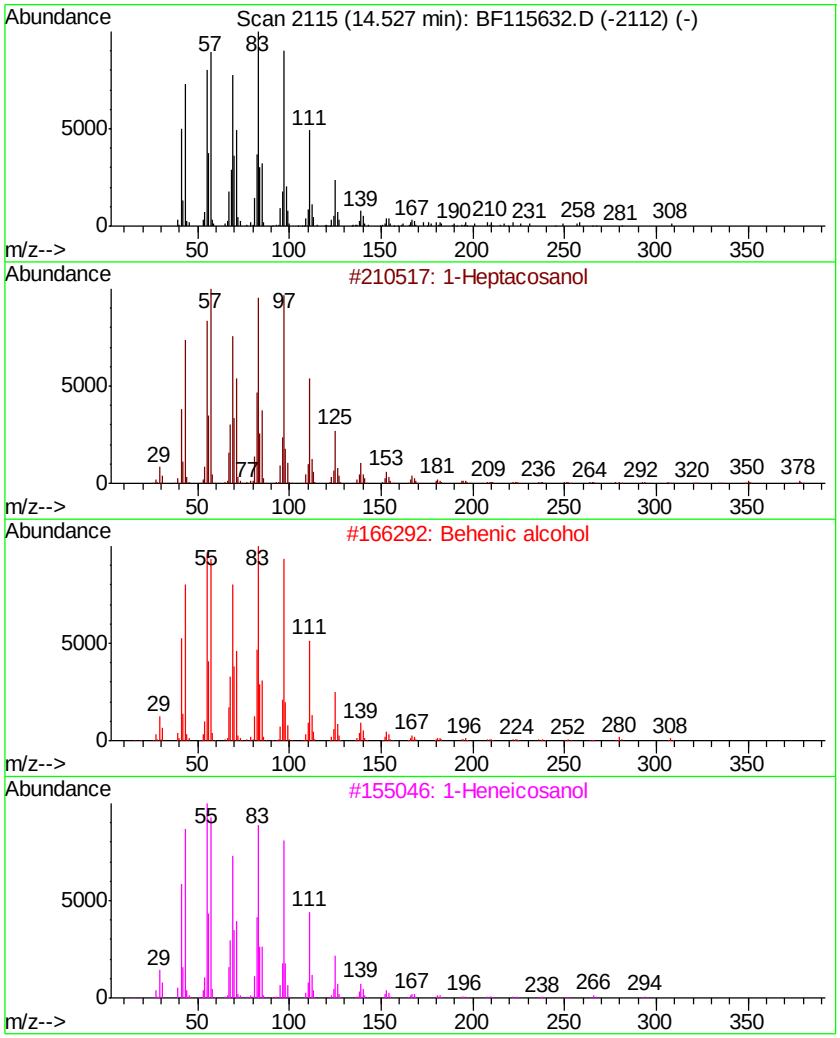
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

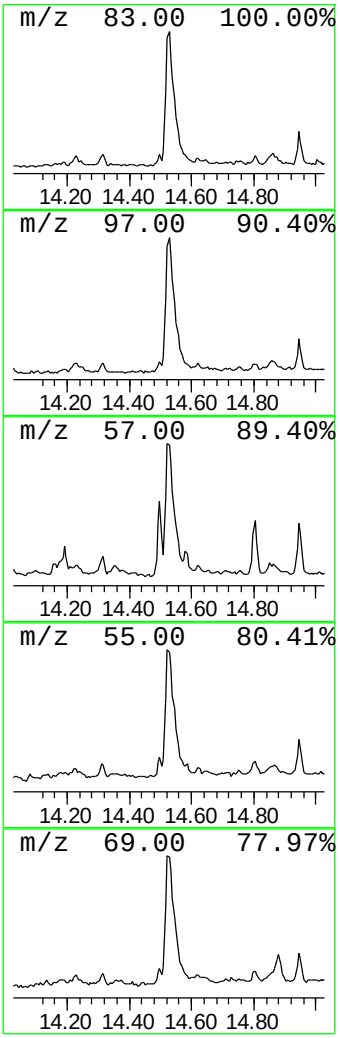
****

Peak Number 7 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	11.48 ng	566975	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
5	1-Docosene	308	C22H44	001599-67-3	95





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
Misc :
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Instrument : BNA_F
ClientSampleId : SB-11(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

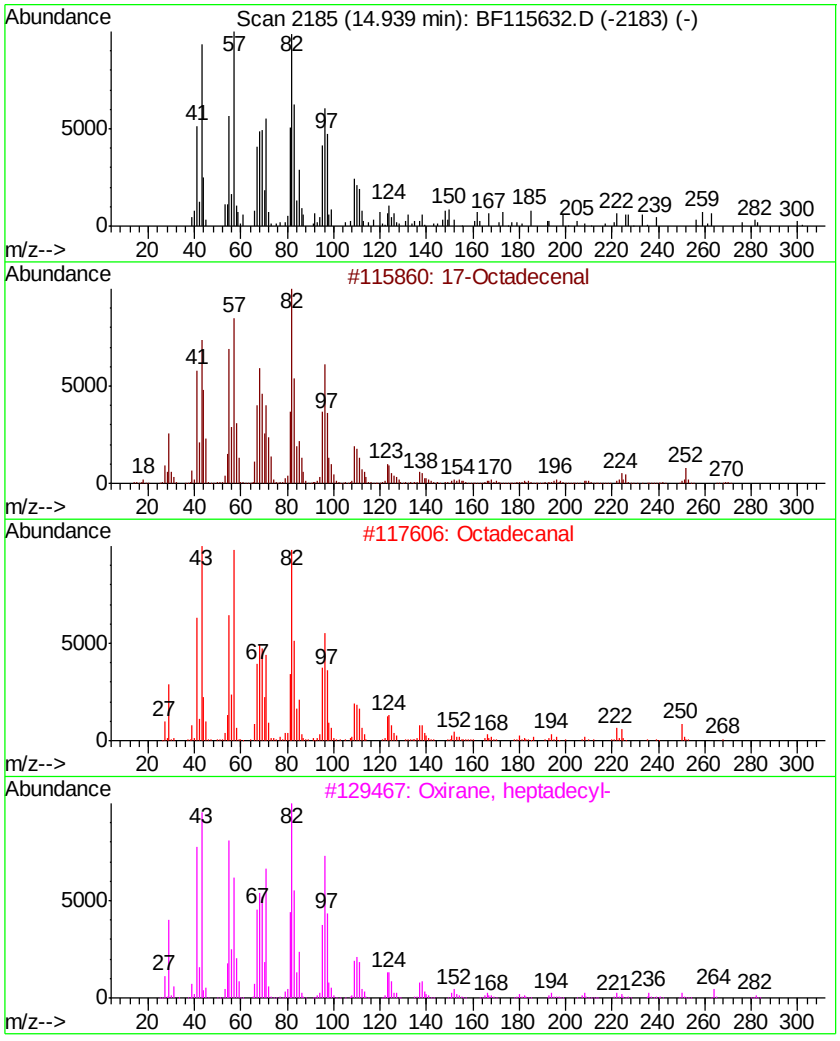
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

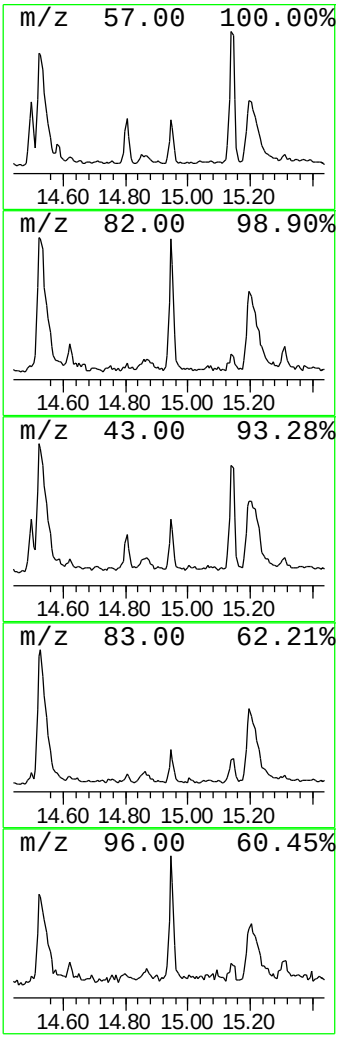
****

Peak Number 8 17-Octadecenal Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	2.72 ng	126898	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Octadecenal	266	C18H34O	056554-86-0	91
2	Octadecanal	268	C18H36O	000638-66-4	91
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
5	Pentadecanal-	226	C15H30O	002765-11-9	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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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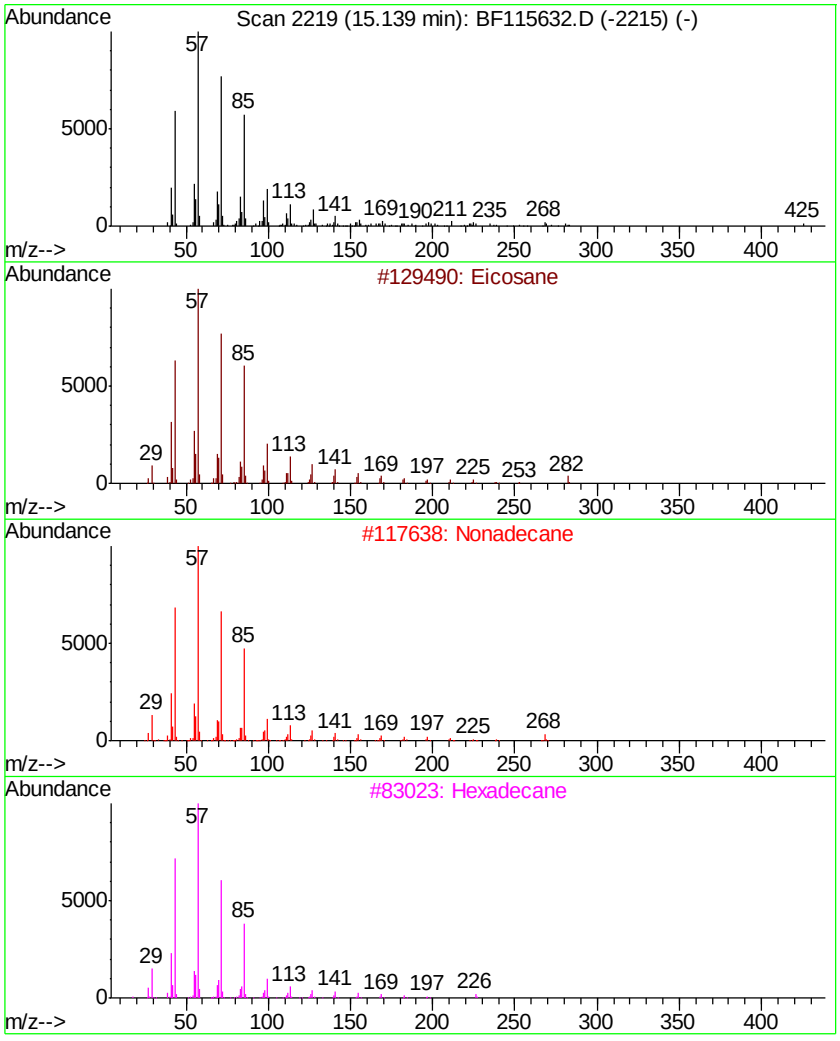
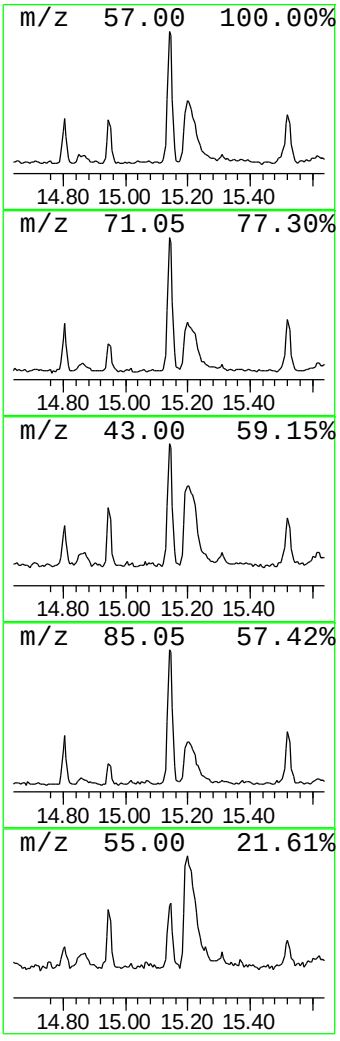
Peak Number 9 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	5.04 ng	234719	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Nonadecane	268	C19H40	000629-92-5	94
3	Hexadecane	226	C16H34	000544-76-3	94
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptadecane	240	C17H36	000629-78-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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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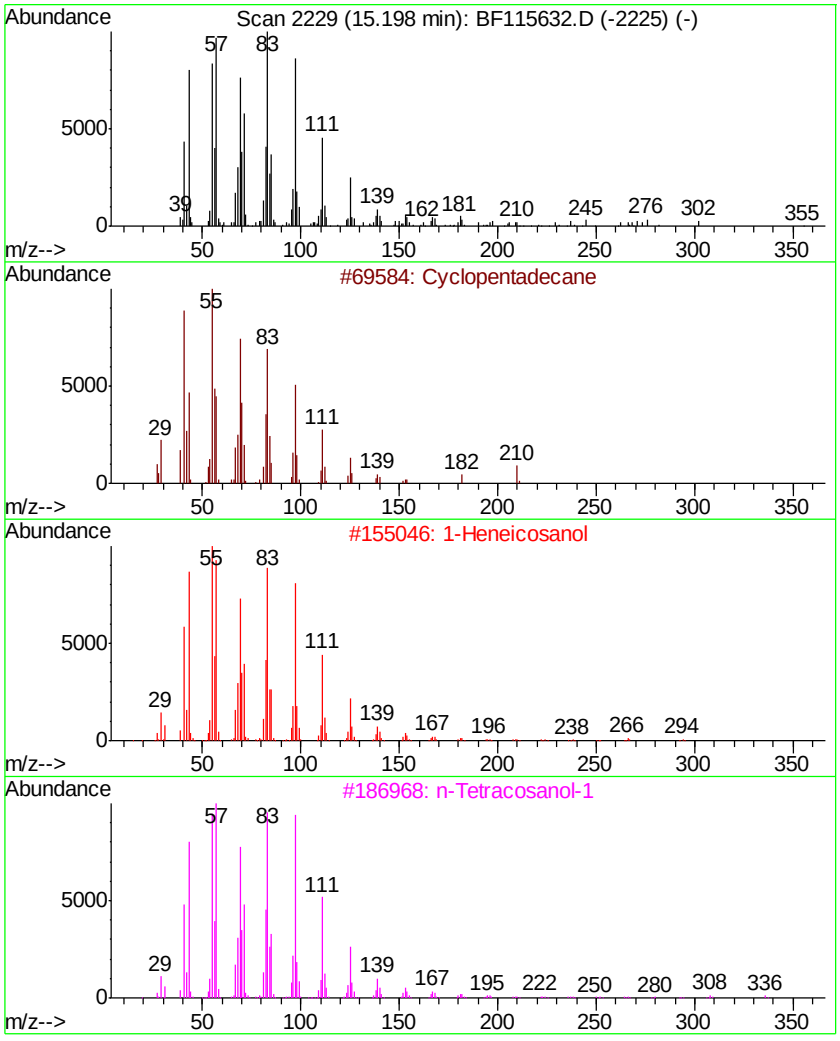
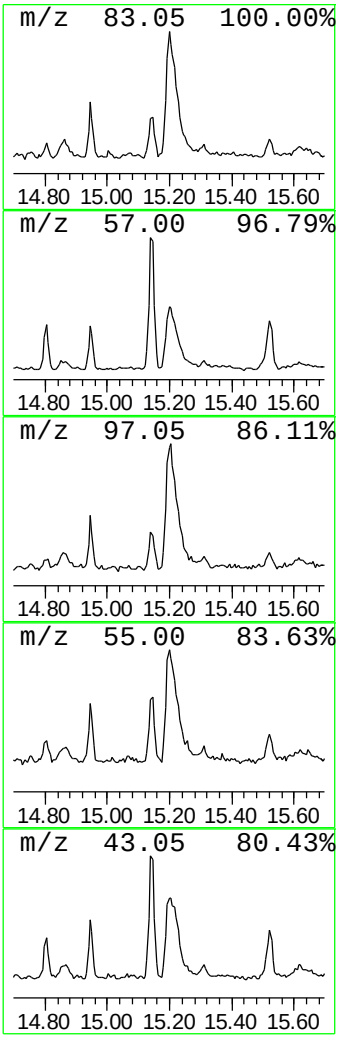
Peak Number 10 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	10.92 ng	508953	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	1-Heptacosanol	396	C27H56O	002004-39-9	95
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	95





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Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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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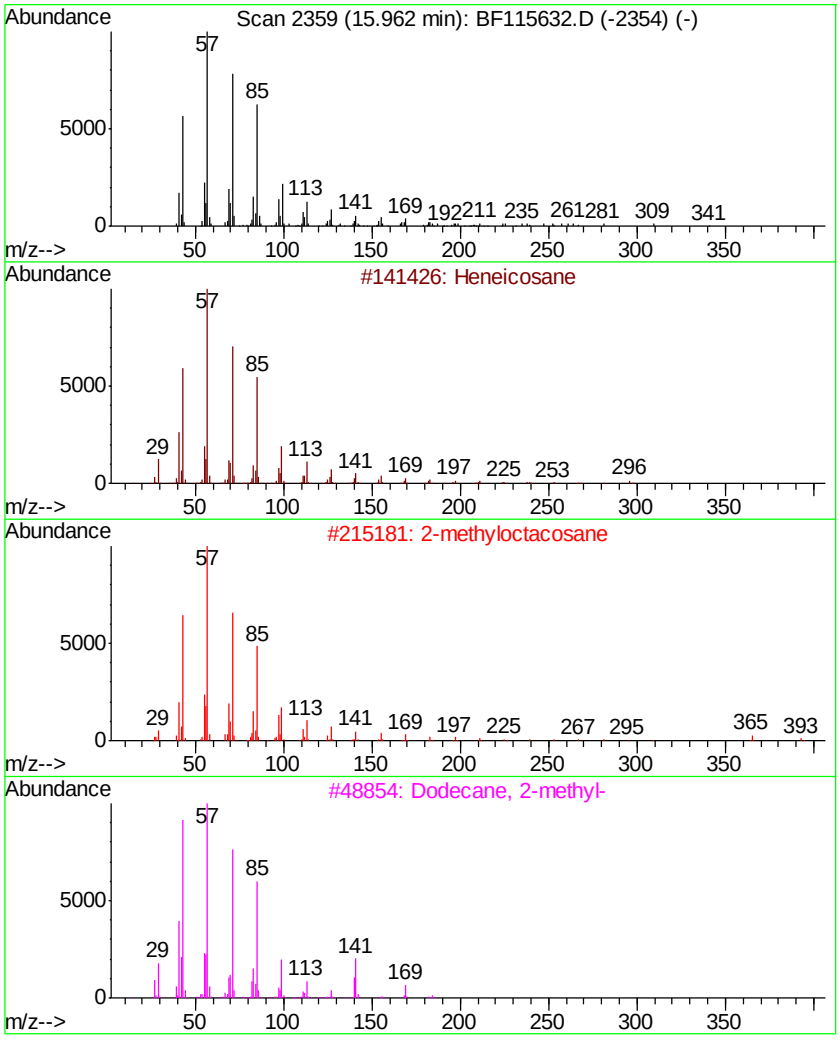
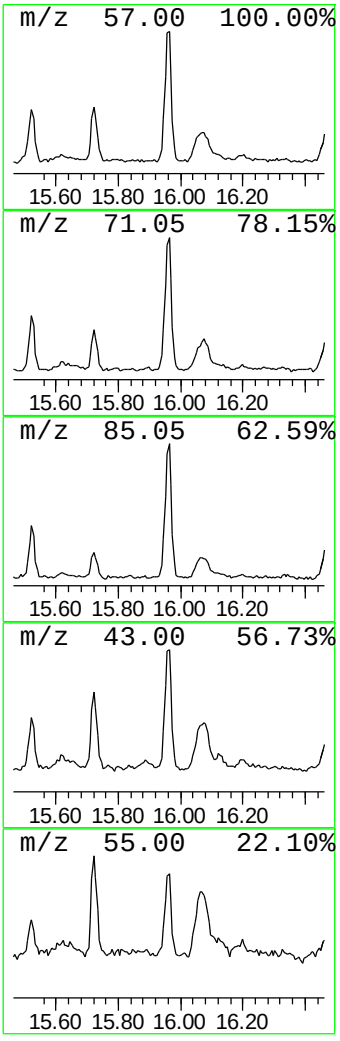
Peak Number 12 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	5.48 ng	255177	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Hentriacontane	437	C31H64	000630-04-6	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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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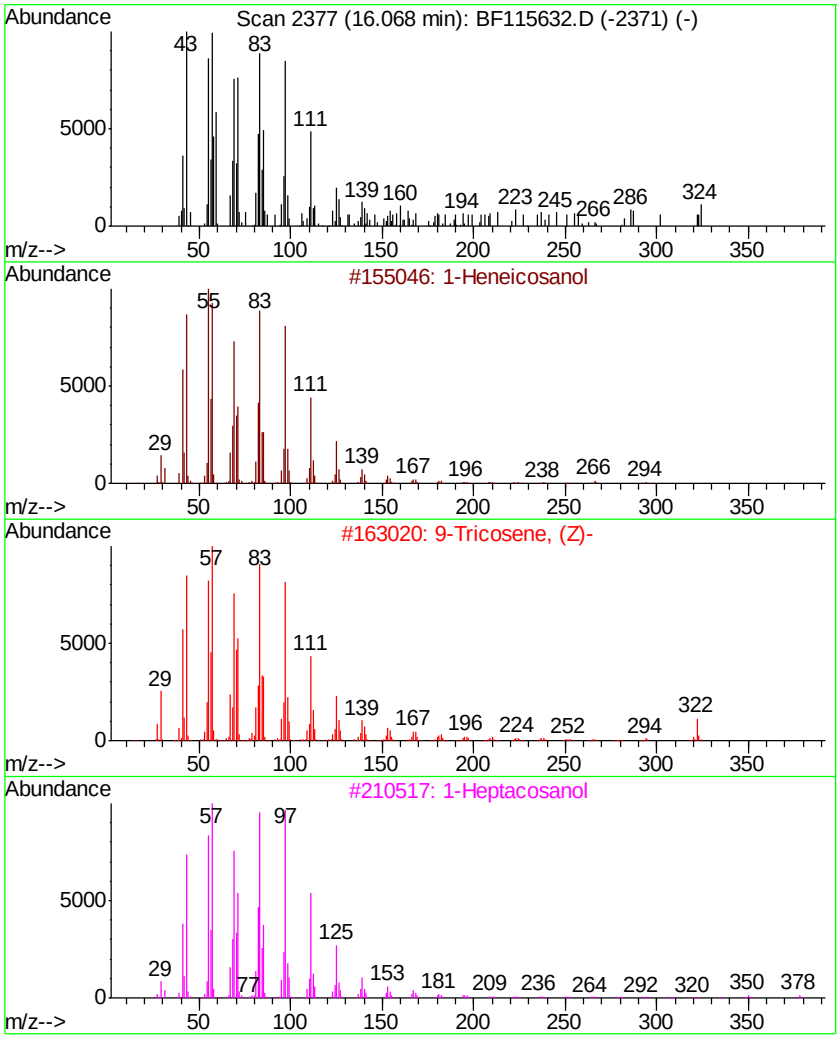
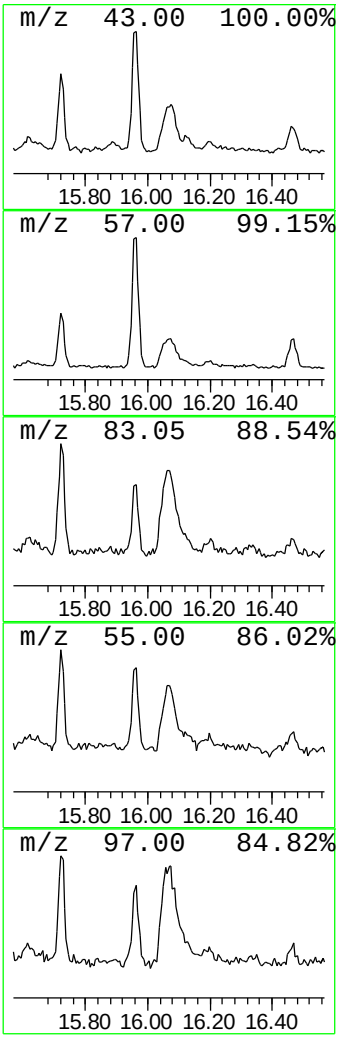
Peak Number 13 1-Heneicosanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	4.48 ng	208838	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	92
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	89
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	70
5	1-Nonadecene	266	C19H38	018435-45-5	68





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071719\
Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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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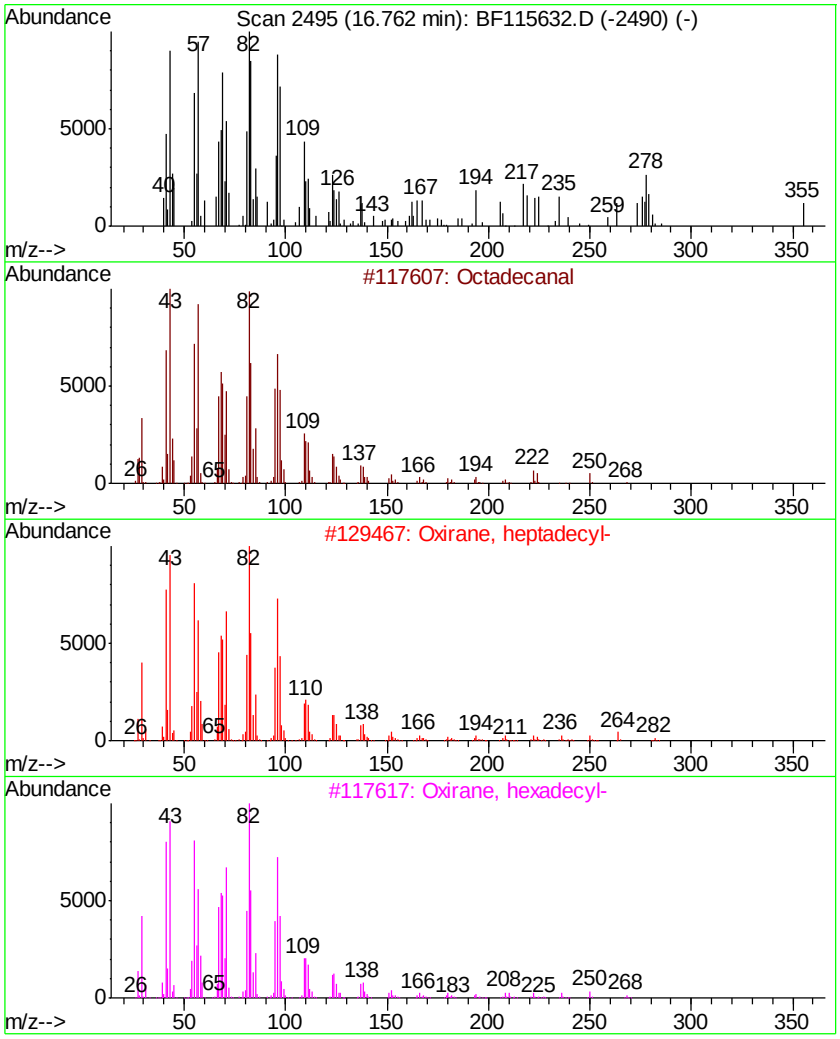
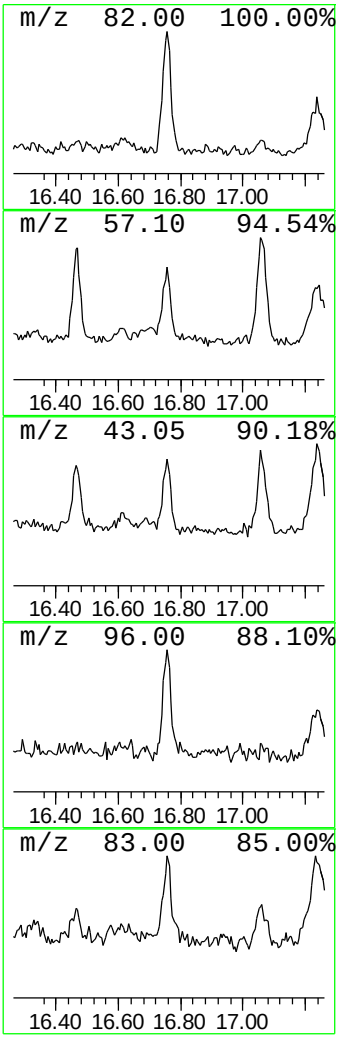
Peak Number 14 Octadecanal Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.76	2.70 ng	125859	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	80
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	72
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	64
4	11-Tetradecen-1-ol, acetate, (Z)-	254	C16H30O2	020711-10-8	53
5	1-Dodecen-1-ol, acetate	226	C14H26O2	056438-08-5	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071719\
Data File : BF115632.D
Acq On : 17 Jul 2019 19:52
Operator : HP/JU
Sample : K3835-29
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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
Butane, 2-methoxy...	2.22	13.4	ng	758634	1	6.88	1129990	20.0
unknown6.65	6.65	57.9	ng	3269120	1	6.88	1129990	20.0
n-Hexadecanoic acid	11.92	6.7	ng	412737	4	11.39	1231410	20.0
Octadecanoic acid	12.70	2.2	ng	135487	4	11.39	1231410	20.0
Behenic alcohol	13.89	9.7	ng	479801	5	14.03	988135	20.0
1-Heptacosanol	14.53	11.5	ng	566975	5	14.03	988135	20.0
17-Octadecenal	14.94	2.7	ng	126898	6	15.49	931968	20.0
Eicosane	15.14	5.0	ng	234719	6	15.49	931968	20.0
Cyclopentadecane	15.20	10.9	ng	508953	6	15.49	931968	20.0
Heneicosane	15.96	5.5	ng	255177	6	15.49	931968	20.0
1-Heneicosanol	16.07	4.5	ng	208838	6	15.49	931968	20.0
Octadecanal	16.76	2.7	ng	125859	6	15.49	931968	20.0