LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF010518\
Data File : BF101923.D
Acq On : 5 Jan 2018 12:19
Operator : SJ/JU
Sample : J1027-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR251608

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:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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	4.998	491	495	515	rBV	224161	463452	12.95%	1.716%
2	5.398	560	563	589	rBV	2042319	3580090	100.00%	13.252%
3	6.428	734	738	755	rBV	2044594	3342181	93.35%	12.372%
4	6.545	755	758	764	rVV	2542761	3001335	83.83%	11.110%
5	6.769	793	796	804	rBV	710567	786430	21.97%	2.911%
6	6.928	819	823	843	rVB	2168890	2399680	67.03%	8.883%
7	7.345	891	894	910	rBV	1619090	2013218	56.23%	7.452%
8	8.022	1006	1009	1011	rBV	41822	41394	1.16%	0.153%
9	8.057	1011	1015	1027	rVV	740986	877222	24.50%	3.247%
10	8.328	1053	1061	1067	rBV6	22273	49344	1.38%	0.183%
11	8.628	1106	1112	1115	rBV	54488	49787	1.39%	0.184%
12	9.122	1193	1196	1205	rBV	2483142	2468243	68.94%	9.137%
13	9.192	1205	1208	1211	rVB	78693	79460	2.22%	0.294%
14	9.504	1258	1261	1263	rBV	40878	48222	1.35%	0.179%
15	9.528	1263	1265	1270	rVB	157324	143251	4.00%	0.530%
16	9.716	1292	1297	1301	rVB	124134	102969	2.88%	0.381%
17	9.810	1309	1313	1324	rVB	697461	730750	20.41%	2.705%
18	10.216	1379	1382	1385	rVB	133631	101144	2.83%	0.374%
19	10.433	1415	1419	1422	rBV	36664	42167	1.18%	0.156%
20	10.610	1445	1449	1460	rBV	1035141	1236359	34.53%	4.577%
21	10.686	1460	1462	1471	rVB	98593	133310	3.72%	0.493%
22	11.304	1563	1567	1578	rBV	677087	689951	19.27%	2.554%
23	11.745	1637	1642	1645	rBV4	26686	38965	1.09%	0.144%
24	11.810	1651	1653	1667	rBV	167846	194353	5.43%	0.719%
25	12.533	1769	1776	1784	rBV2	34798	71789	2.01%	0.266%
26	12.592	1784	1786	1795	rBV2	92774	131253	3.67%	0.486%
27	12.880	1831	1835	1839	rBV	2338244	2194870	61.31%	8.125%
28	13.351	1911	1915	1918	rBV2	47674	53545	1.50%	0.198%
29	13.751	1980	1983	1991	rBV	143098	175428	4.90%	0.649%
30	13.957	2014	2018	2027	rBV	794608	870820	24.32%	3.223%
31	14.998	2192	2195	2199	rBV2	124213	147229	4.11%	0.545%
32	15.427	2264	2268	2276	rBV2	430858	593229	16.57%	2.196%
33	15.768	2323	2326	2333	rVB	118771	163405	4.56%	0.605%

LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF010518\
Data File : BF101923.D
Acq On : 5 Jan 2018 12:19
Operator : SJ/JU
Sample : J1027-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR251608

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:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 27014845

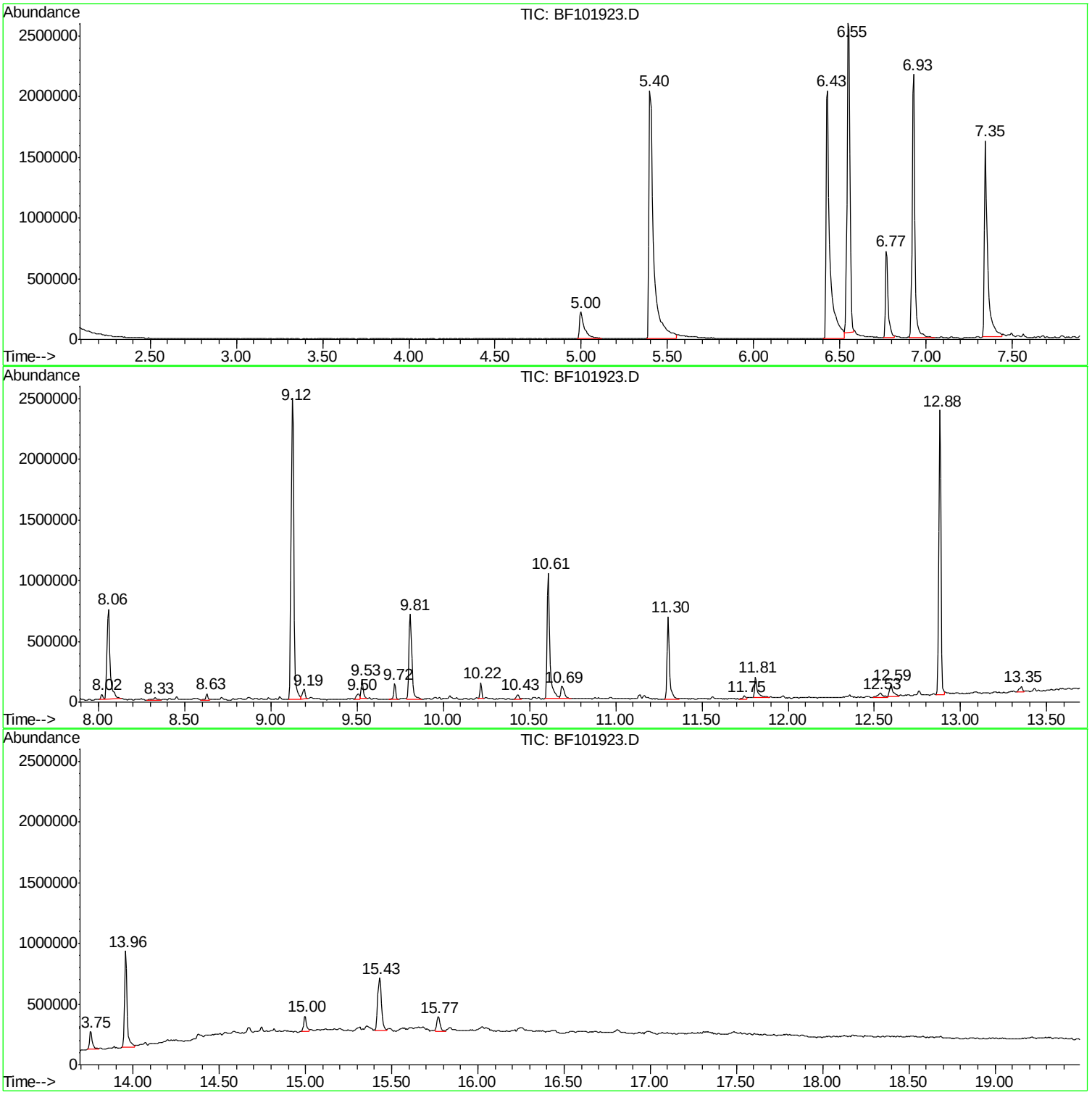
LSC Report - Integrated Chromatogram

Data Path : U:\HPCHEM1\BNA F\DATA\BF010518\
Data File : BF101923.D
Acq On : 5 Jan 2018 12:19
Operator : SJ/JU
Sample : J1027-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR251608

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA F\DATA\BF010518\
Data File : BF101923.D
Acq On : 5 Jan 2018 12:19
Operator : SJ/JU
Sample : J1027-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR251608

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

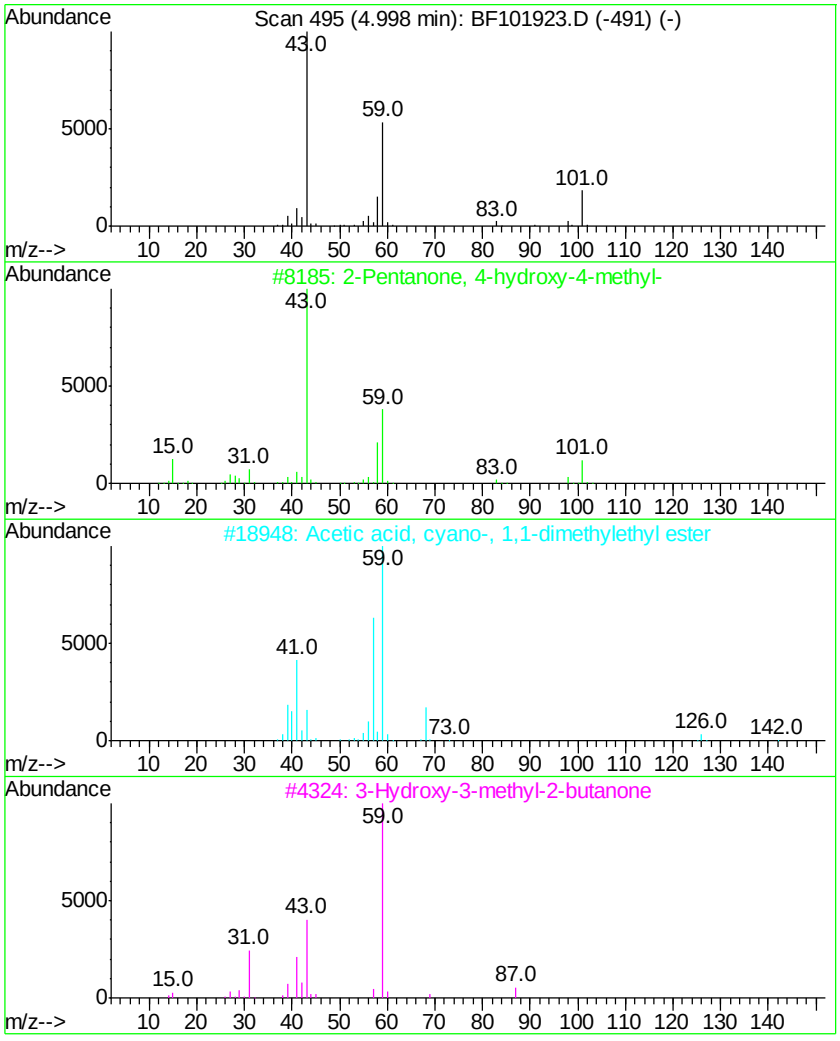
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

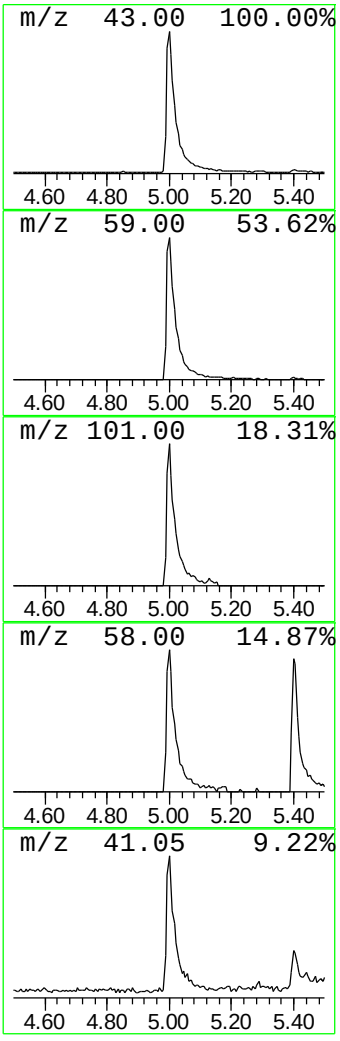
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	11.79 ng	463452	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF010518\
Data File : BF101923.D
Acq On : 5 Jan 2018 12:19
Operator : SJ/JU
Sample : J1027-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR251608

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

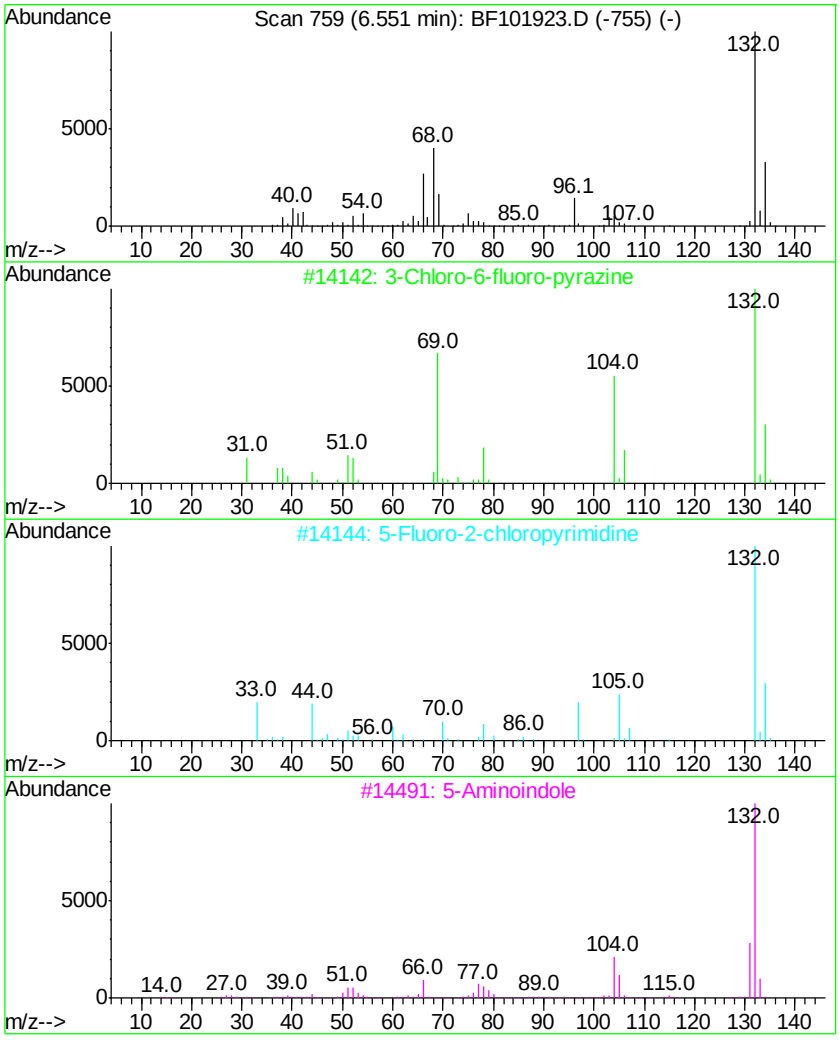
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

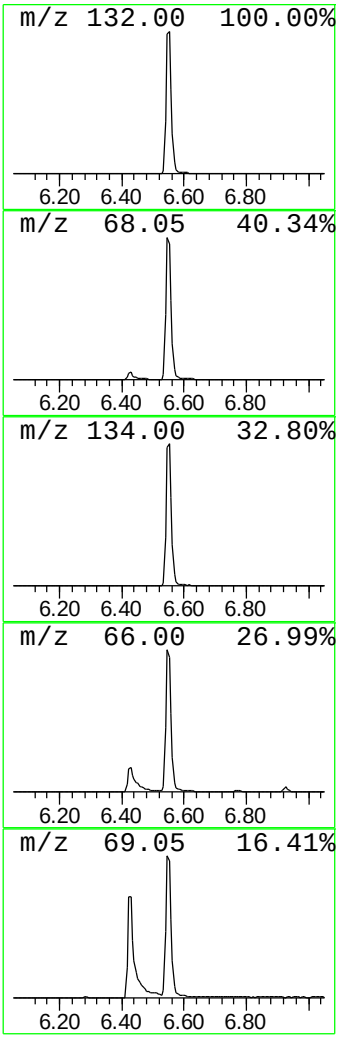
****

Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	76.33 ng	3001340	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF010518\
Data File : BF101923.D
Acq On : 5 Jan 2018 12:19
Operator : SJ/JU
Sample : J1027-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR251608

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

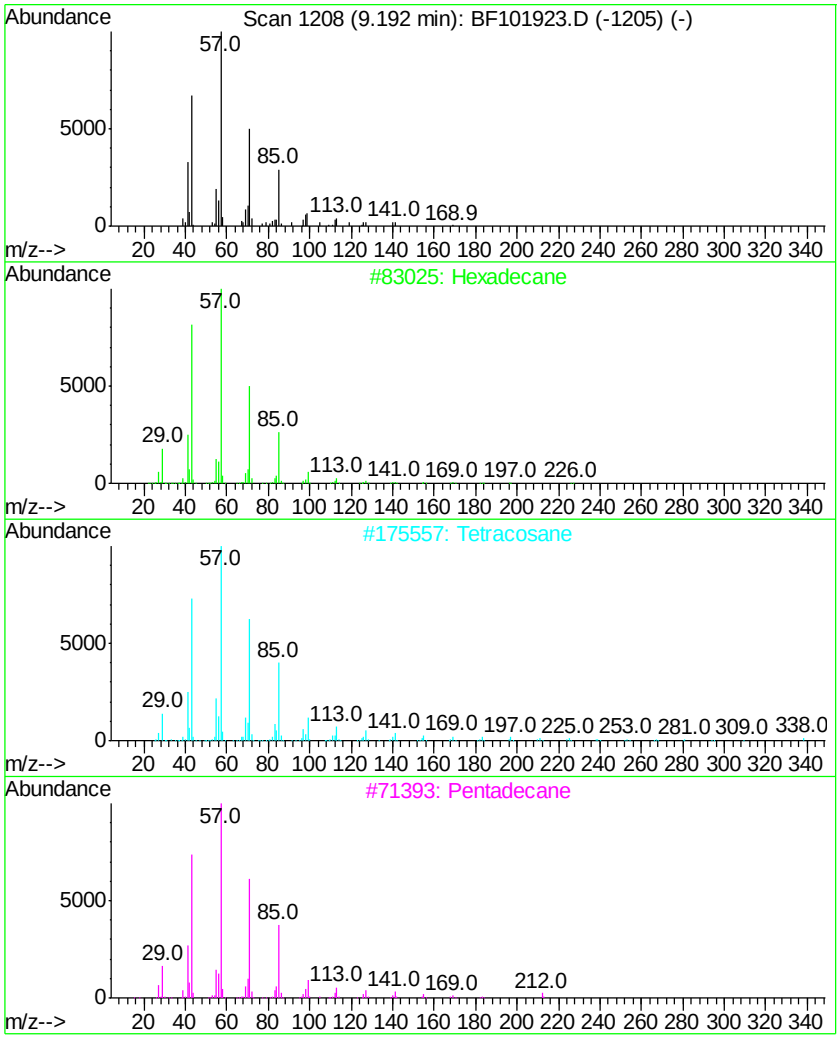
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

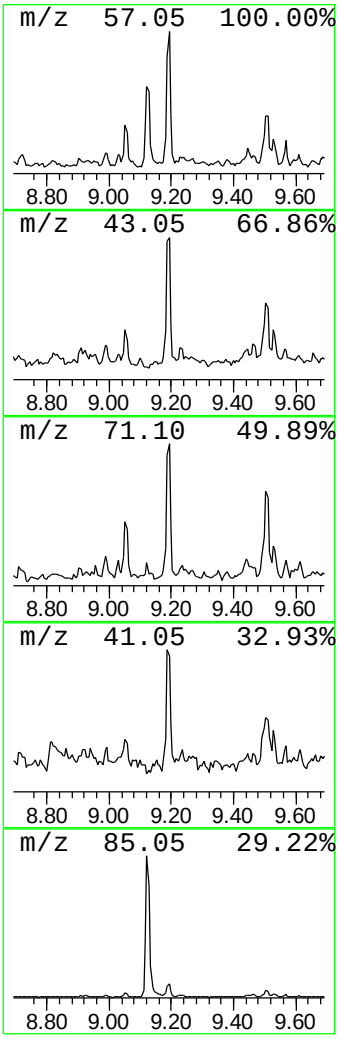
****

Peak Number 4 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.19	2.17 ng	79460	Acenaphthene-d10	9.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Tetracosane	338	C24H50	000646-31-1	80
3	Pentadecane	212	C15H32	000629-62-9	78
4	Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	78
5	Heneicosane	296	C21H44	000629-94-7	72





Data Path : U:\HPCHEM1\BNA F\DATA\BF010518\
Data File : BF101923.D
Acq On : 5 Jan 2018 12:19
Operator : SJ/JU
Sample : J1027-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR251608

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

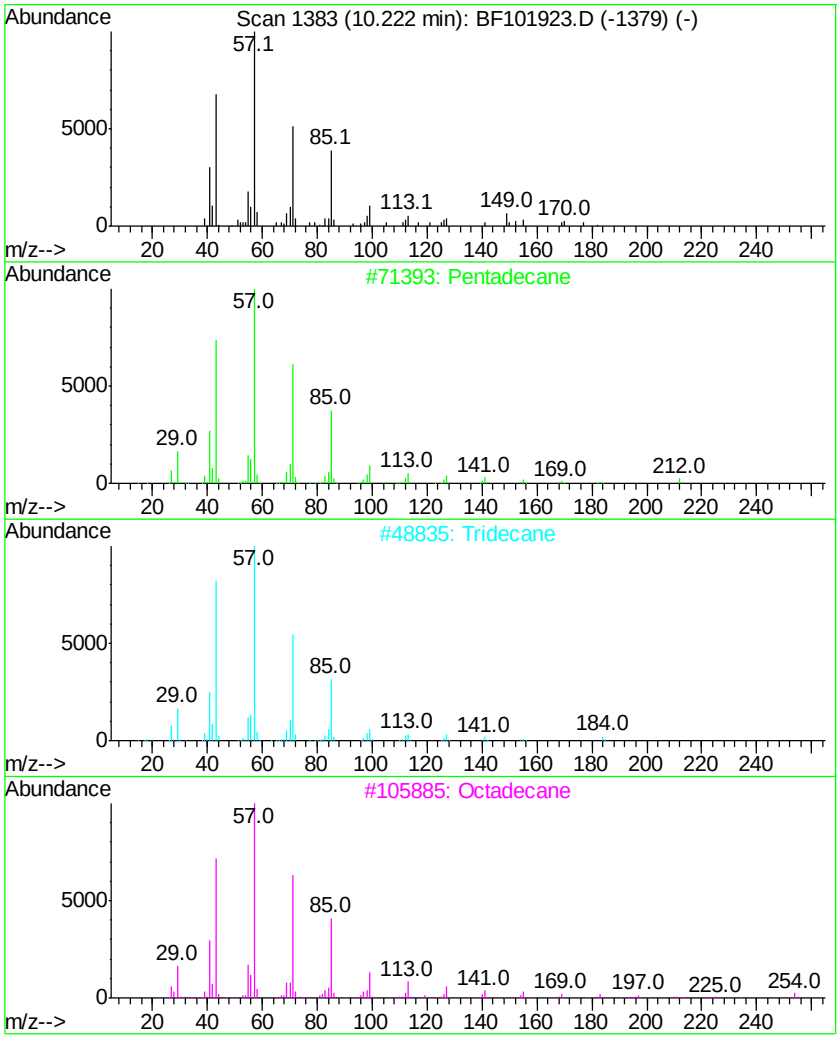
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

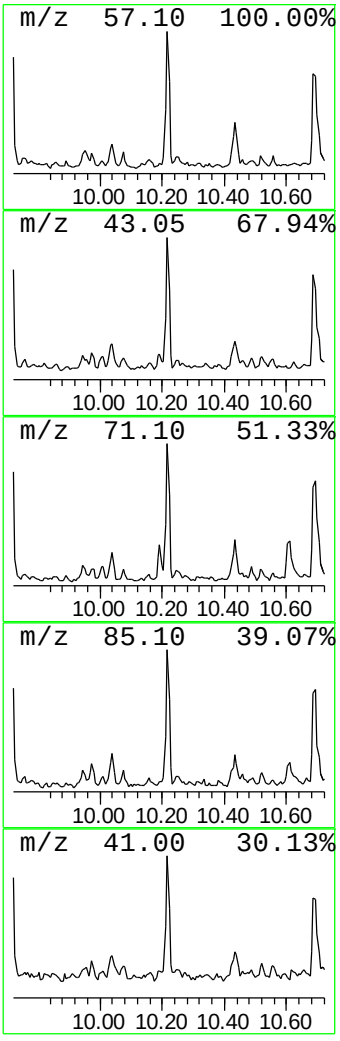
****

Peak Number 6 Pentadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.22	2.77 ng	101144	Acenaphthene-d10	9.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Tridecane	184	C13H28	000629-50-5	86
3	Octadecane	254	C18H38	000593-45-3	86
4	Tetradecane	198	C14H30	000629-59-4	80
5	Hexadecane	226	C16H34	000544-76-3	80





Data Path : U:\HPCHEM1\BNA F\DATA\BF010518\
Data File : BF101923.D
Acq On : 5 Jan 2018 12:19
Operator : SJ/JU
Sample : J1027-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR251608

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

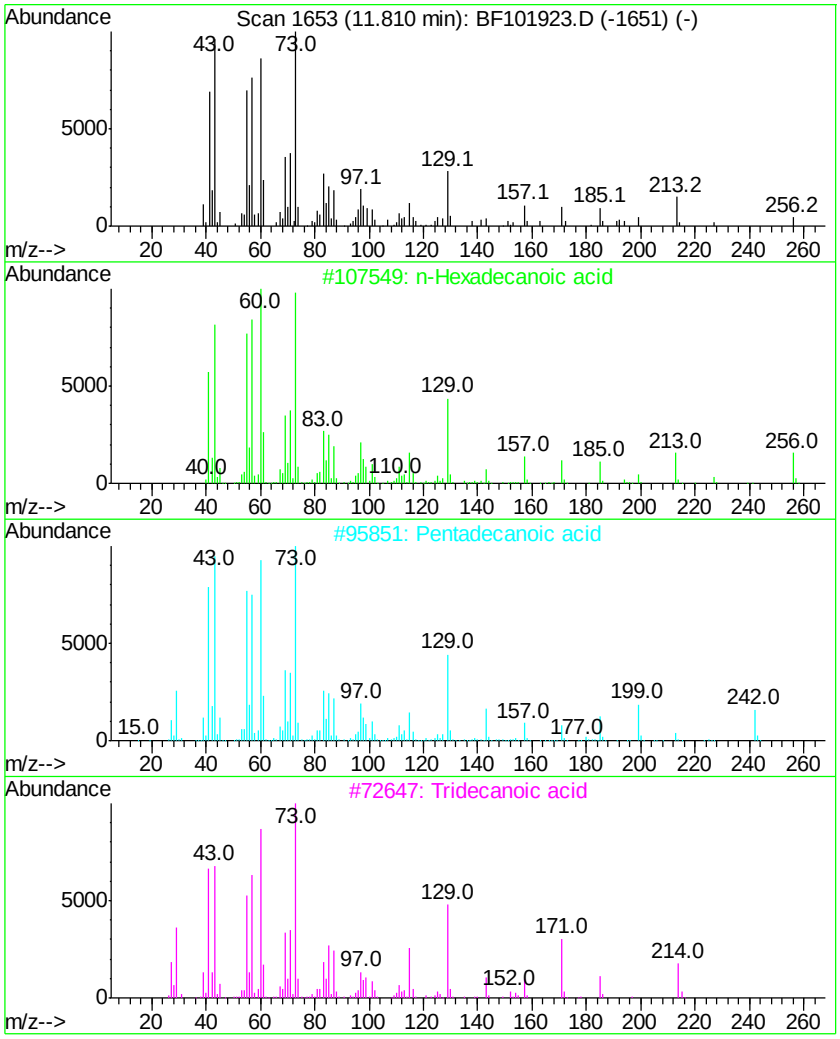
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

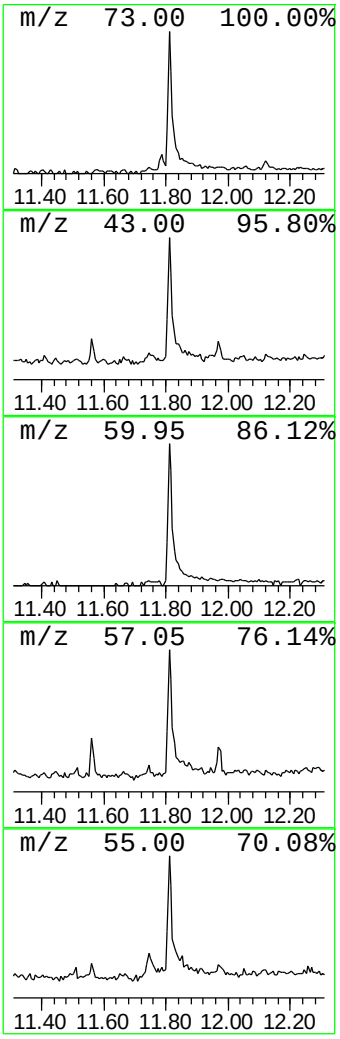
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	5.63 ng	194353	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





Data Path : U:\HPCHEM1\BNA F\DATA\BF010518\
Data File : BF101923.D
Acq On : 5 Jan 2018 12:19
Operator : SJ/JU
Sample : J1027-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR251608

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

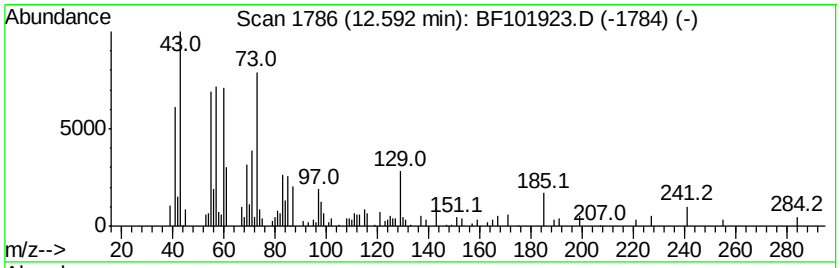
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

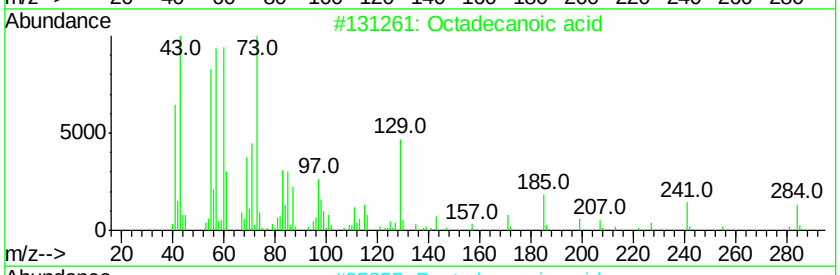
****

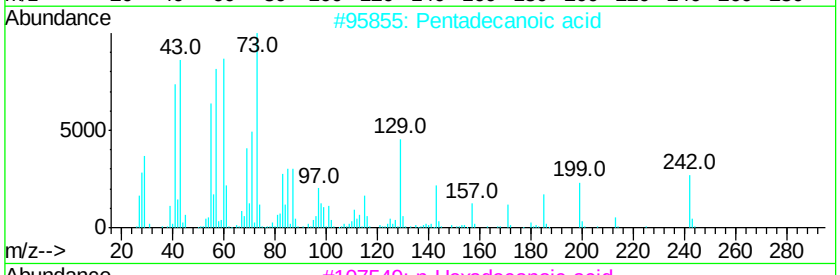
Peak Number 10 Octadecanoic acid Concentration Rank 9

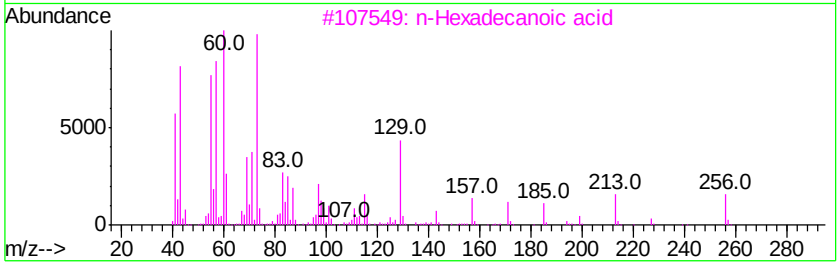
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	3.80 ng	131253	Phenanthrene-d10	11.30

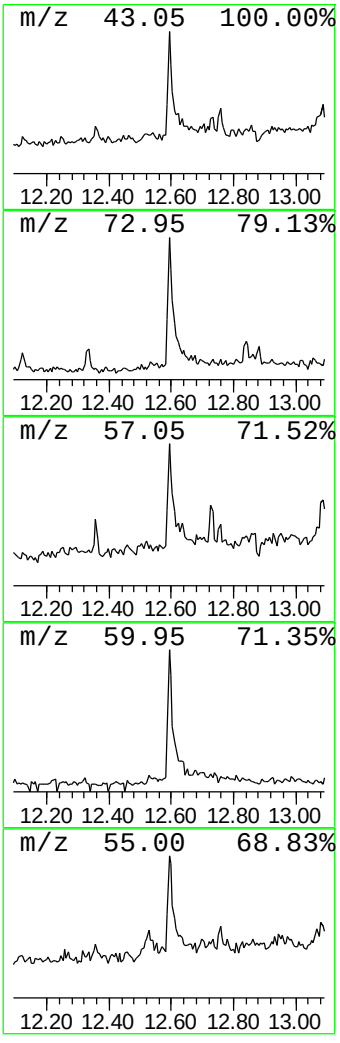
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	25











Data Path : U:\HPCHEM1\BNA F\DATA\BF010518\
Data File : BF101923.D
Acq On : 5 Jan 2018 12:19
Operator : SJ/JU
Sample : J1027-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR251608

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

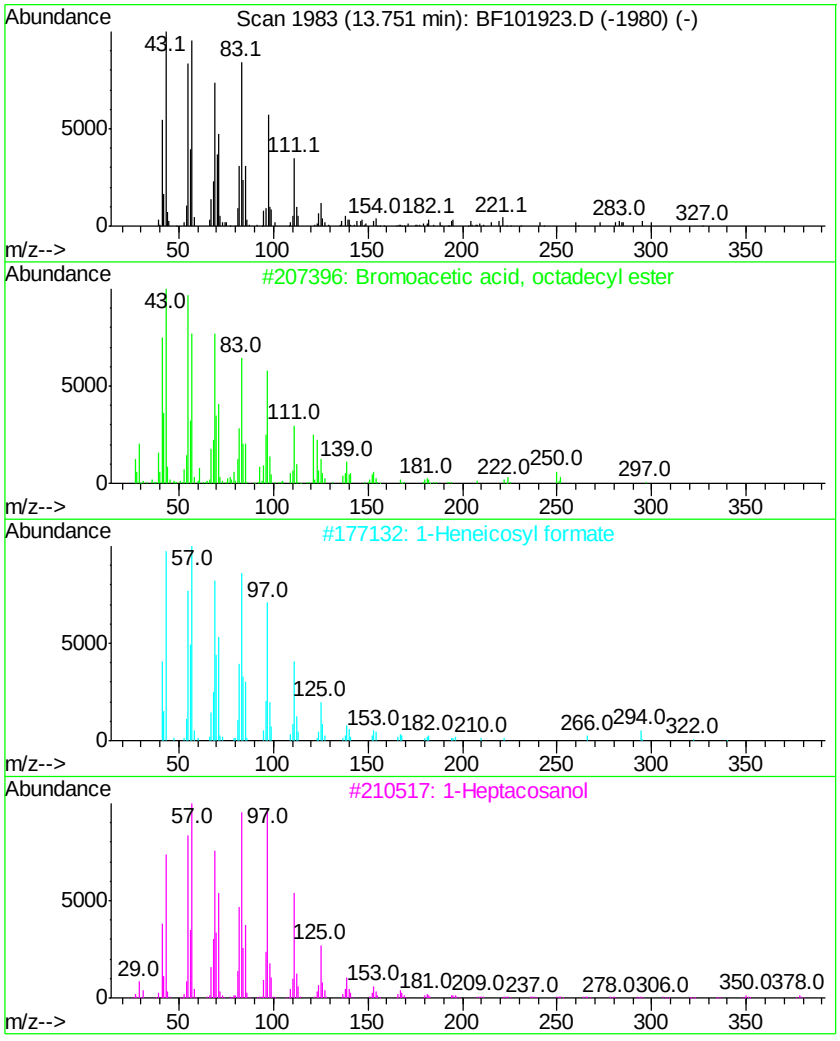
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

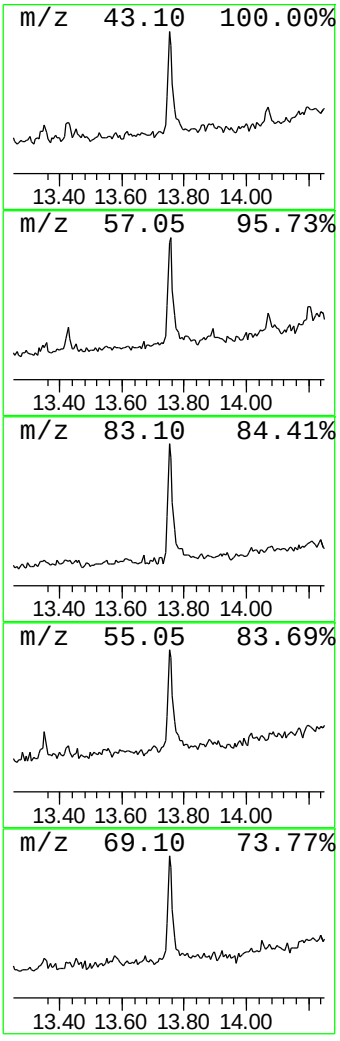
****

Peak Number 11 Bromoacetic acid, octadecyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	4.03 ng	175428	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90





Data Path : U:\HPCHEM1\BNA F\DATA\BF010518\
Data File : BF101923.D
Acq On : 5 Jan 2018 12:19
Operator : SJ/JU
Sample : J1027-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR251608

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

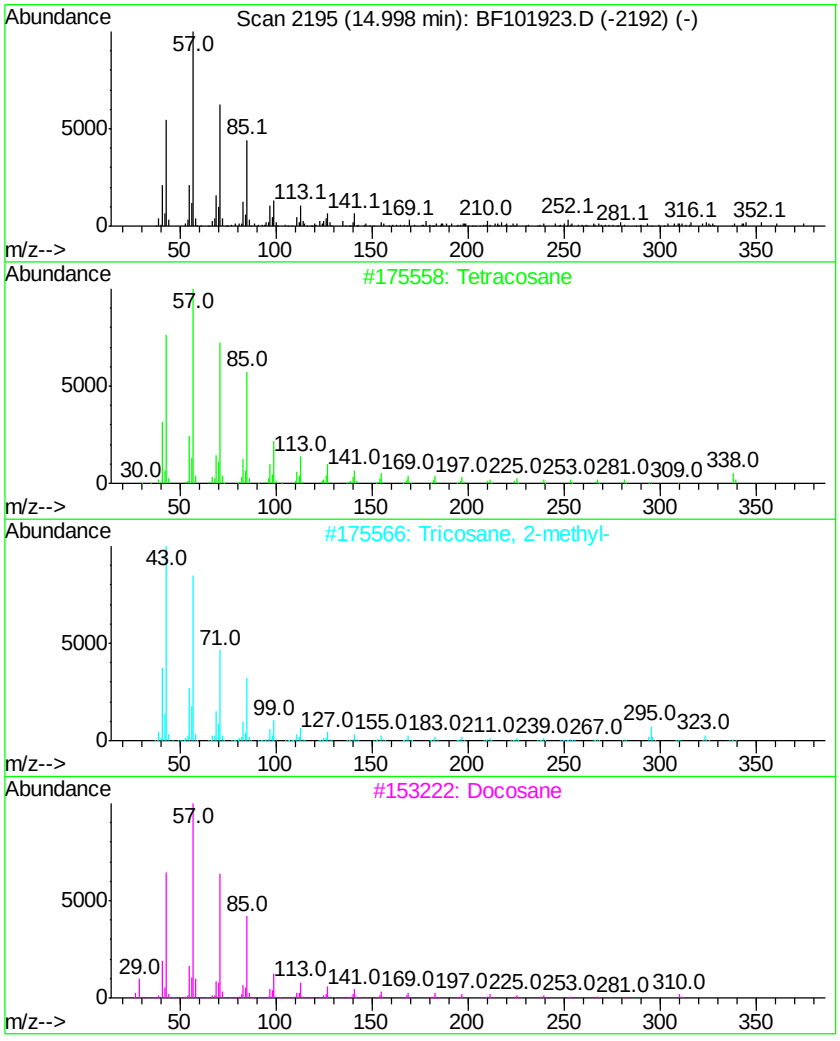
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

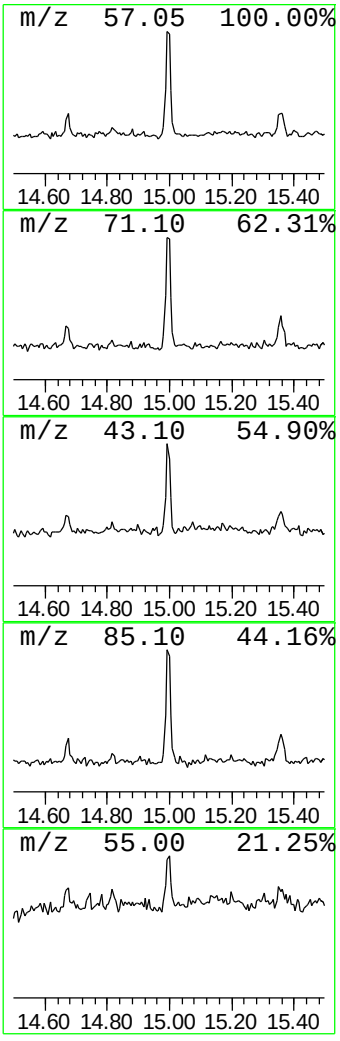
****

Peak Number 12 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	4.96 ng	147229	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	94
2	Tricosane, 2-methyl-	338	C24H50	001928-30-9	93
3	Docosane	310	C22H46	000629-97-0	93
4	Pentacosane	352	C25H52	000629-99-2	93
5	Octadecane	254	C18H38	000593-45-3	91





Data Path : U:\HPCHEM1\BNA F\DATA\BF010518\
Data File : BF101923.D
Acq On : 5 Jan 2018 12:19
Operator : SJ/JU
Sample : J1027-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR251608

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

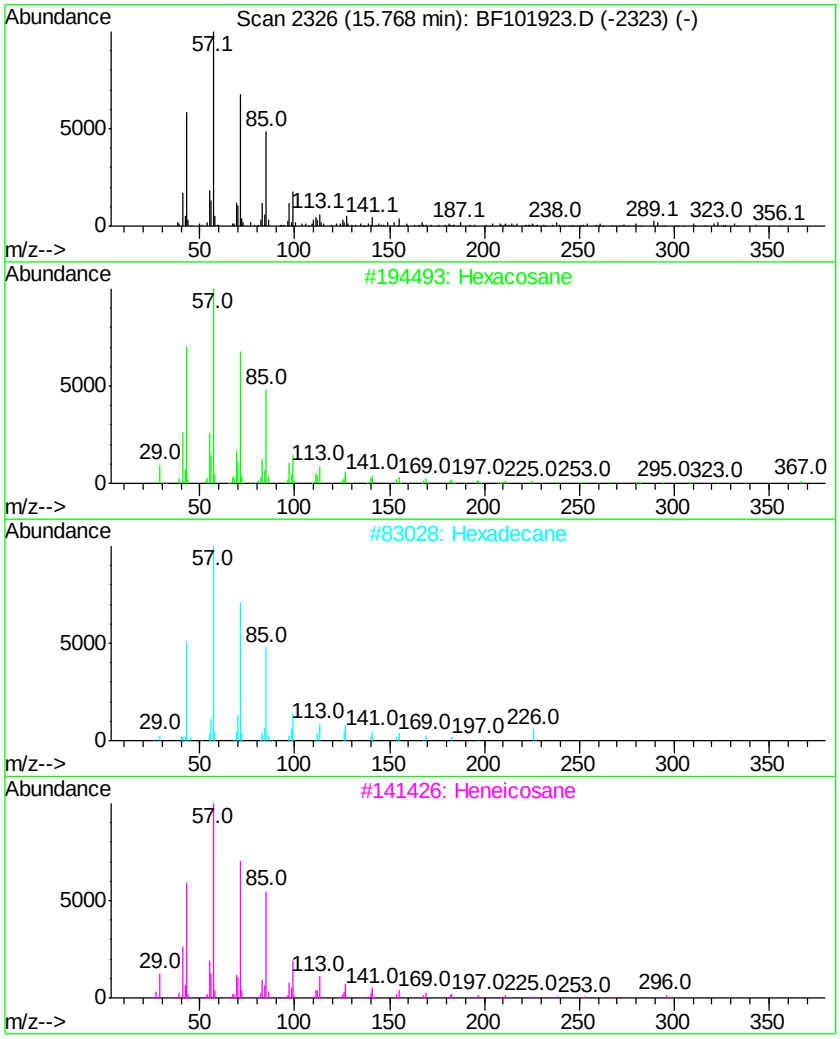
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

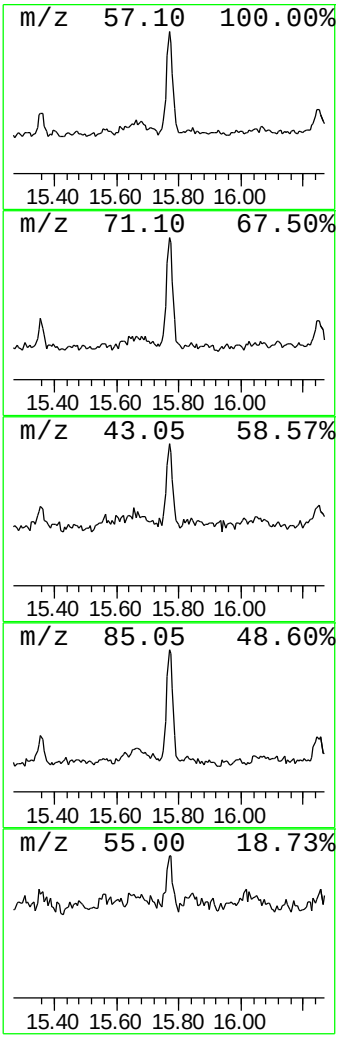
****

Peak Number 13 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	5.51 ng	163405	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Nonadecane	268	C19H40	000629-92-5	80
5	Tetracosane	338	C24H50	000646-31-1	72





Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_F\DATA\BF010518\
Data File : BF101923.D
Acq On : 5 Jan 2018 12:19
Operator : SJ/JU
Sample : J1027-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR251608

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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
2-Pentanone, 4-hy...	5.00	11.8	ng	463452	1	6.77	786430	20.0
unknown6.55	6.55	76.3	ng	3001340	1	6.77	786430	20.0
Hexadecane	9.19	2.2	ng	79460	3	9.81	730750	20.0
Pentadecane	10.22	2.8	ng	101144	3	9.81	730750	20.0
n-Hexadecanoic acid	11.81	5.6	ng	194353	4	11.30	689951	20.0
Octadecanoic acid	12.59	3.8	ng	131253	4	11.30	689951	20.0
Bromoacetic acid,...	13.75	4.0	ng	175428	5	13.96	870820	20.0
Tetracosane	15.00	5.0	ng	147229	6	15.43	593229	20.0
Hexacosane	15.77	5.5	ng	163405	6	15.43	593229	20.0