LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102309.D
Acq On : 22 Jan 2018 19:49
Operator : SJ/JU
Sample : J1116-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-3.5-4.0

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-BF012218.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	4.916	477	481	490	rBV	162224	241415	7.08%	0.801%
2	5.328	545	551	554	rBV	3082543	3268075	95.88%	10.840%
3	6.357	720	726	743	rBV	3001000	3408567	100.00%	11.306%
4	6.486	743	748	751	rBV	3489331	3362944	98.66%	11.155%
5	6.710	783	786	794	rBV	898731	805598	23.63%	2.672%
6	6.869	809	813	816	rBV	2723485	2392739	70.20%	7.937%
7	7.281	878	883	886	rBV	2171161	2107186	61.82%	6.989%
8	7.998	1000	1005	1019	rBV	1098477	1107650	32.50%	3.674%
9	9.075	1182	1188	1191	rBV	3202576	3086546	90.55%	10.238%
10	9.469	1251	1255	1258	rBV	324201	298183	8.75%	0.989%
11	9.680	1287	1291	1294	rVB	117238	91511	2.68%	0.304%
12	9.745	1298	1302	1305	rVV	1286537	1160827	34.06%	3.850%
13	9.769	1305	1306	1309	rVB	57807	41097	1.21%	0.136%
14	10.180	1372	1376	1379	rVB	141486	117694	3.45%	0.390%
15	10.398	1408	1413	1415	rBV	40661	47035	1.38%	0.156%
16	10.539	1430	1437	1440	rBV	2171350	2085798	61.19%	6.919%
17	10.651	1453	1456	1465	rVB	127175	133429	3.91%	0.443%
18	11.098	1529	1532	1535	rBV	51316	42264	1.24%	0.140%
19	11.233	1551	1555	1558	rBV	1243941	1113327	32.66%	3.693%
20	12.639	1790	1794	1797	rBV	210378	160892	4.72%	0.534%
21	12.821	1820	1825	1828	rBV	2541383	2524009	74.05%	8.372%
22	13.345	1911	1914	1917	rBV	130665	112103	3.29%	0.372%
23	13.710	1973	1976	1987	rVB	245046	278839	8.18%	0.925%
24	13.868	1997	2003	2006	rBV	962359	891648	26.16%	2.958%
25	14.033	2028	2031	2034	rBV	35814	36218	1.06%	0.120%
26	14.339	2080	2083	2087	rBV3	37619	46902	1.38%	0.156%
27	14.639	2131	2134	2143	rBV4	45817	75123	2.20%	0.249%
28	14.774	2155	2157	2162	rVB2	45411	44398	1.30%	0.147%
29	14.957	2185	2188	2190	rBV	49520	47891	1.41%	0.159%
30	15.292	2240	2245	2252	rVB	615206	800830	23.49%	2.656%
31	15.721	2315	2318	2321	rBV2	38409	51217	1.50%	0.170%
32	15.774	2323	2327	2334	rVB6	76027	130666	3.83%	0.433%
33	16.192	2395	2398	2401	rBV5	25768	35379	1.04%	0.117%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102309.D
Acq On : 22 Jan 2018 19:49
Operator : SJ/JU
Sample : J1116-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-3.5-4.0

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-BF012218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 30148000

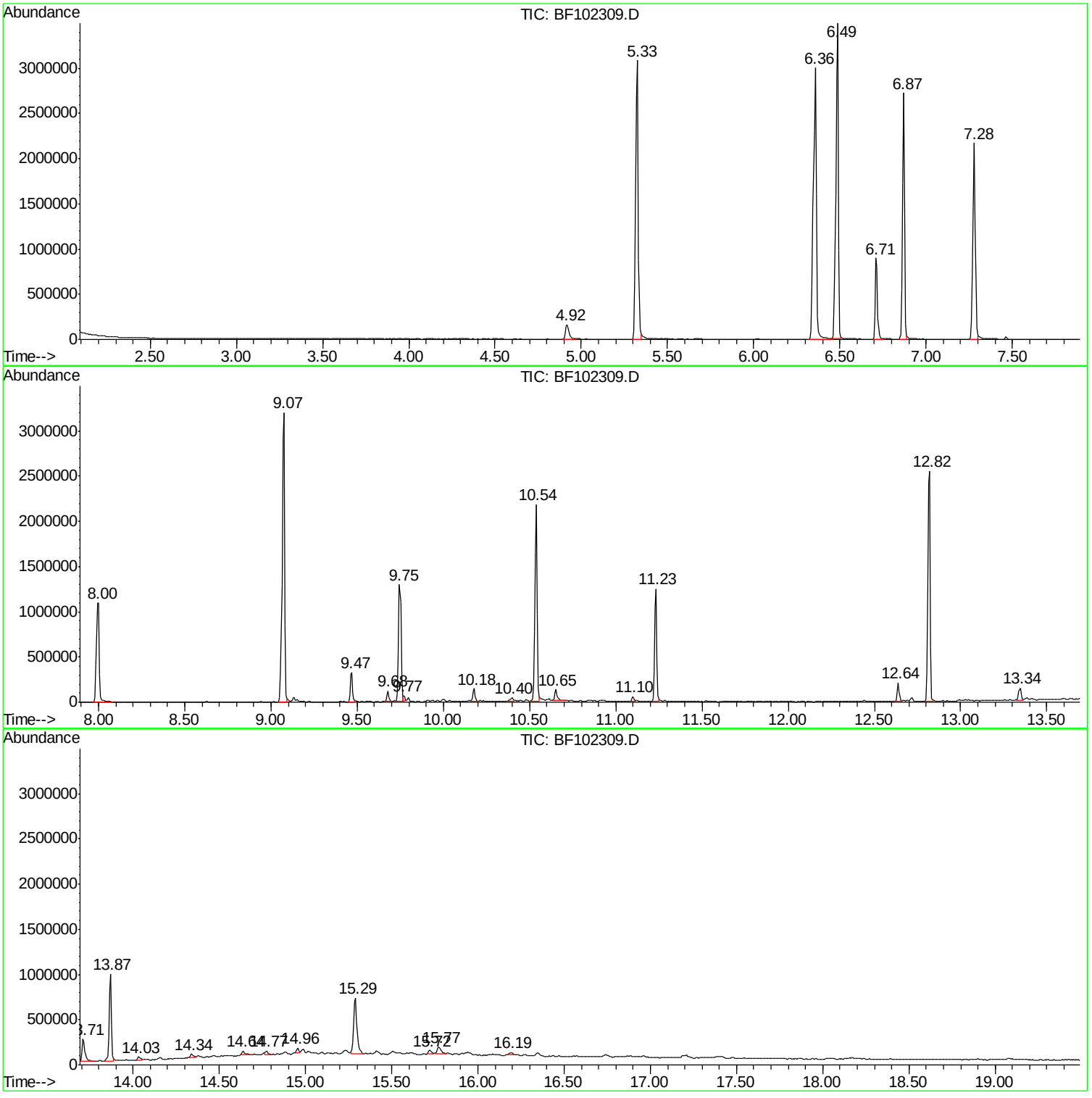
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102309.D
Acq On : 22 Jan 2018 19:49
Operator : SJ/JU
Sample : J1116-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-3.5-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102309.D
Acq On : 22 Jan 2018 19:49
Operator : SJ/JU
Sample : J1116-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-3.5-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

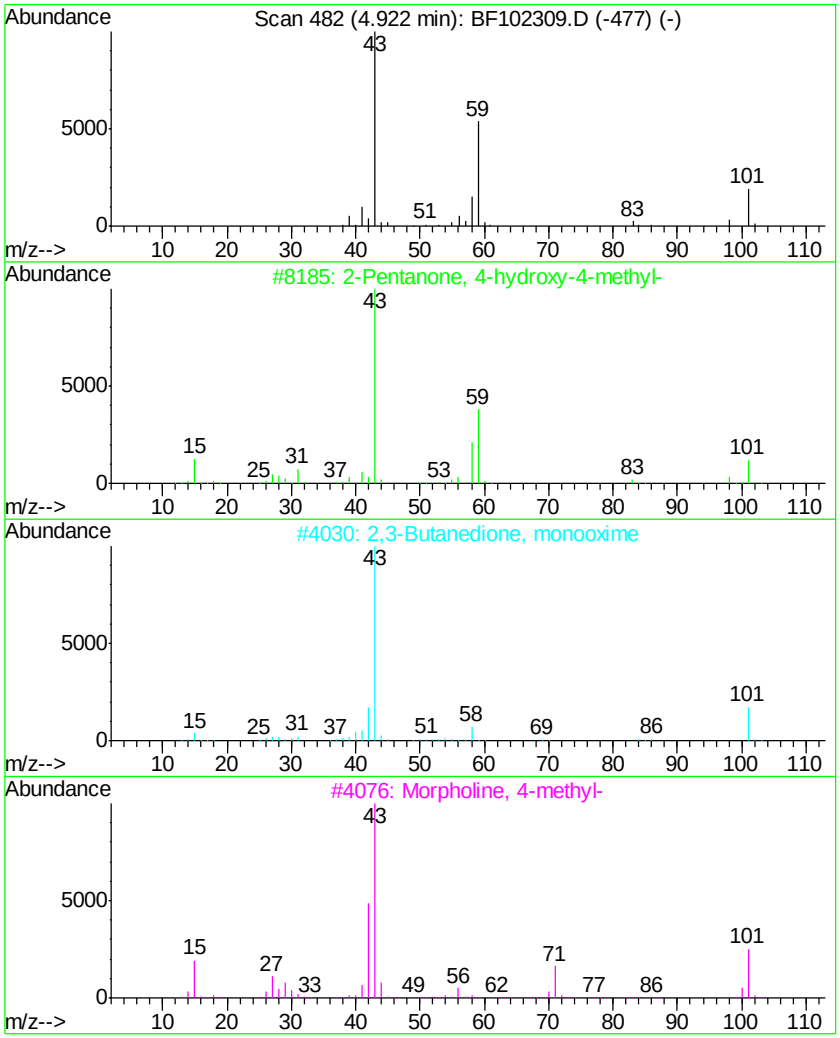
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

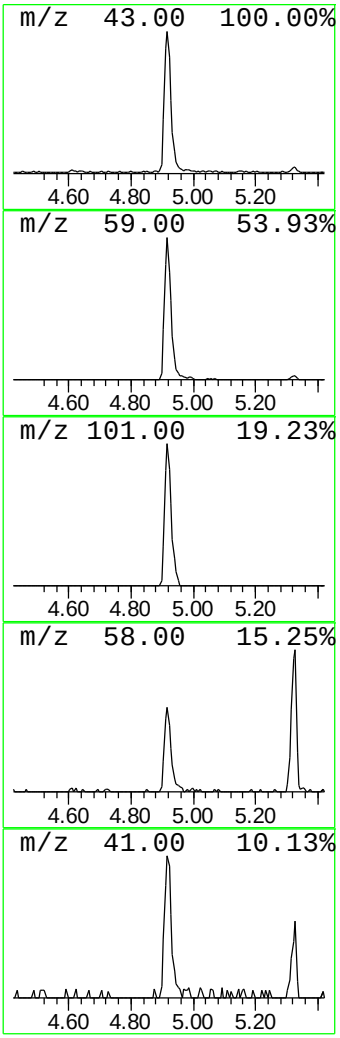
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	5.99 ng	241415	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102309.D
Acq On : 22 Jan 2018 19:49
Operator : SJ/JU
Sample : J1116-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-3.5-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

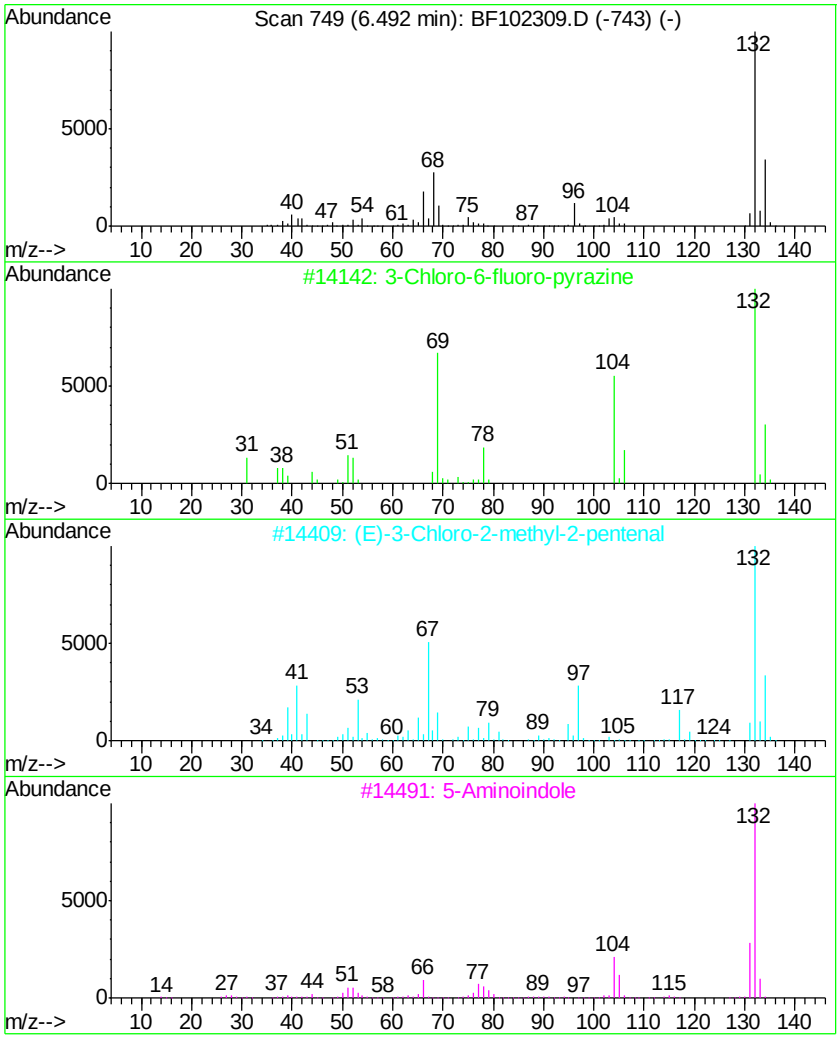
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

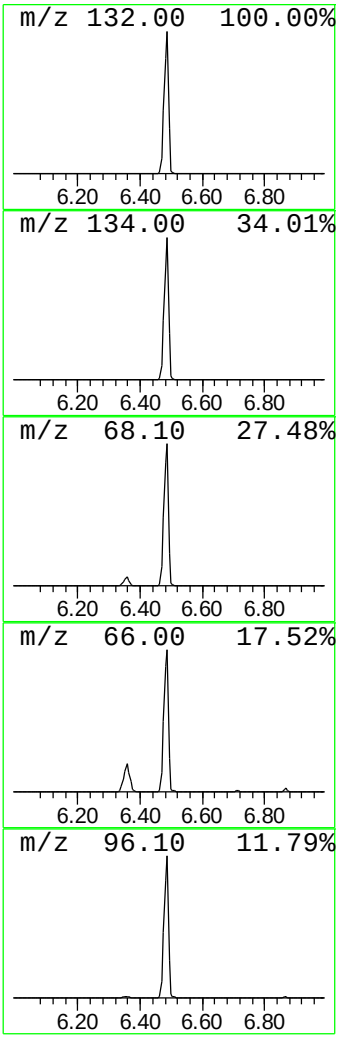
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	83.49 ng	3362940	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102309.D
Acq On : 22 Jan 2018 19:49
Operator : SJ/JU
Sample : J1116-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-3.5-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

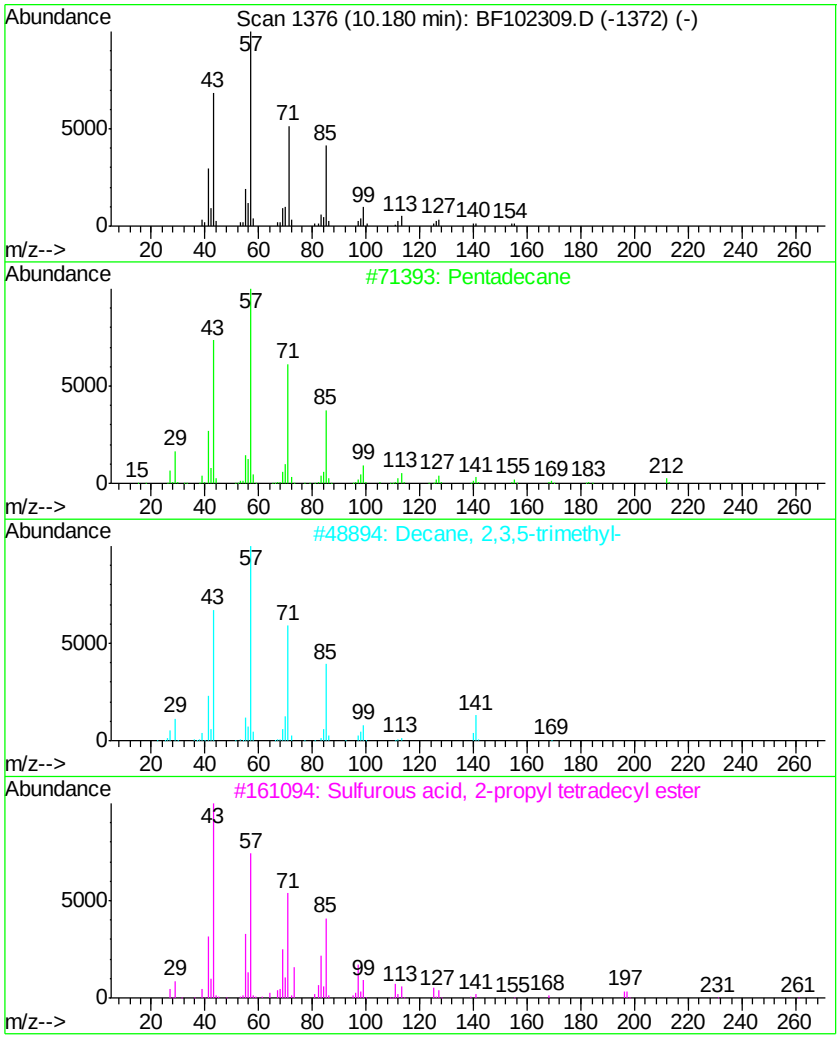
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

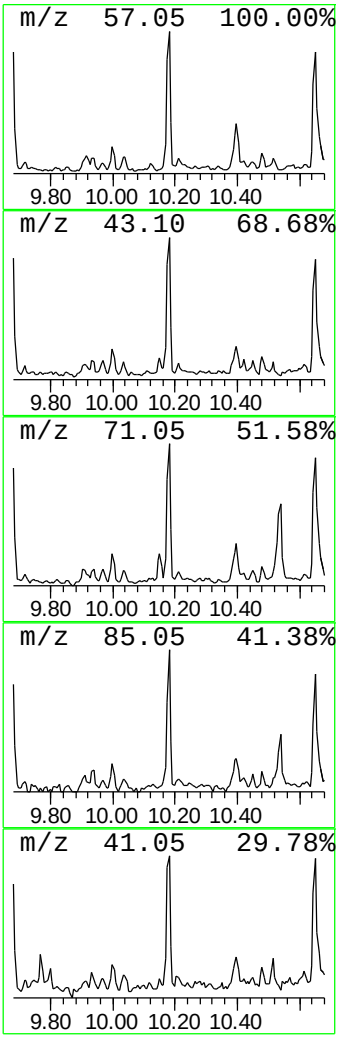
****

Peak Number 4 Pentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.18	2.03 ng	117694	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
3	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	86
4	Tetracosane	338	C24H50	000646-31-1	83
5	Hexadecane	226	C16H34	000544-76-3	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102309.D
Acq On : 22 Jan 2018 19:49
Operator : SJ/JU
Sample : J1116-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-3.5-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

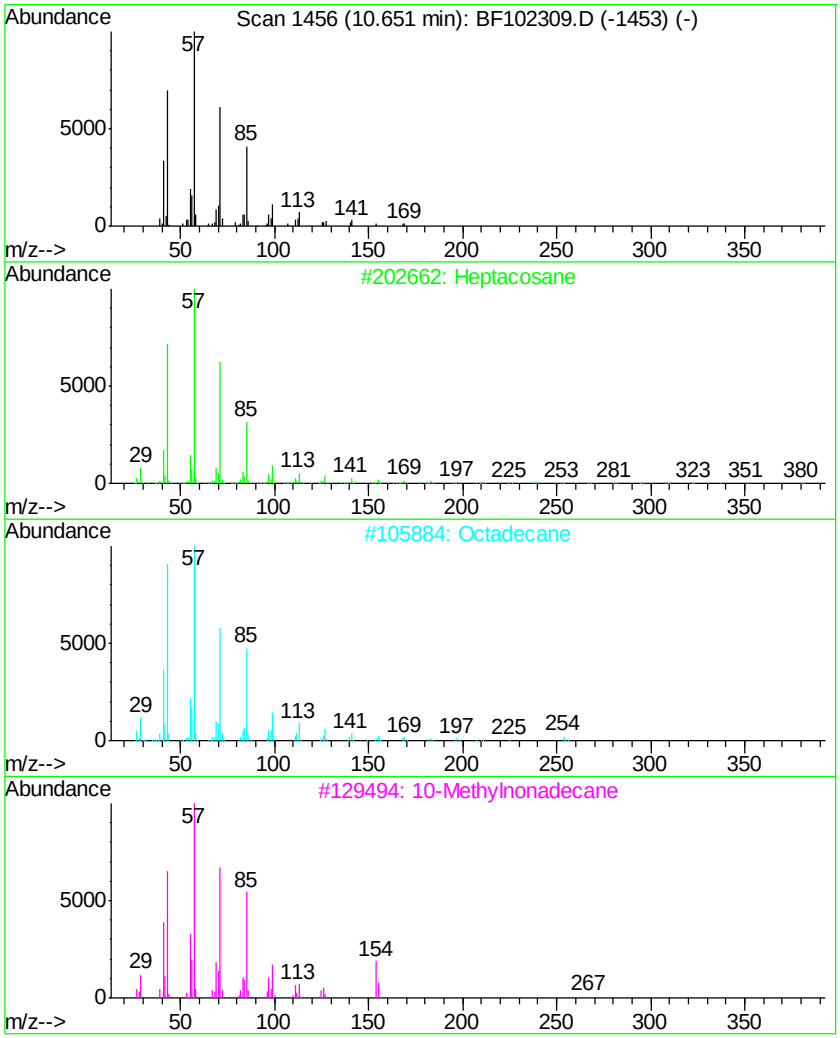
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

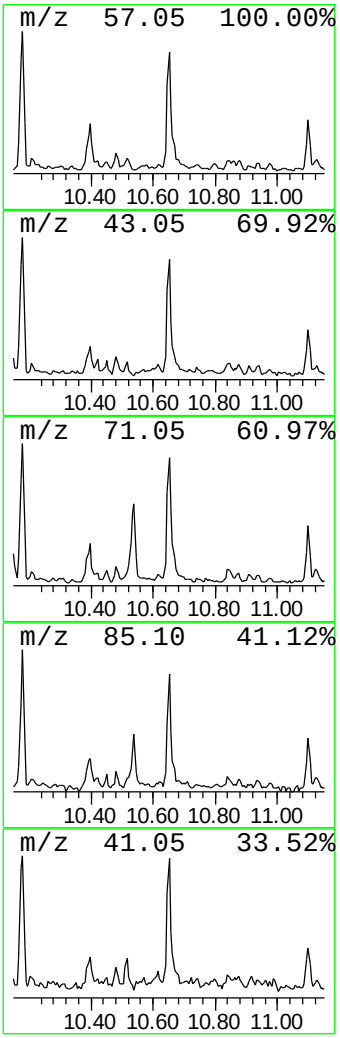
****

Peak Number 5 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	2.40 ng	133429	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Octadecane	254	C18H38	000593-45-3	91
3	10-Methylnonadecane	282	C20H42	056862-62-5	90
4	Hexadecane	226	C16H34	000544-76-3	86
5	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102309.D
Acq On : 22 Jan 2018 19:49
Operator : SJ/JU
Sample : J1116-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-3.5-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

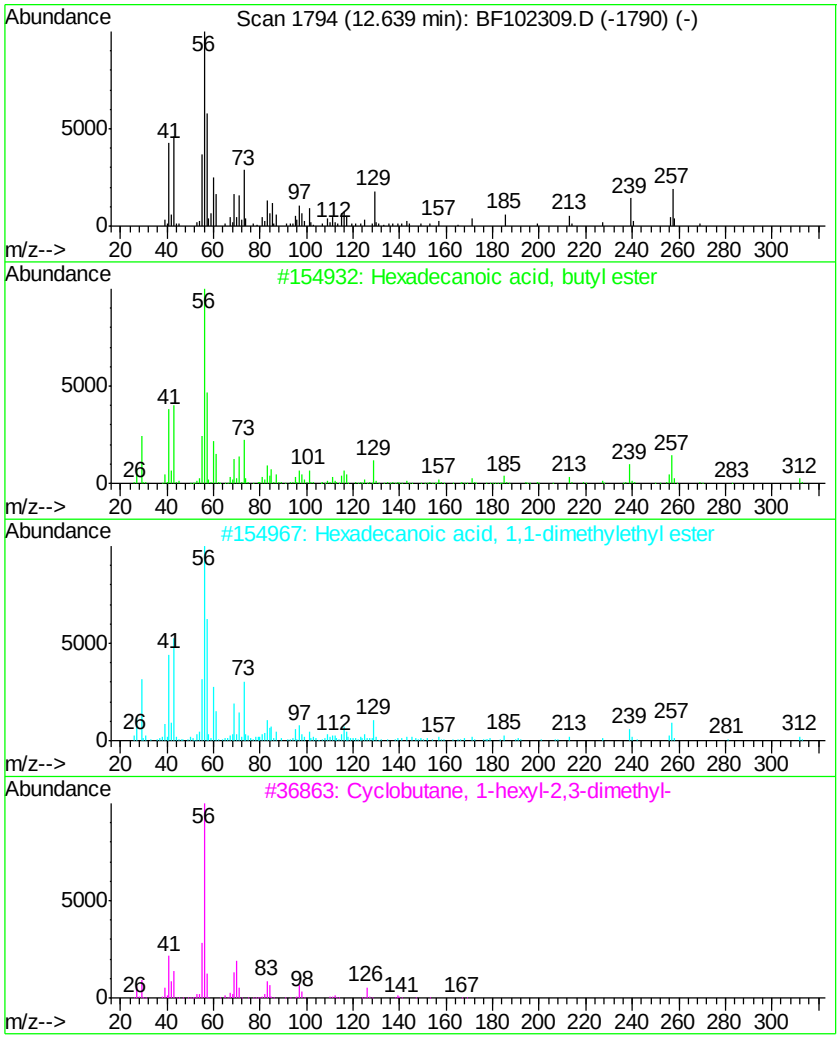
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

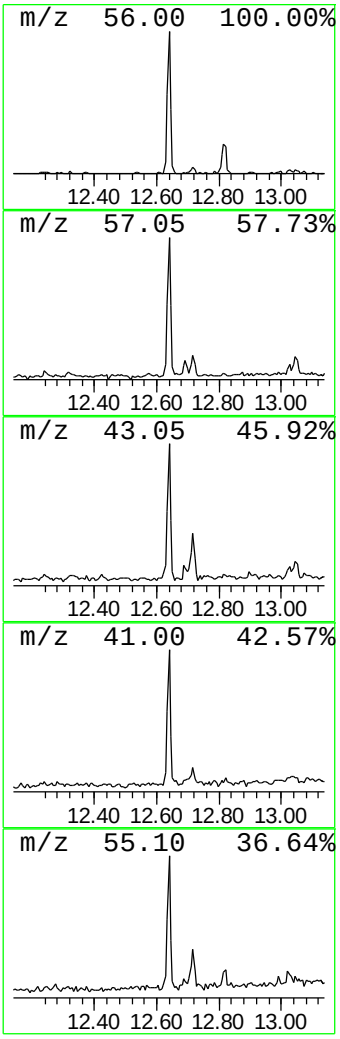
****

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	3.61 ng	160892	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
3	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5	Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	32





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102309.D
Acq On : 22 Jan 2018 19:49
Operator : SJ/JU
Sample : J1116-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-3.5-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

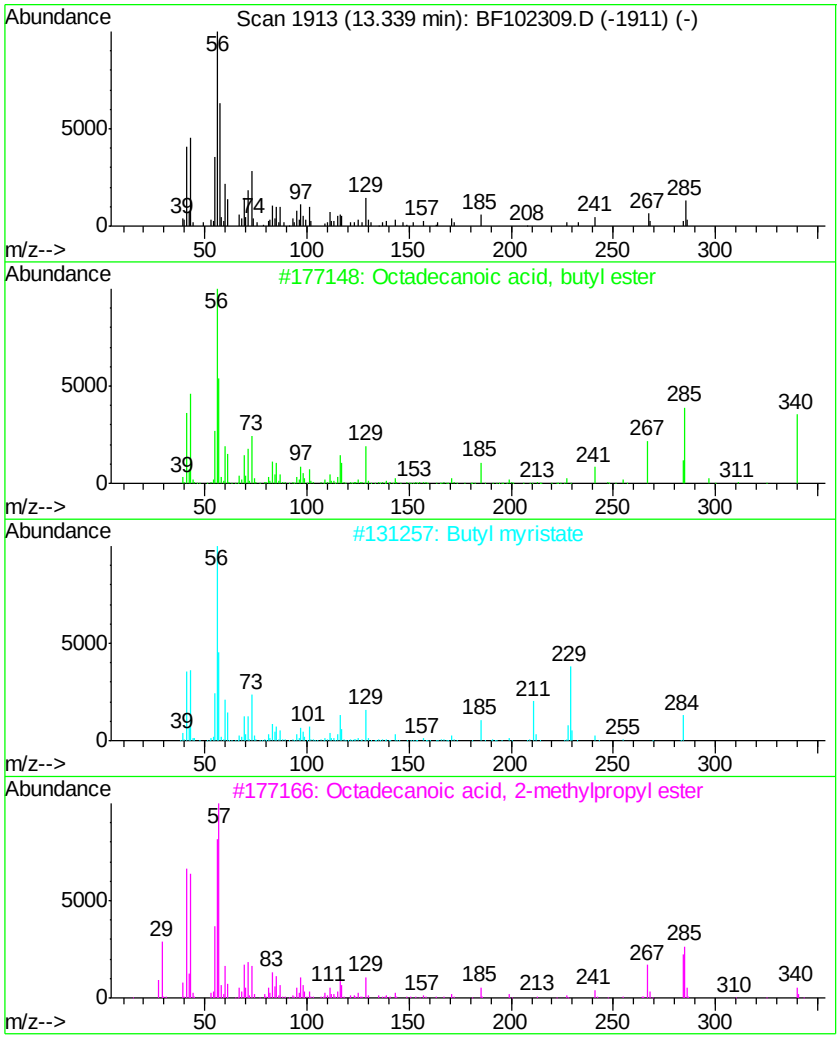
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

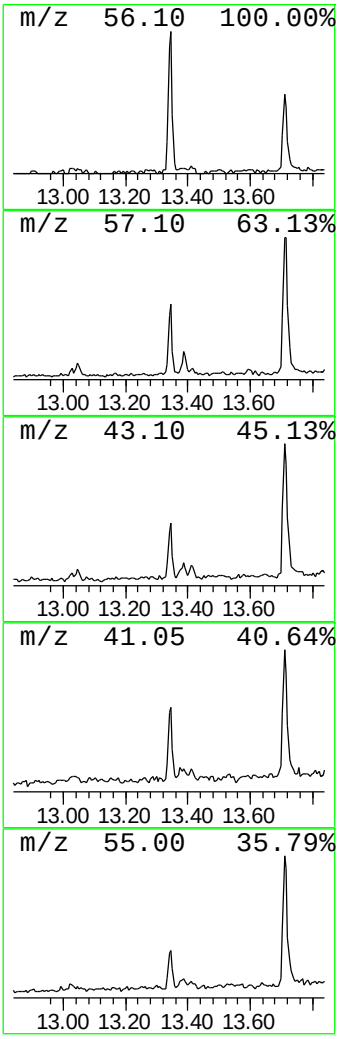
****

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	2.51 ng	112103	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2	Butyl myristate	284	C18H36O2	000110-36-1	64
3	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	43
4	Cyclopentanone, 2,2,5-trimethyl-	126	C8H14O	004573-09-5	35
5	2-Methyl-1-octadecene	266	C19H38	061868-20-0	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102309.D
Acq On : 22 Jan 2018 19:49
Operator : SJ/JU
Sample : J1116-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-3.5-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

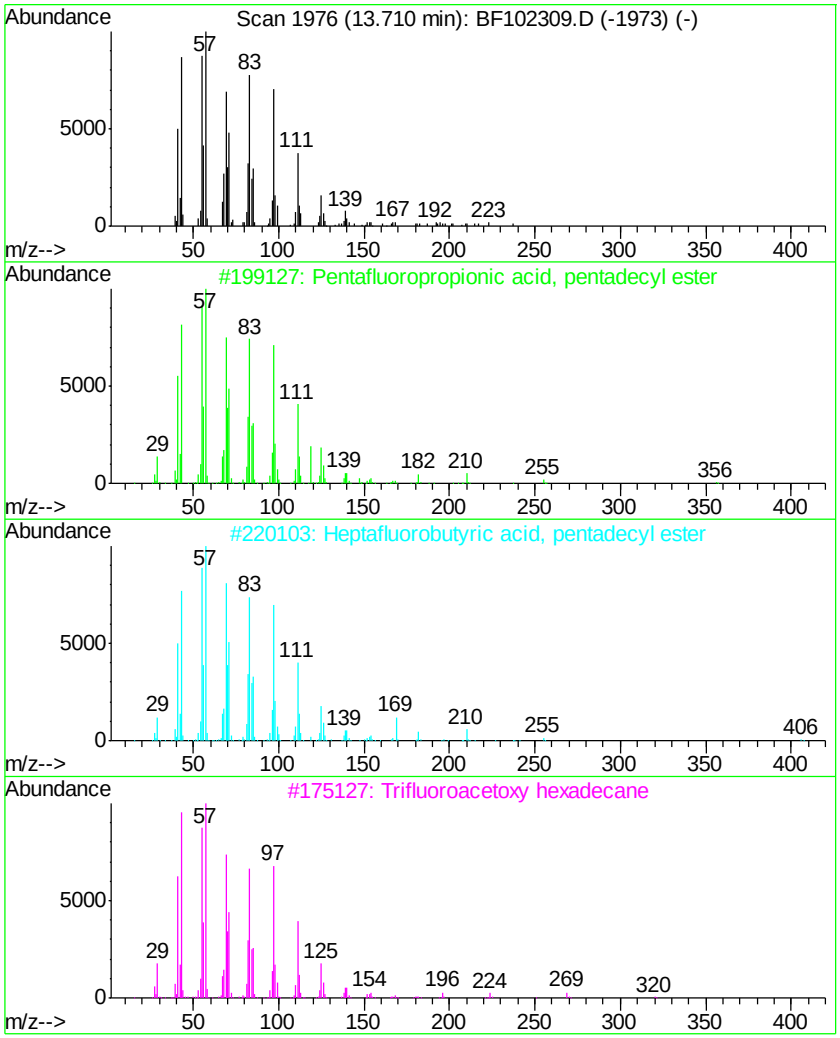
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

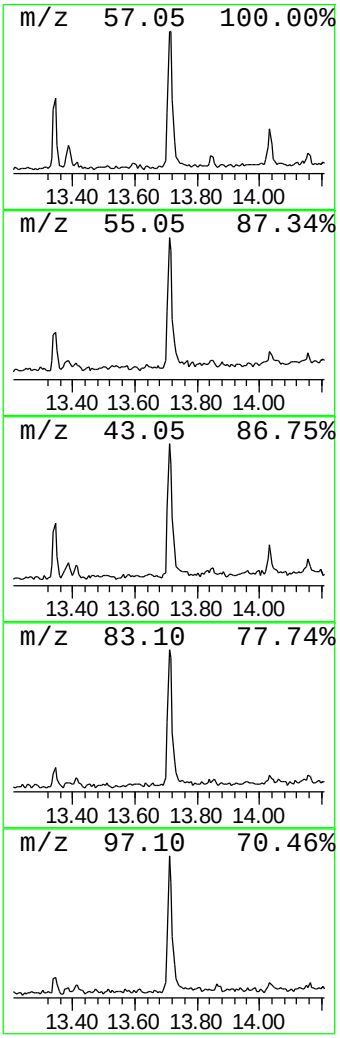
****

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	6.25 ng	278839	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102309.D
Acq On : 22 Jan 2018 19:49
Operator : SJ/JU
Sample : J1116-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-3.5-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

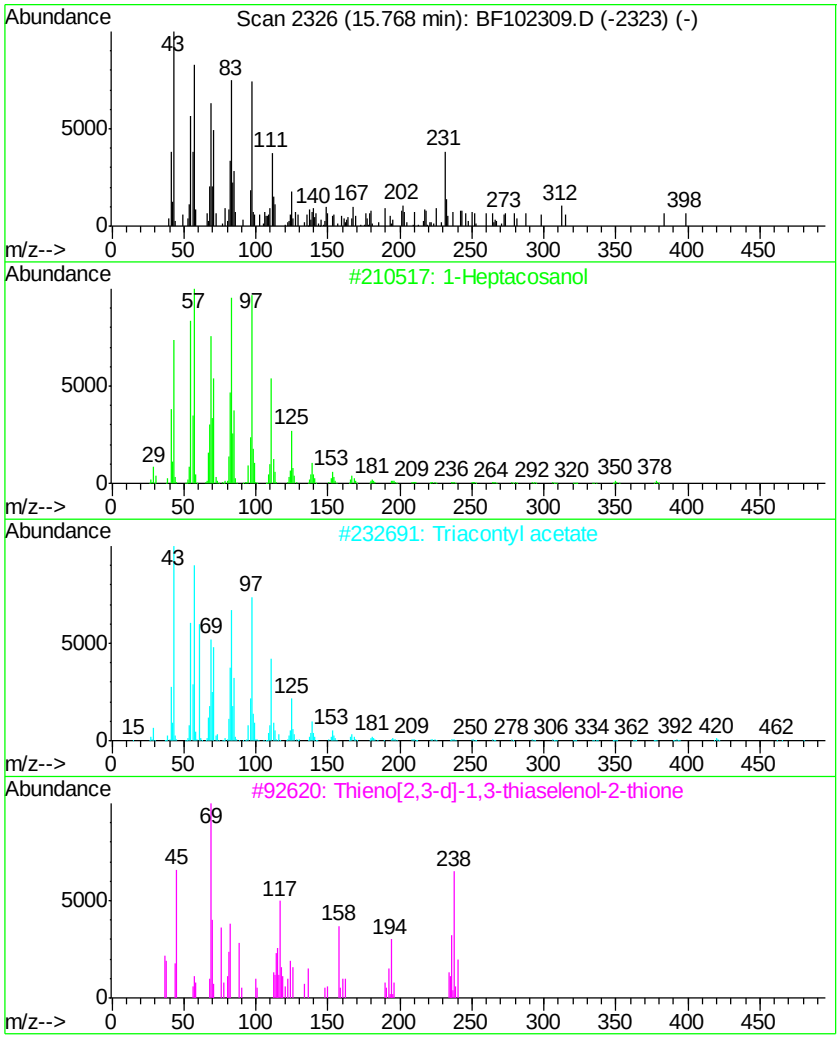
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

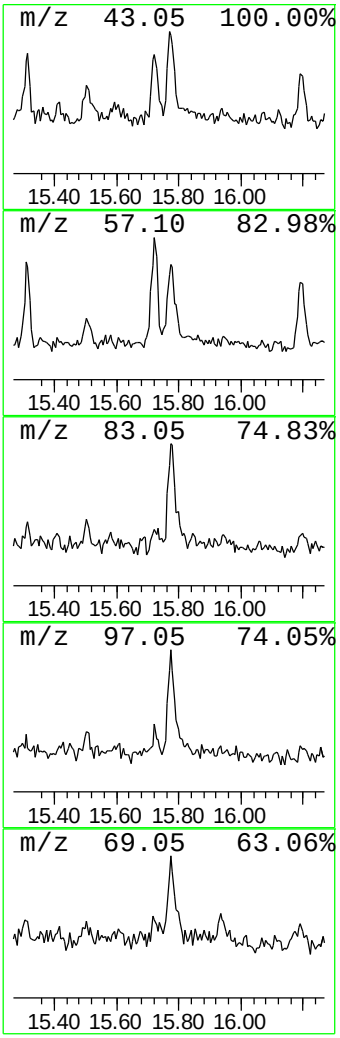
****

Peak Number 9 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	3.26 ng	130666	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	72
2	Triacontyl acetate	480	C32H64O2	041755-58-2	55
3	Thieno[2,3-d]-1,3-thiaselenol-2-...	238	C5H2S3Se	081803-09-0	53
4	Octacosanol	410	C28H58O	000557-61-9	53
5	1-Nonadecene	266	C19H38	018435-45-5	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012218\
Data File : BF102309.D
Acq On : 22 Jan 2018 19:49
Operator : SJ/JU
Sample : J1116-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-3.5-4.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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...	4.92	6.0	ng	241415	1	6.71	805598	20.0
unknown6.49	6.49	83.5	ng	3362940	1	6.71	805598	20.0
Pentadecane	10.18	2.0	ng	117694	3	9.75	1160830	20.0
Heptacosane	10.65	2.4	ng	133429	4	11.23	1113330	20.0
Hexadecanoic acid...	12.64	3.6	ng	160892	5	13.87	891648	20.0
Octadecanoic acid...	13.34	2.5	ng	112103	5	13.87	891648	20.0
Pentafluoropropio...	13.71	6.3	ng	278839	5	13.87	891648	20.0
1-Heptacosanol	15.77	3.3	ng	130666	6	15.29	800830	20.0