LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102156.D
Acq On : 17 Jan 2018 18:06
Operator : SJ/JU
Sample : J1152-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LTP-3

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-BF010918.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	4.934	477	484	492	rBV	197206	291263	7.55%	0.859%
2	5.334	547	552	555	rBV	3328433	3751590	97.21%	11.064%
3	6.363	720	727	730	rBV	3279548	3859103	100.00%	11.381%
4	6.492	744	749	752	rBV	3937132	3815833	98.88%	11.253%
5	6.722	784	788	791	rBV	1030744	906119	23.48%	2.672%
6	6.875	810	814	817	rBV	3095674	2790899	72.32%	8.230%
7	7.287	878	884	887	rBV	2428810	2414455	62.57%	7.120%
8	7.998	1001	1005	1009	rBV	1312682	1218374	31.57%	3.593%
9	8.557	1095	1100	1104	rBV	212976	175243	4.54%	0.517%
10	9.081	1183	1189	1192	rBV	4052198	3595903	93.18%	10.604%
11	9.475	1251	1256	1259	rBV	463485	434860	11.27%	1.282%
12	9.751	1299	1303	1307	rVB	1360933	1228232	31.83%	3.622%
13	10.404	1409	1414	1418	rBV	60750	70210	1.82%	0.207%
14	10.469	1420	1425	1428	rBV	682663	546643	14.17%	1.612%
15	10.545	1433	1438	1441	rBV	2183060	2183072	56.57%	6.438%
16	10.669	1455	1459	1466	rVB	138991	155839	4.04%	0.460%
17	11.133	1535	1538	1543	rVB	70719	73073	1.89%	0.215%
18	11.233	1551	1555	1558	rBV	1200699	1061208	27.50%	3.130%
19	11.257	1558	1559	1563	rVB	175919	105296	2.73%	0.311%
20	11.763	1642	1645	1649	rBV	94780	92036	2.38%	0.271%
21	12.439	1757	1760	1763	rBV	157477	142942	3.70%	0.422%
22	12.669	1793	1799	1802	rBV	136866	142438	3.69%	0.420%
23	12.821	1820	1825	1828	rBV	2572703	2363344	61.24%	6.970%
24	13.292	1902	1905	1908	rBV	255172	224418	5.82%	0.662%
25	13.710	1973	1976	1983	rVB	138109	152340	3.95%	0.449%
26	13.863	1997	2002	2005	rBV	783522	856517	22.19%	2.526%
27	13.892	2005	2007	2009	rVB	66658	54892	1.42%	0.162%
28	14.345	2081	2084	2087	rBV3	38188	42967	1.11%	0.127%
29	14.621	2127	2131	2135	rBV	193820	223311	5.79%	0.659%
30	14.874	2171	2174	2177	rBV	75247	105510	2.73%	0.311%
31	15.221	2230	2233	2238	rBV	46114	52573	1.36%	0.155%
32	15.280	2238	2243	2248	rBV	620630	778766	20.18%	2.297%

LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102156.D
Acq On : 17 Jan 2018 18:06
Operator : SJ/JU
Sample : J1152-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LTP-3

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-BF010918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 33909269

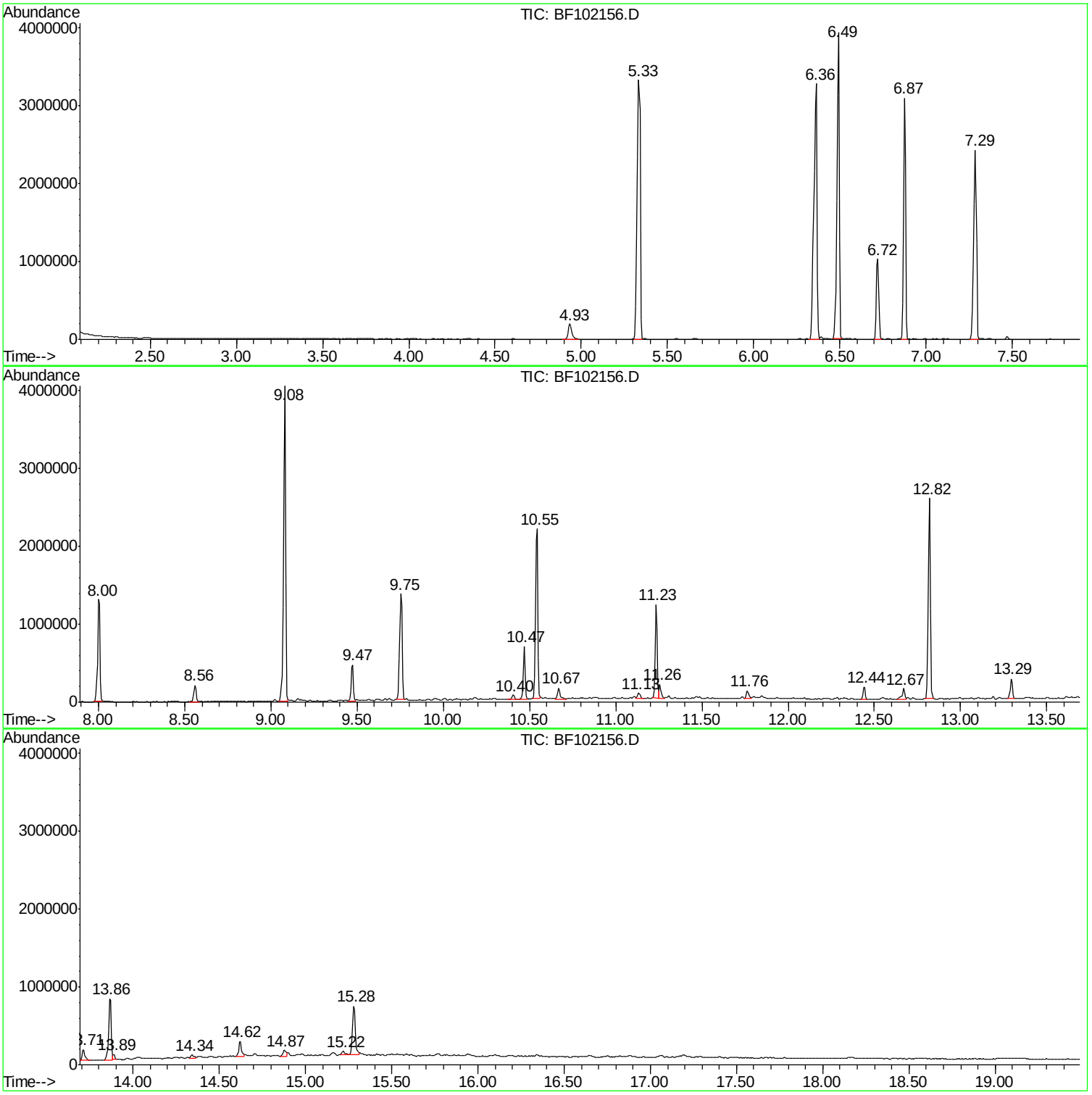
LSC Report - Integrated Chromatogram

Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102156.D
Acq On : 17 Jan 2018 18:06
Operator : SJ/JU
Sample : J1152-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LTP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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 : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102156.D
Acq On : 17 Jan 2018 18:06
Operator : SJ/JU
Sample : J1152-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LTP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

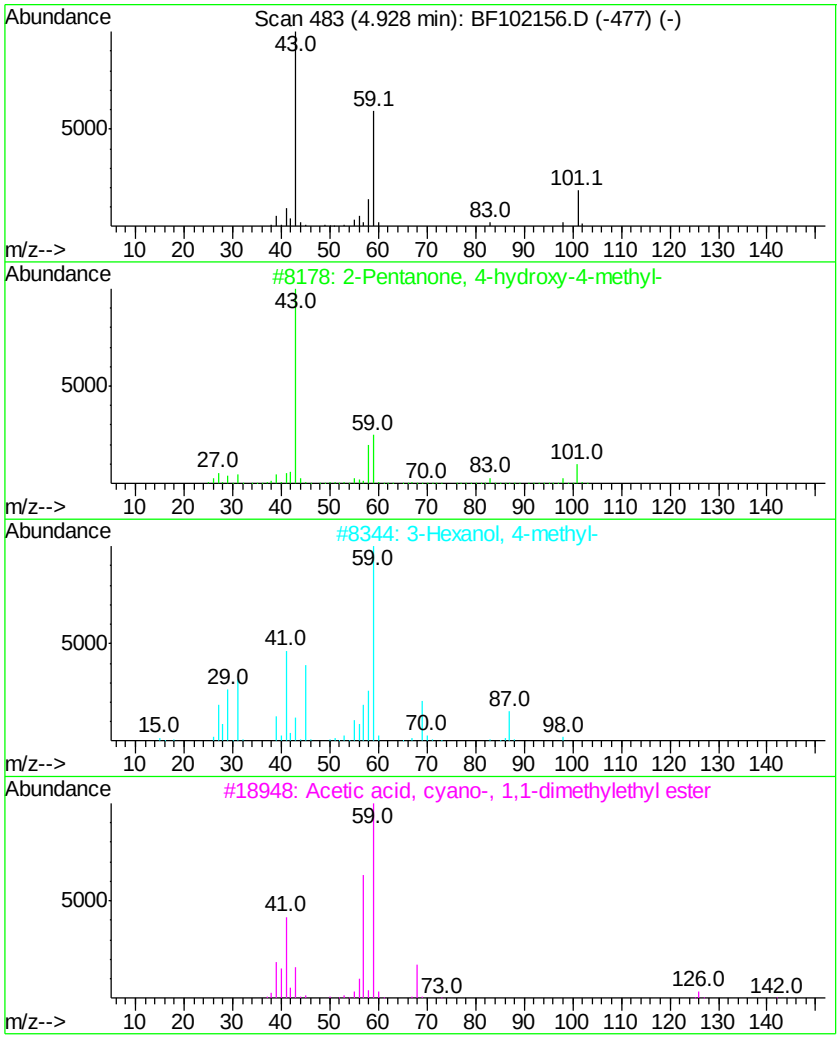
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

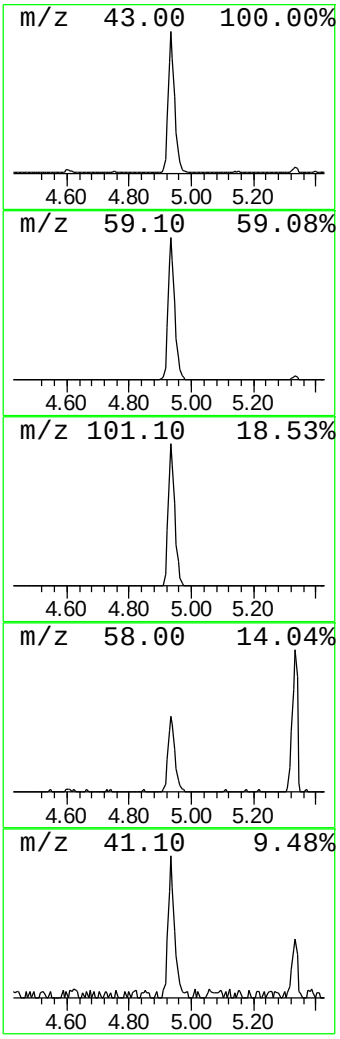
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	6.43 ng	291263	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102156.D
Acq On : 17 Jan 2018 18:06
Operator : SJ/JU
Sample : J1152-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LTP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

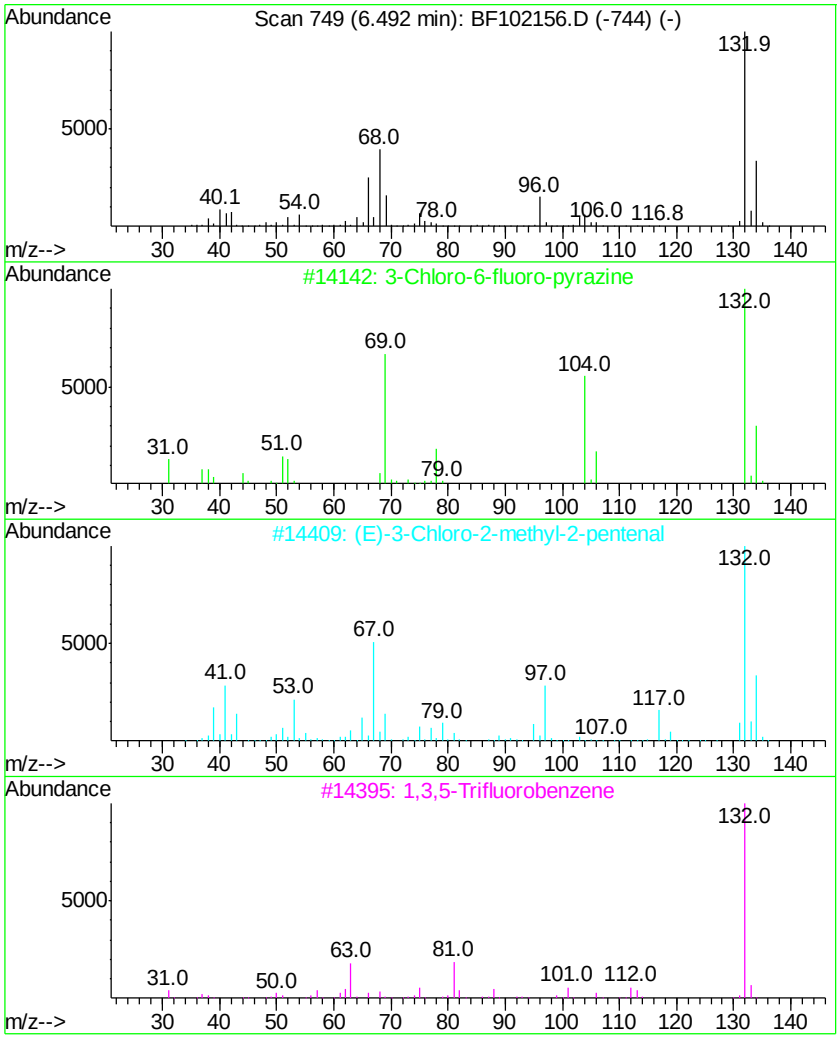
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

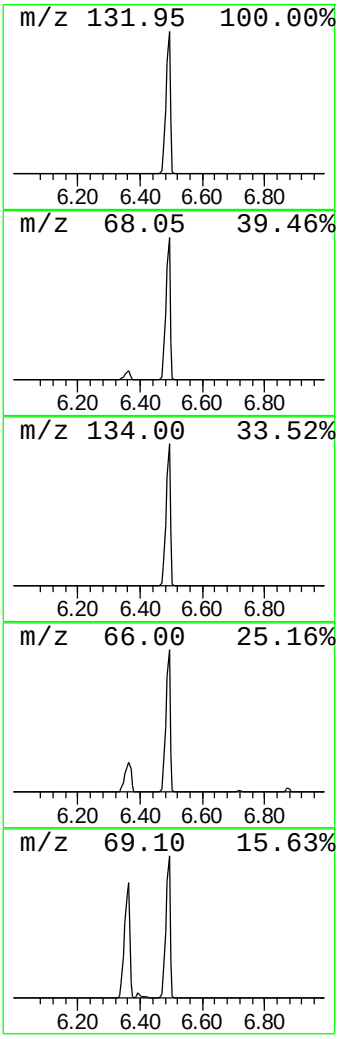
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	84.22 ng	3815830	1,4-Dichlorobenzene-d4	6.72

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	16
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102156.D
Acq On : 17 Jan 2018 18:06
Operator : SJ/JU
Sample : J1152-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LTP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

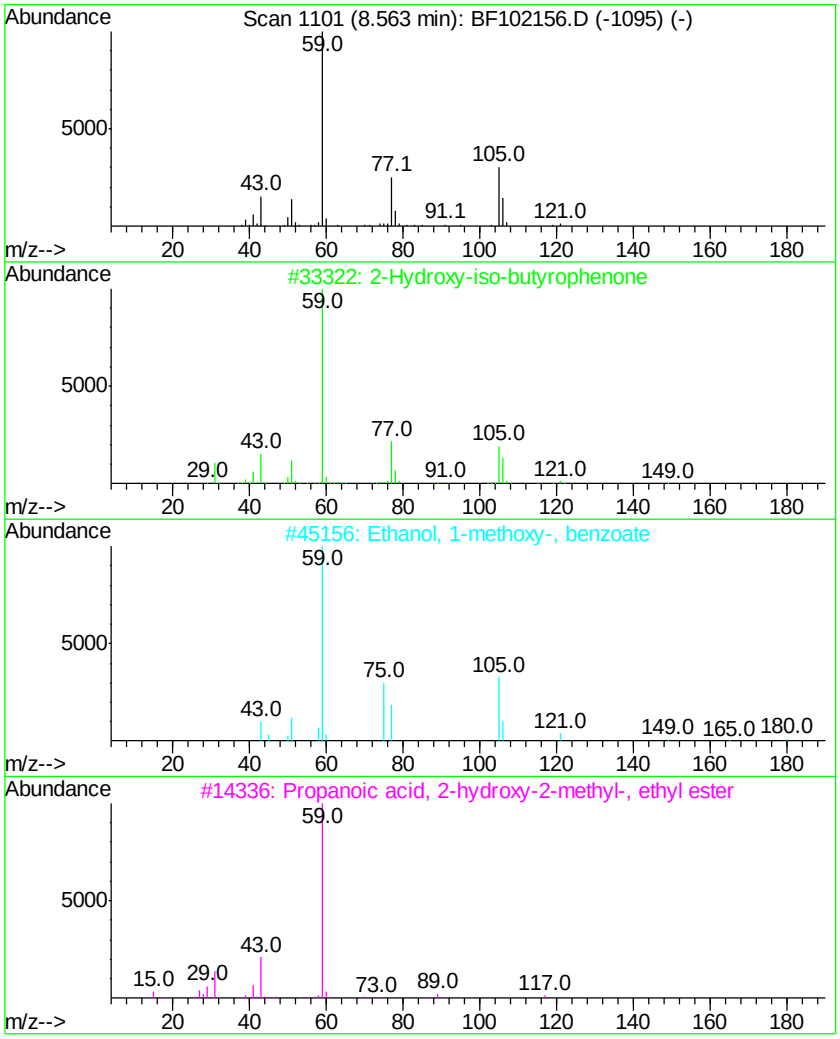
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

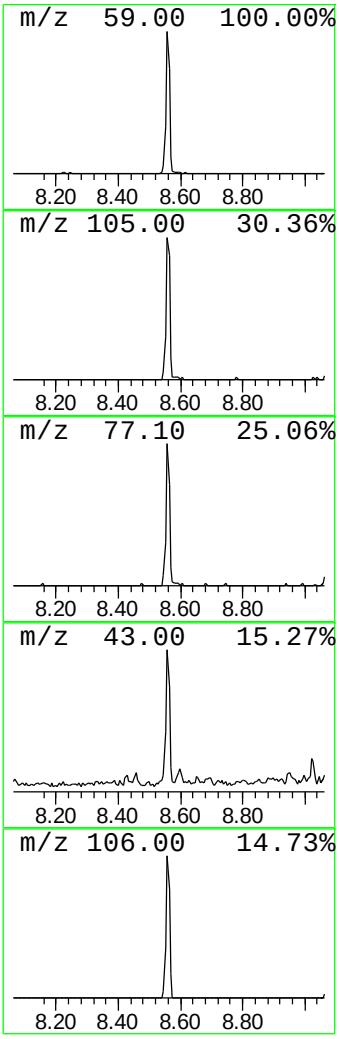
****

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.56	2.88 ng	175243	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3	Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	9
4	Guanidine	59	CH5N3	000113-00-8	7
5	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	7





Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102156.D
Acq On : 17 Jan 2018 18:06
Operator : SJ/JU
Sample : J1152-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LTP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

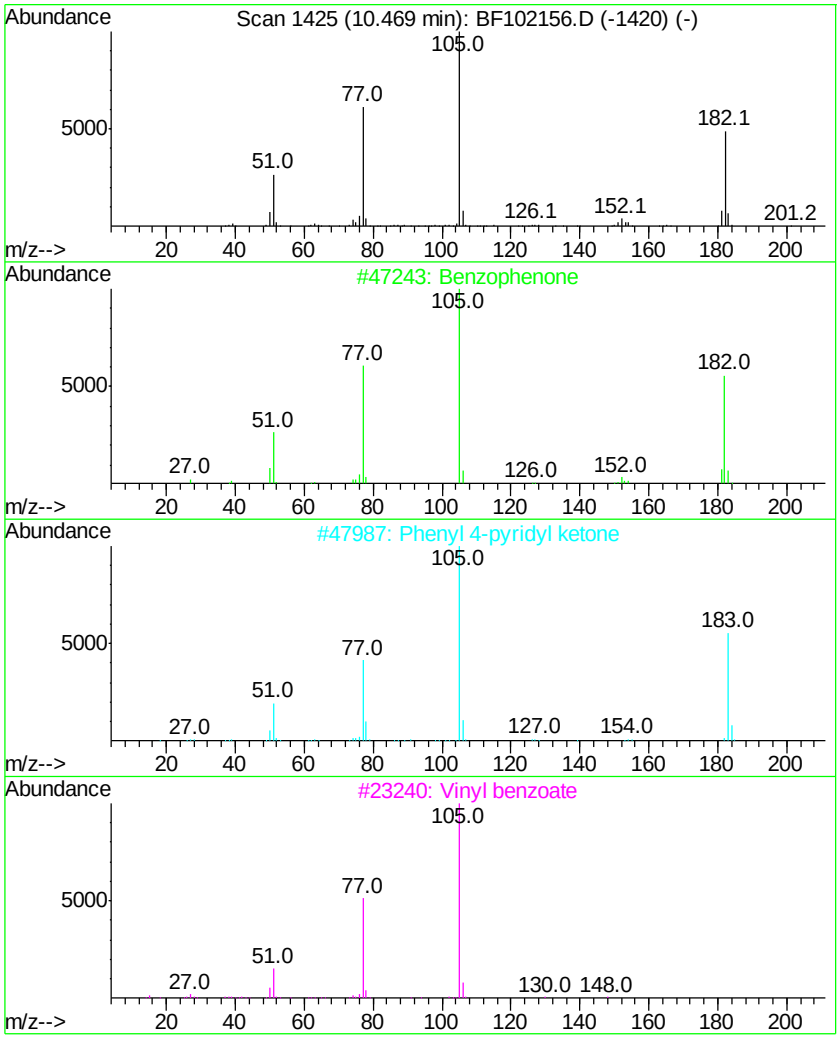
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

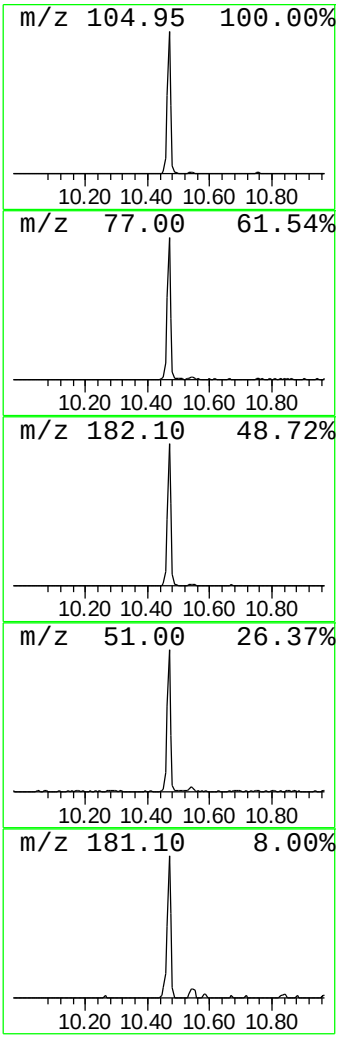
****

Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.47	8.90 ng	546643	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3	Vinyl benzoate	148	C9H8O2	000769-78-8	47
4	Benzenebutanoic acid, .gamma.-ox...	192	C11H12O3	025333-24-8	47
5	5-[N-Benzoylaminomethyl]tetrazole	203	C9H9N5O	1000227-36-3	47





Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
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Acq On : 17 Jan 2018 18:06
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Sample : J1152-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LTP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

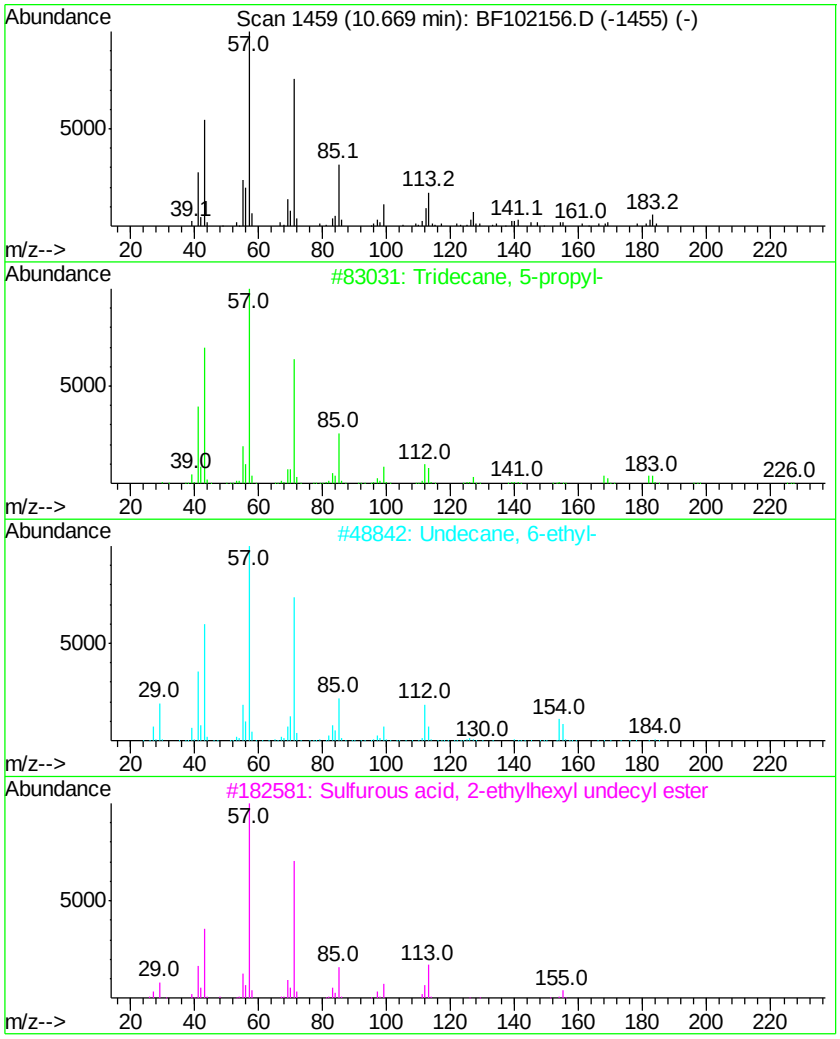
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

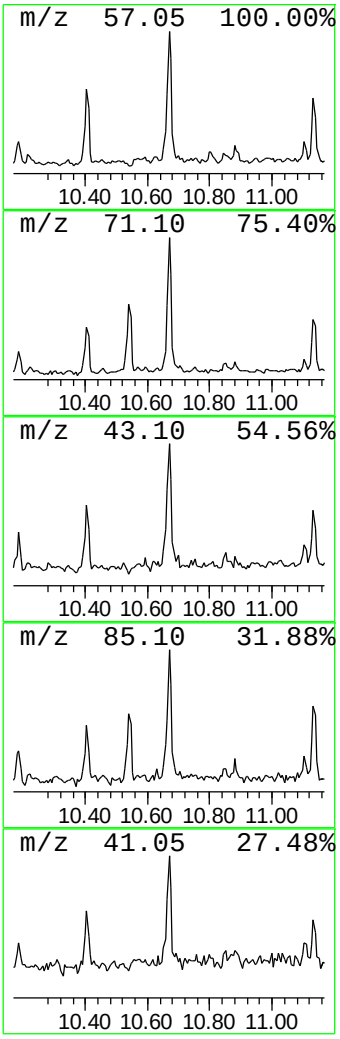
****

Peak Number 6 Tridecane, 5-propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.94 ng	155839	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 5-propyl-	226	C16H34	055045-11-9	80
2	Undecane, 6-ethyl-	184	C13H28	017312-60-6	74
3	Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	72
4	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	72
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72





Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102156.D
Acq On : 17 Jan 2018 18:06
Operator : SJ/JU
Sample : J1152-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LTP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

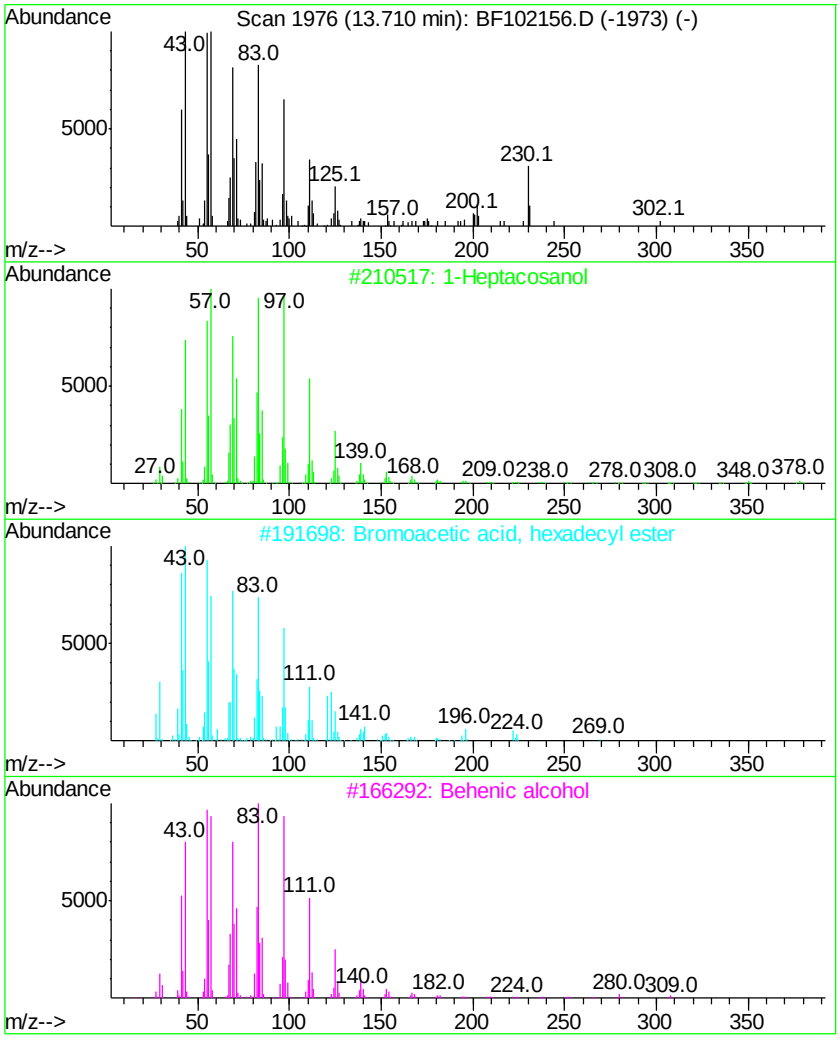
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

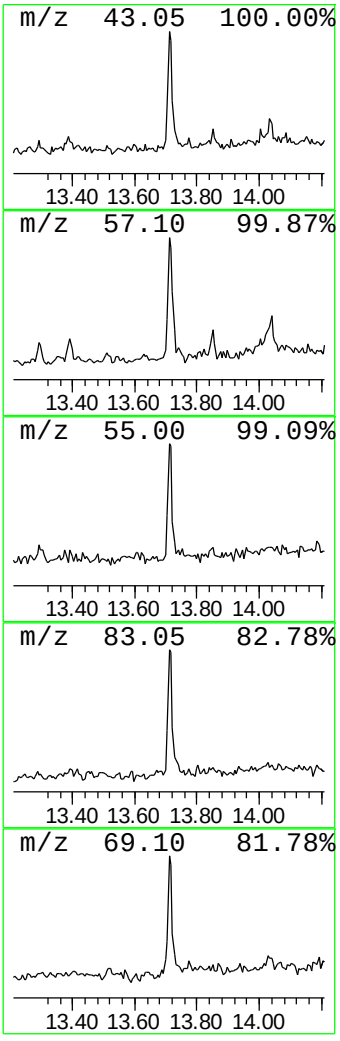
****

Peak Number 7 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	3.56 ng	152340	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	87
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
3	Behenic alcohol	326	C22H46O	000661-19-8	87
4	1-Heneicosanol	312	C21H44O	015594-90-8	87
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	87





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Acq On : 17 Jan 2018 18:06
Operator : SJ/JU
Sample : J1152-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LTP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

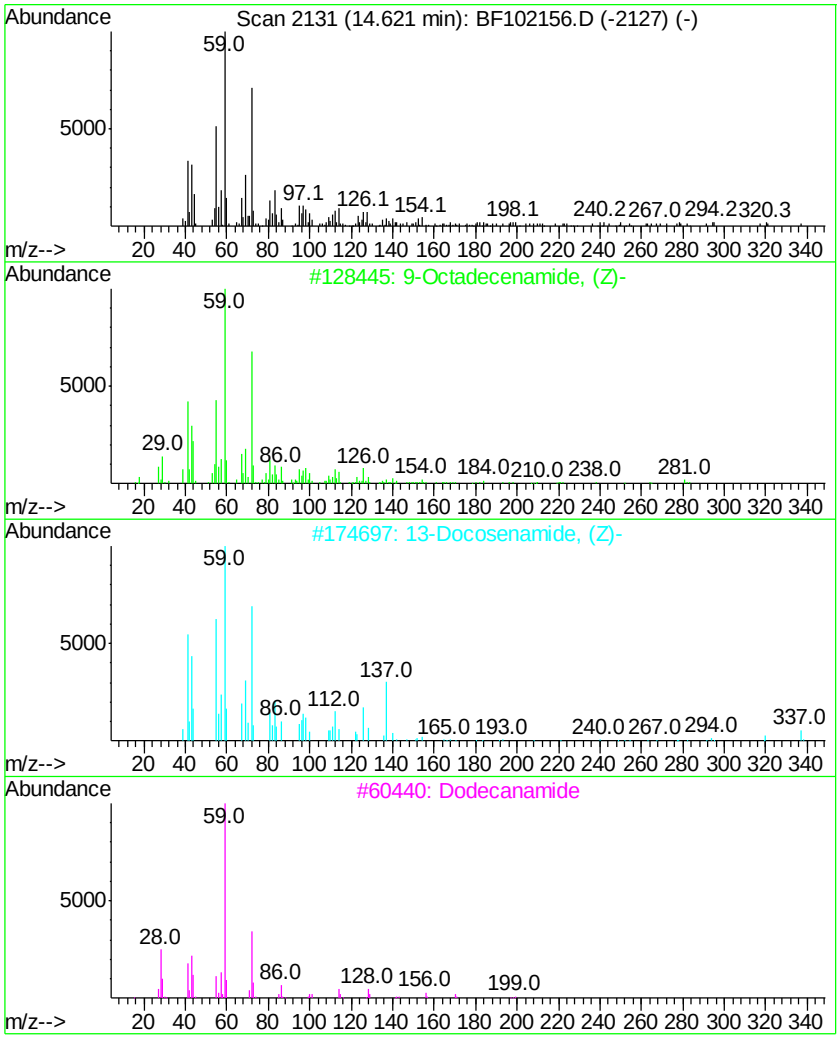
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

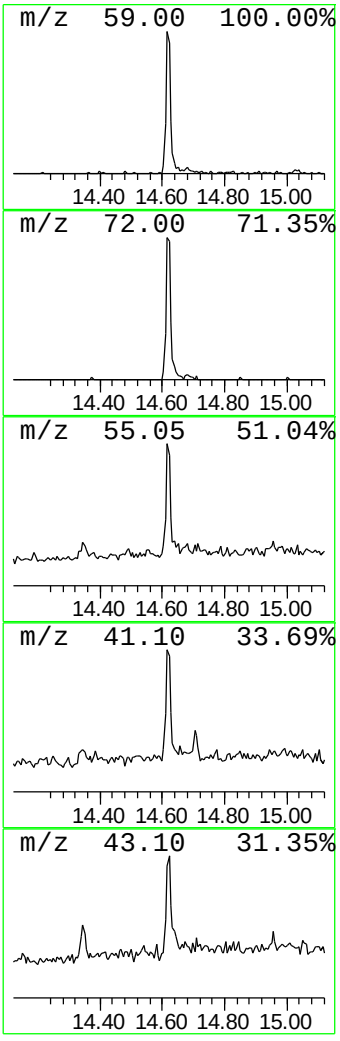
****

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	5.74 ng	223311	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	72
3	Dodecanamide	199	C12H25NO	001120-16-7	62
4	Octadecanamide	283	C18H37NO	000124-26-5	58
5	Octanamide	143	C8H17NO	000629-01-6	53





Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_F\DATA\BF011718\
Data File : BF102156.D
Acq On : 17 Jan 2018 18:06
Operator : SJ/JU
Sample : J1152-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LTP-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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...	4.93	6.4	ng	291263	1	6.72	906119	20.0
unknown6.49	6.49	84.2	ng	3815830	1	6.72	906119	20.0
2-Hydroxy-iso-but...	8.56	2.9	ng	175243	2	8.00	1218370	20.0
Benzophenone	10.47	8.9	ng	546643	3	9.75	1228230	20.0
Tridecane, 5-propyl-	10.67	2.9	ng	155839	4	11.23	1061210	20.0
1-Heptacosanol	13.71	3.6	ng	152340	5	13.87	856517	20.0
9-Octadecenamide,...	14.62	5.7	ng	223311	6	15.28	778766	20.0