LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF120117\
Data File : BF101075.D
Acq On : 1 Dec 2017 20:38
Operator : SJ/JU
Sample : I6622-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBNW1B-4-9

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-BF113017.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	5.081	506	509	521	rBV	62111	87503	6.17%	0.760%
2	5.469	570	575	578	rBV	1301601	1334443	94.08%	11.594%
3	6.487	742	748	759	rBV	1246454	1418392	99.99%	12.323%
4	6.622	766	771	774	rBV	1505559	1418474	100.00%	12.324%
5	6.845	806	809	813	rBV	371102	294340	20.75%	2.557%
6	7.004	832	836	839	rBV	1261911	1025176	72.27%	8.907%
7	7.416	900	906	909	rBV	885132	844747	59.55%	7.339%
8	8.128	1023	1027	1031	rBV	473807	372044	26.23%	3.232%
9	9.204	1205	1210	1213	rBV	1733974	1415095	99.76%	12.295%
10	9.592	1273	1276	1279	rBV	98625	83842	5.91%	0.728%
11	9.804	1309	1312	1316	rBV	35401	26949	1.90%	0.234%
12	9.886	1322	1326	1329	rBV	462424	400968	28.27%	3.484%
13	10.304	1395	1397	1400	rVB	34789	25244	1.78%	0.219%
14	10.675	1456	1460	1463	rBV	792152	662912	46.73%	5.760%
15	10.775	1474	1477	1483	rBV	22572	23099	1.63%	0.201%
16	11.375	1575	1579	1582	rBV	407945	342041	24.11%	2.972%
17	12.957	1844	1848	1851	rBV	1155598	1003335	70.73%	8.717%
18	13.845	1995	1999	2004	rVB	32878	40132	2.83%	0.349%
19	14.016	2024	2028	2034	rVB	363378	306535	21.61%	2.663%
20	14.757	2150	2154	2161	rBV	125741	124551	8.78%	1.082%
21	15.486	2273	2278	2284	rBV	223432	259836	18.32%	2.258%

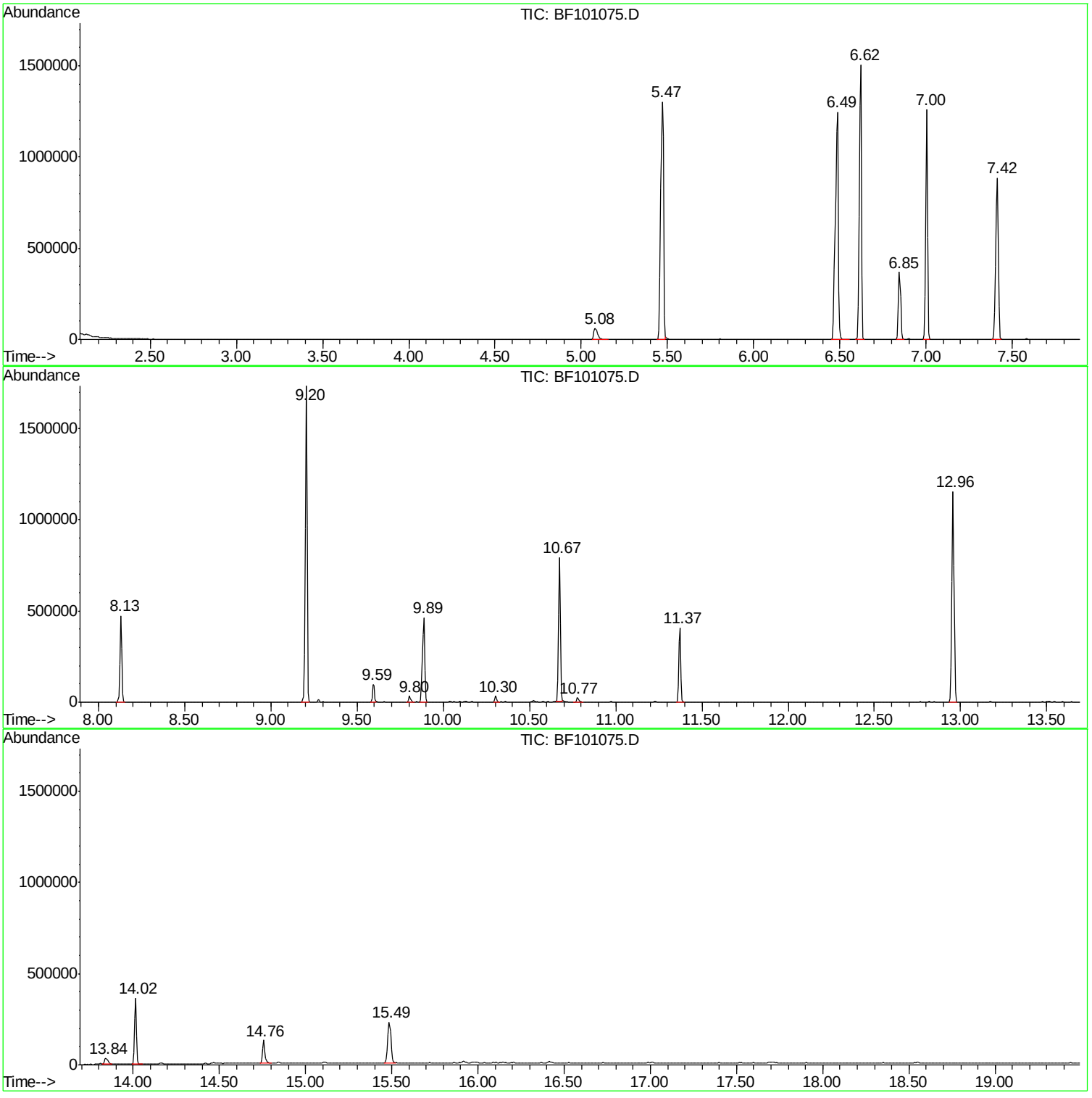
Sum of corrected areas: 11509658

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF120117\
Data File : BF101075.D
Acq On : 1 Dec 2017 20:38
Operator : SJ/JU
Sample : I6622-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DBNW1B-4-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF120117\
Data File : BF101075.D
Acq On : 1 Dec 2017 20:38
Operator : SJ/JU
Sample : I6622-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBNW1B-4-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

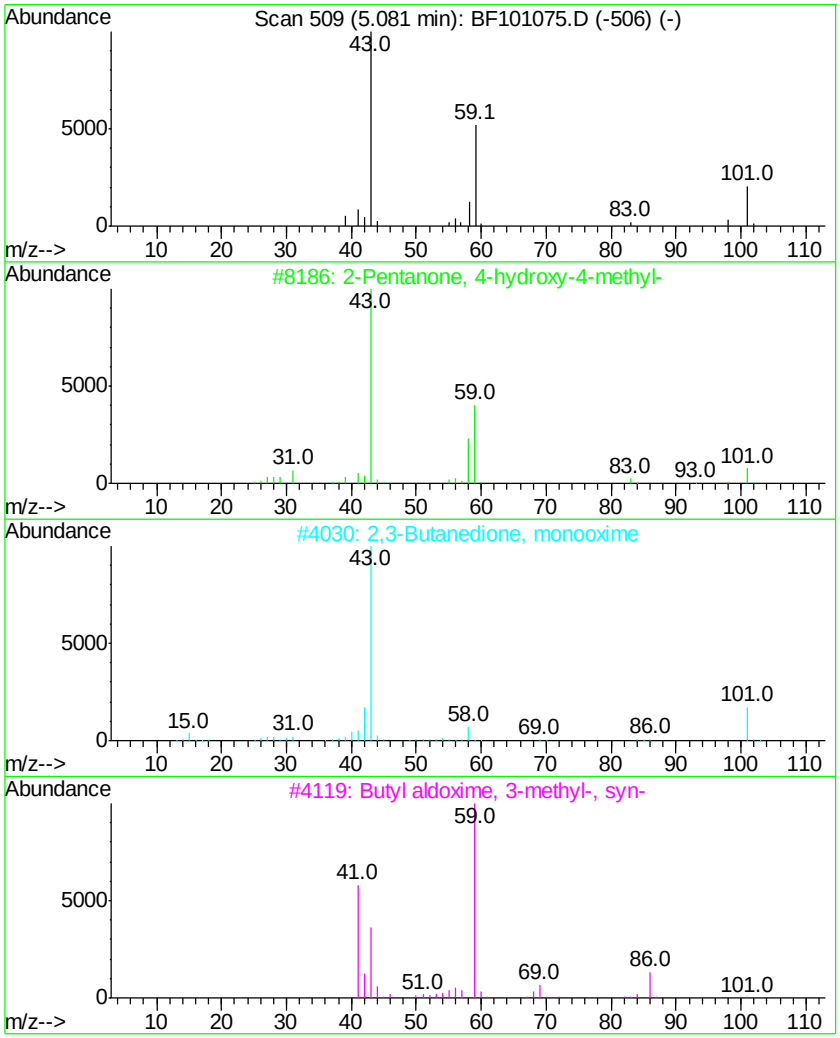
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

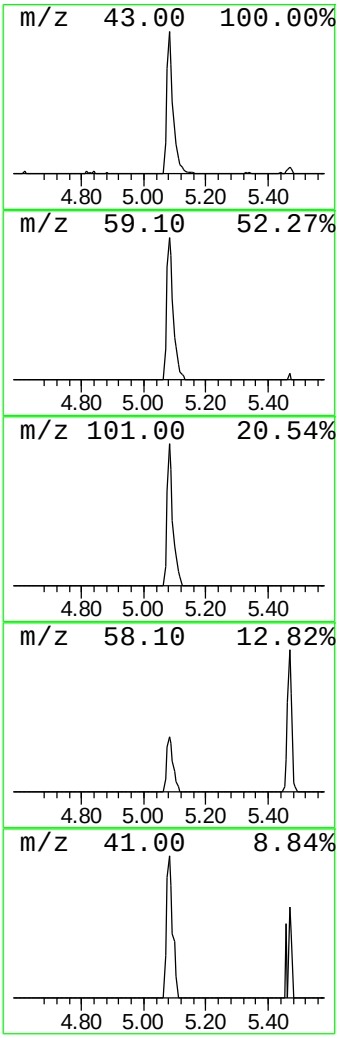
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	5.95 ng	87503	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF120117\
Data File : BF101075.D
Acq On : 1 Dec 2017 20:38
Operator : SJ/JU
Sample : I6622-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBNW1B-4-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

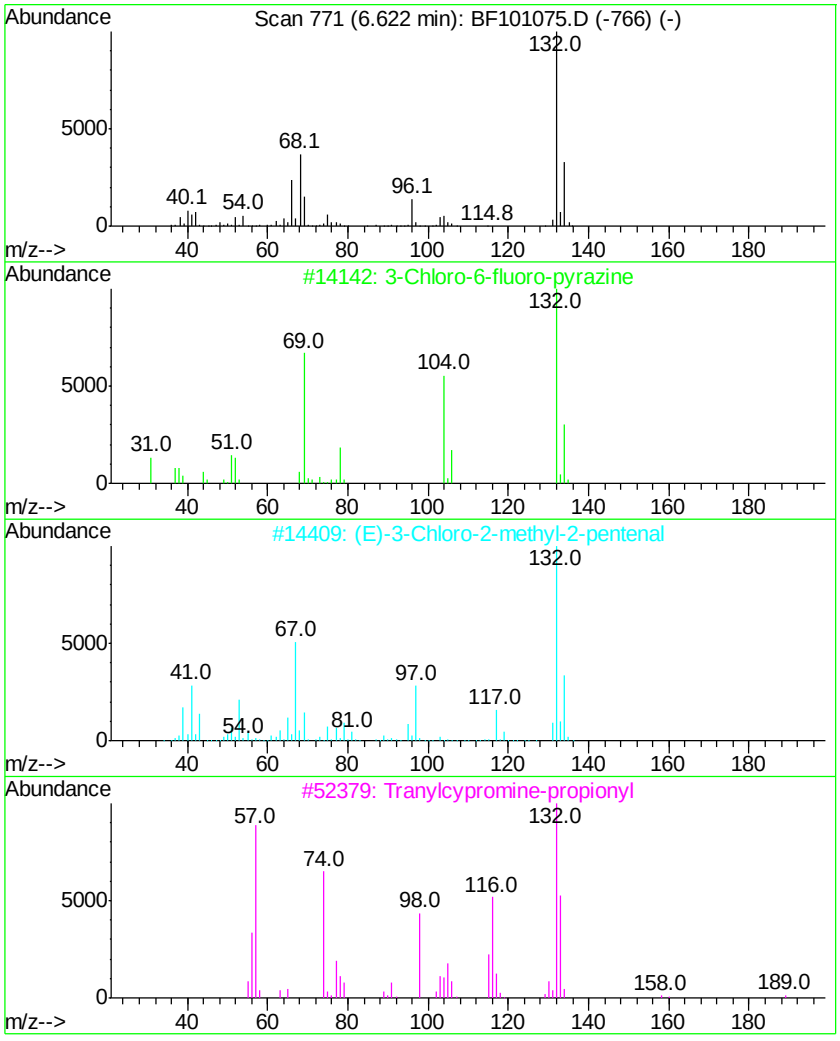
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

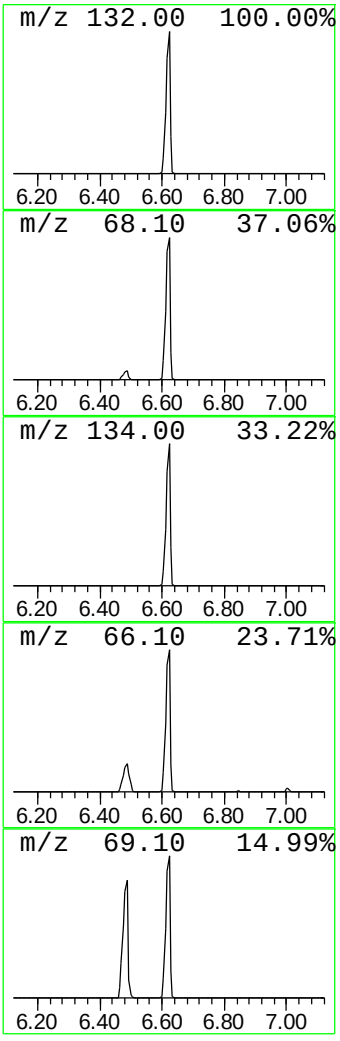
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	96.38 ng	1418470	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF120117\
Data File : BF101075.D
Acq On : 1 Dec 2017 20:38
Operator : SJ/JU
Sample : I6622-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBNW1B-4-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

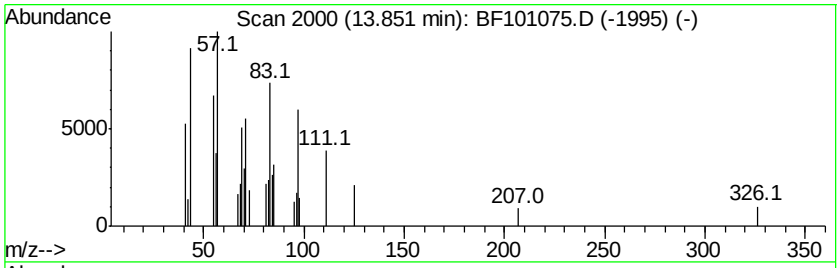
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

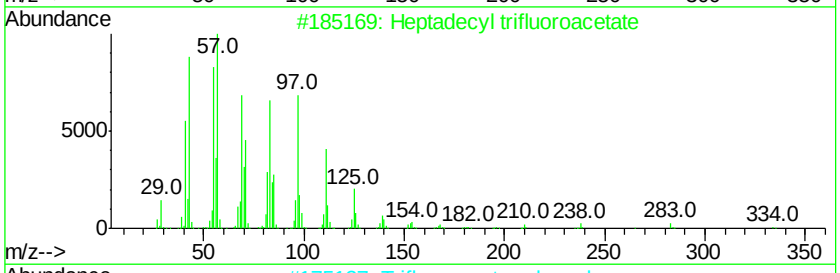
****

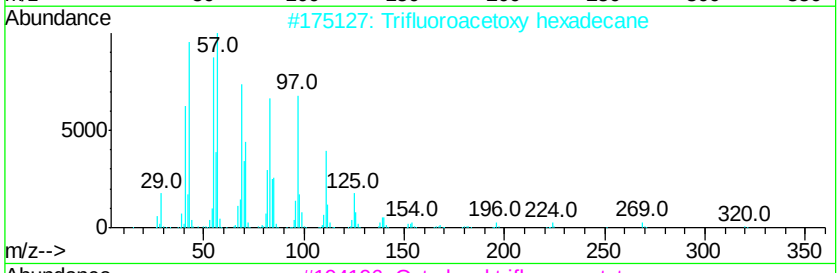
Peak Number 4 Heptadecyl trifluoroacetate Concentration Rank 5

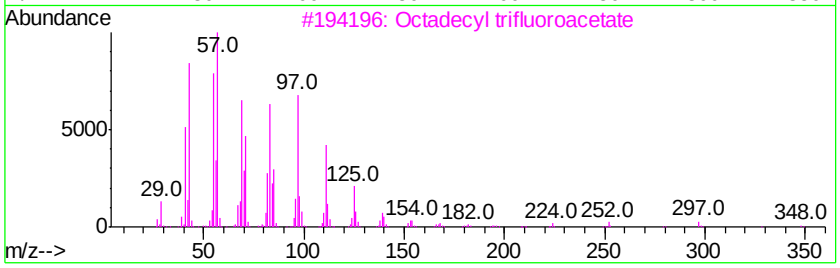
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.62 ng	40132	Chrysene-d12	14.02

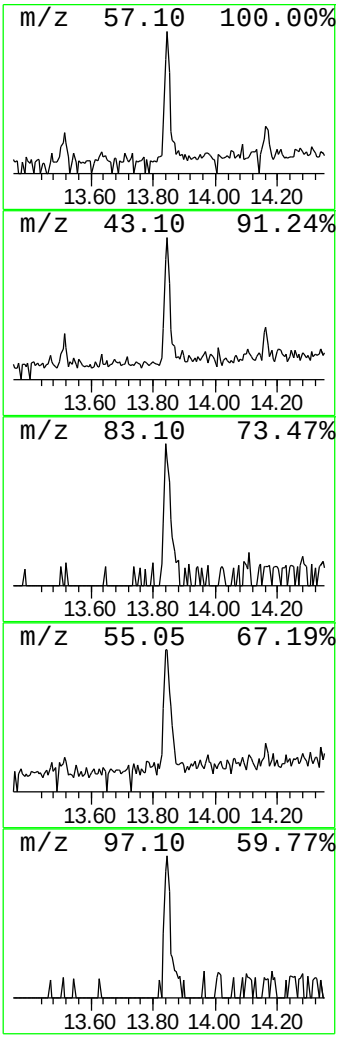
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
4	Octacosanol	410	C28H58O	000557-61-9	87
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87











Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF120117\
Data File : BF101075.D
Acq On : 1 Dec 2017 20:38
Operator : SJ/JU
Sample : I6622-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBNW1B-4-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

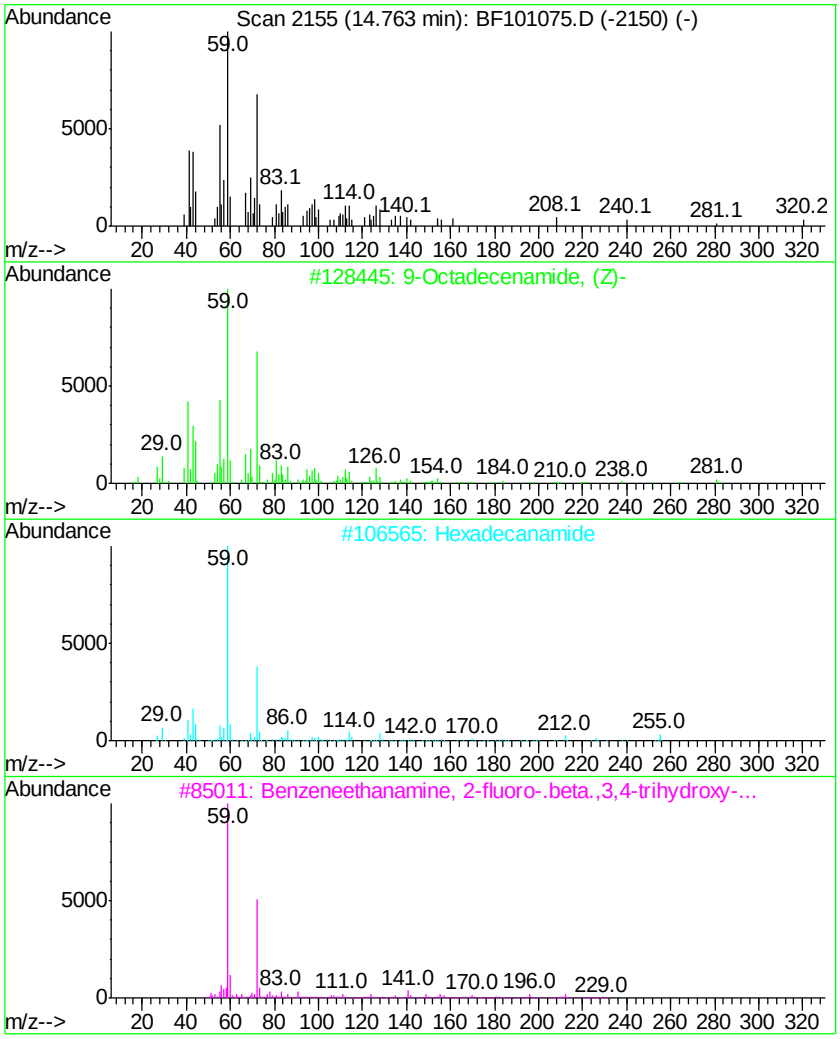
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

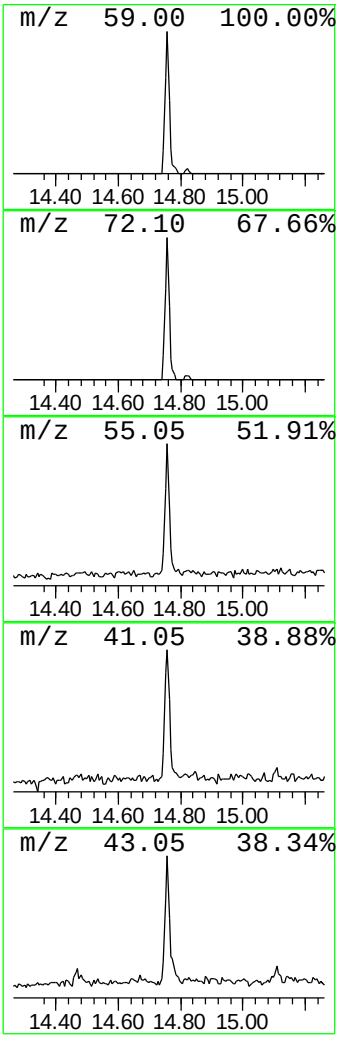
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	9.59 ng	124551	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Hexadecanamide	255	C16H33NO	000629-54-9	64
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59
4	Tetradecanamide	227	C14H29NO	000638-58-4	53
5	Methyl 15-methoxyhexadecanoate	300	C18H36O3	1000110-17-9	50





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF120117\
Data File : BF101075.D
Acq On : 1 Dec 2017 20:38
Operator : SJ/JU
Sample : I6622-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBNW1B-4-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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...	5.08	6.0	ng	87503	1	6.85	294340	20.0
unknown6.62	6.62	96.4	ng	1418470	1	6.85	294340	20.0
Heptadecyl triflu...	13.85	2.6	ng	40132	5	14.02	306535	20.0
9-Octadecenamide,...	14.76	9.6	ng	124551	6	15.49	259836	20.0