LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
Data File : BF118157.D
Acq On : 9 Dec 2019 21:12
Operator : JU
Sample : K6119-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(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-BF120619.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	5.075	504	508	521	rVB	277879	336222	15.33%	1.697%
2	5.481	573	577	597	rVB	1845196	1845701	84.17%	9.314%
3	6.498	745	750	767	rBV	2039202	1919144	87.52%	9.684%
4	6.640	770	774	777	rBV	2359696	2048582	93.43%	10.338%
5	6.869	809	813	816	rBV	693690	553515	25.24%	2.793%
6	7.028	836	840	843	rBV	1841157	1697061	77.39%	8.564%
7	7.428	904	908	919	rVB	1211151	1128502	51.47%	5.695%
8	8.151	1028	1031	1045	rVB	696959	644137	29.38%	3.250%
9	9.228	1211	1214	1225	rBV	2349503	2192741	100.00%	11.065%
10	9.622	1278	1281	1291	rVB	276670	256460	11.70%	1.294%
11	9.916	1327	1331	1341	rVB	689255	644847	29.41%	3.254%
12	10.704	1461	1465	1476	rBV	1377677	1240736	56.58%	6.261%
13	11.404	1581	1584	1588	rBV	619587	590362	26.92%	2.979%
14	11.933	1670	1674	1681	rBV	376230	413783	18.87%	2.088%
15	12.627	1788	1792	1793	rBV	101473	108835	4.96%	0.549%
16	12.639	1793	1794	1804	rVV4	105177	181495	8.28%	0.916%
17	12.721	1804	1808	1815	rVV2	140023	175741	8.01%	0.887%
18	12.857	1828	1831	1837	rBV2	31859	49505	2.26%	0.250%
19	12.998	1851	1855	1858	rBV	2438975	2111981	96.32%	10.657%
20	13.898	2005	2008	2013	rVB3	181741	215231	9.82%	1.086%
21	14.057	2032	2035	2039	rBV	699986	694918	31.69%	3.507%
22	15.557	2286	2290	2299	rVB	509817	767430	35.00%	3.873%

Sum of corrected areas: 19816929

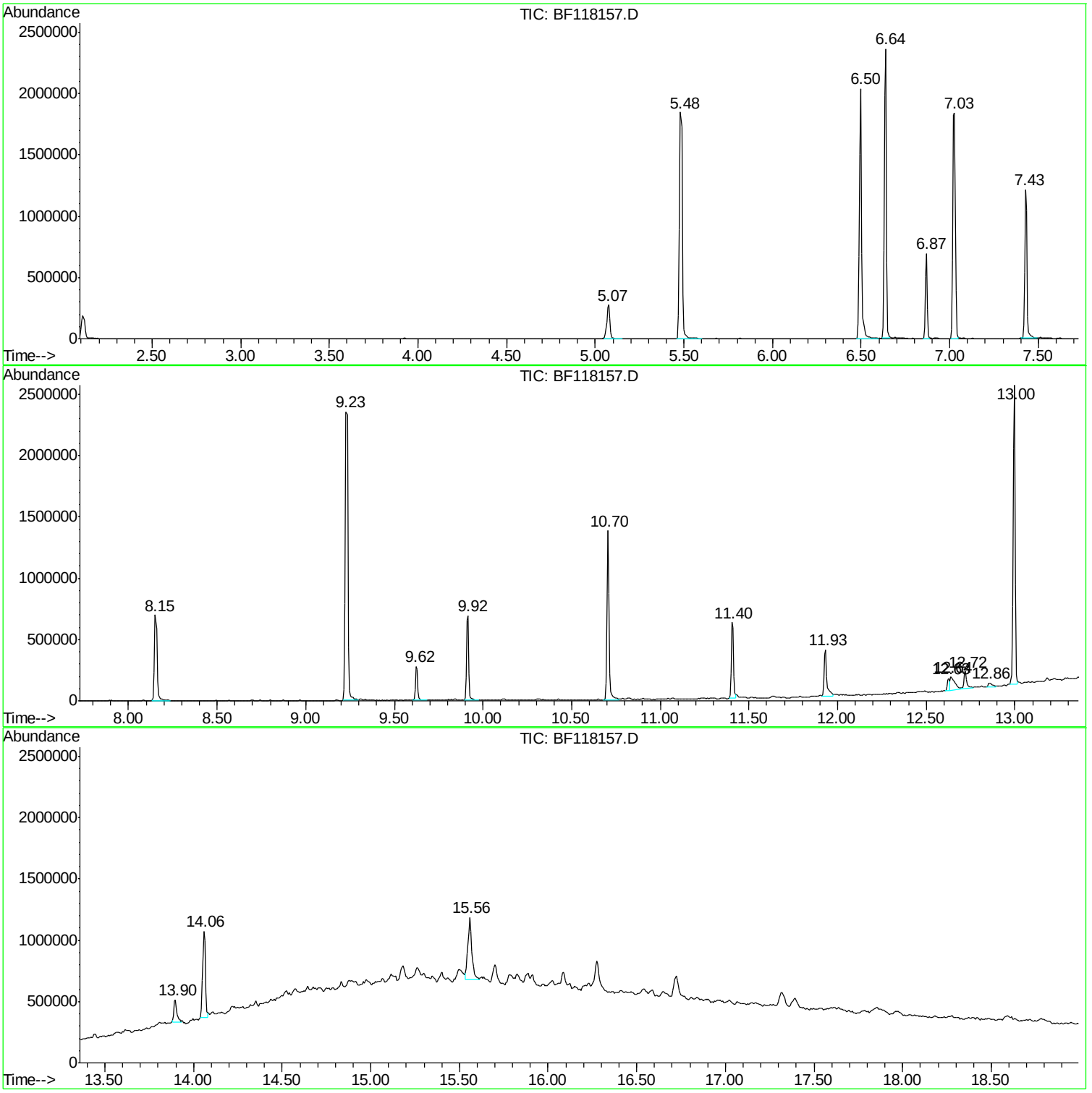
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
Data File : BF118157.D
Acq On : 9 Dec 2019 21:12
Operator : JU
Sample : K6119-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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\BF120919\
Data File : BF118157.D
Acq On : 9 Dec 2019 21:12
Operator : JU
Sample : K6119-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

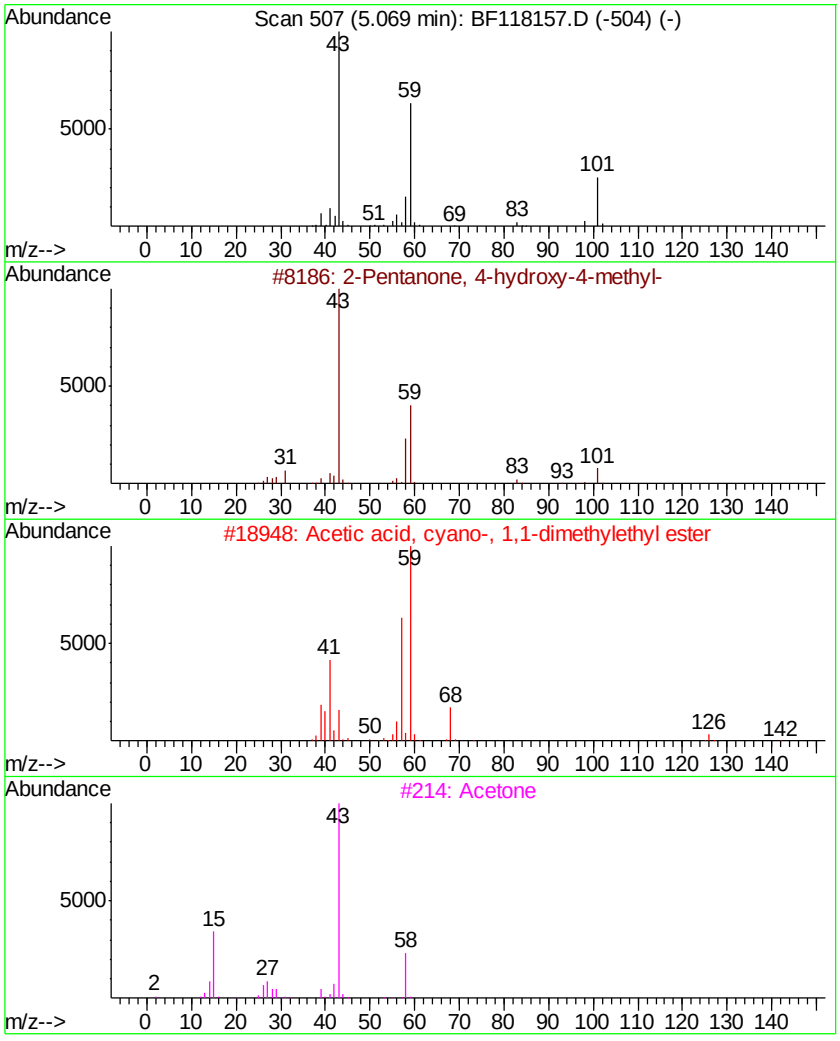
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

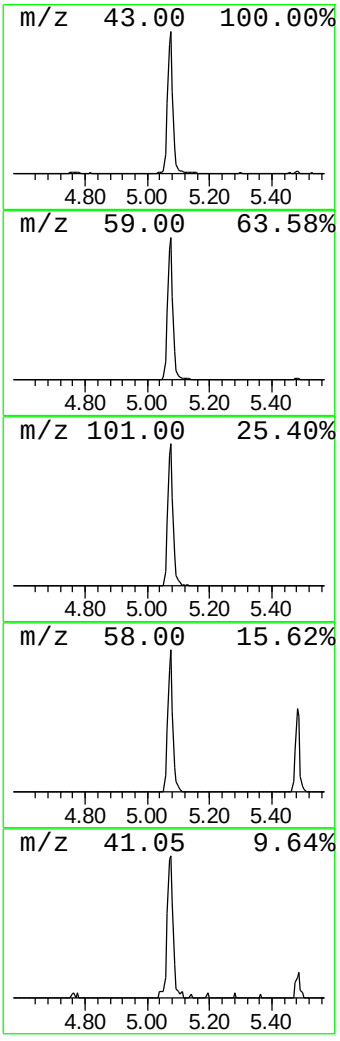
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	12.15 ng	336222	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Acetone	58	C3H6O	000067-64-1	10
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
Data File : BF118157.D
Acq On : 9 Dec 2019 21:12
Operator : JU
Sample : K6119-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

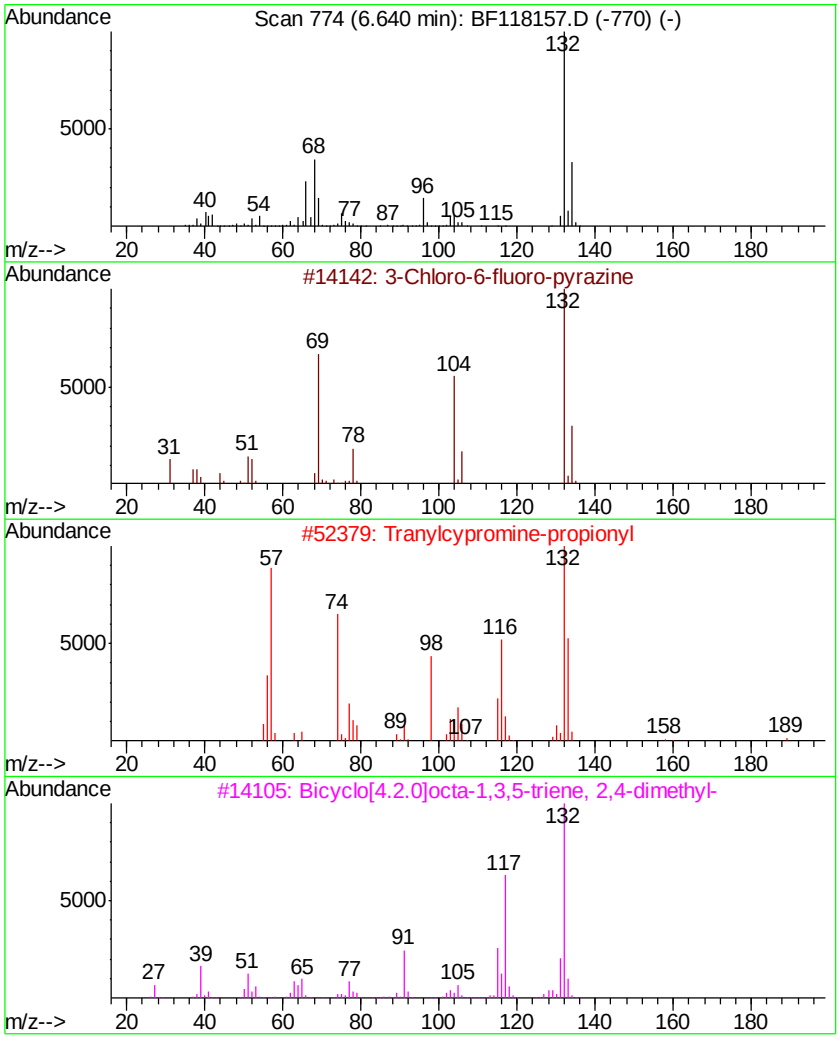
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

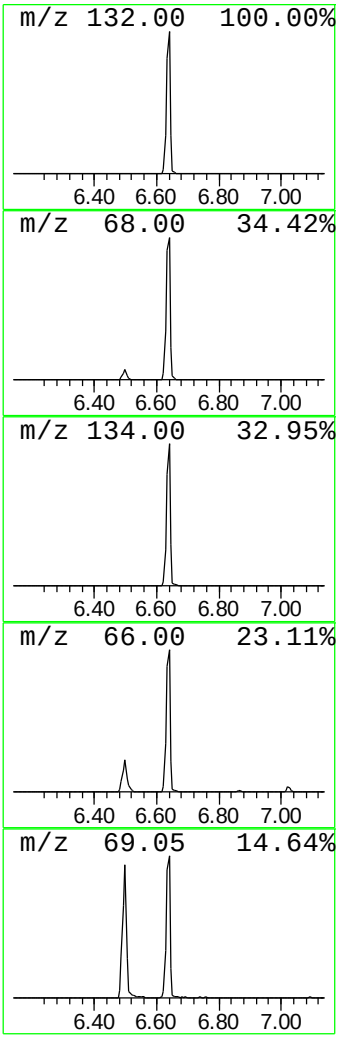
****

Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	74.02 ng	2048580	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
Data File : BF118157.D
Acq On : 9 Dec 2019 21:12
Operator : JU
Sample : K6119-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

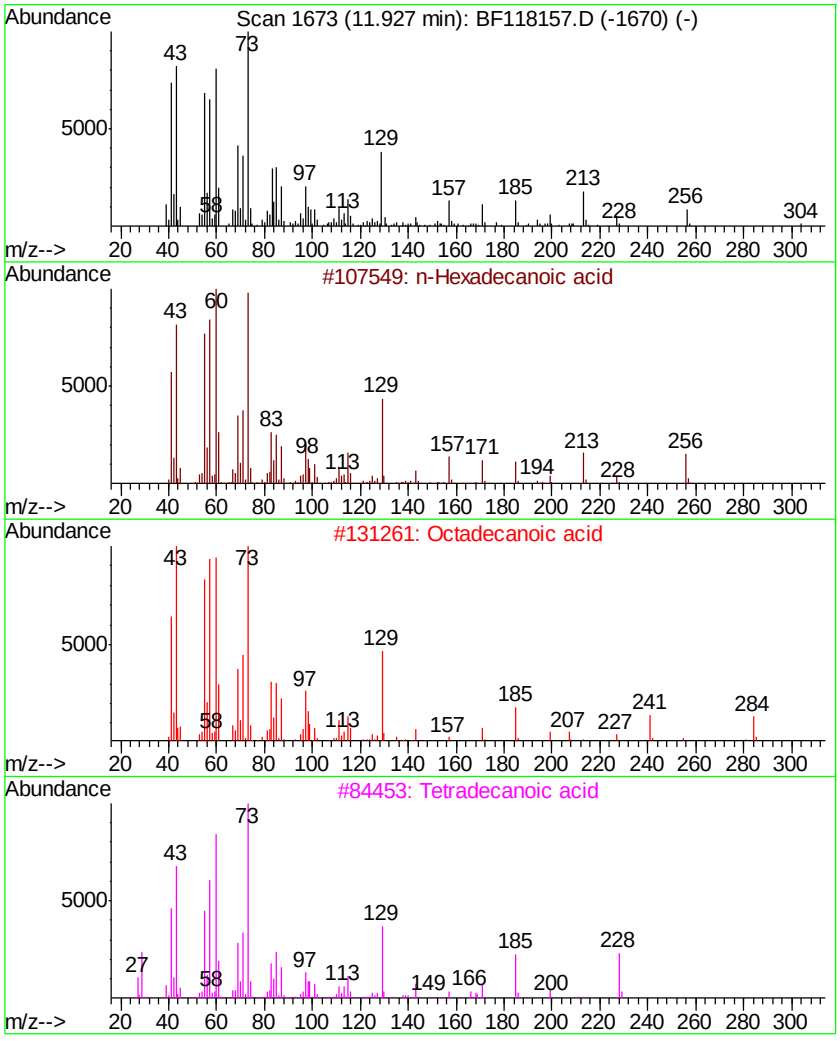
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

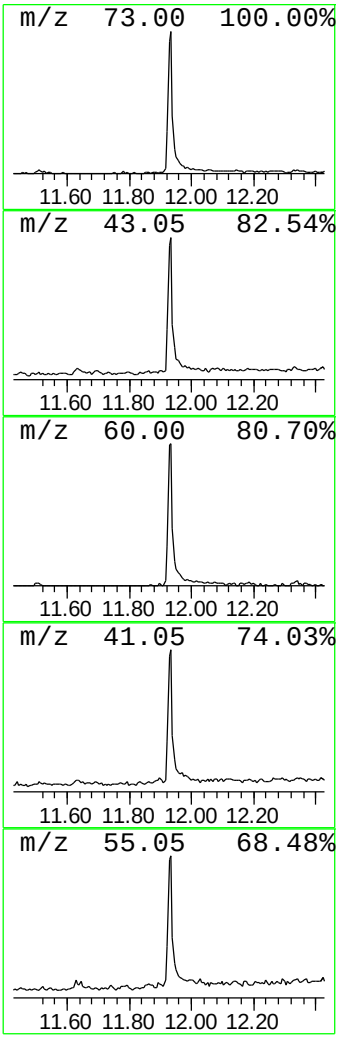
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	14.02 ng	413783	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
Data File : BF118157.D
Acq On : 9 Dec 2019 21:12
Operator : JU
Sample : K6119-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

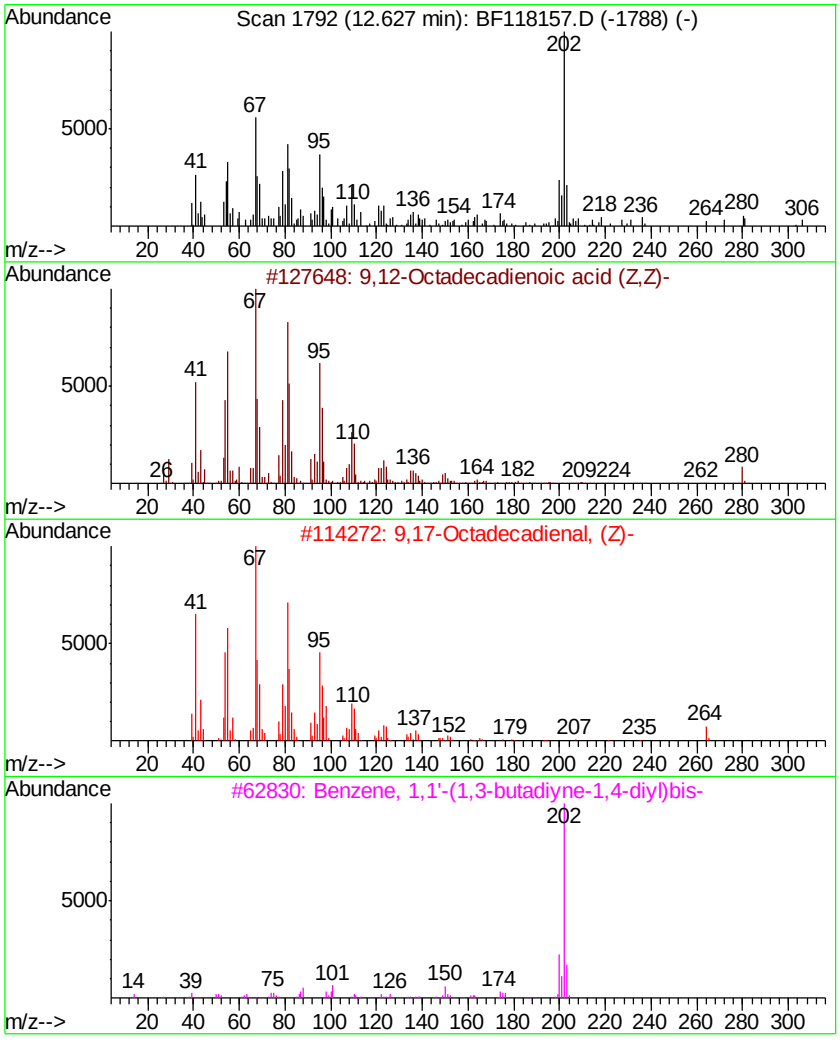
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

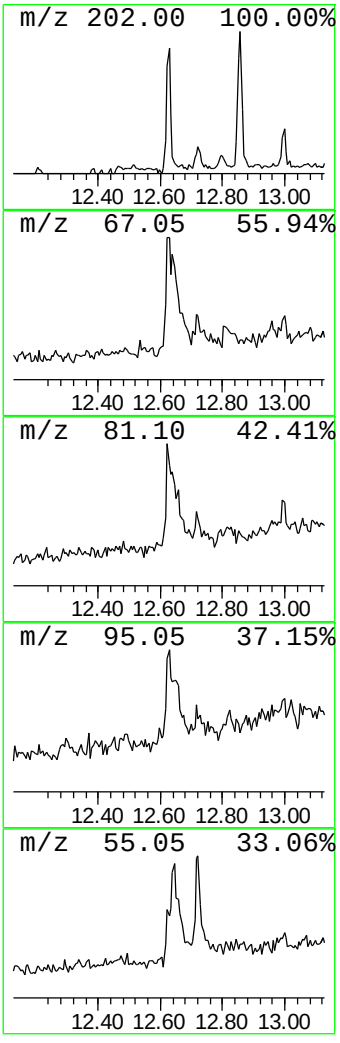
****

Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	3.69 ng	108835	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	83
2	9,17-Octadecadienal, (Z)-	264	C18H32O	056554-35-9	59
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	55
4	Fluoranthene	202	C16H10	000206-44-0	42
5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	30





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
Data File : BF118157.D
Acq On : 9 Dec 2019 21:12
Operator : JU
Sample : K6119-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

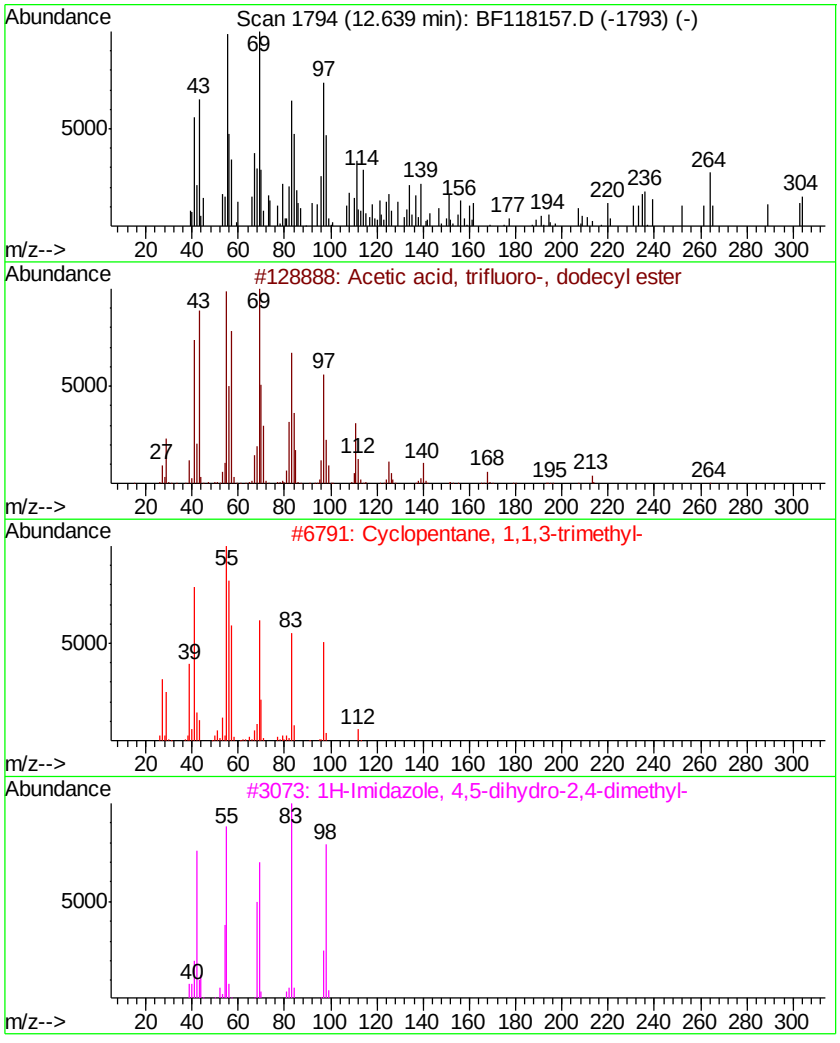
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

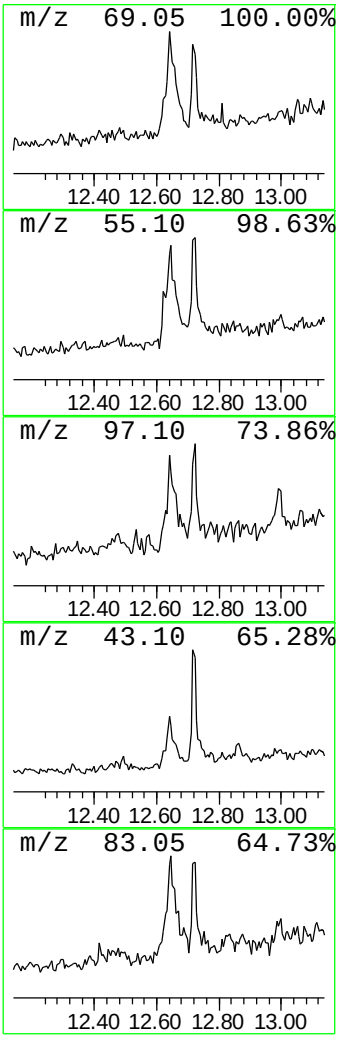
****

Peak Number 6 Acetic acid, trifluoro-, do... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	6.15 ng	181495	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	52
2	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	46
3	1H-Imidazole, 4,5-dihydro-2,4-di...	98	C5H10N2	000930-61-0	30
4	2-Hexenal, (E)-	98	C6H10O	006728-26-3	30
5	Octadec-9-enoic acid	282	C18H34O2	1000190-13-7	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120919\
Data File : BF118157.D
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Operator : JU
Sample : K6119-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

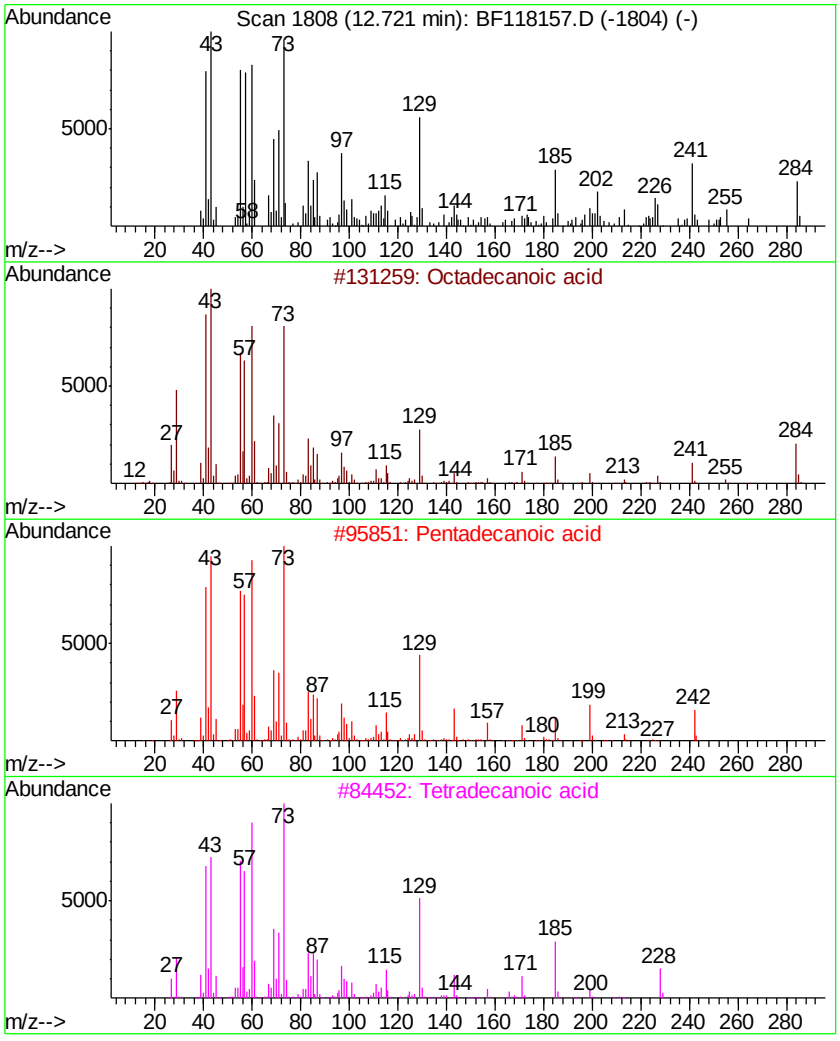
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

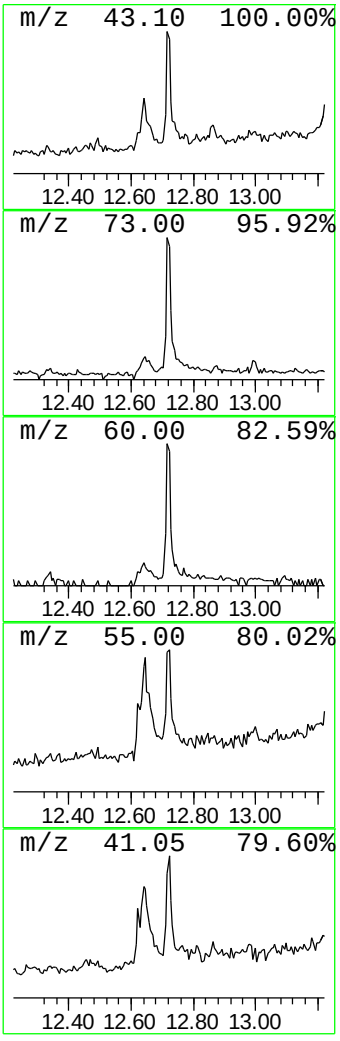
****

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	5.95 ng	175741	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4	n-Decanoic acid	172	C10H20O2	000334-48-5	55
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53





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Misc :
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Instrument : BNA_F
ClientSampleId : SB-4-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

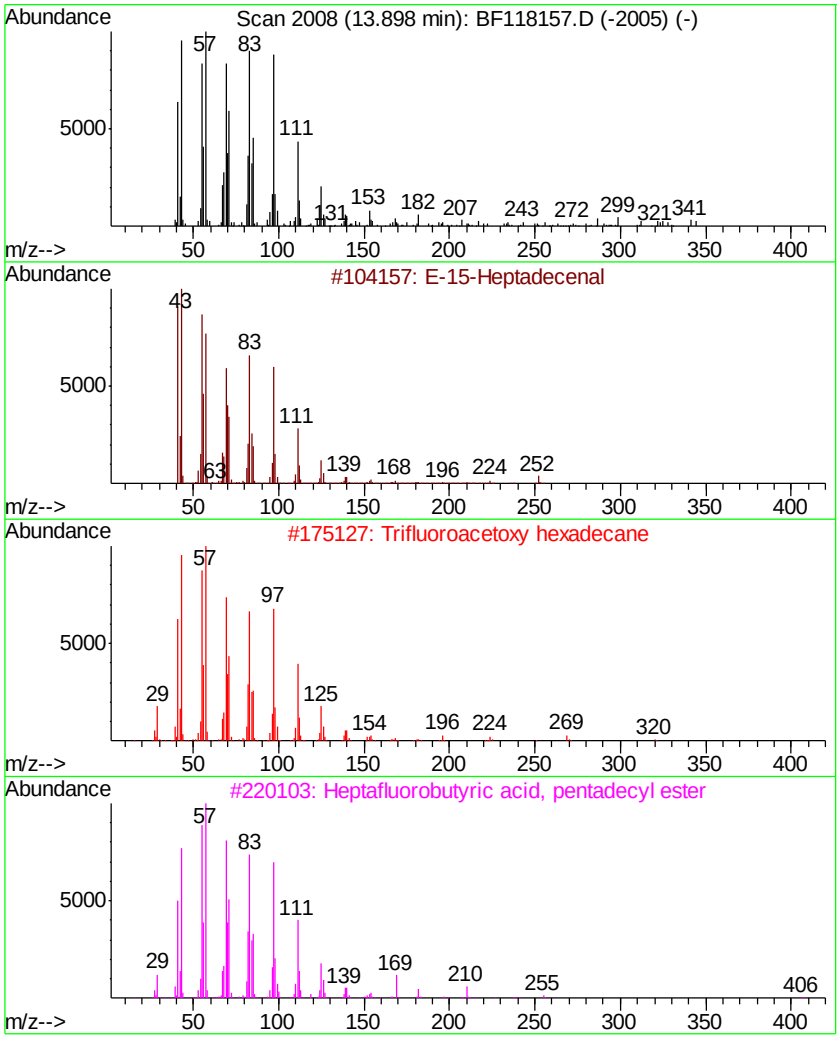
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

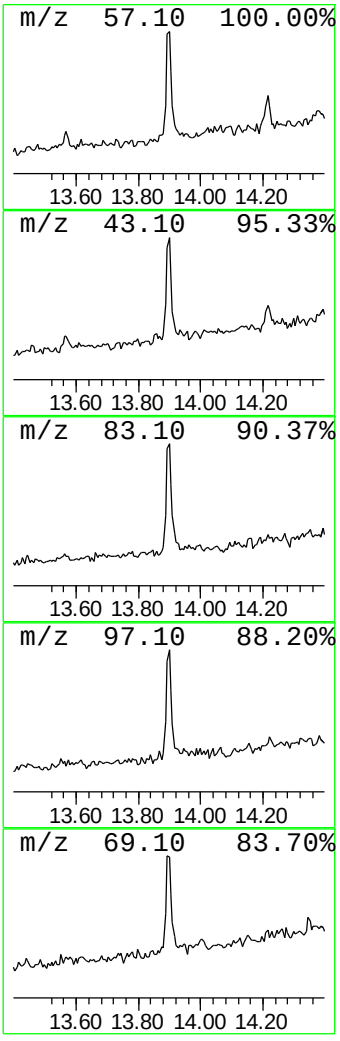
****

Peak Number 8 E-15-Heptadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	6.19 ng	215231	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	96
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	1-Tricosene	322	C23H46	018835-32-0	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120919\
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Operator : JU
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
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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...	5.07	12.2	ng	336222	1	6.87	553515	20.0
unknown6.64	6.64	74.0	ng	2048580	1	6.87	553515	20.0
n-Hexadecanoic acid	11.93	14.0	ng	413783	4	11.40	590362	20.0
9,12-Octadecadien...	12.63	3.7	ng	108835	4	11.40	590362	20.0
Acetic acid, trif...	12.64	6.2	ng	181495	4	11.40	590362	20.0
Octadecanoic acid	12.72	6.0	ng	175741	4	11.40	590362	20.0
E-15-Heptadecenal	13.90	6.2	ng	215231	5	14.06	694918	20.0