LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101847.D
Acq On : 2 Jan 2018 13:29
Operator : SJ/JU
Sample : I7100-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(5-10)

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	5.004	492	496	511	rBV	223220	422037	13.31%	1.592%
2	5.404	561	564	595	rBV	2182067	3169741	100.00%	11.953%
3	6.428	735	738	756	rBV	2340261	3139442	99.04%	11.839%
4	6.551	756	759	771	rVB	2694828	2960054	93.38%	11.163%
5	6.775	794	797	807	rBV	740372	798024	25.18%	3.009%
6	6.933	820	824	846	rBV	2238486	2287097	72.15%	8.625%
7	7.351	891	895	915	rBV	1761241	1978823	62.43%	7.462%
8	8.063	1012	1016	1029	rBV	940783	1025438	32.35%	3.867%
9	8.622	1108	1111	1120	rBV	209476	215458	6.80%	0.813%
10	9.133	1194	1198	1206	rBV	3067518	2722739	85.90%	10.268%
11	9.533	1262	1266	1272	rBV	380852	357549	11.28%	1.348%
12	9.816	1310	1314	1321	rVB	1062220	964587	30.43%	3.638%
13	10.527	1432	1435	1443	rBV	752021	623555	19.67%	2.351%
14	10.616	1446	1450	1462	rBV	1298736	1384900	43.69%	5.223%
15	11.310	1564	1568	1575	rBV	827242	782361	24.68%	2.950%
16	11.821	1651	1655	1666	rBV2	171491	208179	6.57%	0.785%
17	12.604	1785	1788	1793	rBV	104188	116188	3.67%	0.438%
18	12.886	1832	1836	1840	rBV	1819695	1723093	54.36%	6.498%
19	13.762	1982	1985	1991	rBV	169679	174437	5.50%	0.658%
20	13.962	2015	2019	2027	rBV	706376	770907	24.32%	2.907%
21	15.433	2265	2269	2278	rBV	475515	692889	21.86%	2.613%

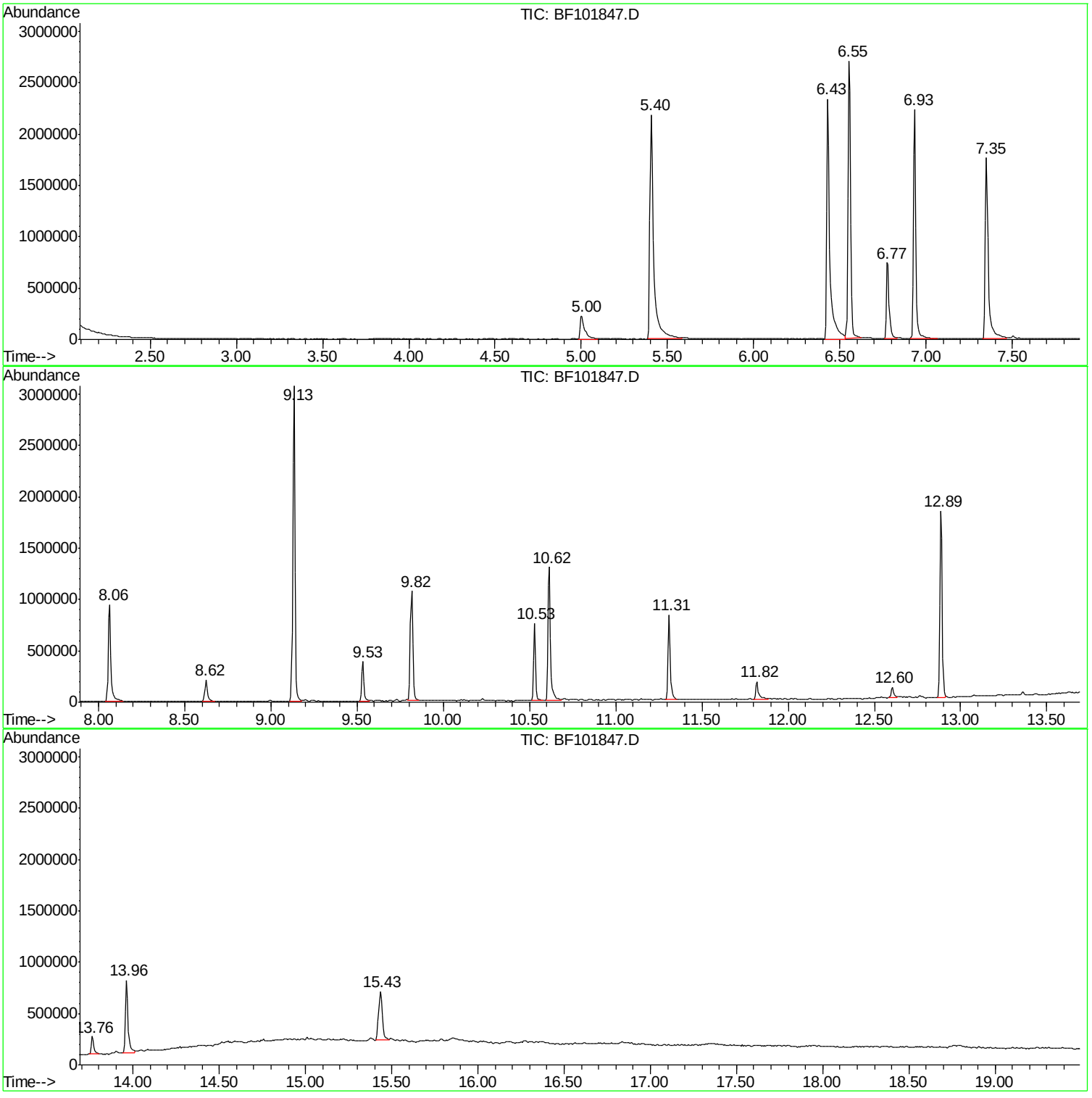
Sum of corrected areas: 26517498

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101847.D
Acq On : 2 Jan 2018 13:29
Operator : SJ/JU
Sample : I7100-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(5-10)

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



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Data File : BF101847.D
Acq On : 2 Jan 2018 13:29
Operator : SJ/JU
Sample : I7100-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(5-10)

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

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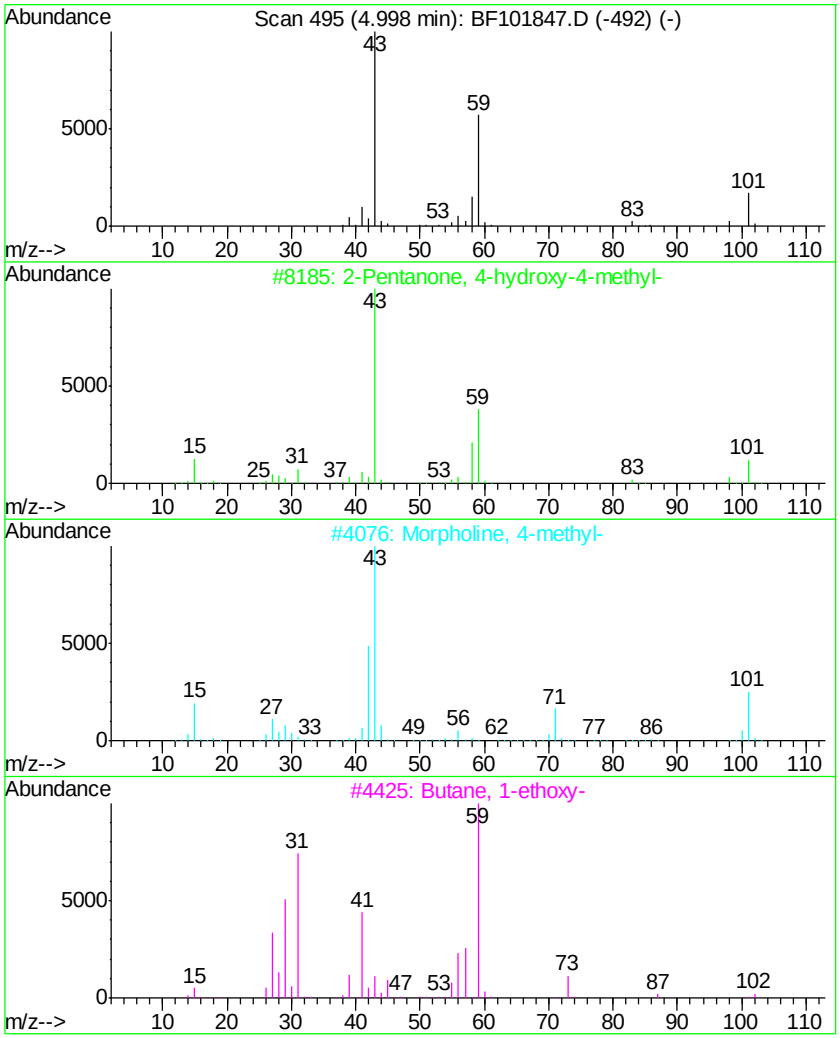
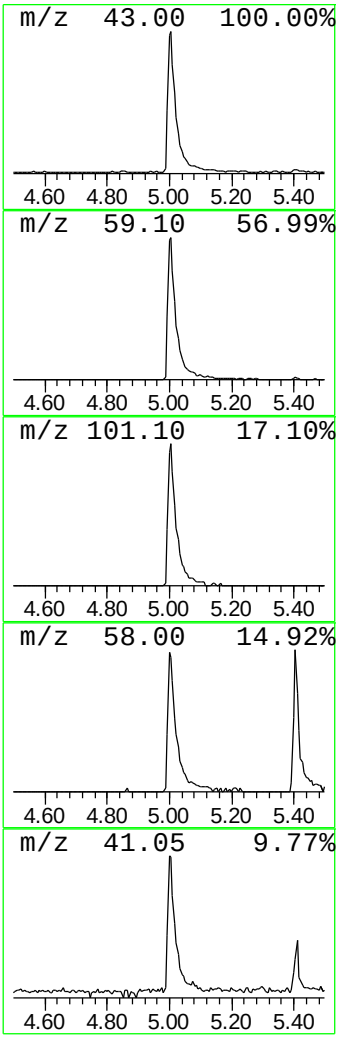
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	10.58 ng	422037	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101847.D
Acq On : 2 Jan 2018 13:29
Operator : SJ/JU
Sample : I7100-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(5-10)

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

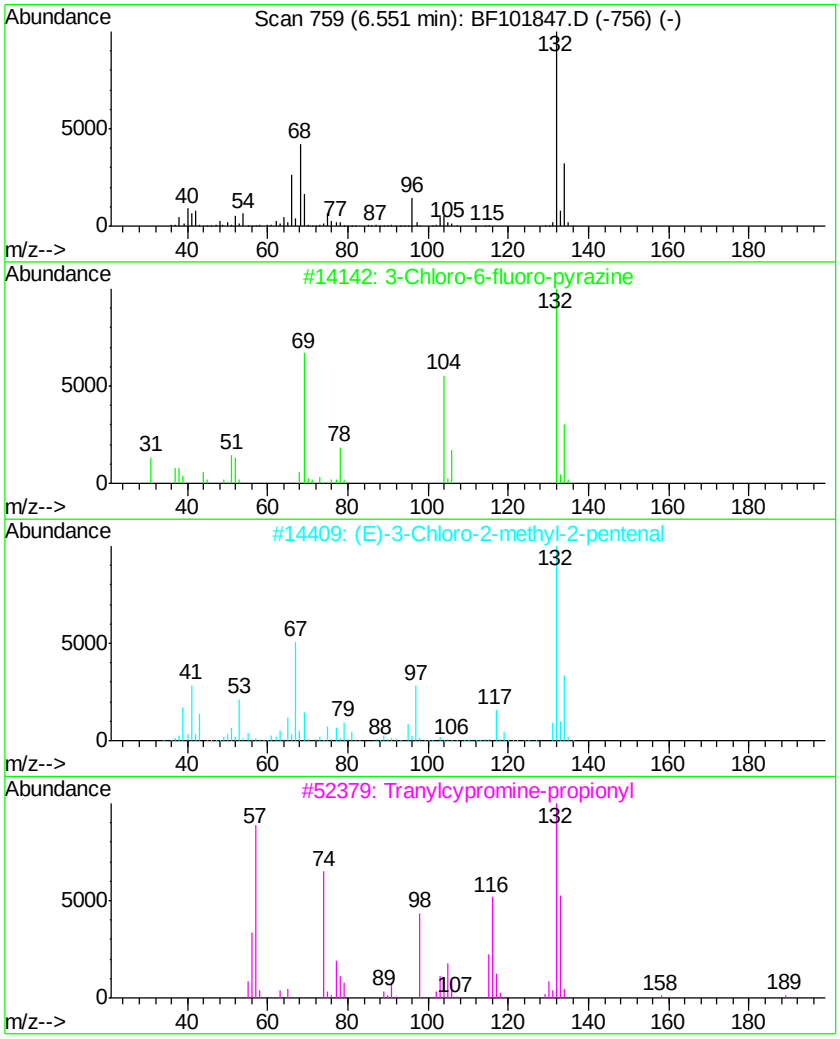
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

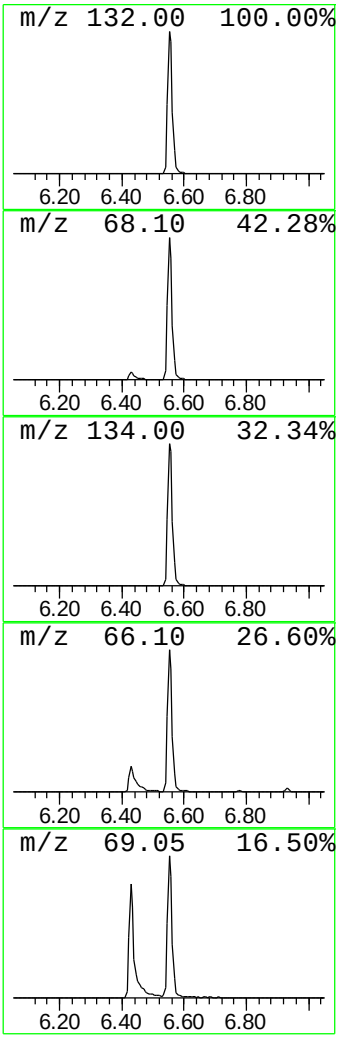
****

Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	74.18 ng	2960050	1,4-Dichlorobenzene-d4	6.78

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	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101847.D
Acq On : 2 Jan 2018 13:29
Operator : SJ/JU
Sample : I7100-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(5-10)

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

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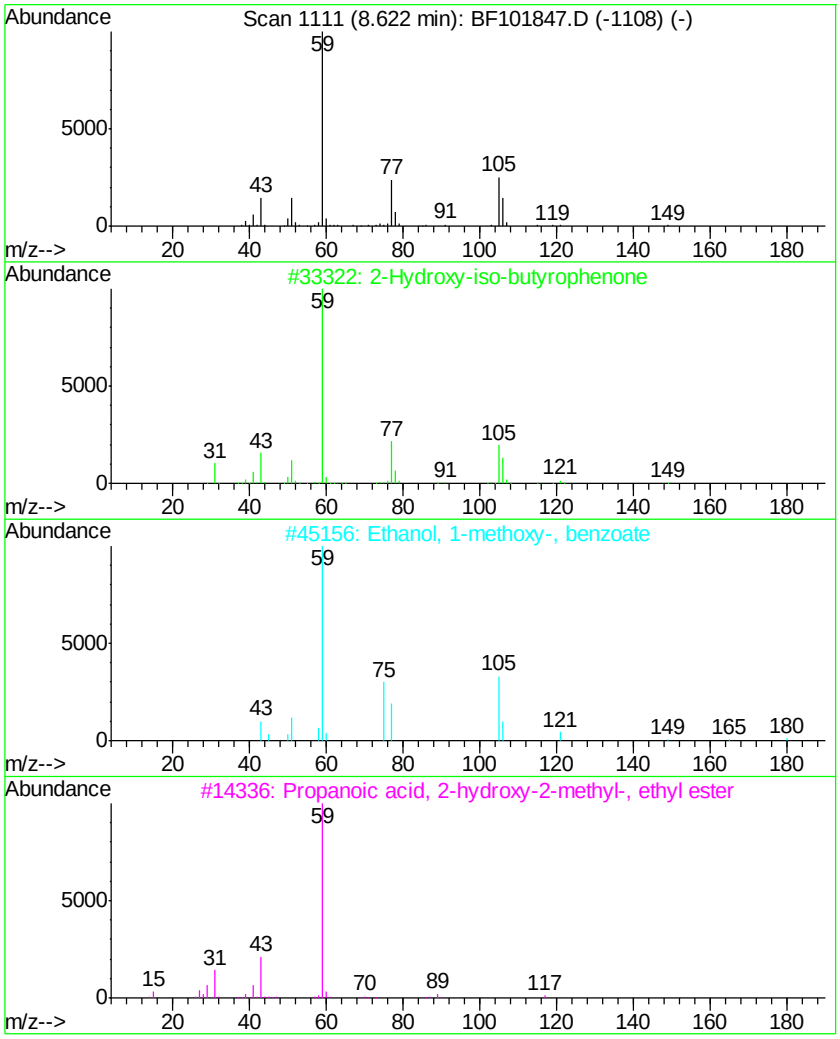
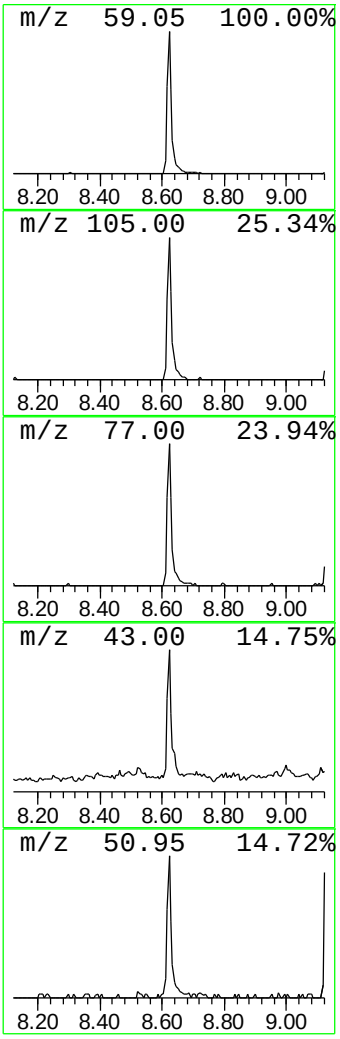
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.62	4.20 ng	215458	Naphthalene-d8	8.06

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	50
3	Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	23
4	Propanedioic acid, (benzoylhydra...	282	C12H14N2O6	1000142-99-9	23
5	Propanoic acid, 2-hydroxy-2-meth...	118	C5H10O3	002110-78-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101847.D
Acq On : 2 Jan 2018 13:29
Operator : SJ/JU
Sample : I7100-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(5-10)

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

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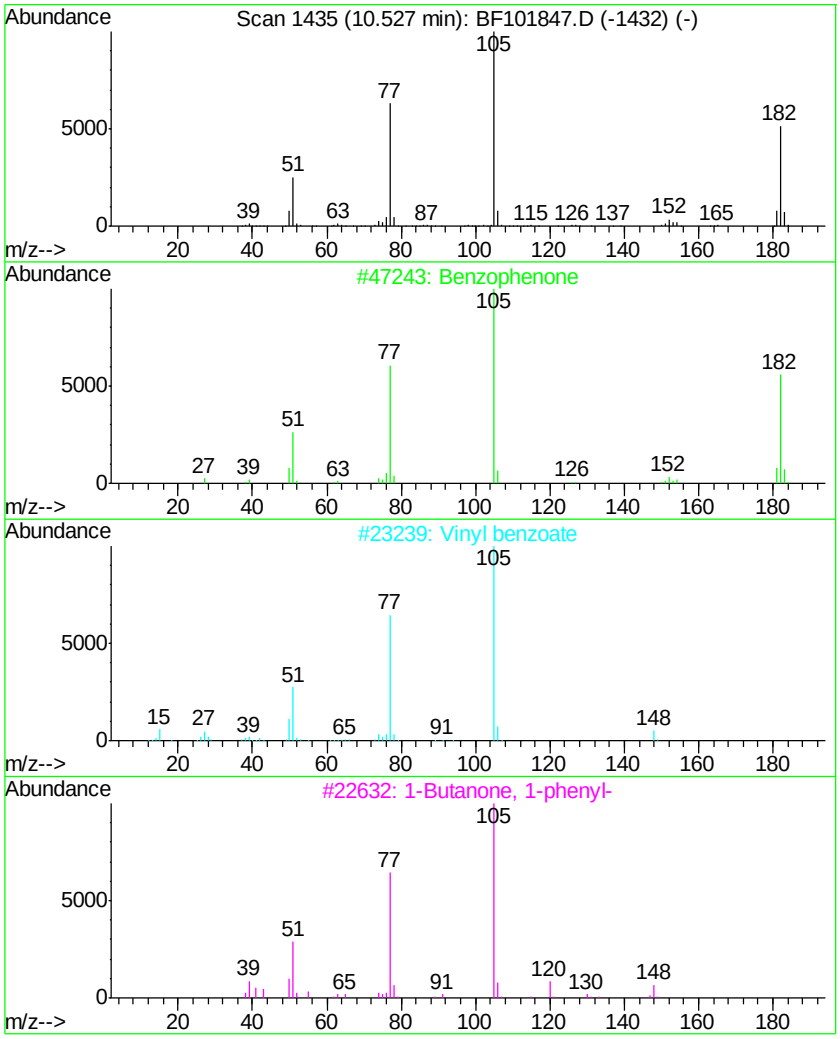
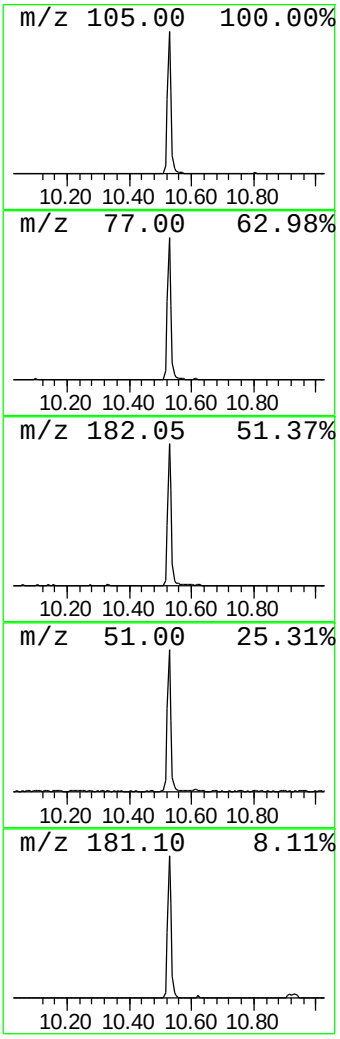
Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	12.93 ng	623555	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Vinyl benzoate	148	C9H8O2	000769-78-8	47
3	1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101847.D
Acq On : 2 Jan 2018 13:29
Operator : SJ/JU
Sample : I7100-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(5-10)

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

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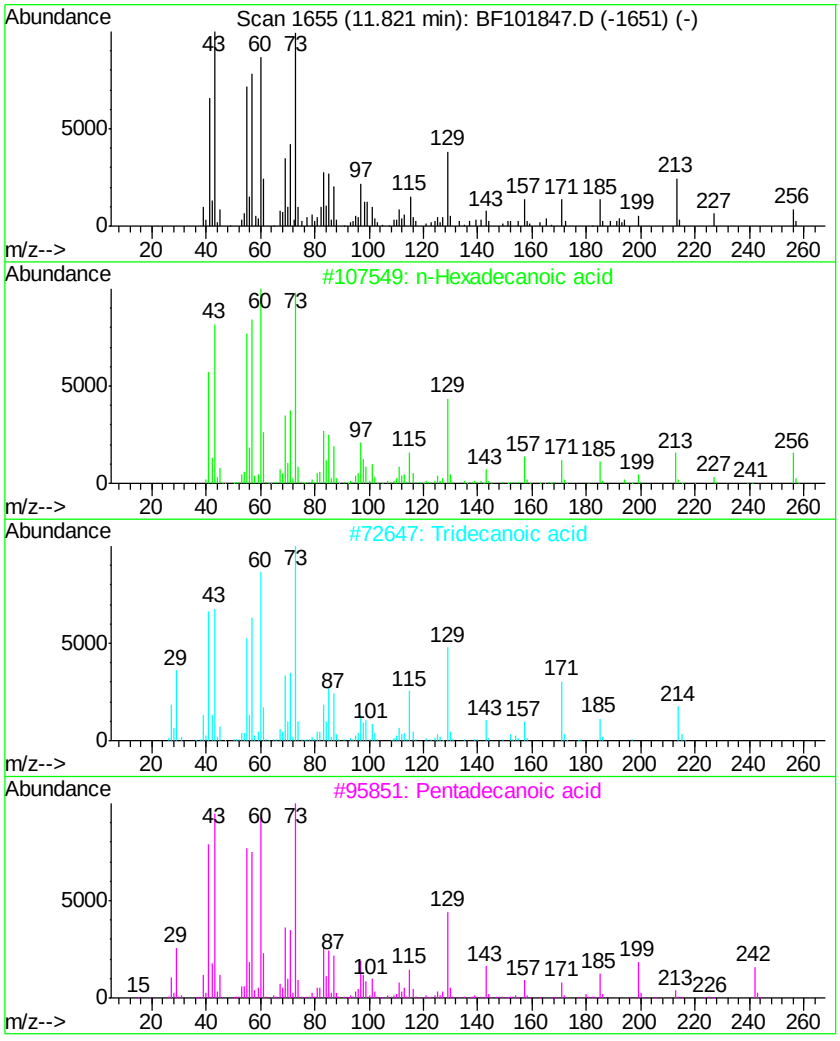
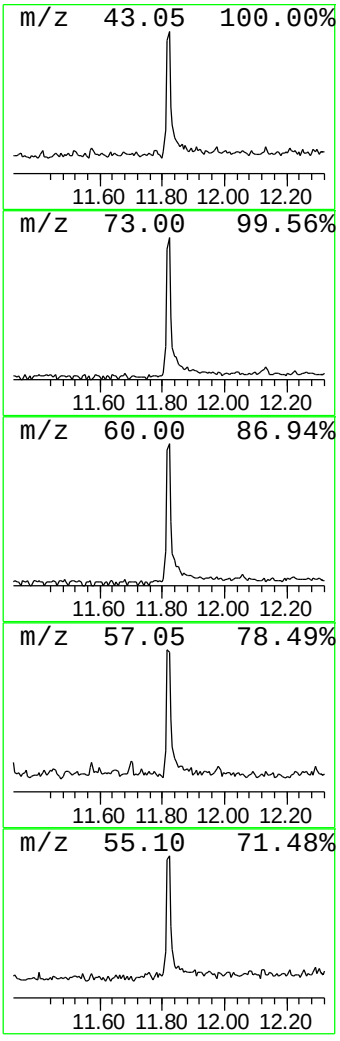
Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	5.32 ng	208179	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101847.D
Acq On : 2 Jan 2018 13:29
Operator : SJ/JU
Sample : I7100-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(5-10)

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

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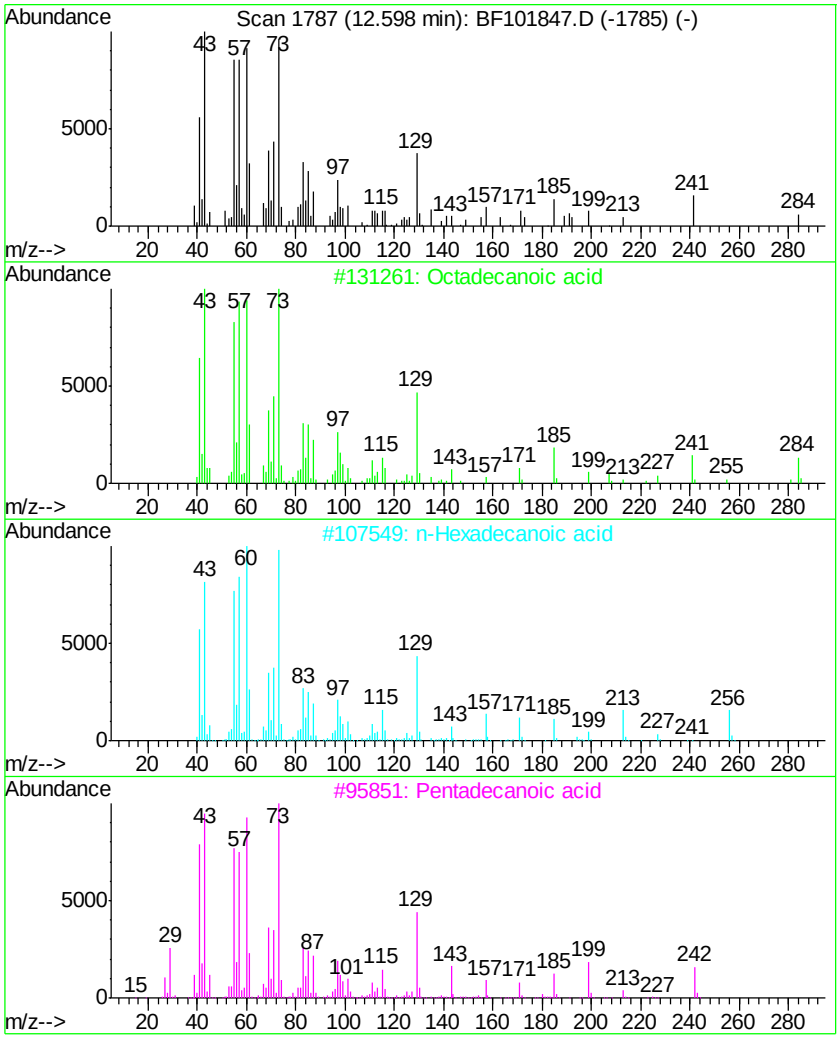
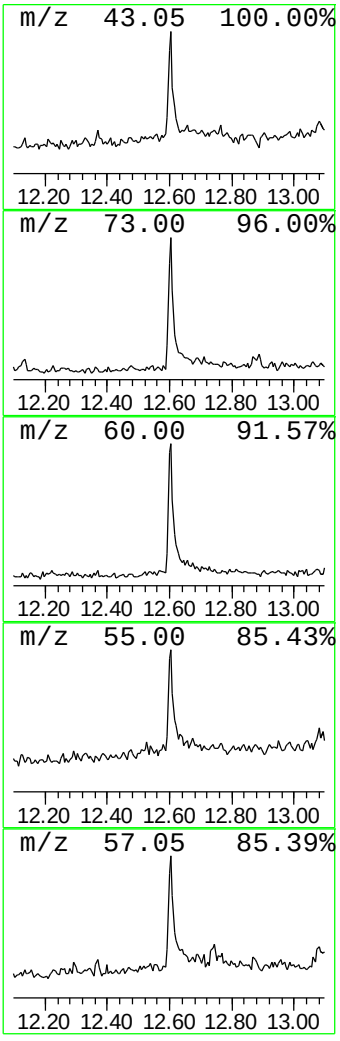
Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.60	2.97 ng	116188	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Undecanoic acid	186	C11H22O2	000112-37-8	60





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Data File : BF101847.D
Acq On : 2 Jan 2018 13:29
Operator : SJ/JU
Sample : I7100-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(5-10)

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

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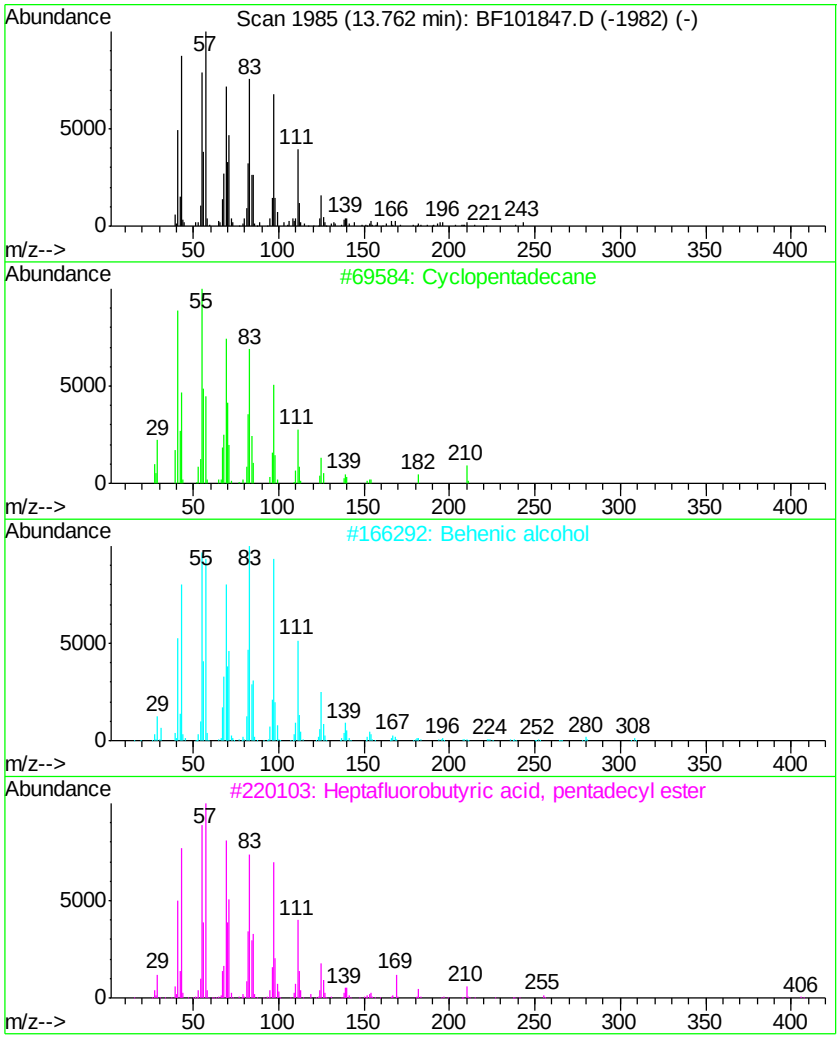
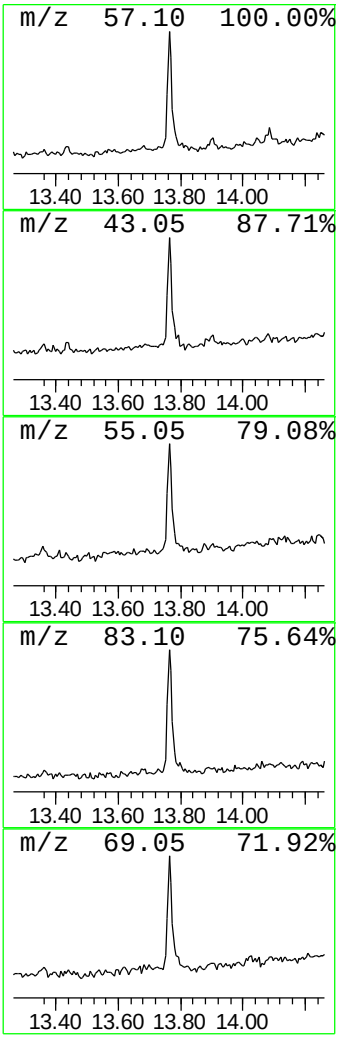
Peak Number 8 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	4.53 ng	174437	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101847.D
Acq On : 2 Jan 2018 13:29
Operator : SJ/JU
Sample : I7100-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(5-10)

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	10.6	ng	422037	1	6.78	798024	20.0
unknown6.55	6.55	74.2	ng	2960050	1	6.78	798024	20.0
2-Hydroxy-iso-but...	8.62	4.2	ng	215458	2	8.06	1025440	20.0
Benzophenone	10.53	12.9	ng	623555	3	9.82	964587	20.0
n-Hexadecanoic acid	11.82	5.3	ng	208179	4	11.31	782361	20.0
Octadecanoic acid	12.60	3.0	ng	116188	4	11.31	782361	20.0
Cyclopentadecane	13.76	4.5	ng	174437	5	13.96	770907	20.0