LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101846.D
Acq On : 2 Jan 2018 13:02
Operator : SJ/JU
Sample : I7100-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(0-5)

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	4.998	491	495	516	rBV	507019	941611	26.66%	3.049%
2	5.404	561	564	593	rBV	2360260	3364330	95.24%	10.893%
3	6.434	735	739	756	rBV	2640752	3532518	100.00%	11.438%
4	6.557	756	760	775	rVB	2859152	3276929	92.76%	10.610%
5	6.775	794	797	806	rBV	807468	857343	24.27%	2.776%
6	6.934	820	824	840	rBV	2638171	2616621	74.07%	8.472%
7	7.351	891	895	918	rBV	2013374	2288107	64.77%	7.408%
8	8.063	1012	1016	1033	rBV	1029641	1113951	31.53%	3.607%
9	8.622	1107	1111	1118	rBV	289388	290666	8.23%	0.941%
10	9.133	1194	1198	1201	rBV	3646728	3359257	95.10%	10.877%
11	9.533	1262	1266	1272	rBV	490113	441440	12.50%	1.429%
12	9.816	1310	1314	1324	rVB	1211799	1068775	30.26%	3.460%
13	10.527	1432	1435	1446	rBV	1028637	843316	23.87%	2.730%
14	10.616	1446	1450	1462	rBV	1288906	1355823	38.38%	4.390%
15	11.310	1564	1568	1578	rBV	926494	919019	26.02%	2.976%
16	11.816	1651	1654	1658	rBV	143386	157334	4.45%	0.509%
17	12.533	1770	1776	1781	rBV	91294	117012	3.31%	0.379%
18	12.604	1785	1788	1794	rVV2	51675	67306	1.91%	0.218%
19	12.763	1813	1815	1820	rVB	96584	93847	2.66%	0.304%
20	12.886	1832	1836	1840	rBV	2171850	2199448	62.26%	7.121%
21	13.763	1982	1985	1992	rBV	329973	360520	10.21%	1.167%
22	13.963	2015	2019	2023	rBV	765284	782119	22.14%	2.532%
23	14.551	2116	2119	2124	rBV	148531	126795	3.59%	0.411%
24	15.433	2265	2269	2279	rVB	535901	711014	20.13%	2.302%

Sum of corrected areas: 30885101

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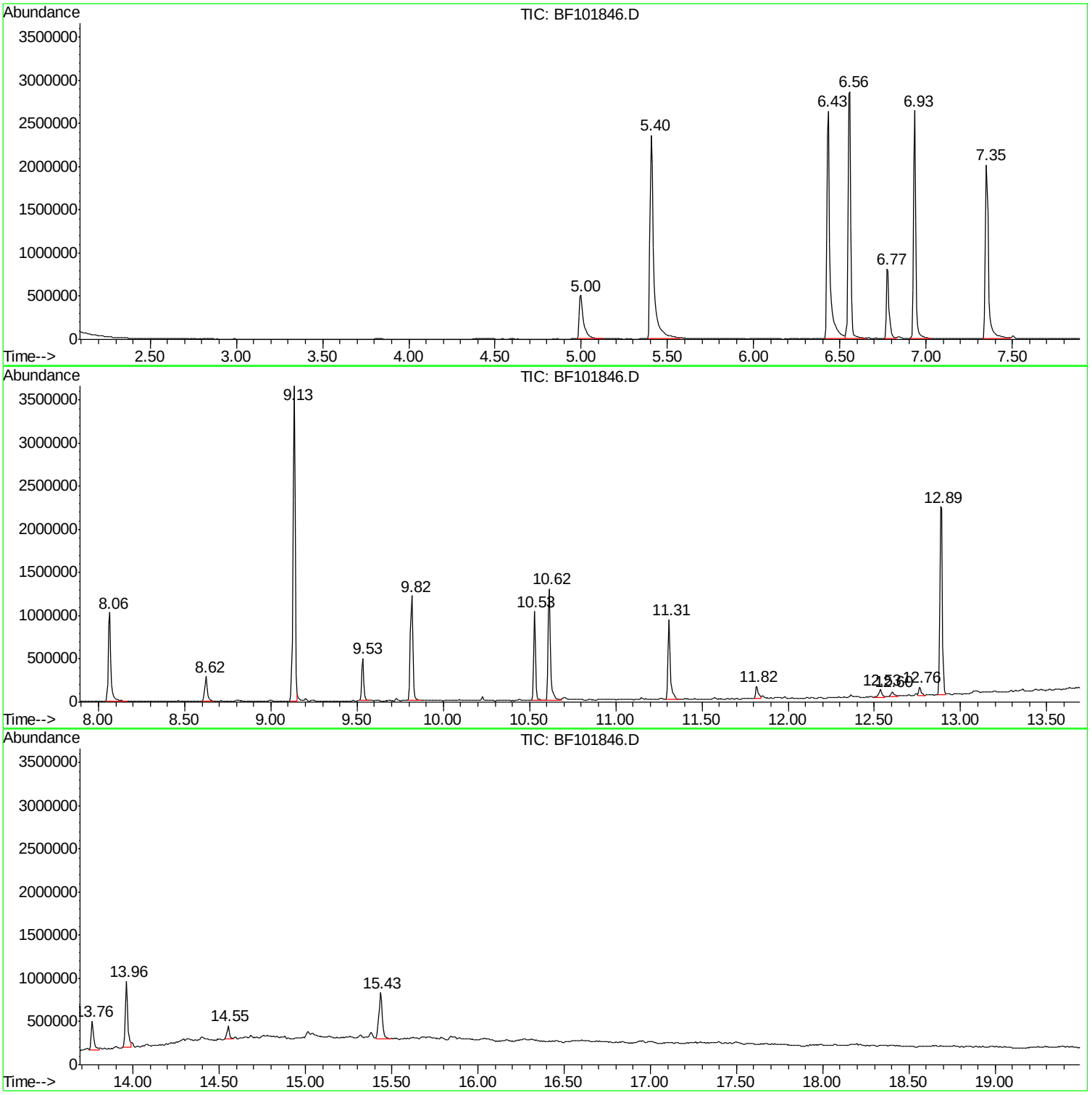
Sample : I7100-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EPE-105-1(0-5)

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101846.D
Acq On : 2 Jan 2018 13:02
Operator : SJ/JU
Sample : I7100-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(0-5)

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

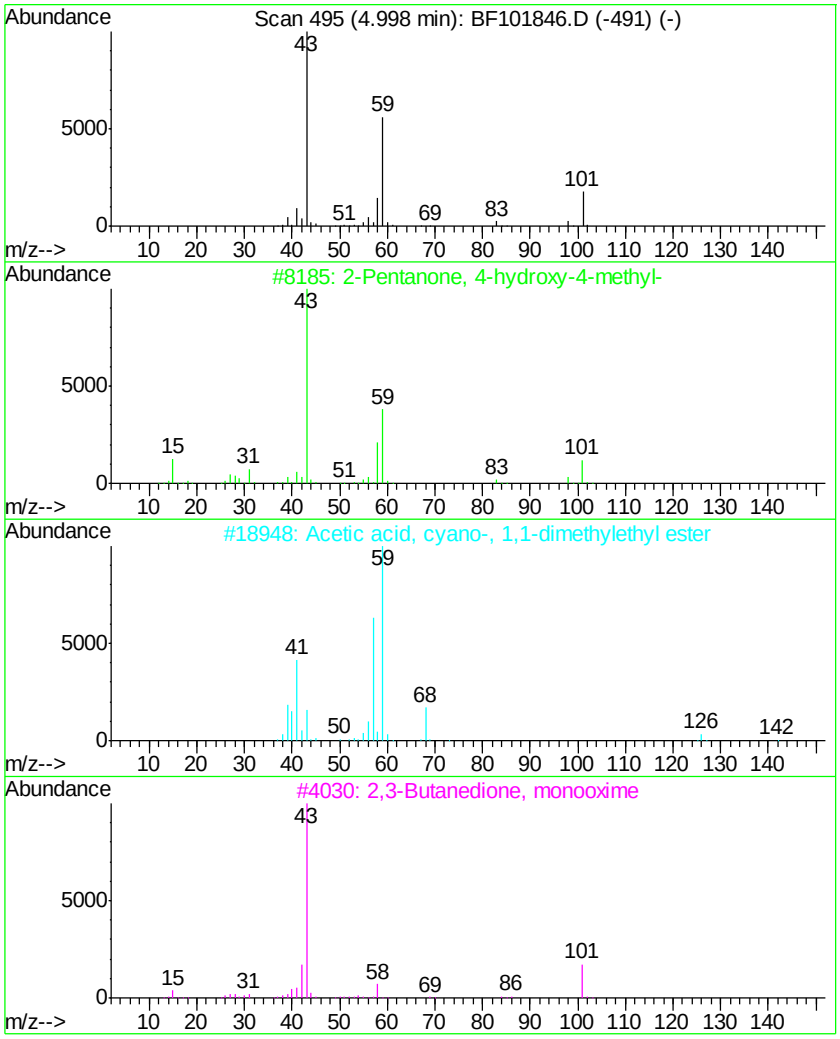
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

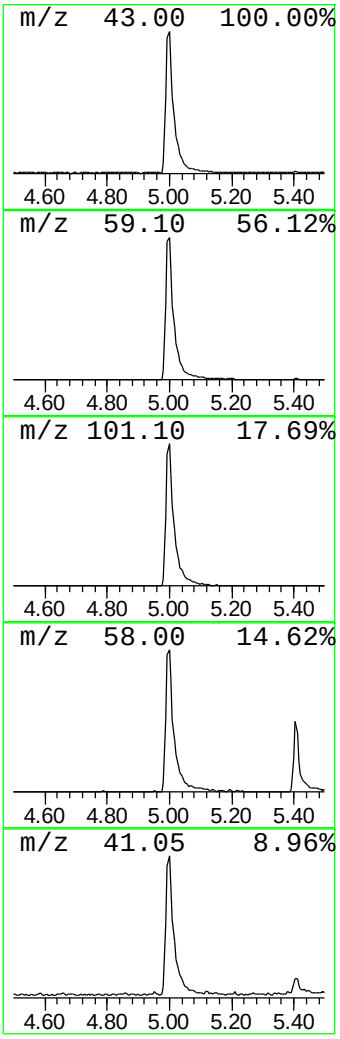
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	21.97 ng	941611	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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101846.D
Acq On : 2 Jan 2018 13:02
Operator : SJ/JU
Sample : I7100-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(0-5)

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

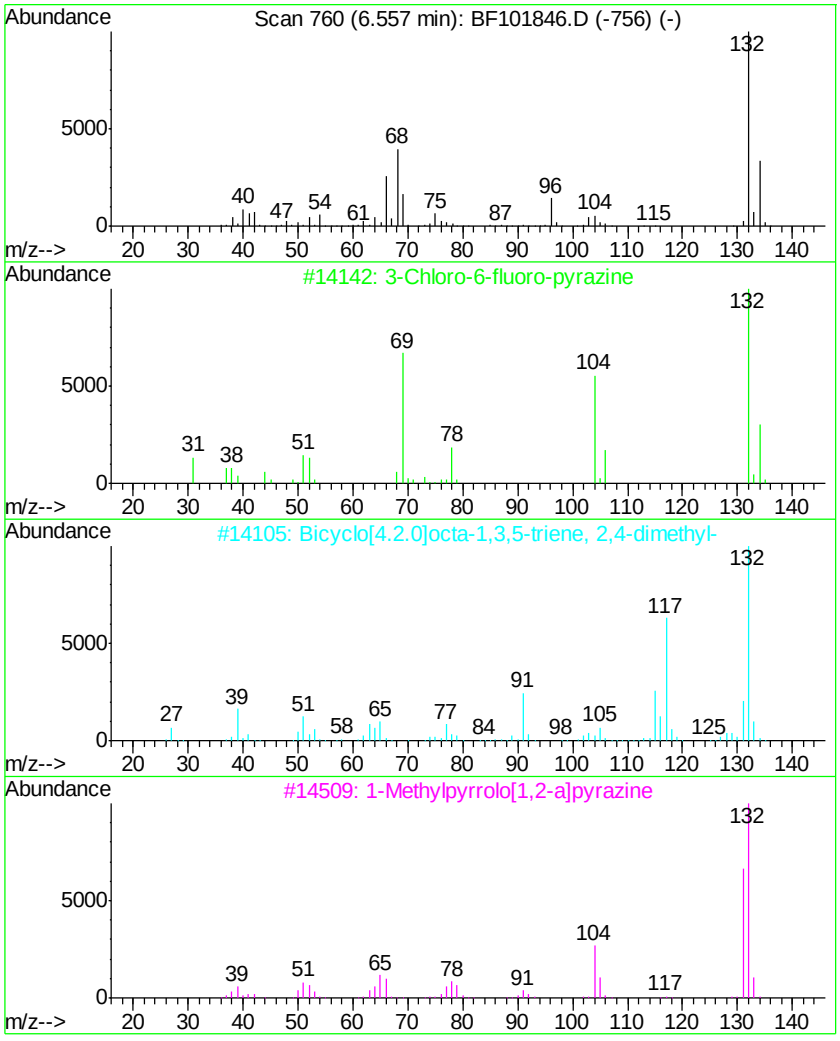
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

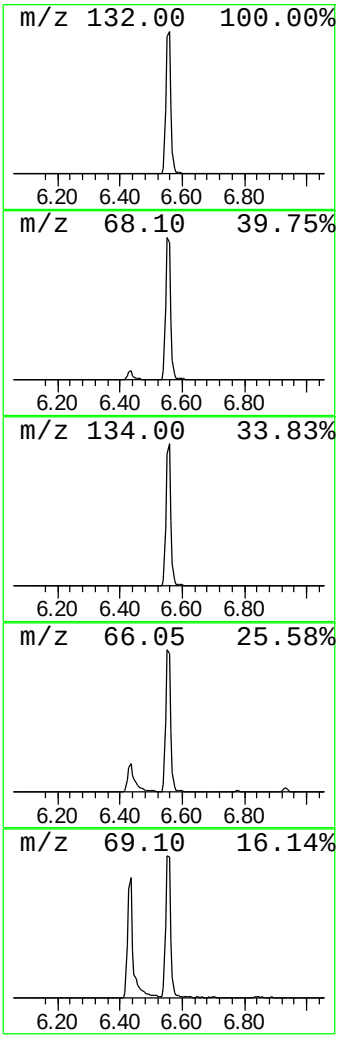
****

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	76.44 ng	3276930	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	27
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	5-Aminoindole	132	C8H8N2	005192-03-0	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101846.D
Acq On : 2 Jan 2018 13:02
Operator : SJ/JU
Sample : I7100-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(0-5)

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

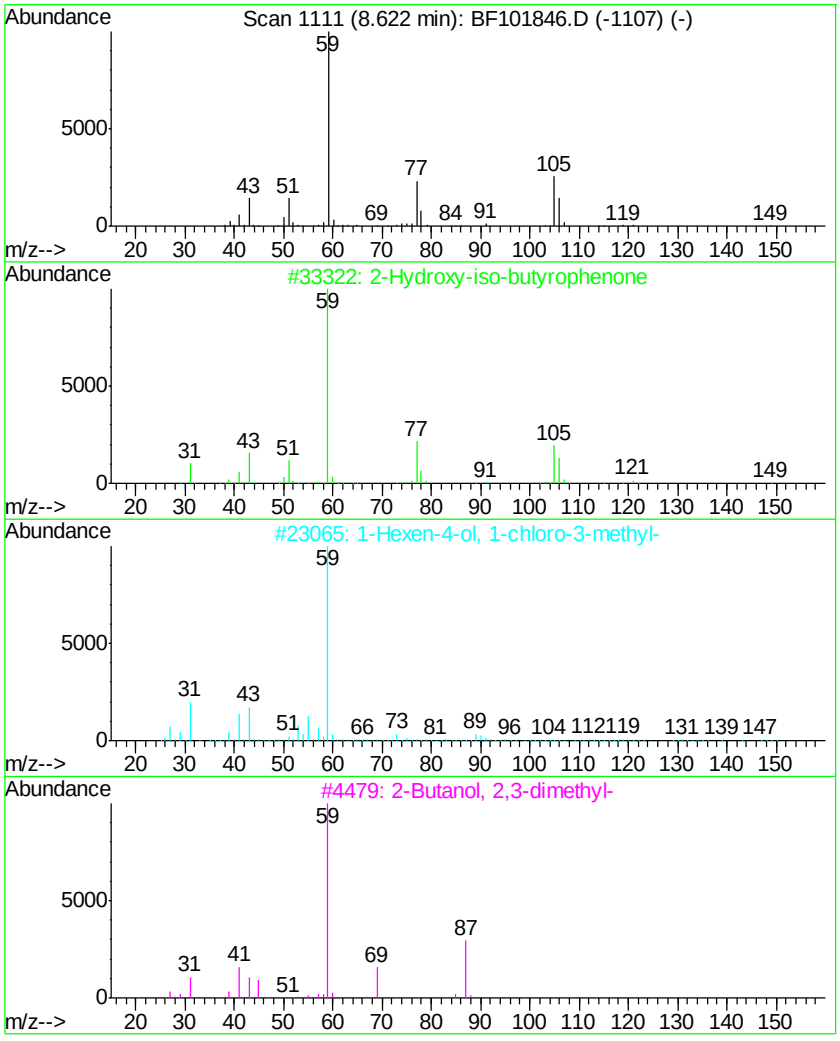
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

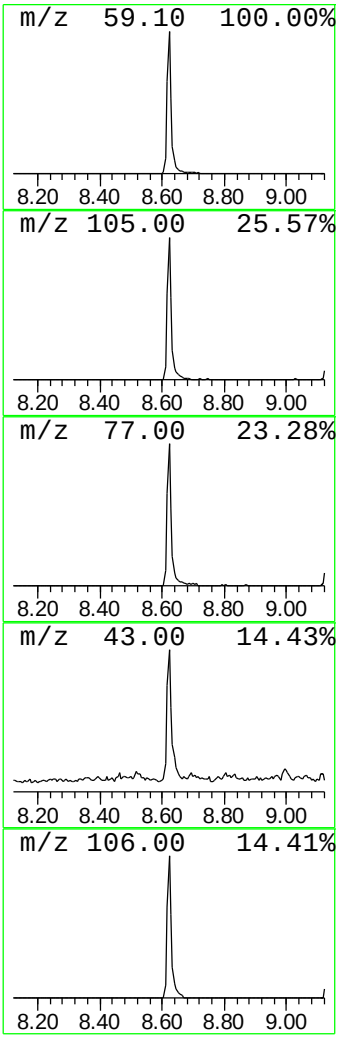
****

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.62	5.22 ng	290666	Naphthalene-d8	8.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	83
2	1-Hexen-4-ol, 1-chloro-3-methyl-	148	C7H13ClO	1000153-35-0	9
3	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	9
4	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	9
5	Ethanone, 2-amino-1-phenyl-	135	C8H9NO	000613-89-8	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101846.D
Acq On : 2 Jan 2018 13:02
Operator : SJ/JU
Sample : I7100-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(0-5)

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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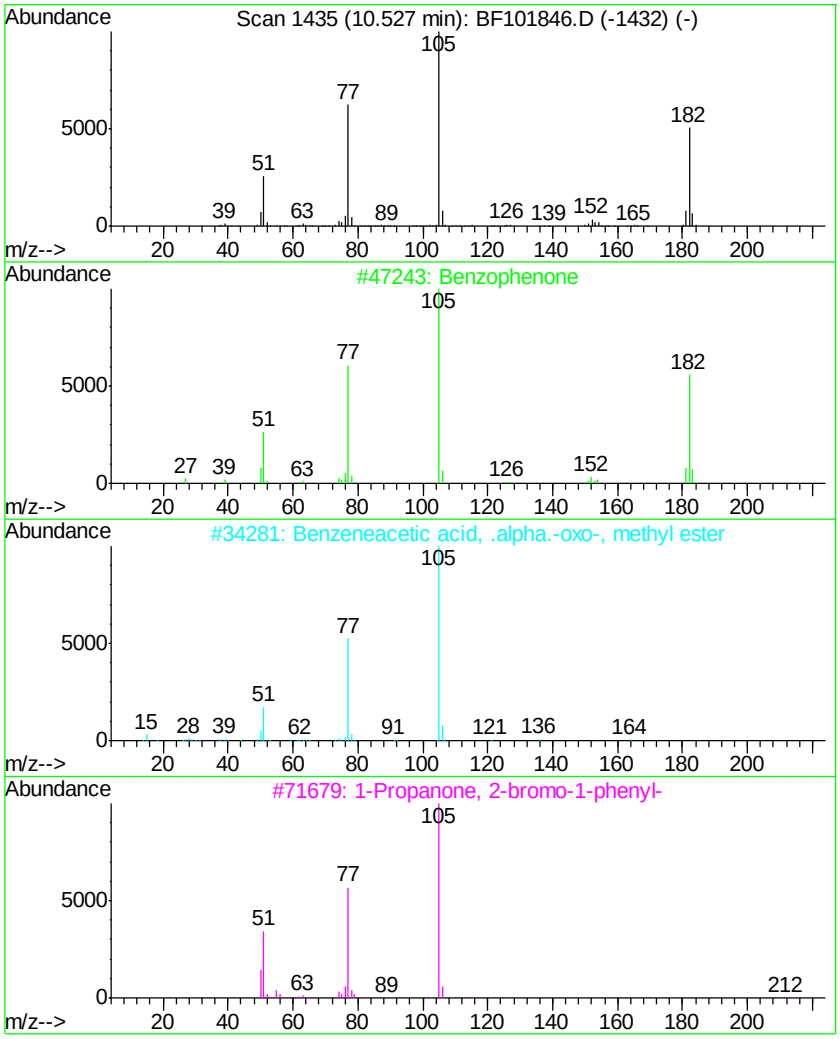
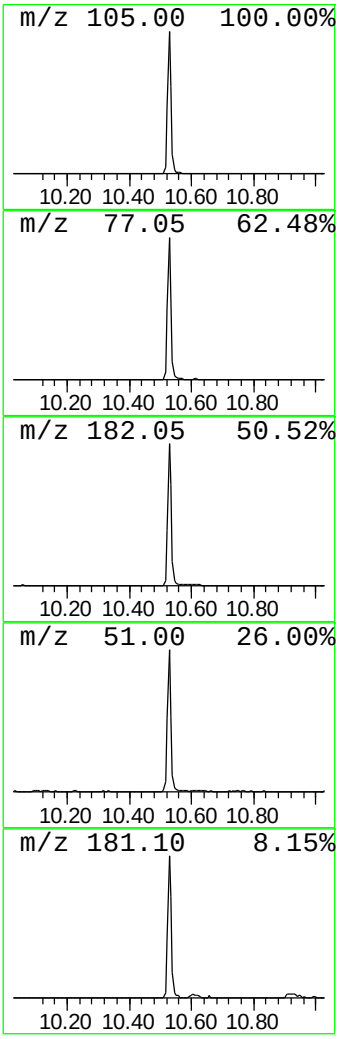
Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	15.78 ng	843316	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101846.D
Acq On : 2 Jan 2018 13:02
Operator : SJ/JU
Sample : I7100-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(0-5)

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

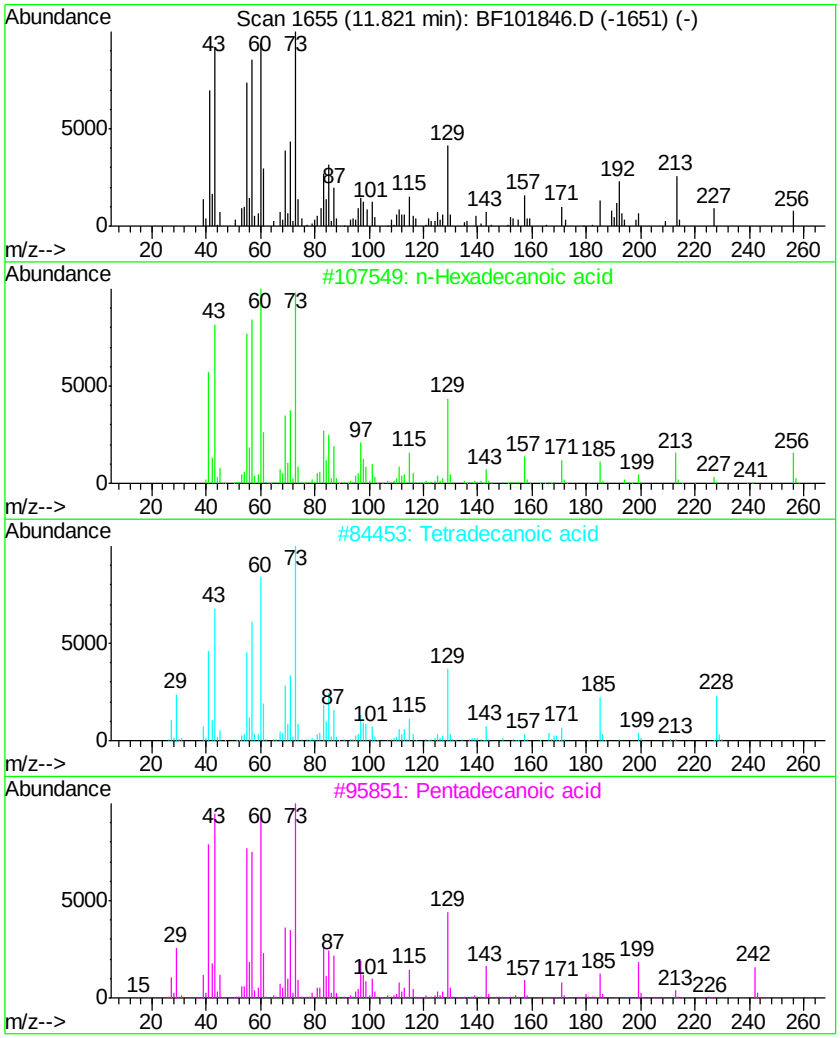
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

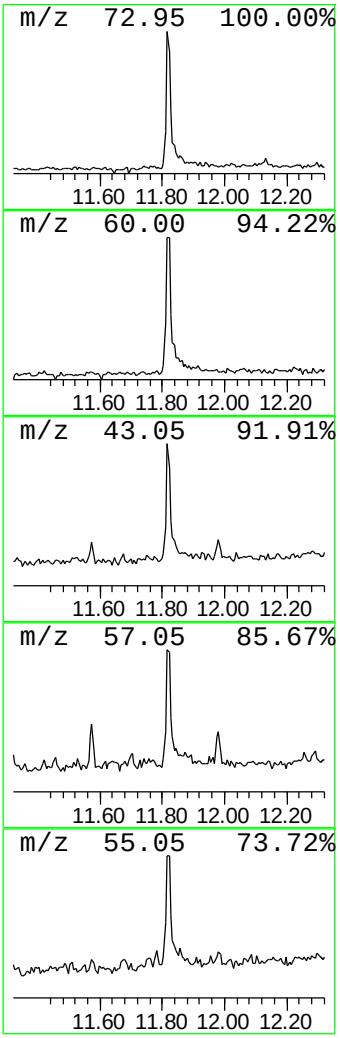
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	3.42 ng	157334	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	15





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101846.D
Acq On : 2 Jan 2018 13:02
Operator : SJ/JU
Sample : I7100-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(0-5)

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

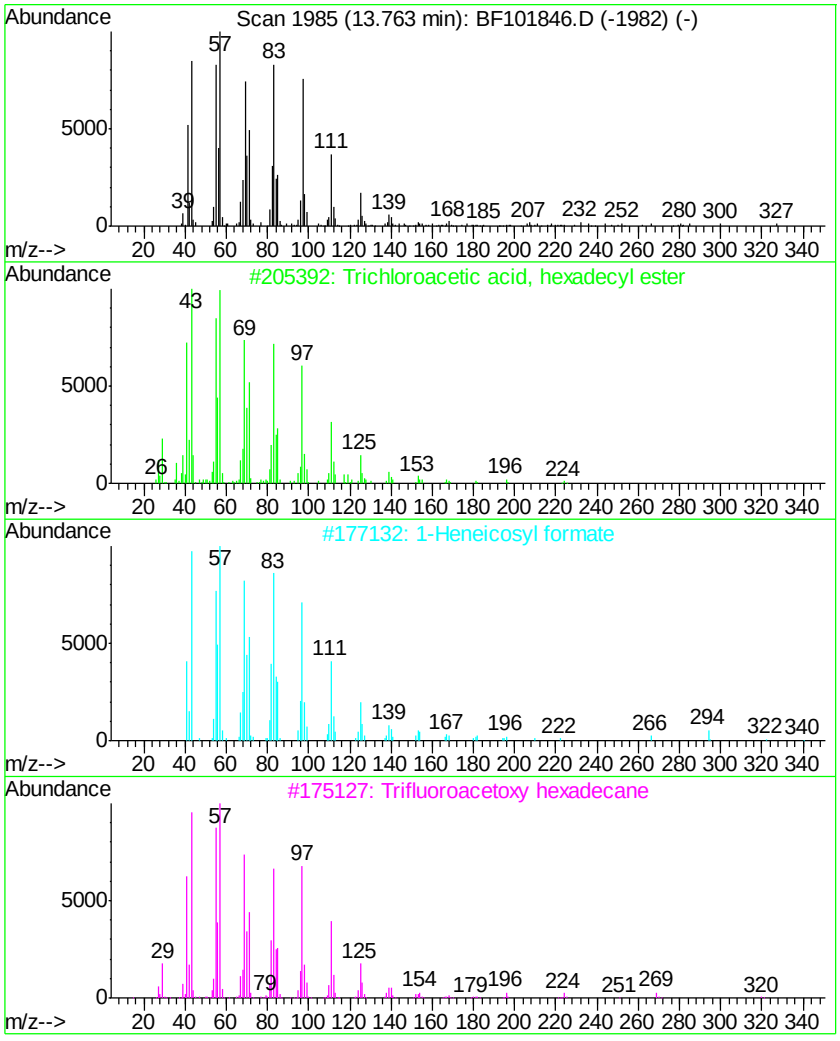
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

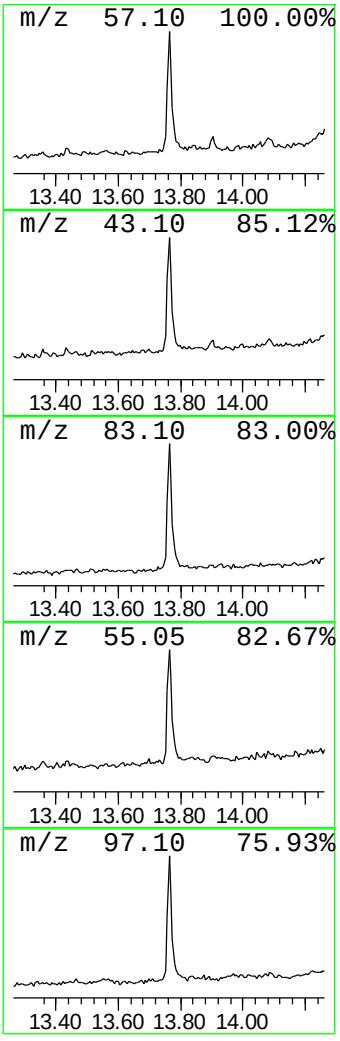
****

Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	9.22 ng	360520	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	1-Nonadecene	266	C19H38	018435-45-5	92
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101846.D
Acq On : 2 Jan 2018 13:02
Operator : SJ/JU
Sample : I7100-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-105-1(0-5)

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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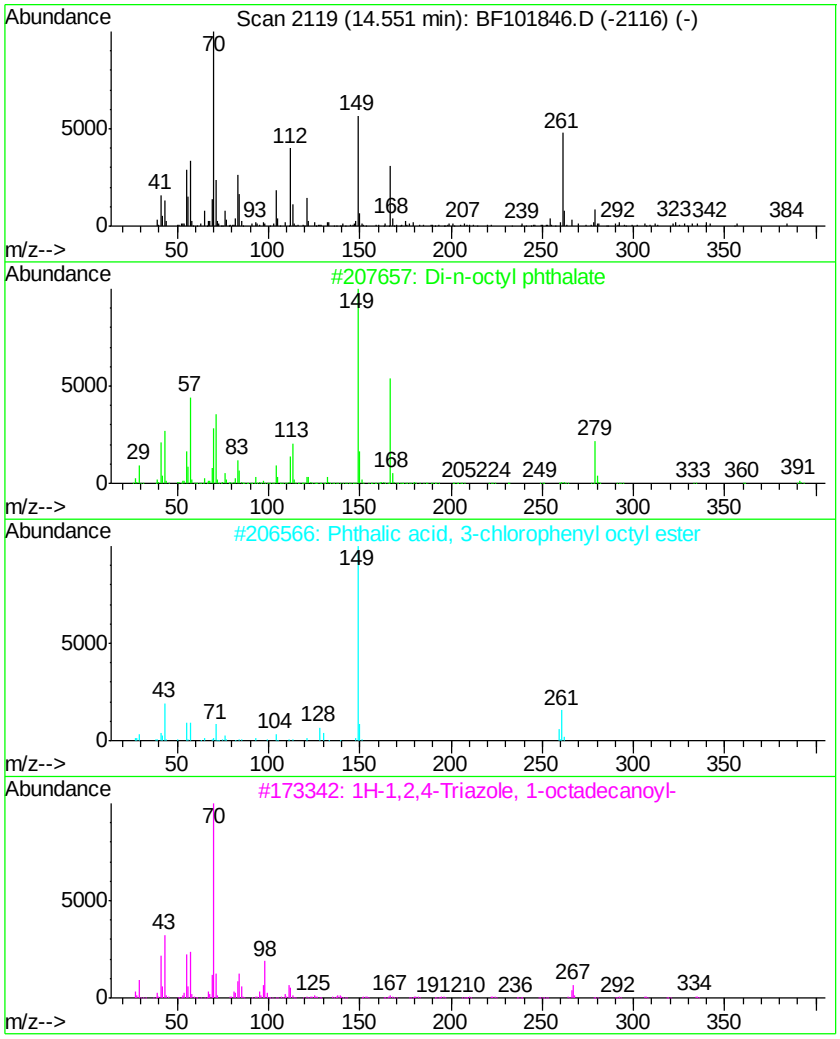
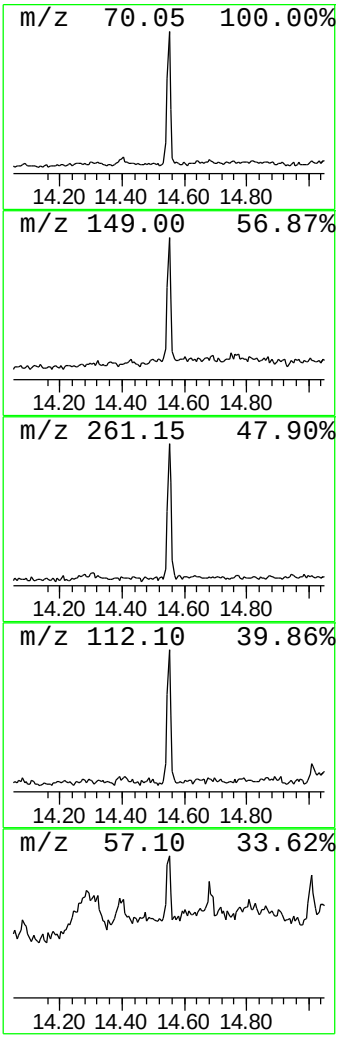
Peak Number 10 unknown14.55 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	3.24 ng	126795	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-n-octyl phthalate	390	C24H38O4	000117-84-0	22
2	Phthalic acid, 3-chlorophenyl oc...	388	C22H25ClO4	1000314-94-5	22
3	1H-1,2,4-Triazole, 1-octadecanoyl-	335	C20H37N3O	060718-55-0	22
4	Octane, 3,4-epoxy-2,2,7,7-tetram...	184	C12H24O	1000163-73-3	14
5	Phthalic acid, 3,5-difluoropheny...	418	C24H28F2O4	1000315-53-1	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010218\
Data File : BF101846.D
Acq On : 2 Jan 2018 13:02
Operator : SJ/JU
Sample : I7100-01
Misc :
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Instrument : BNA_F
ClientSampleId : EPE-105-1(0-5)

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	22.0	ng	941611	1	6.78	857343	20.0
unknown6.56	6.56	76.4	ng	3276930	1	6.78	857343	20.0
2-Hydroxy-iso-but...	8.62	5.2	ng	290666	2	8.06	1113950	20.0
Benzophenone	10.53	15.8	ng	843316	3	9.82	1068780	20.0
n-Hexadecanoic acid	11.82	3.4	ng	157334	4	11.31	919019	20.0
Trichloroacetic a...	13.76	9.2	ng	360520	5	13.96	782119	20.0
unknown14.55	14.55	3.2	ng	126795	5	13.96	782119	20.0