LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102725.D
Acq On : 3 Feb 2018 18:57
Operator : SJ/JU
Sample : J1436-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B12

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-BF020318.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	2.157	7	12	19	rVB	393665	514807	11.38%	1.279%
2	5.110	511	514	520	rVB	167737	198225	4.38%	0.493%
3	5.498	574	580	583	rBV	4128805	4525636	100.00%	11.247%
4	6.504	745	751	755	rBV	4167769	4487674	99.16%	11.153%
5	6.651	770	776	779	rBV	4168288	4425358	97.78%	10.998%
6	6.881	811	815	818	rBV	1506284	1232832	27.24%	3.064%
7	7.039	837	842	845	rVB	3580305	3391930	74.95%	8.430%
8	7.439	905	910	913	rBV	2827814	2806331	62.01%	6.974%
9	8.163	1029	1033	1036	rBV	1864693	1620033	35.80%	4.026%
10	8.710	1123	1126	1130	rBV	102058	88332	1.95%	0.220%
11	9.239	1211	1216	1219	rBV	4501186	4282563	94.63%	10.643%
12	9.627	1278	1282	1285	rBV	595521	459573	10.15%	1.142%
13	9.839	1316	1318	1323	rVB	61718	53381	1.18%	0.133%
14	9.916	1327	1331	1335	rVV2	1889044	1586451	35.05%	3.943%
15	10.221	1377	1383	1396	rBV	72849	196425	4.34%	0.488%
16	10.339	1401	1403	1406	rVB	60951	51329	1.13%	0.128%
17	10.627	1447	1452	1455	rBV	213178	174770	3.86%	0.434%
18	10.704	1460	1465	1468	rBV	2452032	2224446	49.15%	5.528%
19	10.816	1481	1484	1490	rVB	51846	59288	1.31%	0.147%
20	11.398	1580	1583	1587	rBV	1332387	1236262	27.32%	3.072%
21	11.921	1668	1672	1684	rBV	503269	598950	13.23%	1.488%
22	12.627	1787	1792	1794	rBV3	57262	84441	1.87%	0.210%
23	12.704	1802	1805	1815	rBV	212083	278505	6.15%	0.692%
24	12.986	1849	1853	1856	rBV	3045661	2723649	60.18%	6.769%
25	13.257	1897	1899	1901	rBV	58855	54370	1.20%	0.135%
26	13.874	2001	2004	2007	rBV	702478	640471	14.15%	1.592%
27	14.039	2028	2032	2035	rBV	1155232	1012129	22.36%	2.515%
28	14.509	2109	2112	2116	rBV	172342	199162	4.40%	0.495%
29	15.515	2278	2283	2294	rVB	784953	1031317	22.79%	2.563%

Sum of corrected areas: 40238640

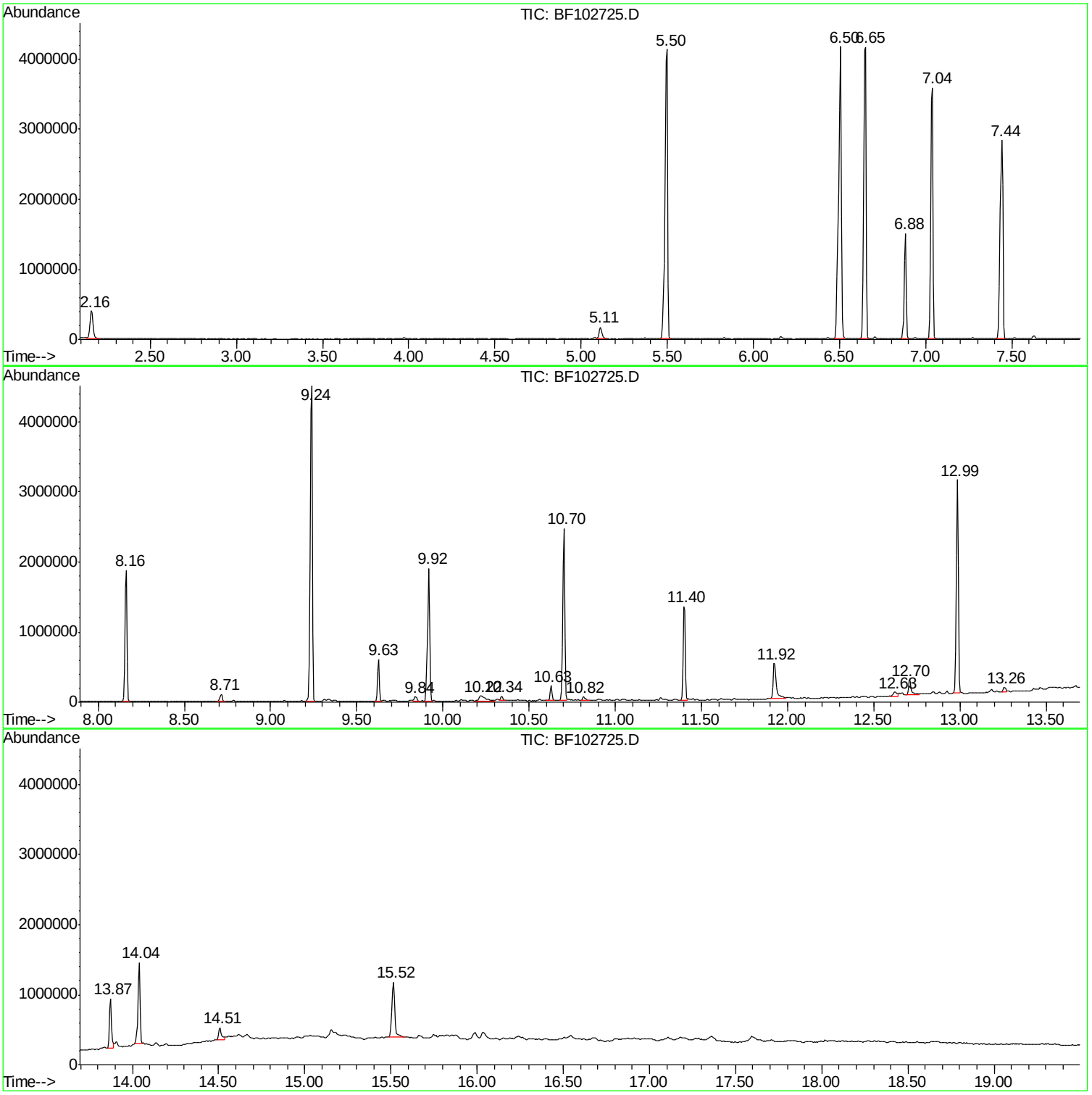
LSC Report - Integrated Chromatogram

Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102725.D
Acq On : 3 Feb 2018 18:57
Operator : SJ/JU
Sample : J1436-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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\BF020318\
Data File : BF102725.D
Acq On : 3 Feb 2018 18:57
Operator : SJ/JU
Sample : J1436-09
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

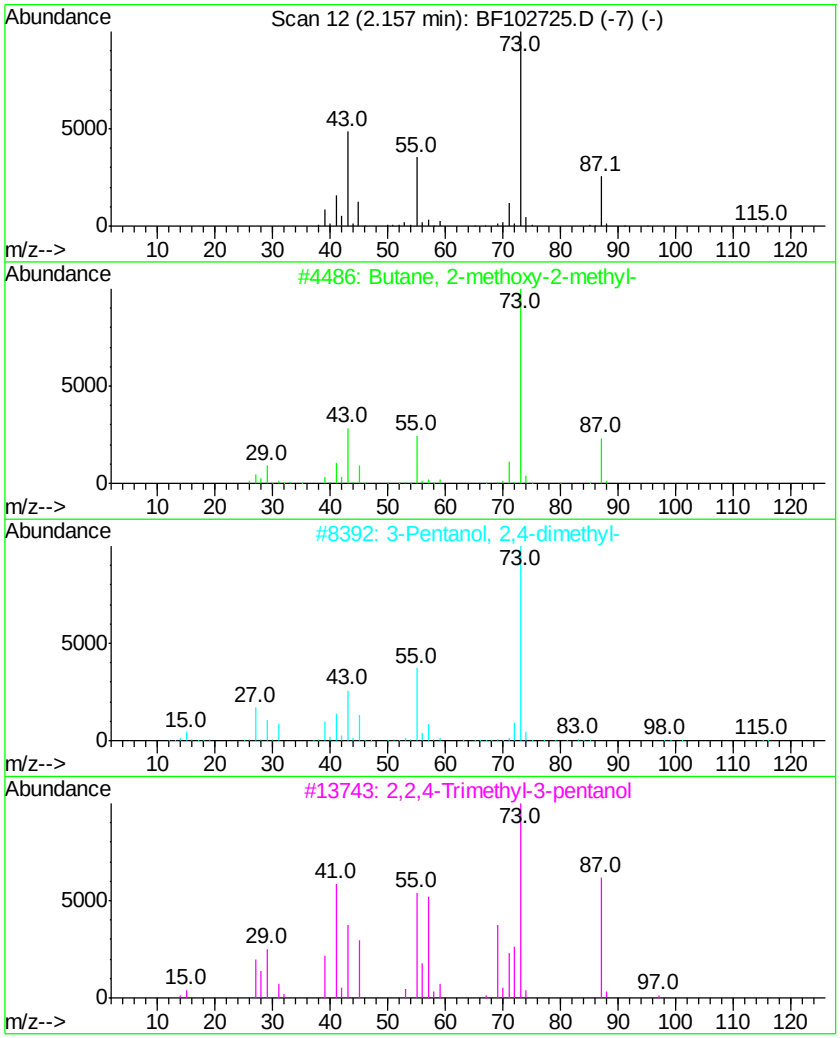
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

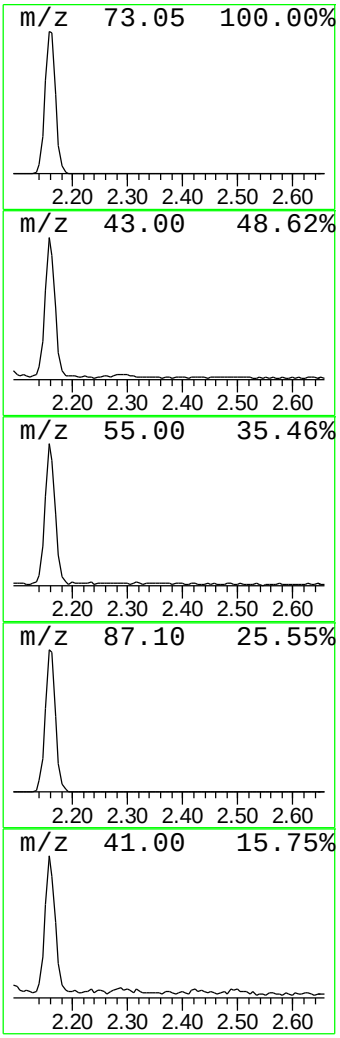
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	8.35 ng	514807	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	33





Library Search Compound Report

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Data File : BF102725.D
Acq On : 3 Feb 2018 18:57
Operator : SJ/JU
Sample : J1436-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

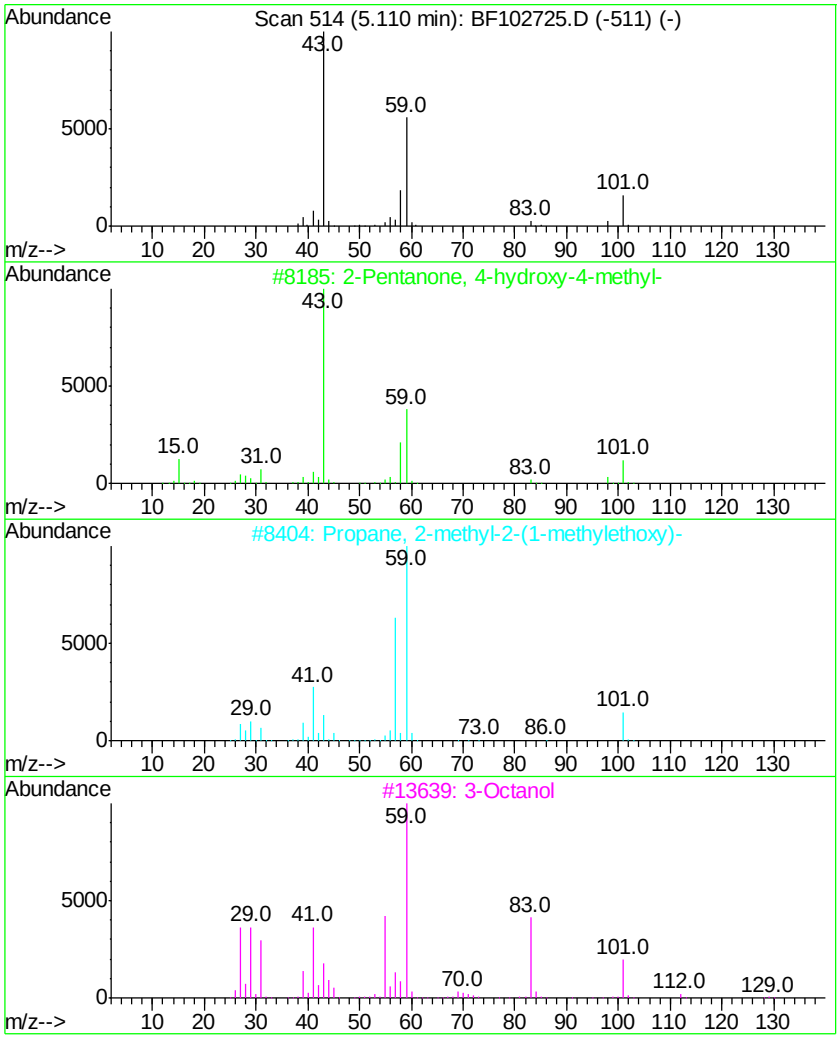
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

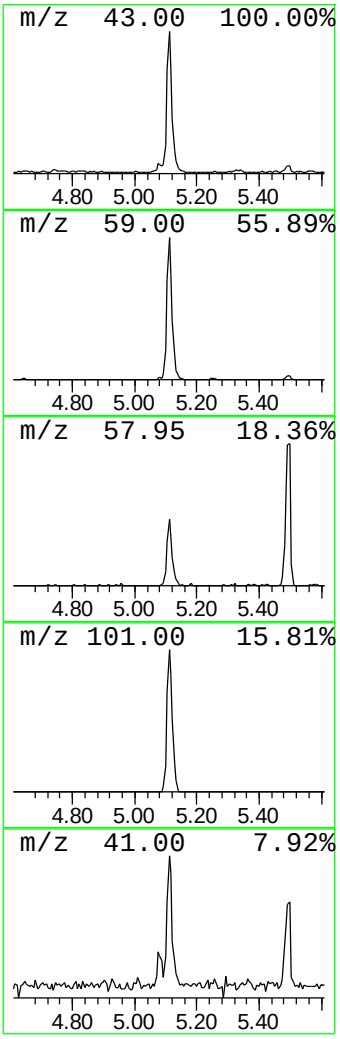
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	3.22 ng	198225	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Octanol	130	C8H18O	000589-98-0	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25





Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102725.D
Acq On : 3 Feb 2018 18:57
Operator : SJ/JU
Sample : J1436-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

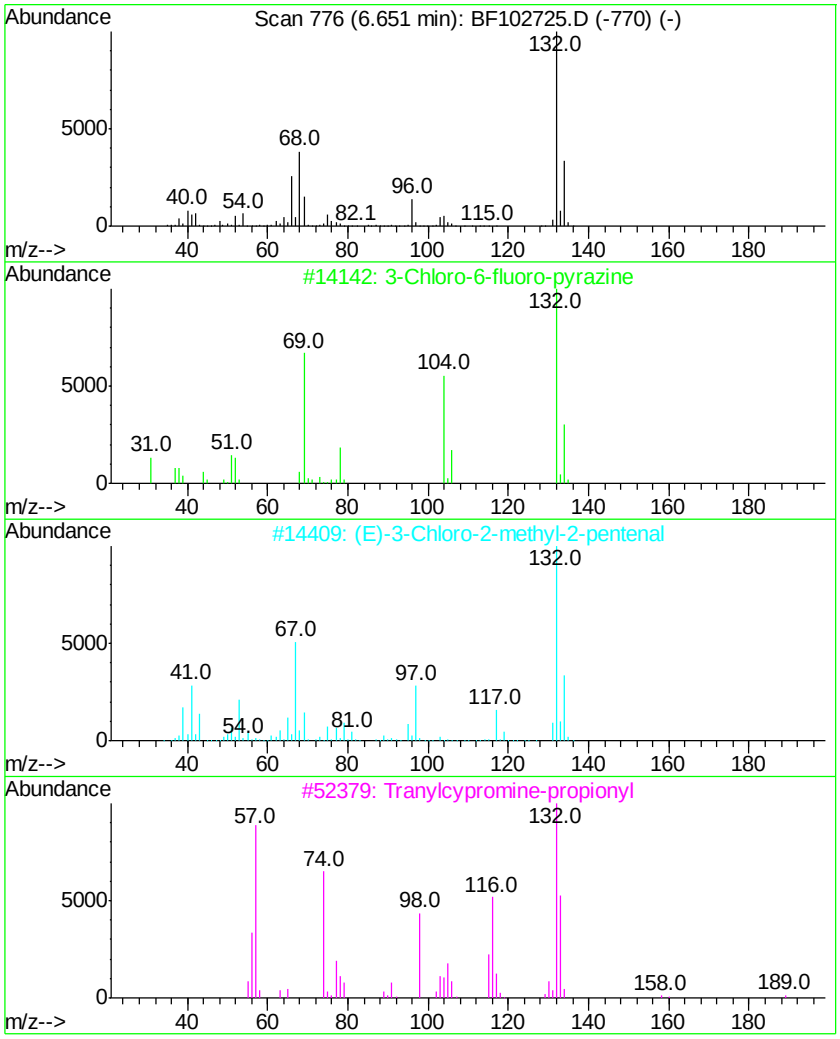
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

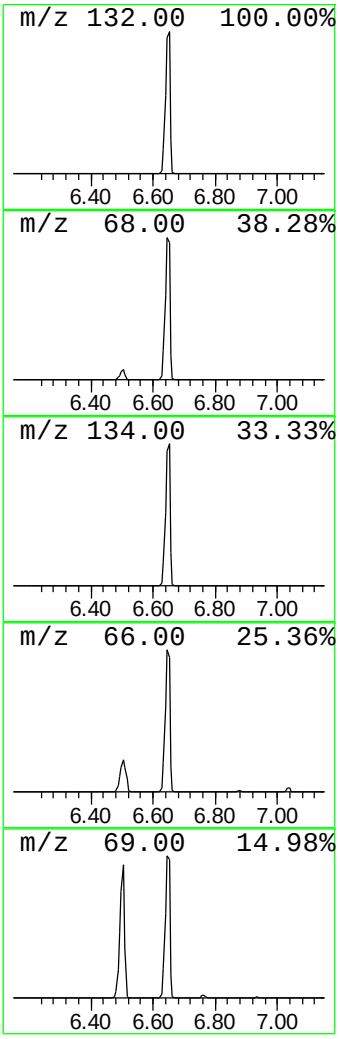
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	71.79 ng	4425360	1,4-Dichlorobenzene-d4	6.88

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	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102725.D
Acq On : 3 Feb 2018 18:57
Operator : SJ/JU
Sample : J1436-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

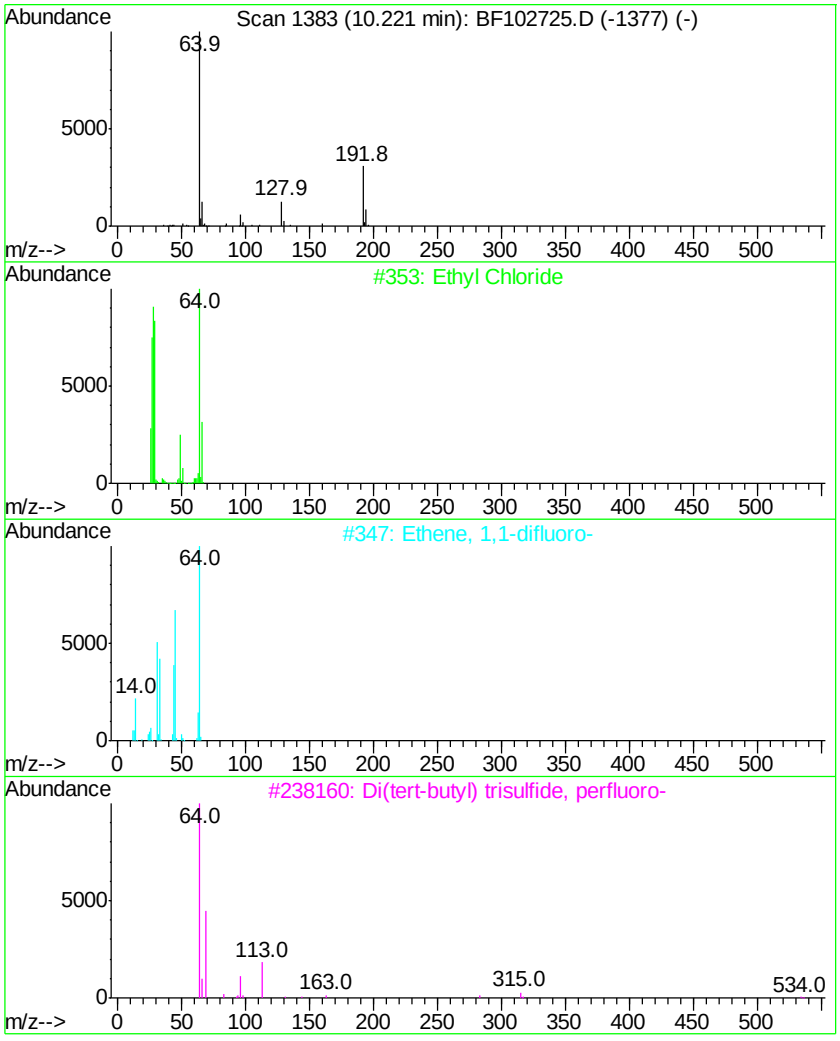
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

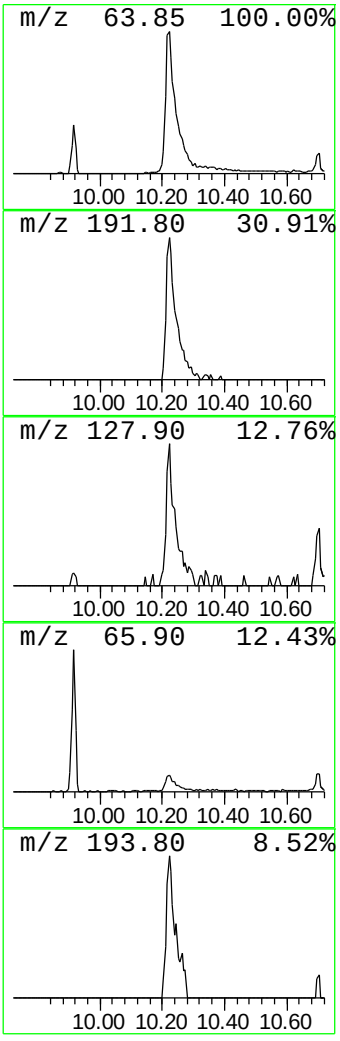
****

Peak Number 5 unknown10.22 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.22	2.48 ng	196425	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl Chloride	64	C2H5Cl	000075-00-3	4
2	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
3	Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	4
4	Pentafluorochlorodimethyl trisul...	250	C2ClF5S3	1000226-65-9	4
5	Sulfur dioxide	64	O2S	007446-09-5	3





Data Path : U:\HPCHEM1\BNA F\DATA\BF020318\
Data File : BF102725.D
Acq On : 3 Feb 2018 18:57
Operator : SJ/JU
Sample : J1436-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

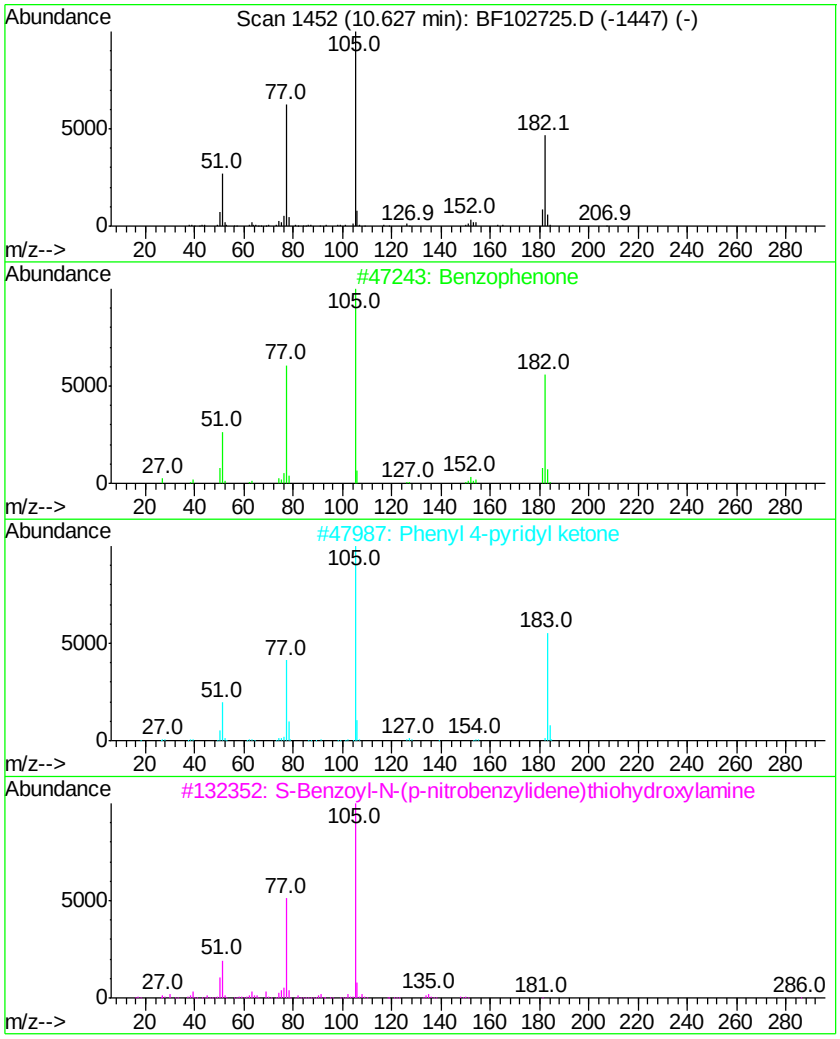
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

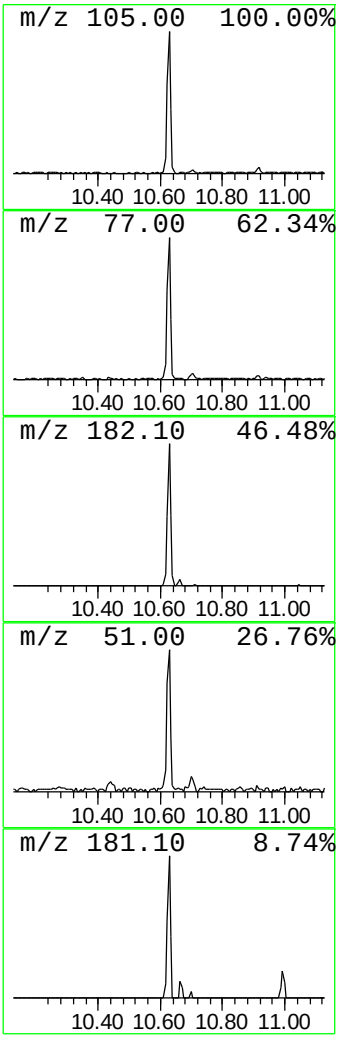
****

Peak Number 6 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	2.20 ng	174770	Acenaphthene-d10	9.92

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	S-Benzoyl-N-(p-nitrobenzylidene)...	286	C14H10N2O3S	139776-09-3	47
4	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47





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Sample : J1436-09
Misc :
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Instrument : BNA_F
ClientSampleId : B12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

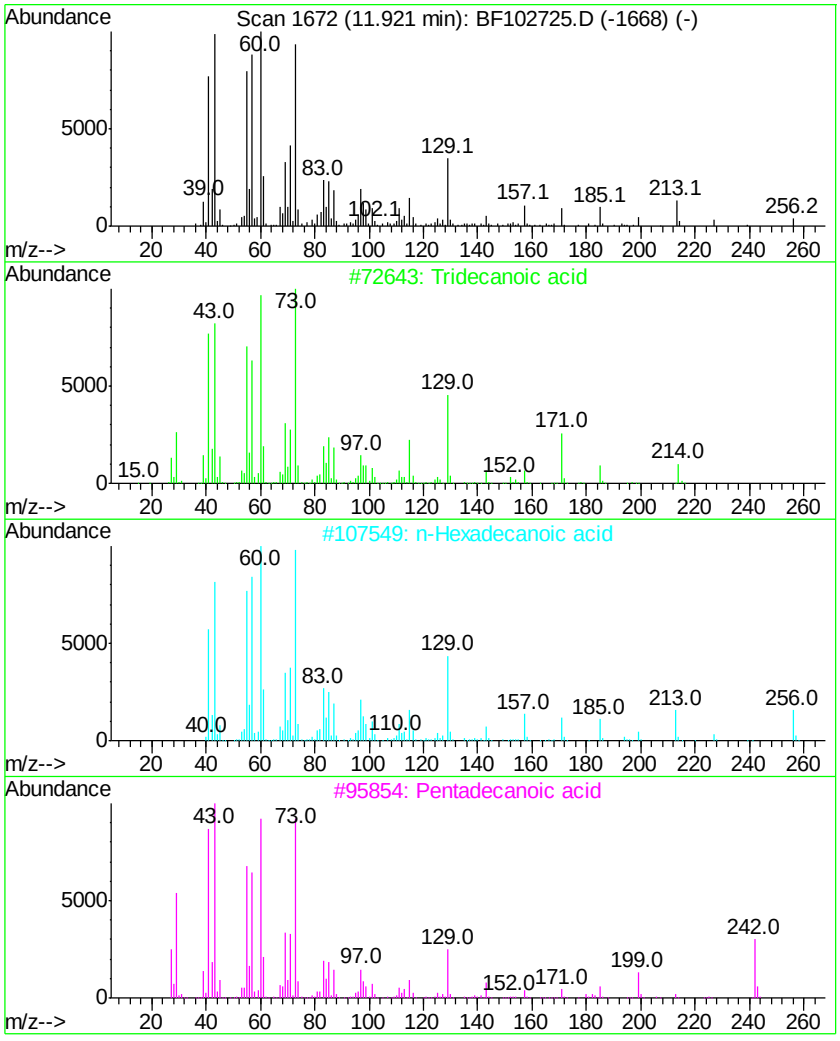
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

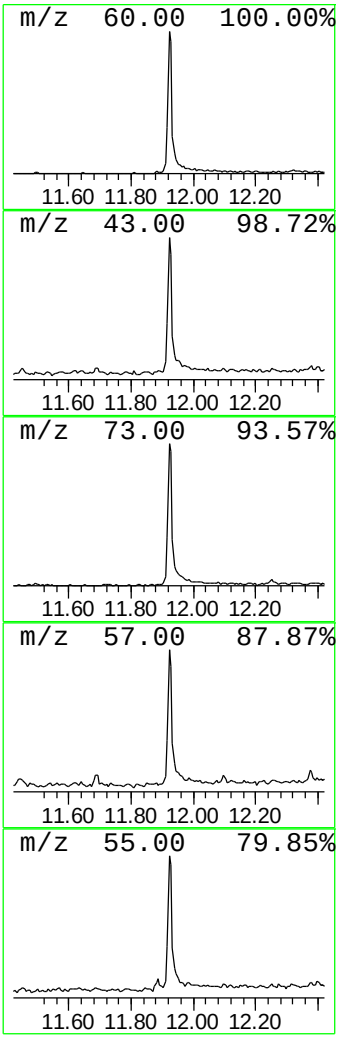
****

Peak Number 7 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	9.69 ng	598950	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Data File : BF102725.D
Acq On : 3 Feb 2018 18:57
Operator : SJ/JU
Sample : J1436-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

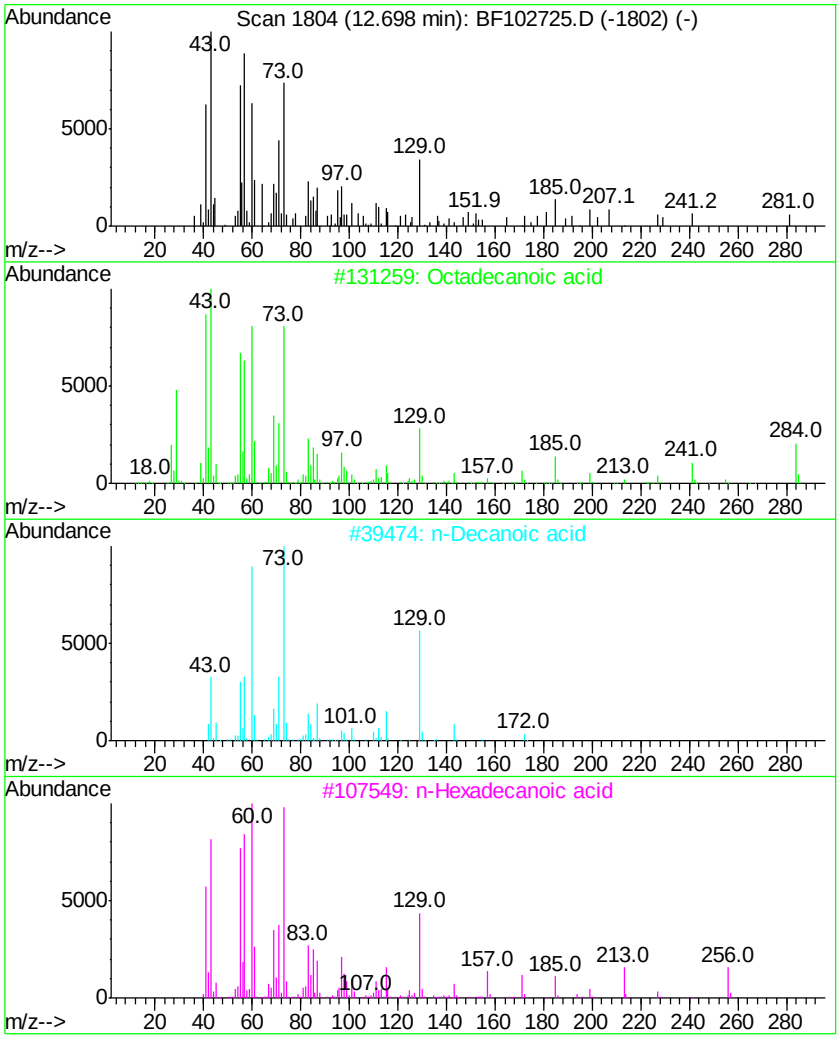
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

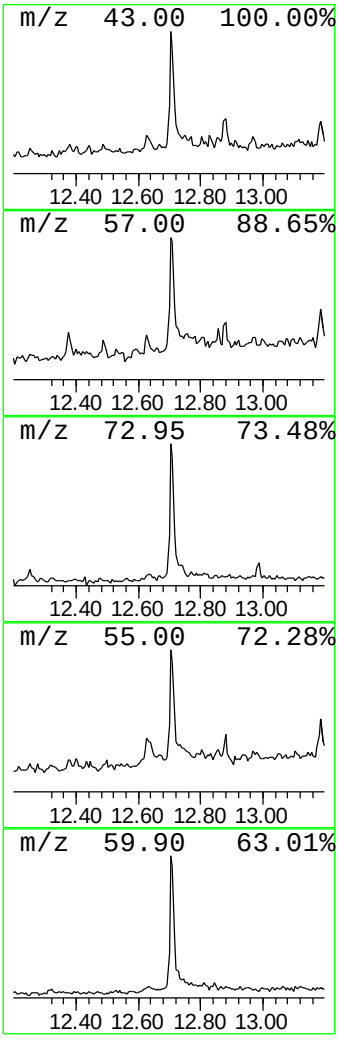
****

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	4.51 ng	278505	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Decanoic acid	172	C10H20O2	000334-48-5	94
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Undecanoic acid	186	C11H22O2	000112-37-8	83





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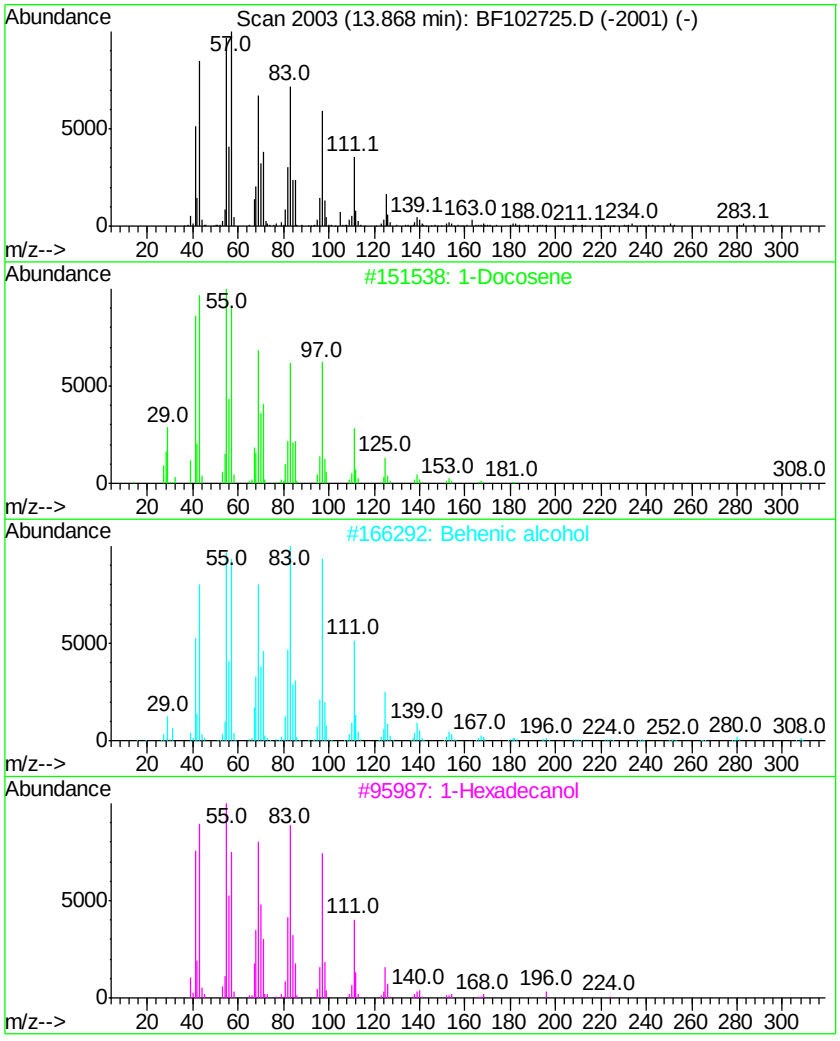
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

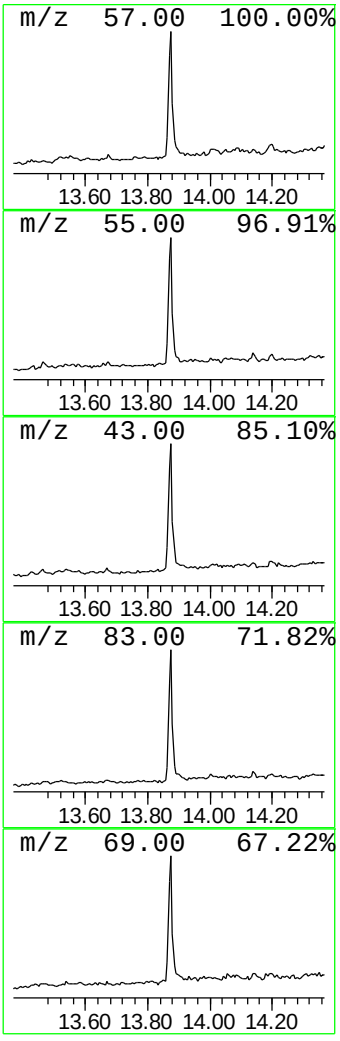
****

Peak Number 9 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	12.66 ng	640471	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	1-Hexadecanol	242	C16H34O	036653-82-4	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





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Operator : SJ/JU
Sample : J1436-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

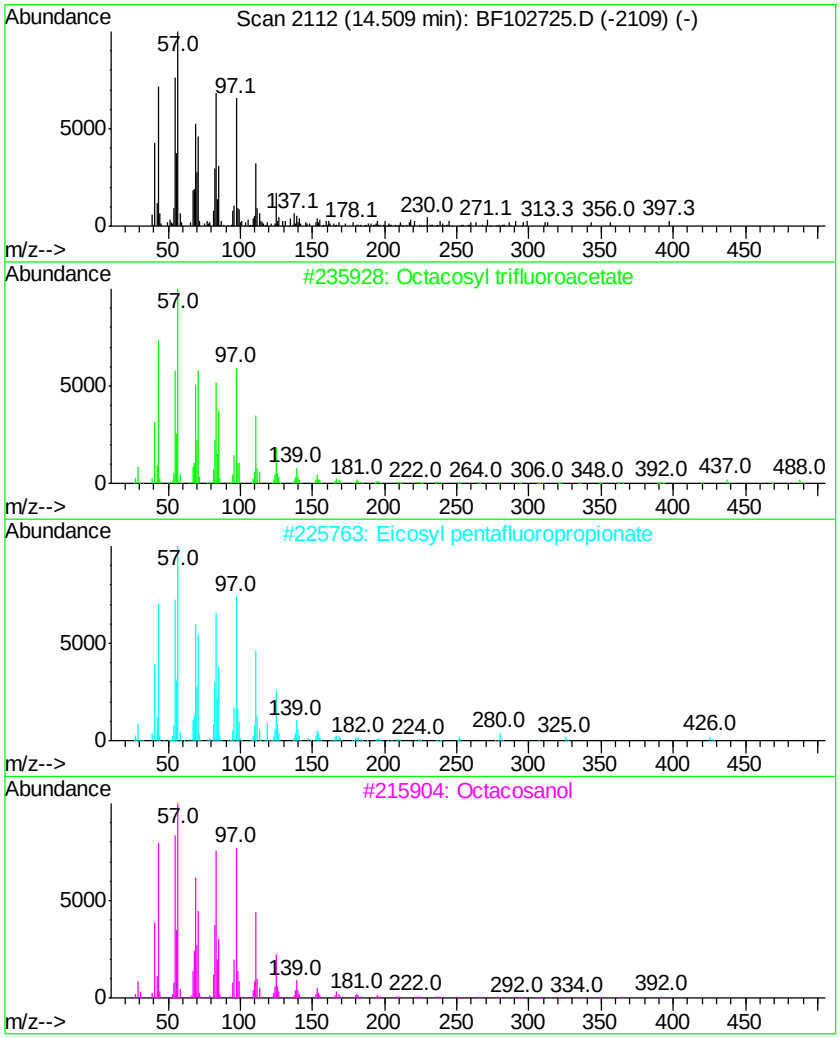
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

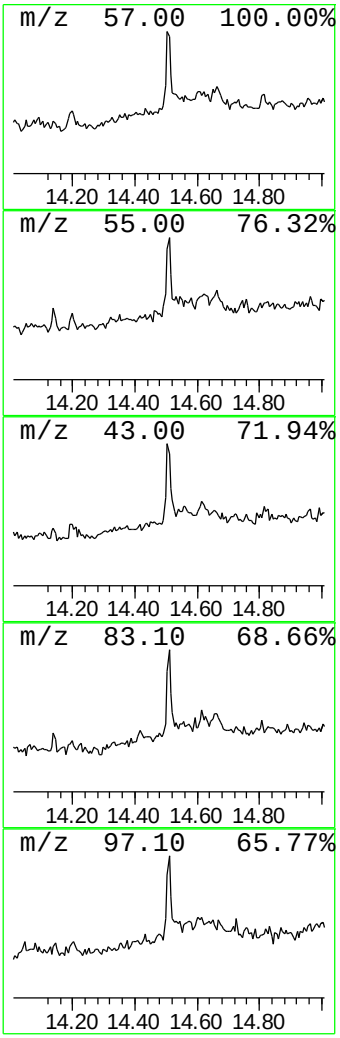
****

Peak Number 10 Octacosyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	3.94 ng	199162	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
3	Octacosanol	410	C28H58O	000557-61-9	87
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	81
5	Behenic alcohol	326	C22H46O	000661-19-8	74





Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_F\DATA\BF020318\
Data File : BF102725.D
Acq On : 3 Feb 2018 18:57
Operator : SJ/JU
Sample : J1436-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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
Butane, 2-methoxy...	2.16	8.3	ng	514807	1	6.88	1232830	20.0
2-Pentanone, 4-hy...	5.11	3.2	ng	198225	1	6.88	1232830	20.0
unknown6.65	6.65	71.8	ng	4425360	1	6.88	1232830	20.0
unknown10.22	10.22	2.5	ng	196425	3	9.92	1586450	20.0
Benzophenone	10.63	2.2	ng	174770	3	9.92	1586450	20.0
Tridecanoic acid	11.92	9.7	ng	598950	4	11.40	1236260	20.0
Octadecanoic acid	12.70	4.5	ng	278505	4	11.40	1236260	20.0
1-Docosene	13.87	12.7	ng	640471	5	14.04	1012130	20.0
Octacosyl trifluo...	14.51	3.9	ng	199162	5	14.04	1012130	20.0