LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100476.D
Acq On : 12 Nov 2017 8:22
Operator : SJ/JU
Sample : I6402-03
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110717-TIDO-F-U-B

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-BF110817.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	2.210	17	21	38	rVB	95426	177744	4.23%	0.706%
2	5.122	512	516	525	rVB	259476	274165	6.53%	1.089%
3	5.516	579	583	586	rBV	1678759	1428017	34.02%	5.674%
4	6.516	749	753	762	rVB	1166625	1007544	24.00%	4.003%
5	6.669	774	779	782	rBV	2605568	2392258	56.99%	9.505%
6	6.898	815	818	822	rBV	938899	856178	20.40%	3.402%
7	7.063	841	846	849	rVB	3040407	3038417	72.39%	12.072%
8	7.469	909	915	918	rBV	2281916	2608346	62.14%	10.363%
9	8.180	1032	1036	1040	rBV	1211280	1056521	25.17%	4.198%
10	9.263	1214	1220	1223	rBV	3999606	4197550	100.00%	16.678%
11	9.645	1282	1285	1289	rBV	94500	74497	1.77%	0.296%
12	9.939	1328	1335	1347	rVB	1113315	1060694	25.27%	4.214%
13	10.604	1445	1448	1451	rBV	66852	47420	1.13%	0.188%
14	10.645	1452	1455	1462	rVB	71566	61198	1.46%	0.243%
15	10.722	1464	1468	1480	rBV	1415982	1387830	33.06%	5.514%
16	11.421	1584	1587	1591	rBV	946954	842824	20.08%	3.349%
17	12.821	1822	1825	1828	rBV	114549	84891	2.02%	0.337%
18	13.010	1852	1857	1860	rBV	3106513	3087772	73.56%	12.268%
19	13.527	1942	1945	1948	rBV	72794	57030	1.36%	0.227%
20	14.062	2032	2036	2043	rVB	875206	775569	18.48%	3.081%
21	14.751	2149	2153	2163	rBV	52459	98561	2.35%	0.392%
22	15.545	2283	2288	2299	rBV	401296	553622	13.19%	2.200%

Sum of corrected areas: 25168648

LSC Report - Integrated Chromatogram

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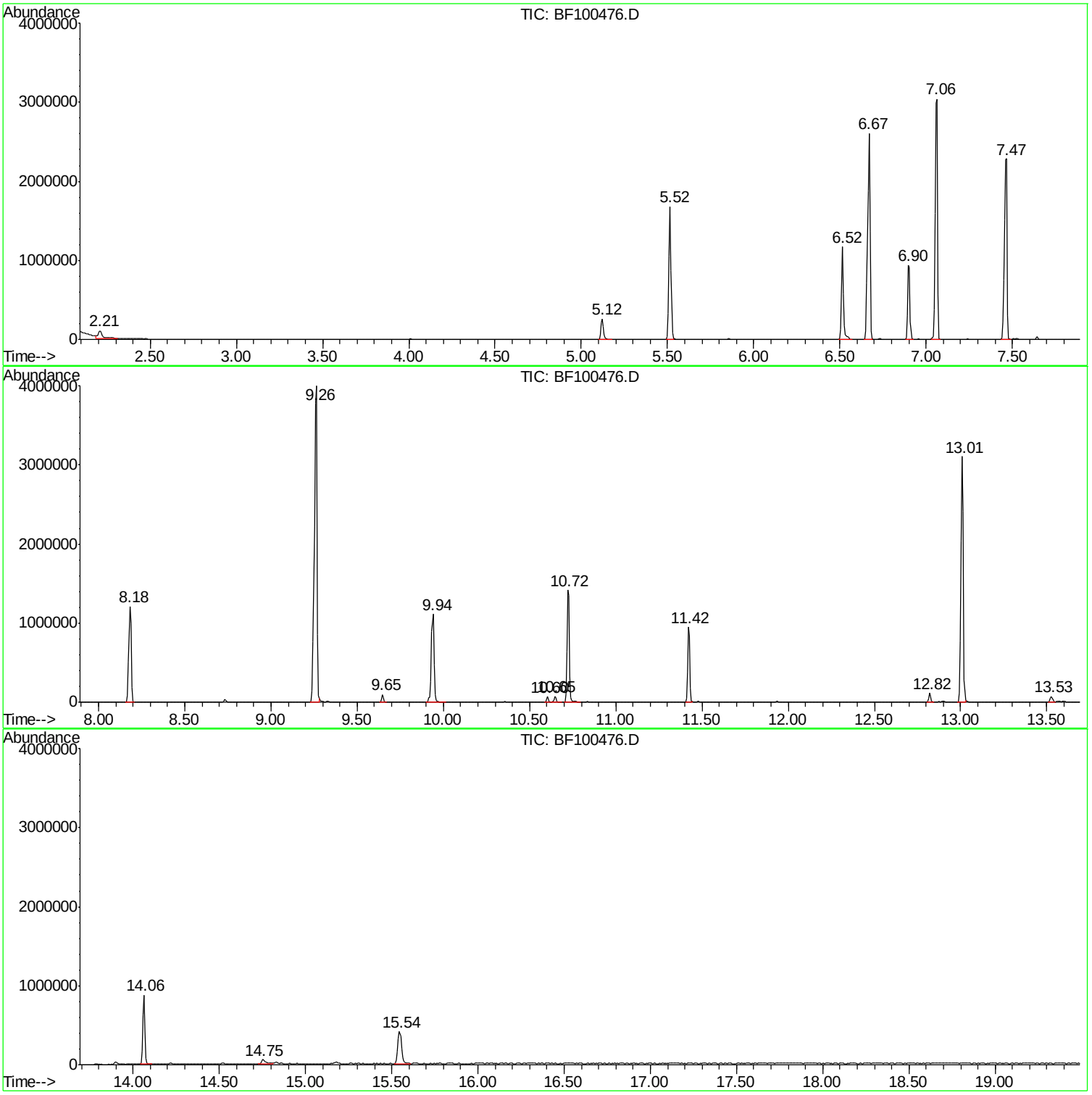
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110717-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100476.D
Acq On : 12 Nov 2017 8:22
Operator : SJ/JU
Sample : I6402-03
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110717-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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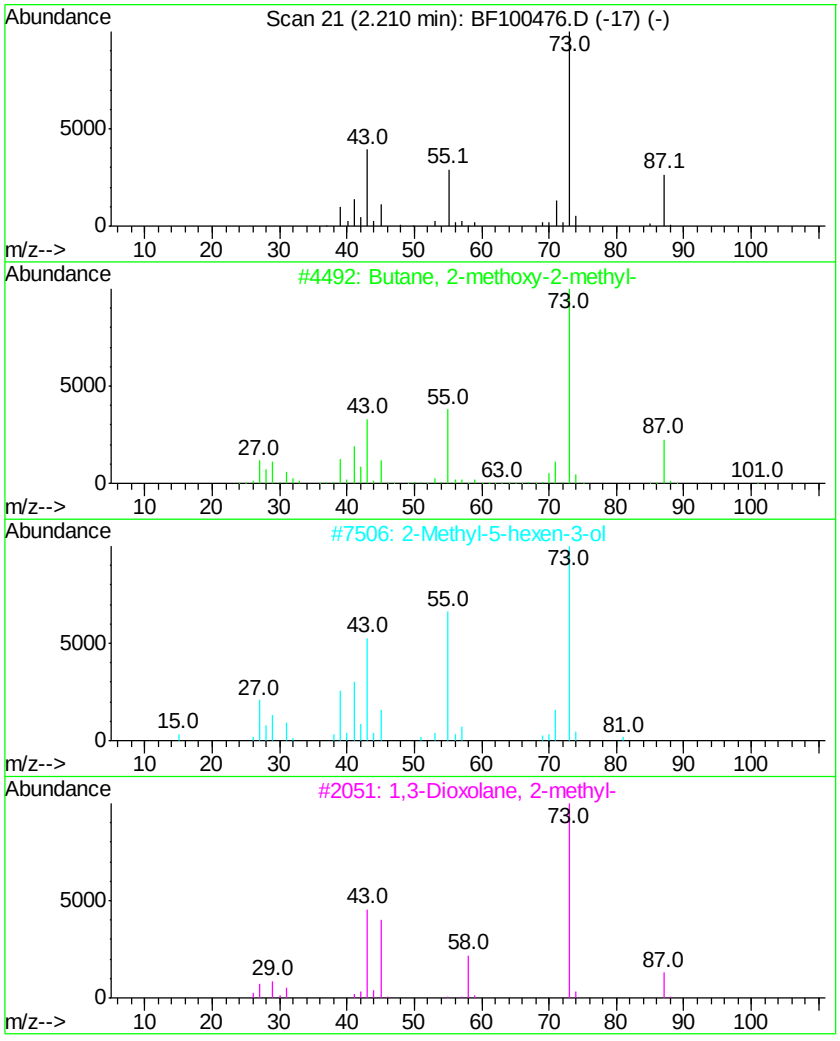
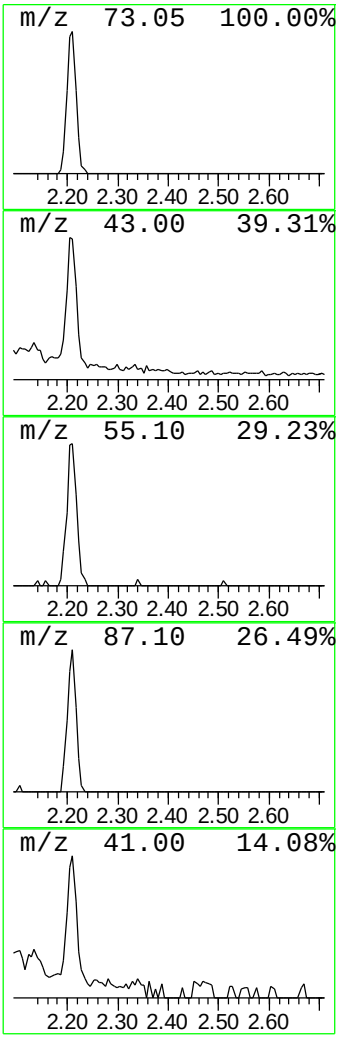
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	4.15 ng	177744	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	35
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	23
5	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	23





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Data File : BF100476.D
Acq On : 12 Nov 2017 8:22
Operator : SJ/JU
Sample : I6402-03
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110717-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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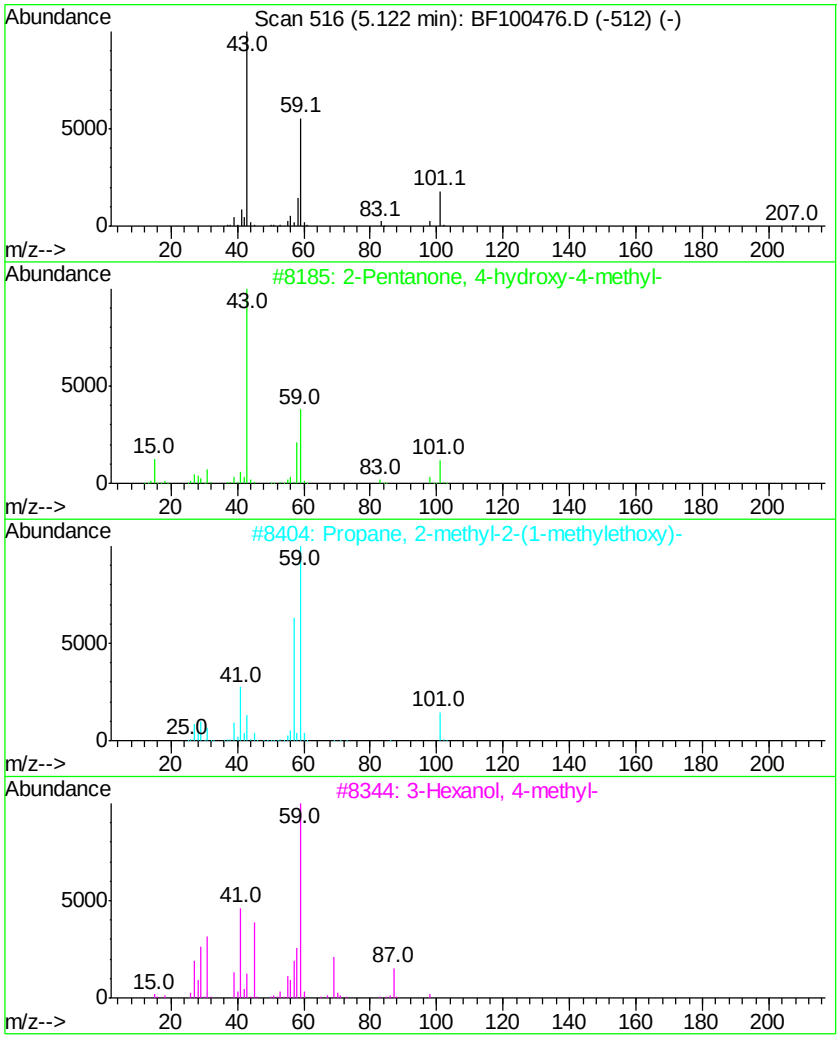
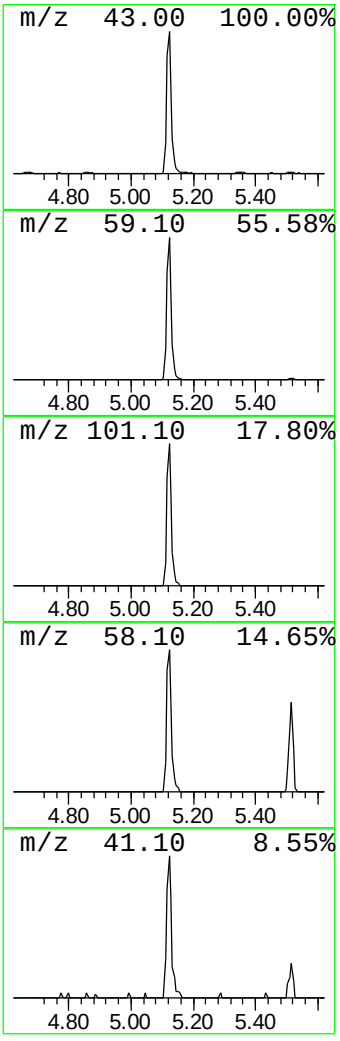
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	6.40 ng	274165	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100476.D
Acq On : 12 Nov 2017 8:22
Operator : SJ/JU
Sample : I6402-03
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110717-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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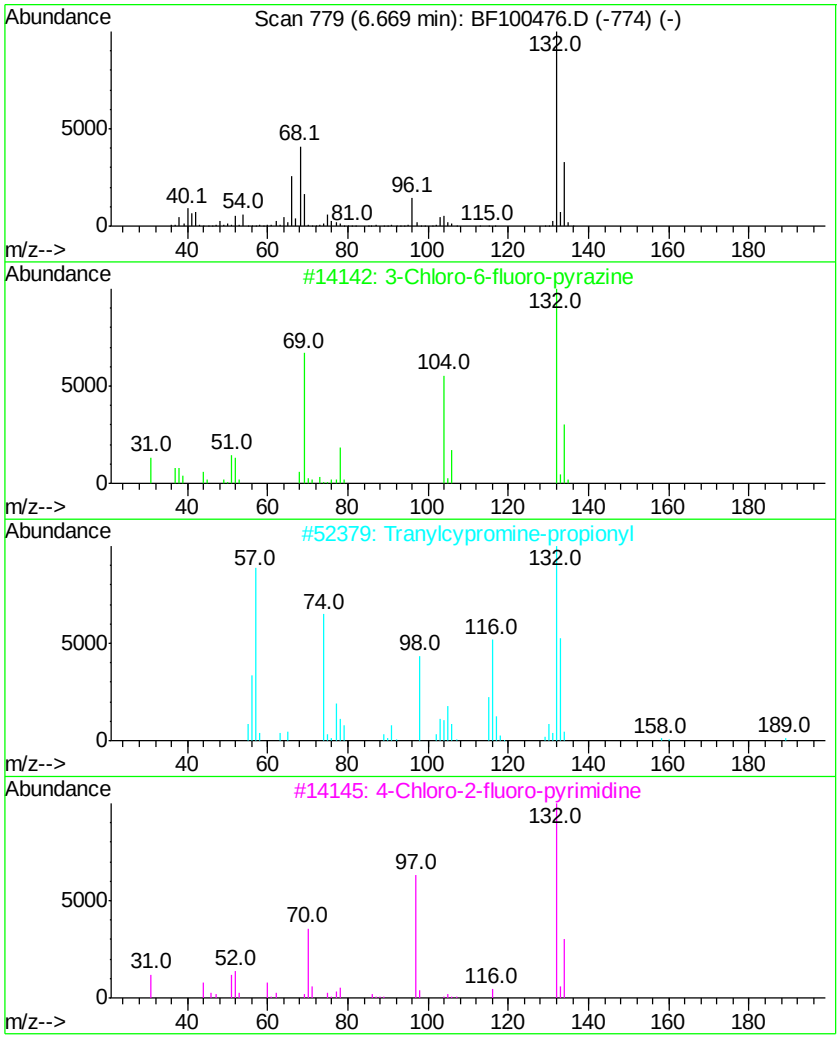
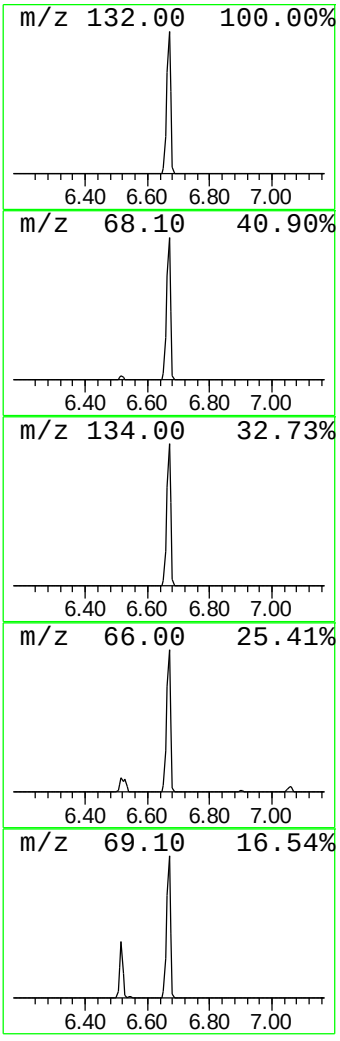
Peak Number 3 unknown6.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	55.88 ng	2392260	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Operator : SJ/JU
Sample : I6402-03
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110717-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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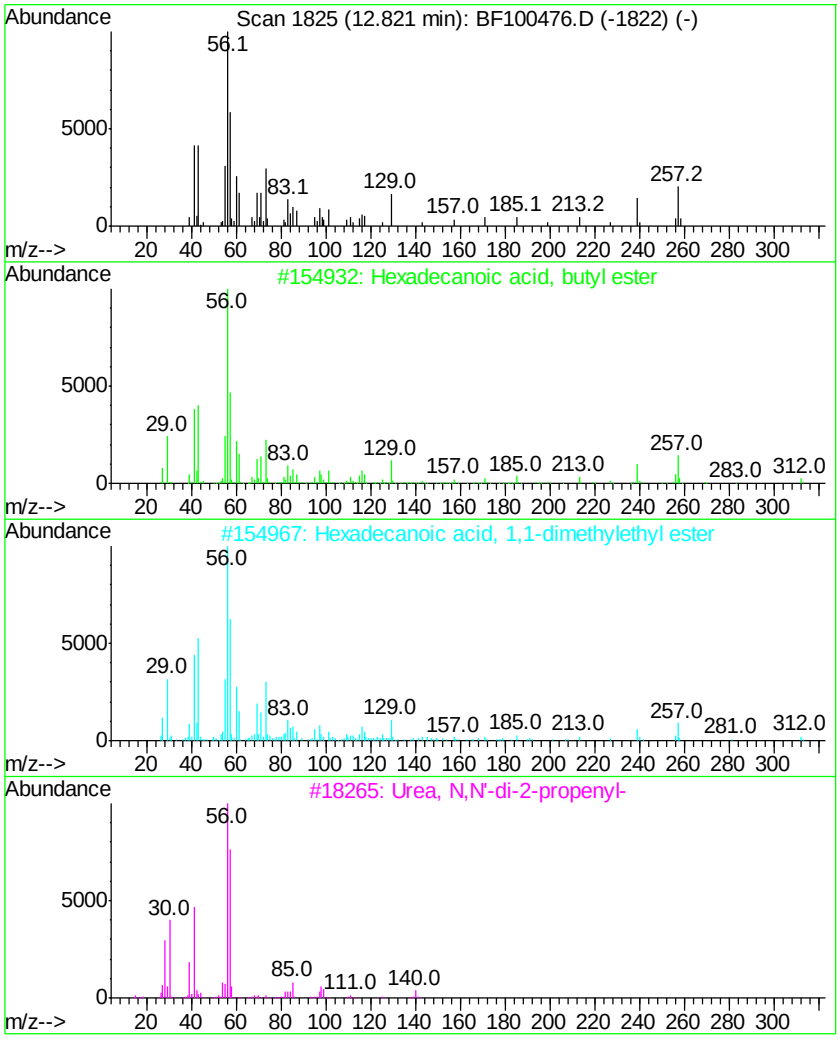
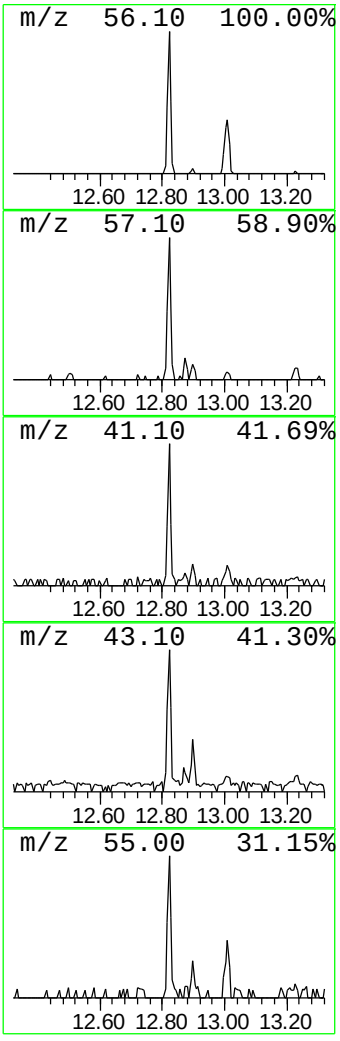
Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	2.19 ng	84891	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35
4	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	32
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	27





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
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Operator : SJ/JU
Sample : I6402-03
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110717-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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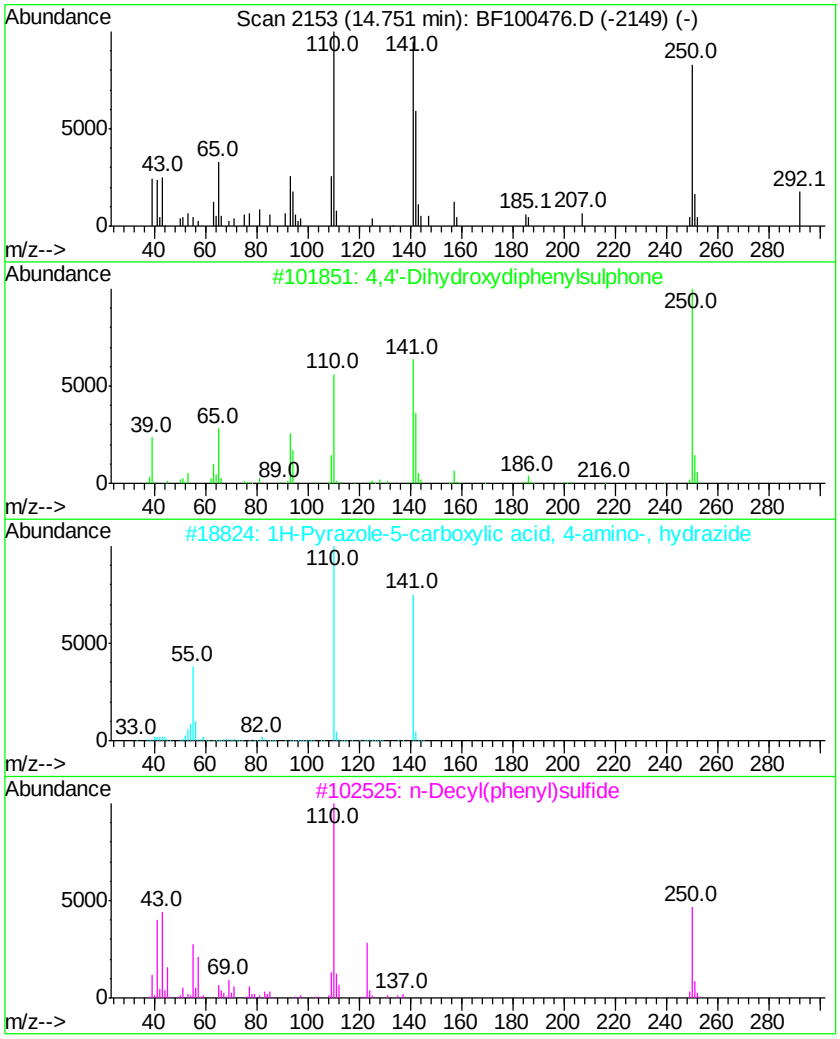
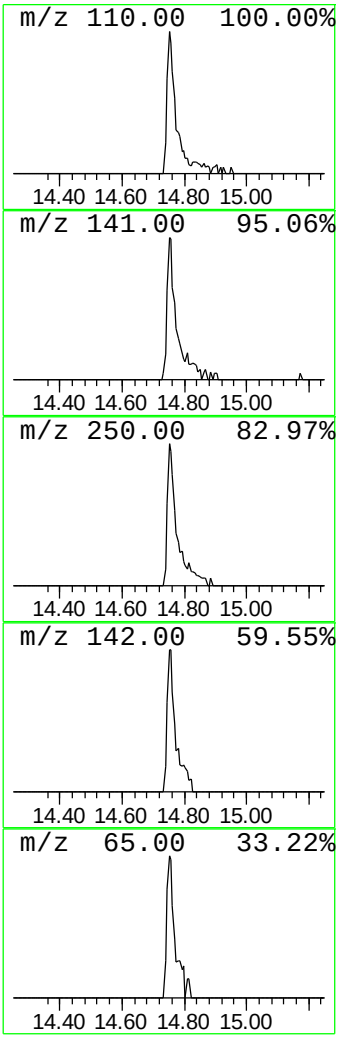
Peak Number 6 4,4'-Dihydroxydiphenylsulphone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	2.54 ng	98561	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	94
2	1H-Pyrazole-5-carboxylic acid, 4...	141	C4H7N5O	1000327-48-2	32
3	n-Decyl(phenyl)sulfide	250	C16H26S	013910-18-4	30
4	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	25
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	22





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.21	4.2	ng	177744	1	6.90	856178	20.0
2-Pentanone, 4-hy...	5.12	6.4	ng	274165	1	6.90	856178	20.0
unknown6.67	6.67	55.9	ng	2392260	1	6.90	856178	20.0
Hexadecanoic acid...	12.82	2.2	ng	84891	5	14.06	775569	20.0
4,4'-Dihydroxydip...	14.75	2.5	ng	98561	5	14.06	775569	20.0