LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111617\
Data File : BF100656.D
Acq On : 17 Nov 2017 3:40
Operator : SJ/JU
Sample : I6491-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 111317-TIDO-E-D-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	2.187	13	17	28	rVB2	49302	83067	2.58%	0.439%
2	4.493	406	409	415	rVB	86204	92439	2.87%	0.488%
3	5.099	508	512	523	rVB	308027	324177	10.08%	1.713%
4	5.498	575	580	583	rBV	1076455	959928	29.85%	5.073%
5	6.498	746	750	758	rBV	769346	632512	19.67%	3.343%
6	6.651	771	776	779	rBV	1818408	1667352	51.85%	8.811%
7	6.881	812	815	819	rVB	753347	603568	18.77%	3.190%
8	7.040	838	842	845	rBV	2466960	2220510	69.05%	11.734%
9	7.445	905	911	914	rBV	1763535	1800641	55.99%	9.516%
10	8.163	1029	1033	1036	rBV	920184	771449	23.99%	4.077%
11	9.239	1210	1216	1219	rBV	3362976	3215862	100.00%	16.994%
12	9.916	1325	1331	1335	rBV	925566	832449	25.89%	4.399%
13	10.704	1461	1465	1475	rBV	1209472	1084393	33.72%	5.731%
14	11.404	1580	1584	1587	rBV	865670	717175	22.30%	3.790%
15	12.986	1849	1853	1856	rBV	2344110	2250421	69.98%	11.892%
16	13.874	2000	2004	2012	rBV	72791	95638	2.97%	0.505%
17	14.039	2028	2032	2036	rVB	645576	561686	17.47%	2.968%
18	14.727	2144	2149	2157	rBV	344054	388401	12.08%	2.053%
19	15.515	2277	2283	2294	rBV	460944	584001	18.16%	3.086%
20	16.474	2441	2446	2453	rBV3	23254	37423	1.16%	0.198%

Sum of corrected areas: 18923092

LSC Report - Integrated Chromatogram

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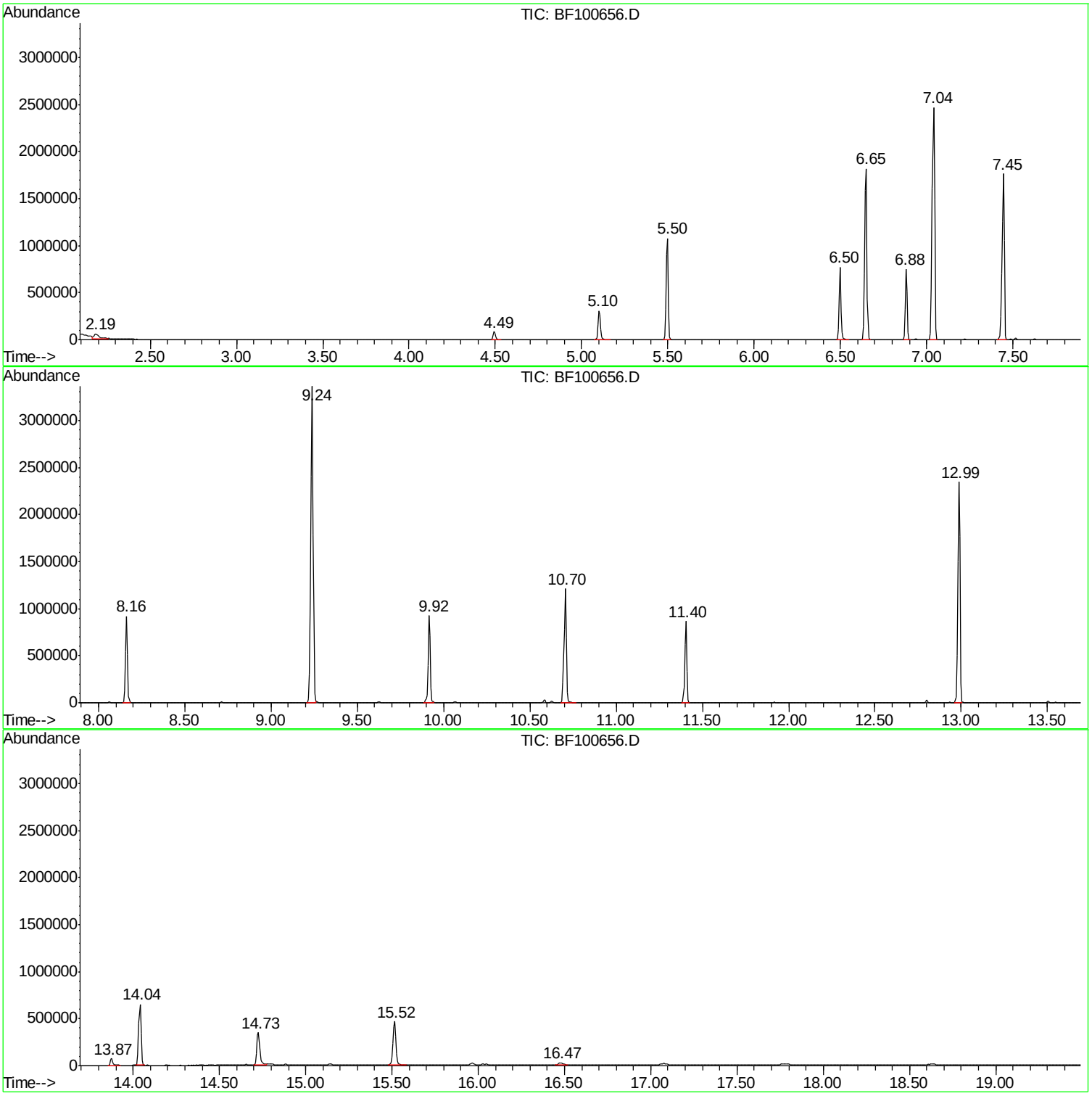
Operator : SJ/JU
Sample : I6491-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
111317-TIDO-E-D-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 : Z:\HPCHEM1\BNA F\DATA\BF111617\
Data File : BF100656.D
Acq On : 17 Nov 2017 3:40
Operator : SJ/JU
Sample : I6491-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 111317-TIDO-E-D-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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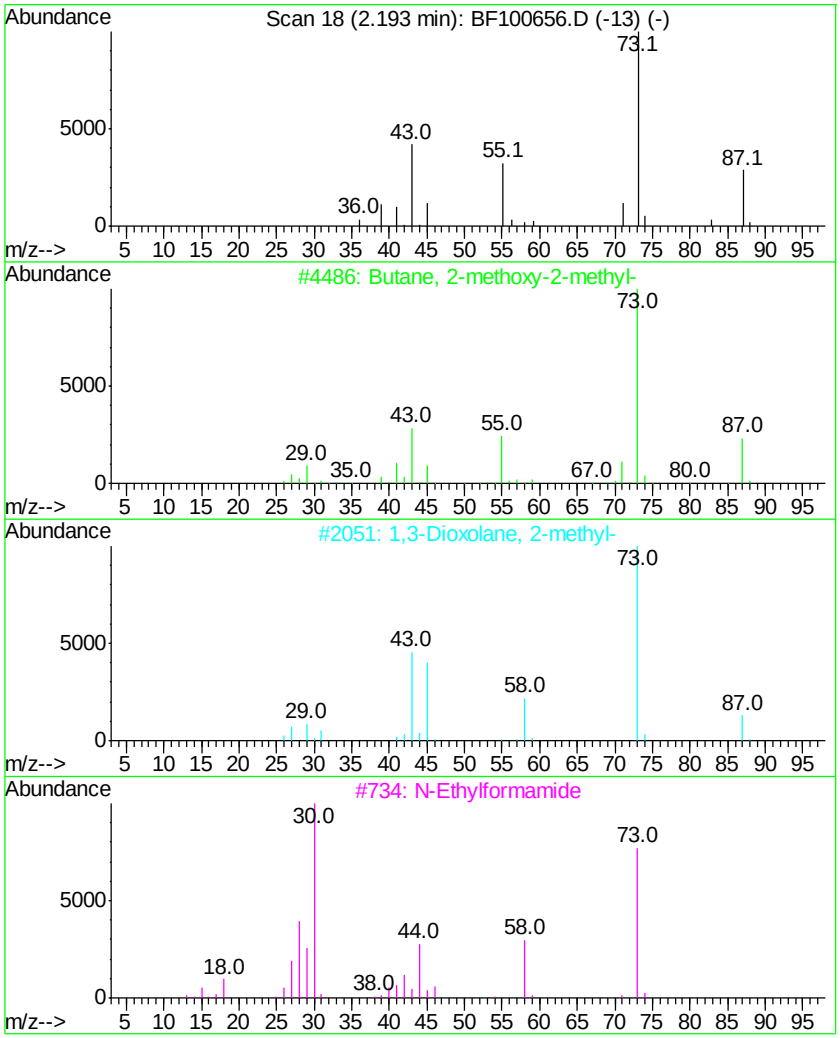
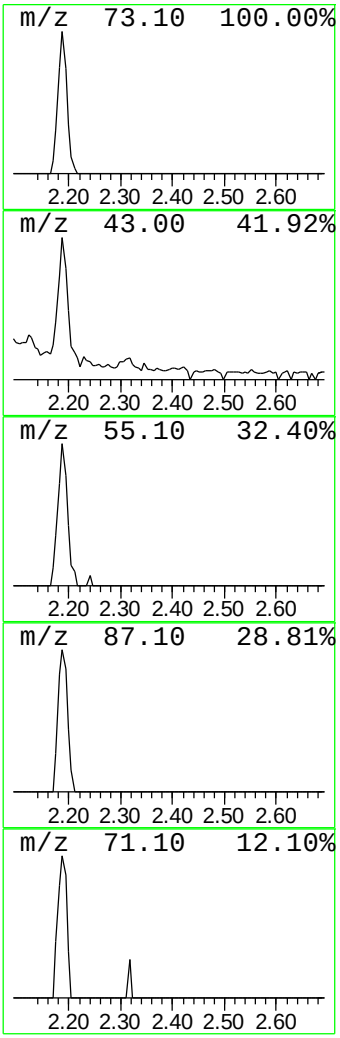
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	2.75 ng	83067	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	74
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	9





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Data File : BF100656.D
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Operator : SJ/JU
Sample : I6491-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 111317-TIDO-E-D-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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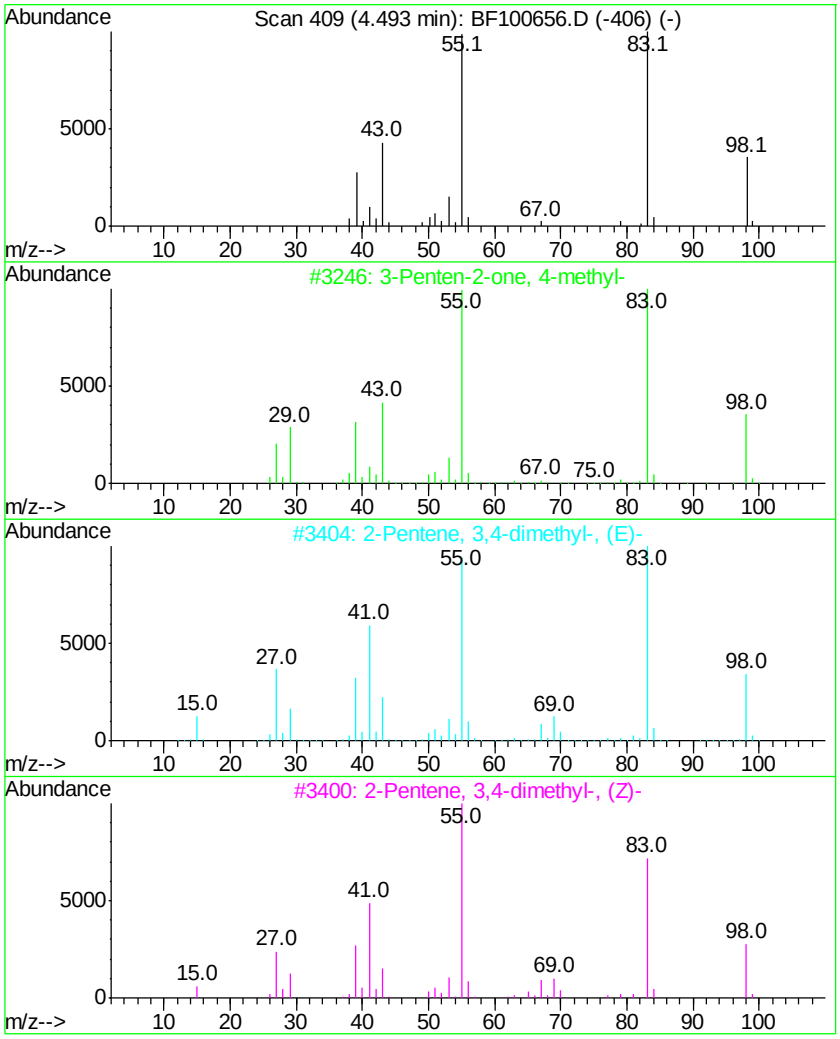
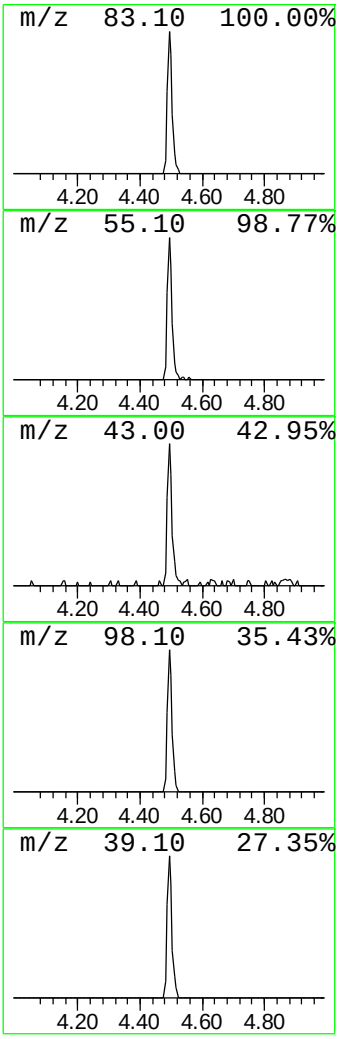
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	3.06 ng	92439	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	3-Hexen-2-one	98	C6H10O	000763-93-9	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111617\
Data File : BF100656.D
Acq On : 17 Nov 2017 3:40
Operator : SJ/JU
Sample : I6491-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 111317-TIDO-E-D-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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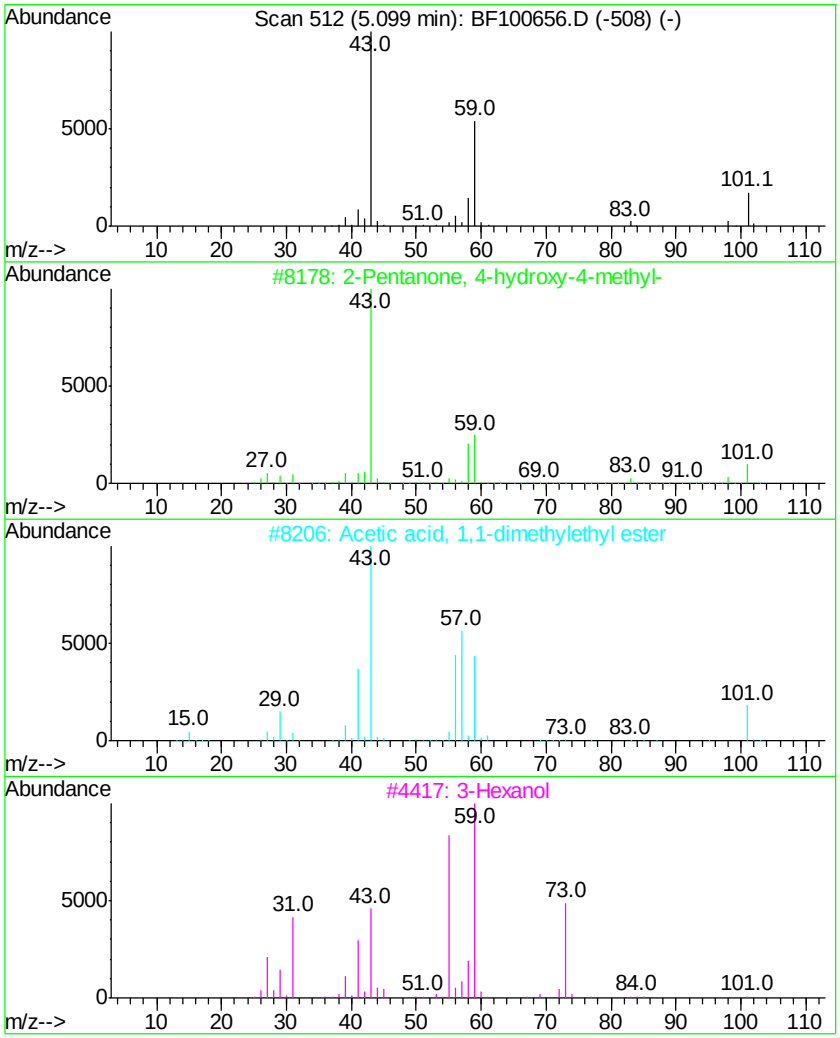
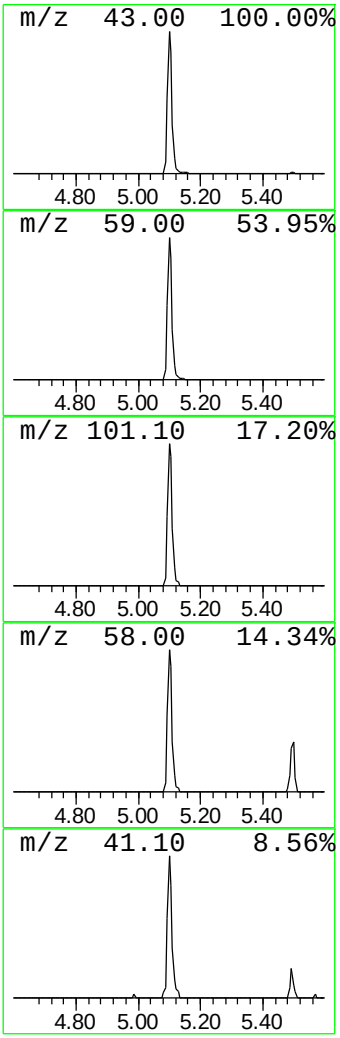
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	10.74 ng	324177	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	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111617\
Data File : BF100656.D
Acq On : 17 Nov 2017 3:40
Operator : SJ/JU
Sample : I6491-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 111317-TIDO-E-D-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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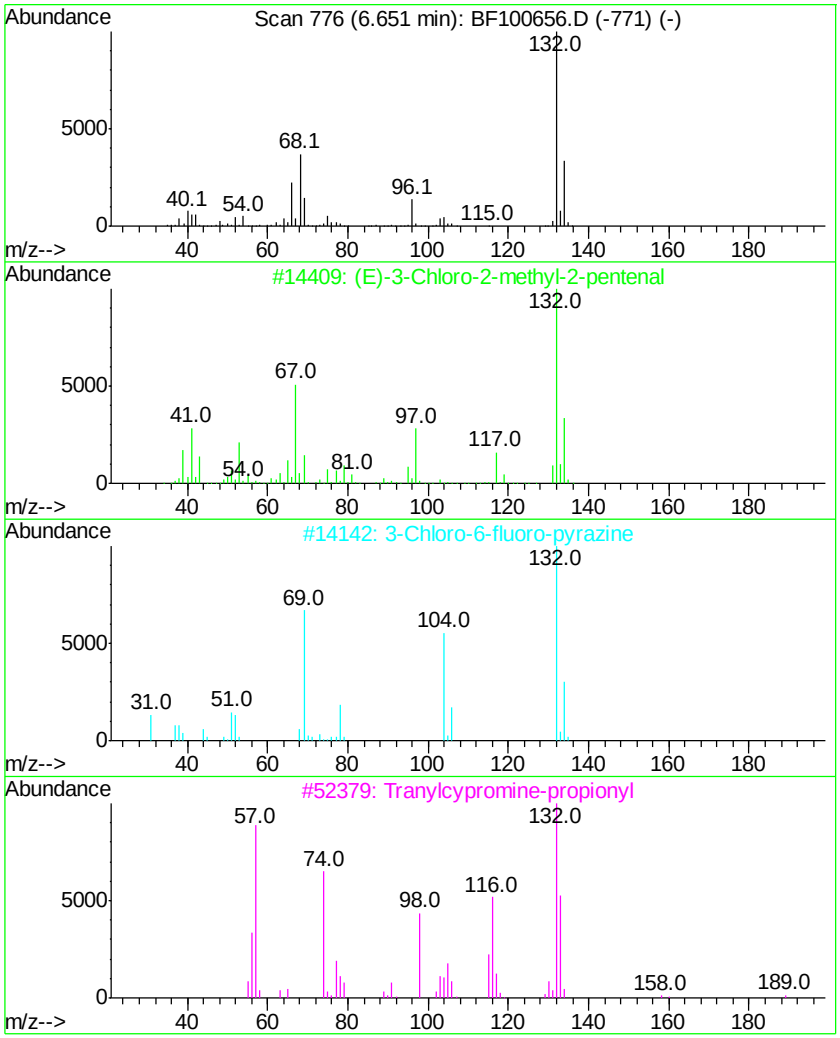
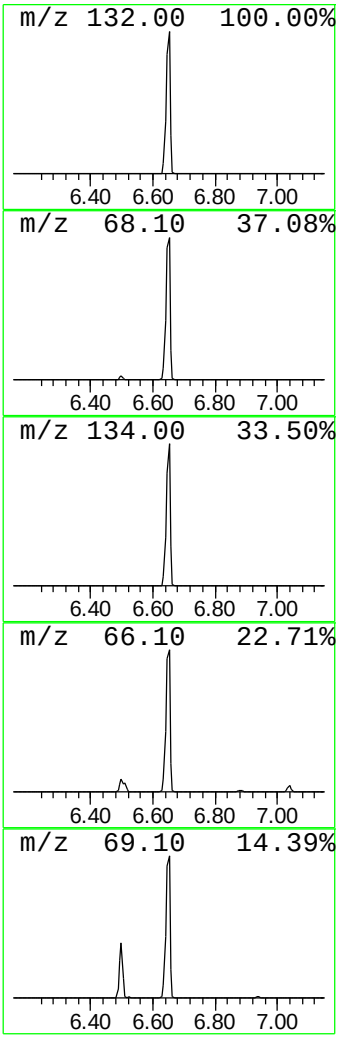
Peak Number 4 unknown6.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	55.25 ng	1667350	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Operator : SJ/JU
Sample : I6491-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 111317-TIDO-E-D-B

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

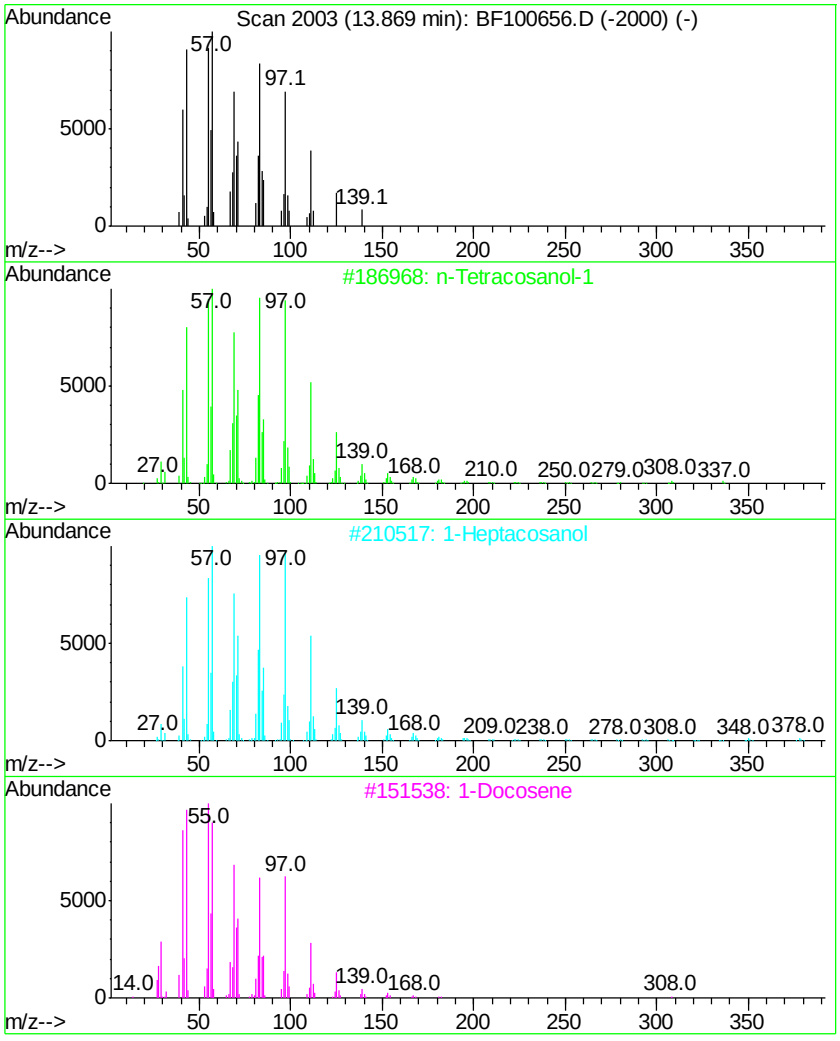
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

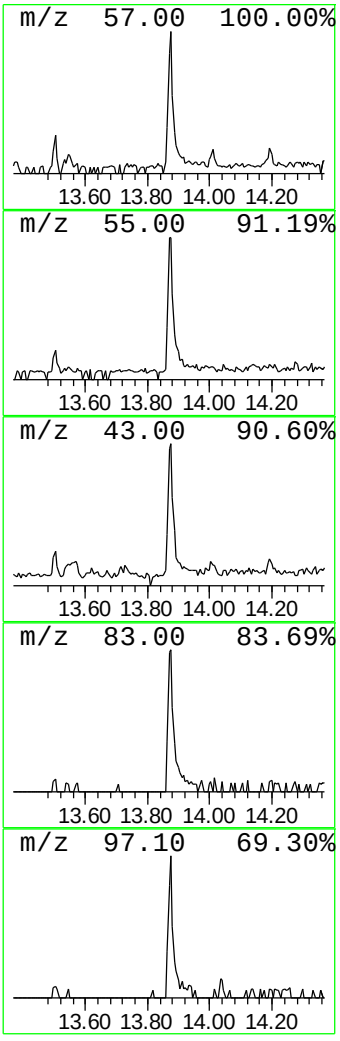
****

Peak Number 6 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	3.41 ng	95638	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	1-Heptacosanol	396	C27H56O	002004-39-9	91
3	1-Docosene	308	C22H44	001599-67-3	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





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Sample : I6491-01
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 111317-TIDO-E-D-B

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

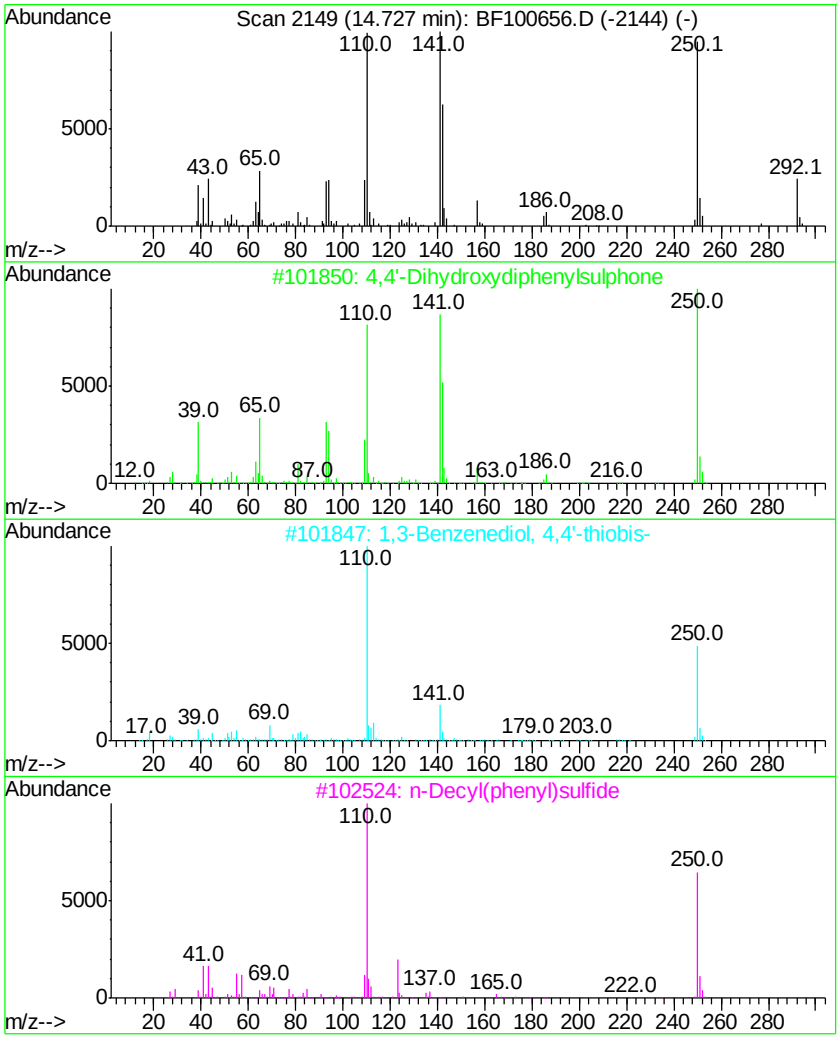
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

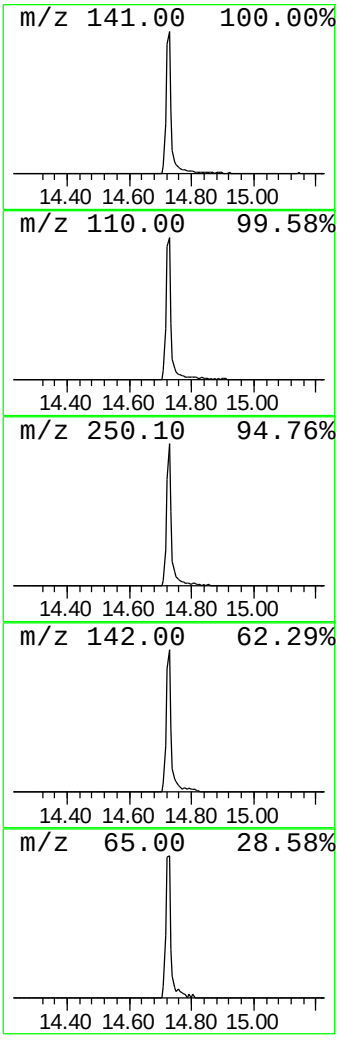
****

Peak Number 7 4,4'-Dihydroxydiphenylsulphone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	13.83 ng	388401	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	98
2	1,3-Benzenediol, 4,4'-thiobis-	250	C12H10O4S	000097-29-0	45
3	n-Decyl(phenyl)sulfide	250	C16H26S	013910-18-4	38
4	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	14
5	1-[5-Nitro-6-uracilyl]-2-[2-chlo...	293	C12H8ClN3O4	296798-53-3	11





Tentatively Identified Compound (LSC) summary

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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.19	2.8	ng	83067	1	6.88	603568	20.0
3-Penten-2-one, 4...	4.49	3.1	ng	92439	1	6.88	603568	20.0
2-Pentanone, 4-hy...	5.10	10.7	ng	324177	1	6.88	603568	20.0
unknown6.65	6.65	55.3	ng	1667350	1	6.88	603568	20.0
n-Tetracosanol-1	13.87	3.4	ng	95638	5	14.04	561686	20.0
4,4'-Dihydroxydip...	14.73	13.8	ng	388401	5	14.04	561686	20.0