LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094718.D
Acq On : 30 Apr 2017 16:53
Operator : SJ/MA
Sample : I2860-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HW-3

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-BF041717.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	3.366	240	243	254	rBV	446207	463509	15.09%	2.245%
2	3.919	331	337	346	rBV	1046642	1223338	39.82%	5.926%
3	4.319	402	405	420	rBV	590164	652175	21.23%	3.159%
4	4.696	466	469	477	rVB	266346	240891	7.84%	1.167%
5	5.390	583	587	600	rBV	314145	408213	13.29%	1.977%
6	5.513	604	608	621	rVB	1438135	1354953	44.11%	6.564%
7	5.760	647	650	660	rVB	666462	605189	19.70%	2.932%
8	5.943	676	681	684	rBV	1882689	1832775	59.66%	8.878%
9	6.413	756	761	764	rBV	1592562	1504462	48.97%	7.288%
10	7.254	900	904	915	rVB	872712	816957	26.59%	3.957%
11	8.578	1124	1129	1133	rBV	3062749	3072062	100.00%	14.881%
12	9.084	1211	1215	1222	rBV	232706	221772	7.22%	1.074%
13	9.389	1260	1267	1277	rBV2	963769	975314	31.75%	4.725%
14	10.366	1429	1433	1447	rBV	1037212	1089082	35.45%	5.276%
15	10.572	1464	1468	1475	rBV	37183	51674	1.68%	0.250%
16	11.213	1573	1577	1587	rBV	994883	966967	31.48%	4.684%
17	11.942	1697	1701	1710	rBV2	22391	36999	1.20%	0.179%
18	12.913	1860	1866	1873	rBV2	21863	31873	1.04%	0.154%
19	13.195	1908	1914	1917	rBV	2725485	3030712	98.65%	14.681%
20	14.354	2108	2111	2119	rBV3	28418	45022	1.47%	0.218%
21	14.466	2125	2130	2135	rBV	777866	829274	26.99%	4.017%
22	14.513	2135	2138	2142	rVB	32732	32369	1.05%	0.157%
23	15.483	2299	2303	2312	rBV	370941	445487	14.50%	2.158%
24	16.089	2402	2406	2413	rBV	487636	602811	19.62%	2.920%
25	16.195	2421	2424	2428	rVB	28291	31615	1.03%	0.153%
26	16.577	2485	2489	2497	rBV3	24644	38890	1.27%	0.188%
27	17.007	2558	2562	2570	rVB5	22050	39180	1.28%	0.190%

Sum of corrected areas: 20643565

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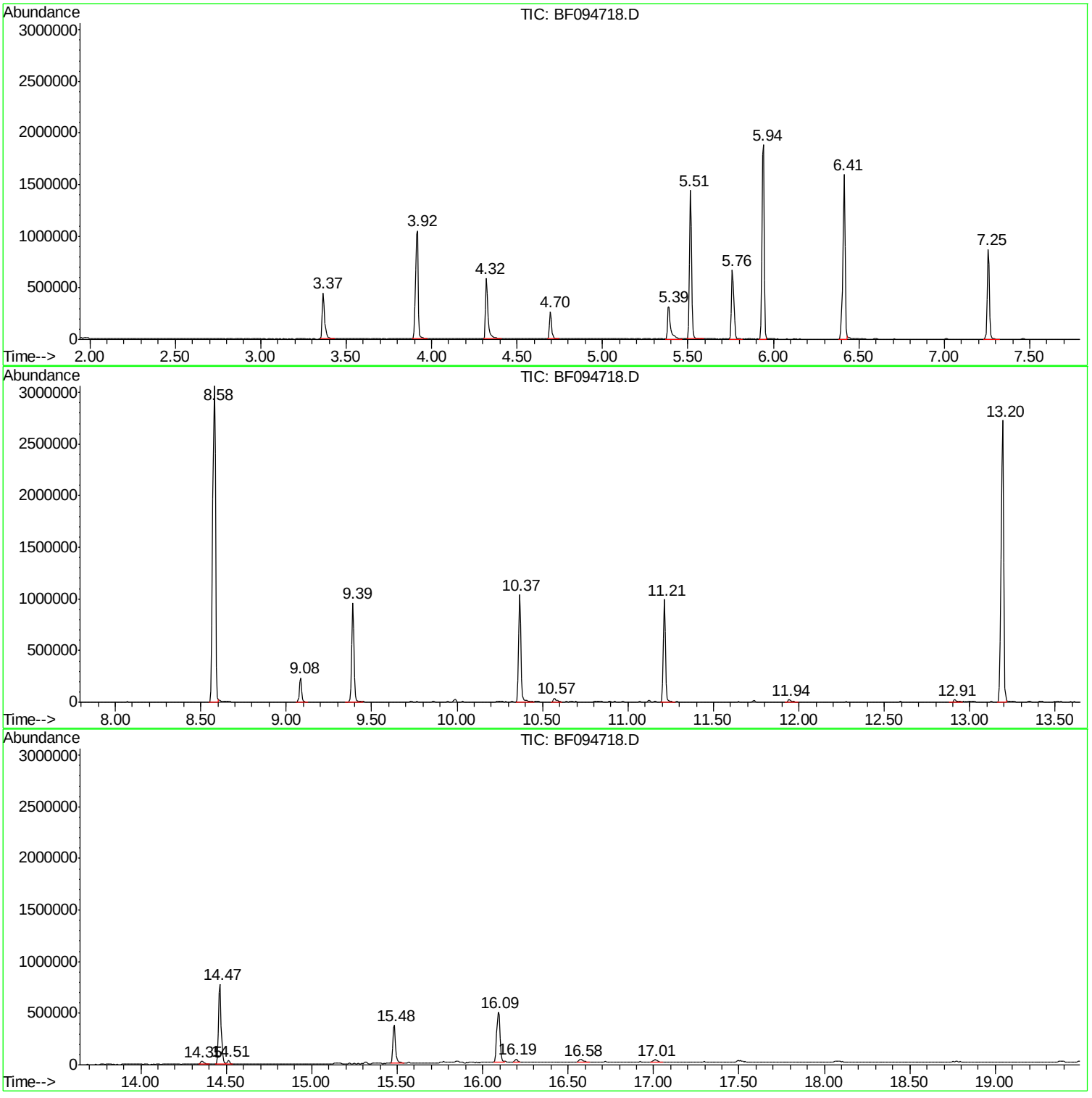
Instrument : BNA_F
ClientSampleId : HW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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\BF043017\
Data File : BF094718.D
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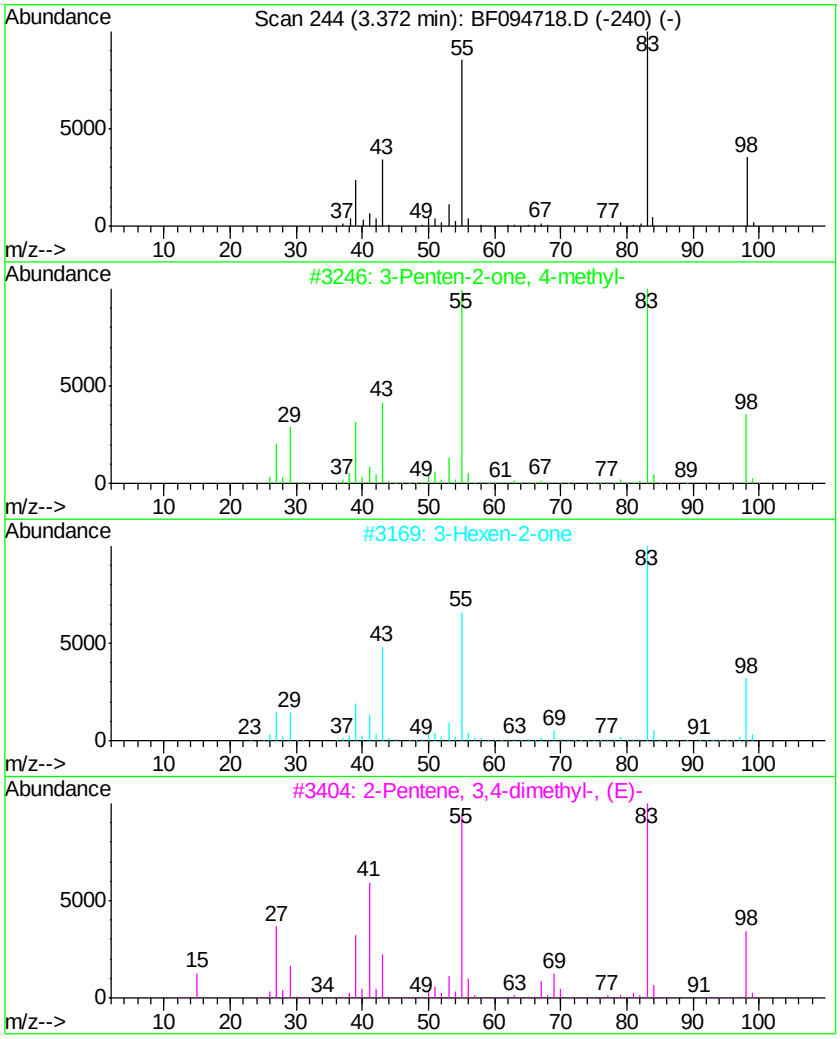
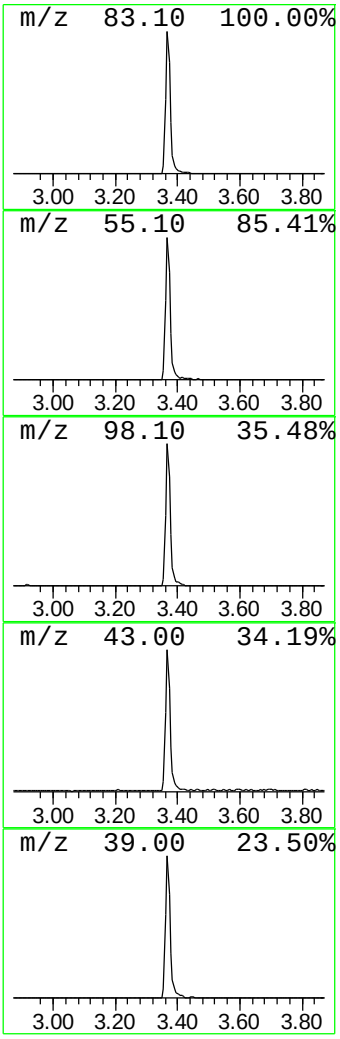
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.37	15.32 ng	463509	1,4-Dichlorobenzene-d4	5.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094718.D
Acq On : 30 Apr 2017 16:53
Operator : SJ/MA
Sample : I2860-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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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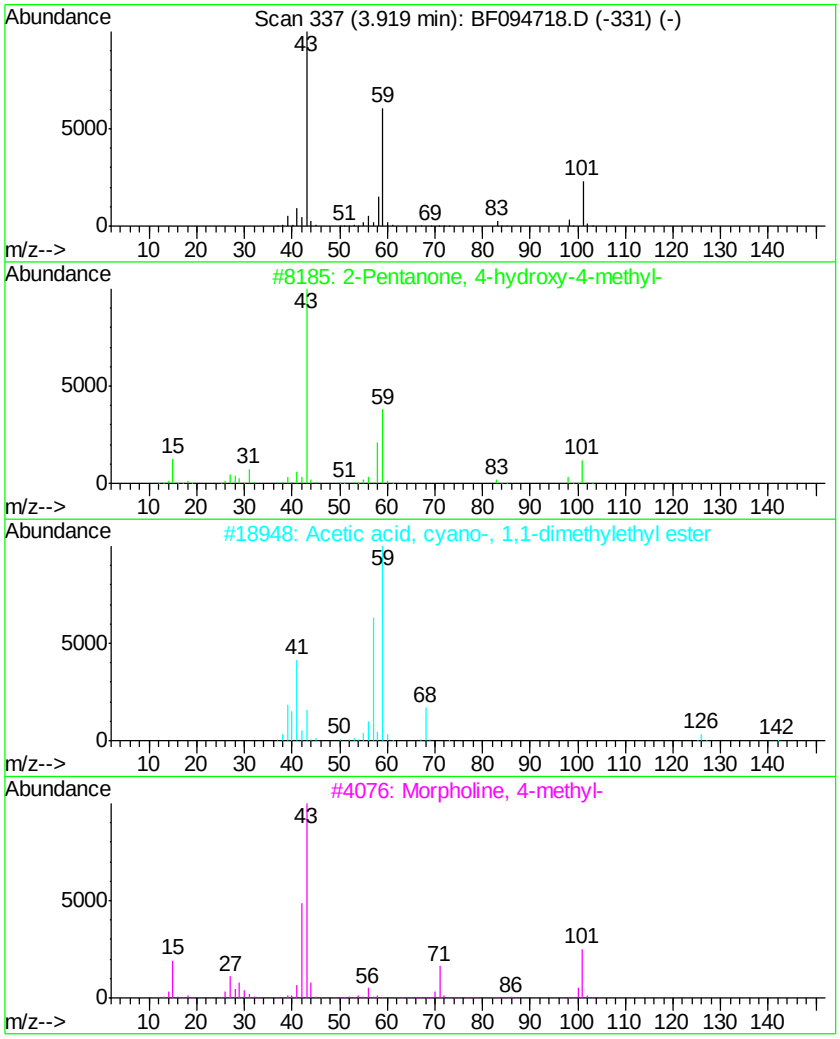
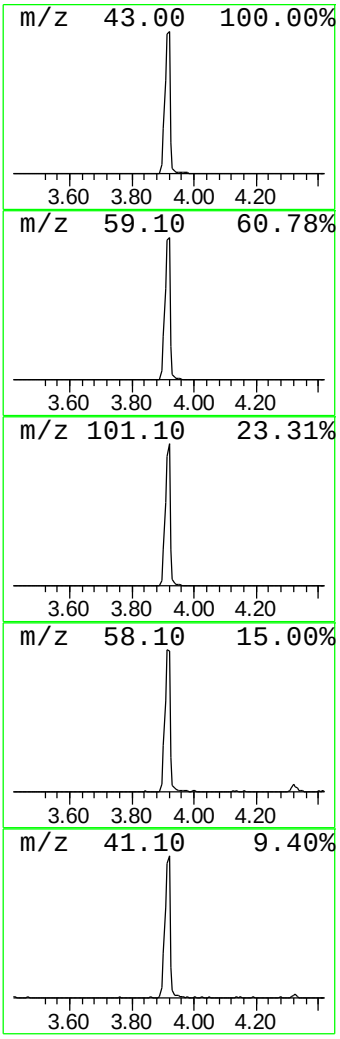
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.92	40.43 ng	1223340	1,4-Dichlorobenzene-d4	5.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
Data File : BF094718.D
Acq On : 30 Apr 2017 16:53
Operator : SJ/MA
Sample : I2860-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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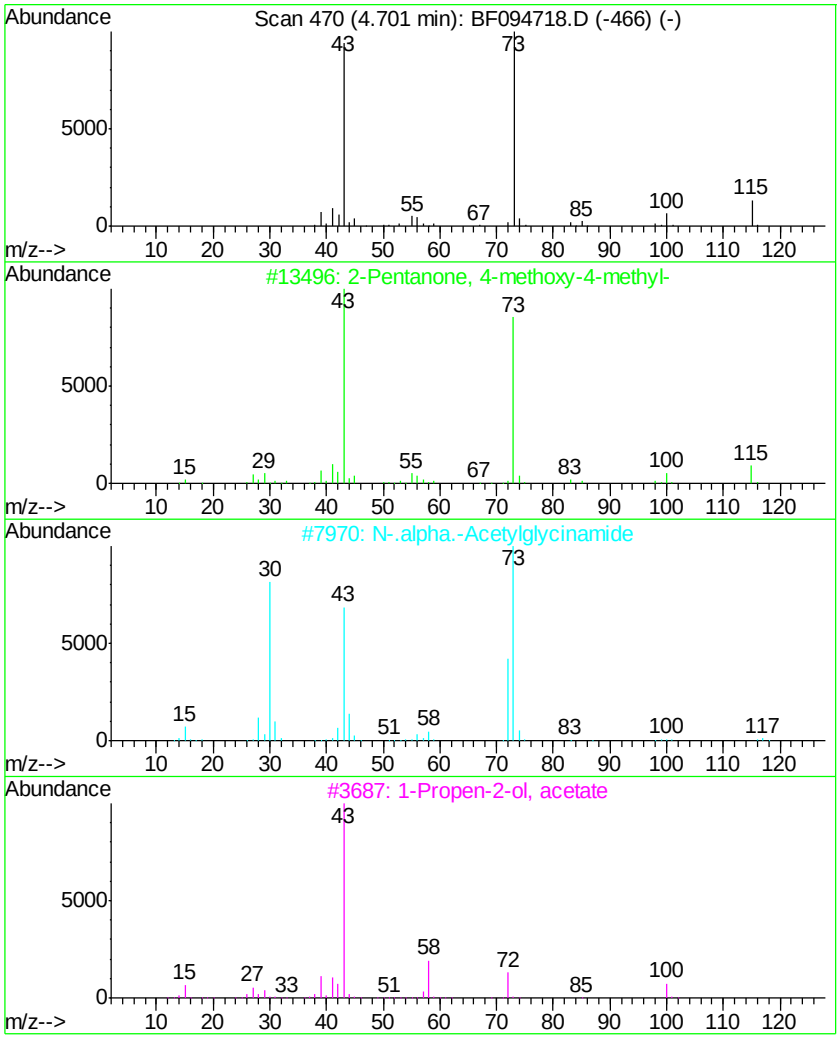
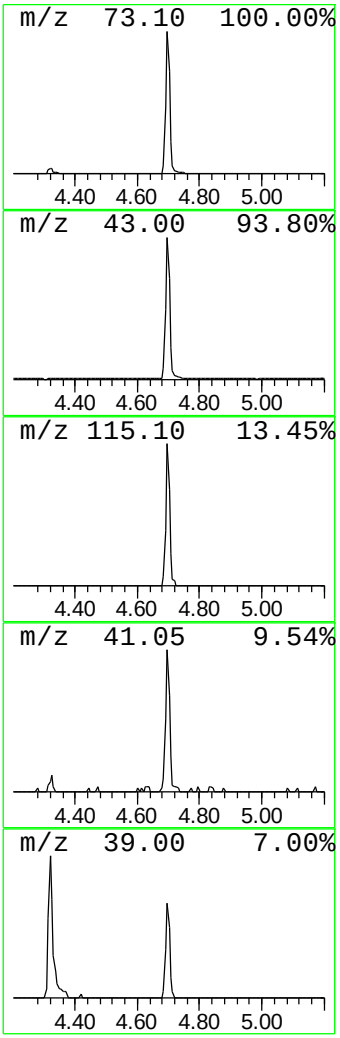
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	7.96 ng	240891	1,4-Dichlorobenzene-d4	5.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
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Acq On : 30 Apr 2017 16:53
Operator : SJ/MA
Sample : I2860-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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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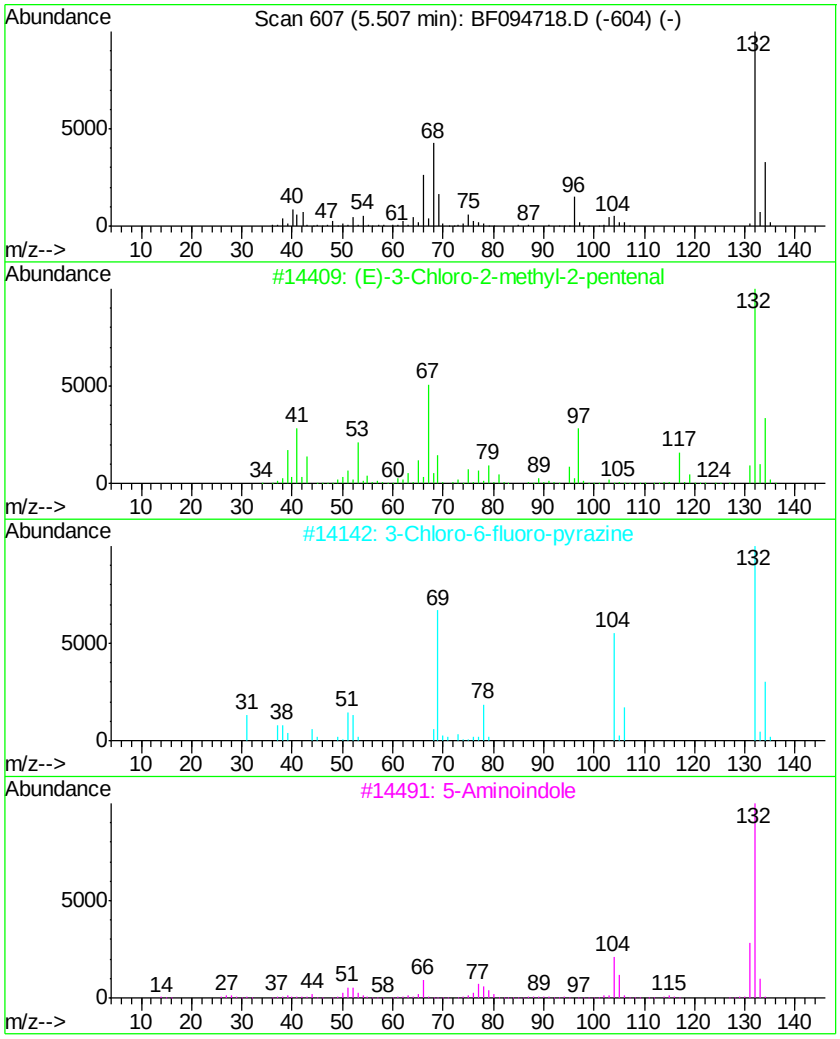
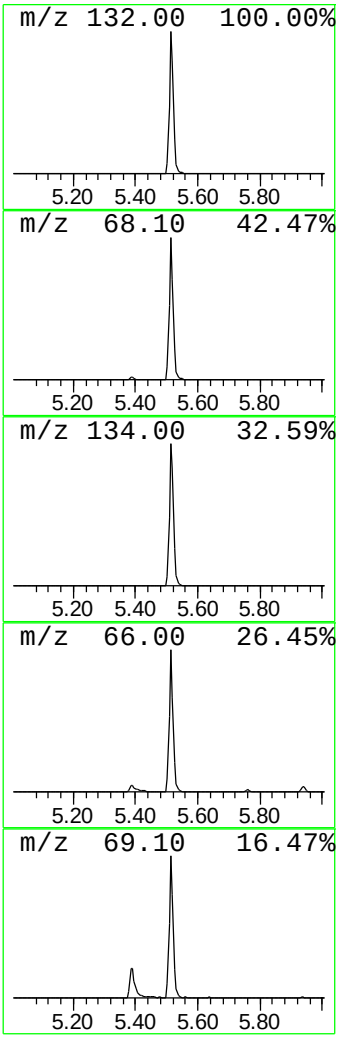
Peak Number 4 unknown5.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	44.78 ng	1354950	1,4-Dichlorobenzene-d4	5.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF043017\
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Operator : SJ/MA
Sample : I2860-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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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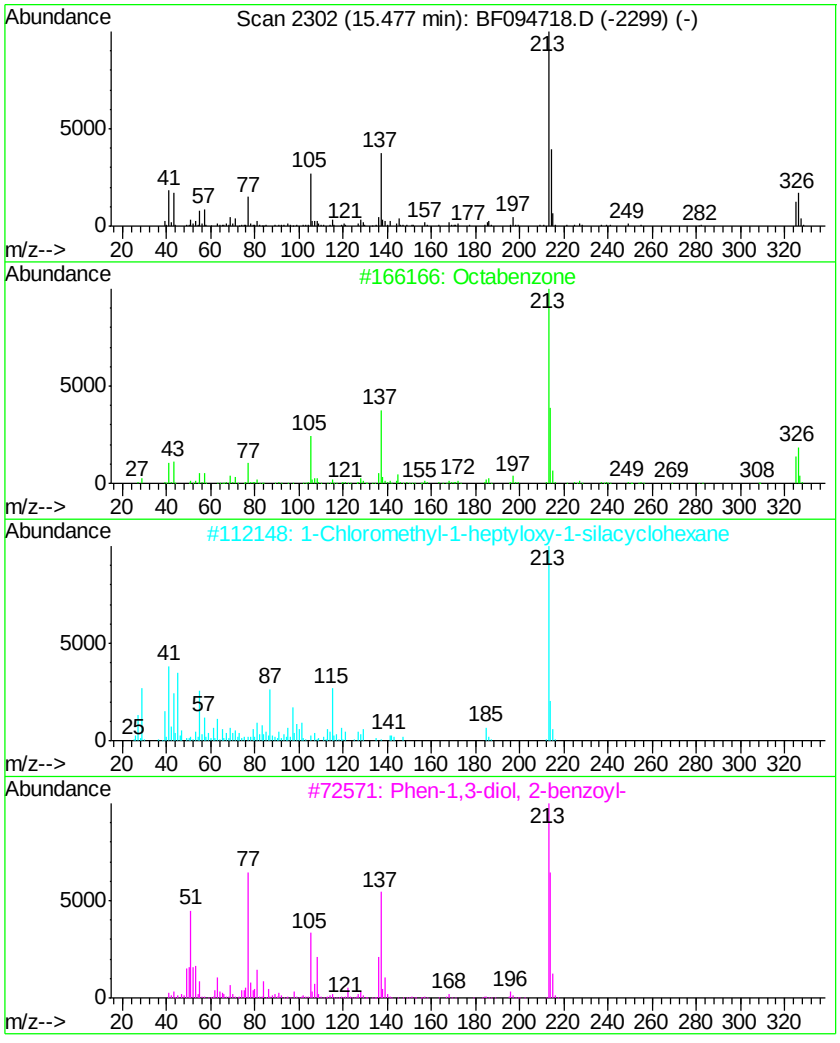
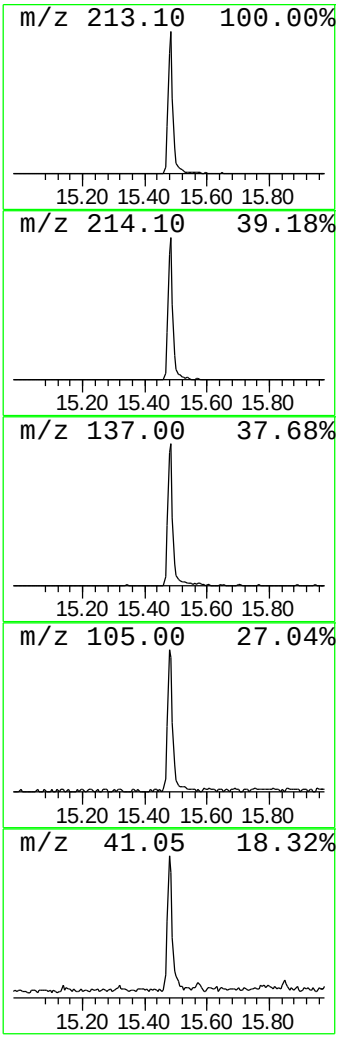
Peak Number 6 Octabenzone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.48	14.78 ng	445487	Perylene-d12	16.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octabenzone	326	C21H26O3	001843-05-6	99
2	1-Chloromethyl-1-heptyloxy-1-sil...	262	C13H27ClOSi	1000279-33-5	23
3	Phen-1,3-diol, 2-benzoyl-	214	C13H10O3	063411-81-4	23
4	1,2,4-Triazine-3,5(2H,4H)-dione,...	213	C4H2F3N3O2S	113307-05-4	12
5	Harmaline	214	C13H14N2O	000304-21-2	10





Tentatively Identified Compound (LSC) summary

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Data File : BF094718.D
Acq On : 30 Apr 2017 16:53
Operator : SJ/MA
Sample : I2860-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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
3-Penten-2-one, 4...	3.37	15.3	ng	463509	1	5.76	605189	20.0
2-Pentanone, 4-hy...	3.92	40.4	ng	1223340	1	5.76	605189	20.0
2-Pentanone, 4-me...	4.70	8.0	ng	240891	1	5.76	605189	20.0
unknown5.51	5.51	44.8	ng	1354950	1	5.76	605189	20.0
Octabenzone	15.48	14.8	ng	445487	6	16.09	602811	20.0