LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081725.D
Acq On : 21 Sep 2015 21:31
Operator : UM/IZ
Sample : G3717-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-9-17-15

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-BF090115.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	1.213	8	11	13	rBV	2878813	3228443	64.02%	15.852%
2	1.441	29	31	37	rBV	189825	502111	9.96%	2.465%
3	1.521	37	38	91	rVB	1401412	5042791	100.00%	24.761%
4	4.424	290	292	315	rBV	91068	246960	4.90%	1.213%
5	5.316	367	370	387	rBV	252584	603543	11.97%	2.963%
6	7.602	567	570	574	rBV	137874	308014	6.11%	1.512%
7	7.682	574	577	590	rVB	732781	1322675	26.23%	6.494%
8	8.162	615	619	625	rVB	140669	256447	5.09%	1.259%
9	8.482	644	647	659	rVB	669757	1183314	23.47%	5.810%
10	9.465	729	733	736	rBV	522126	989820	19.63%	4.860%
11	11.054	869	872	878	rBV	168587	314546	6.24%	1.544%
12	12.288	974	980	987	rVB3	18473	54485	1.08%	0.268%
13	13.705	1100	1104	1107	rBV	967111	1735220	34.41%	8.520%
14	15.191	1230	1234	1244	rVB	205111	408031	8.09%	2.003%
15	16.780	1368	1373	1377	rBV4	19047	66250	1.31%	0.325%
16	17.100	1397	1401	1410	rBV	556948	1157653	22.96%	5.684%
17	18.700	1537	1541	1547	rVB	225913	387429	7.68%	1.902%
18	20.472	1693	1696	1700	rBV2	29337	65684	1.30%	0.323%
19	22.072	1832	1836	1839	rBV	1228404	1795993	35.62%	8.818%
20	22.883	1905	1907	1910	rBV	93507	136351	2.70%	0.669%
21	23.352	1945	1948	1950	rVB	240923	326591	6.48%	1.604%
22	24.781	2071	2073	2078	rVB	178828	233885	4.64%	1.148%

Sum of corrected areas: 20366236

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081725.D
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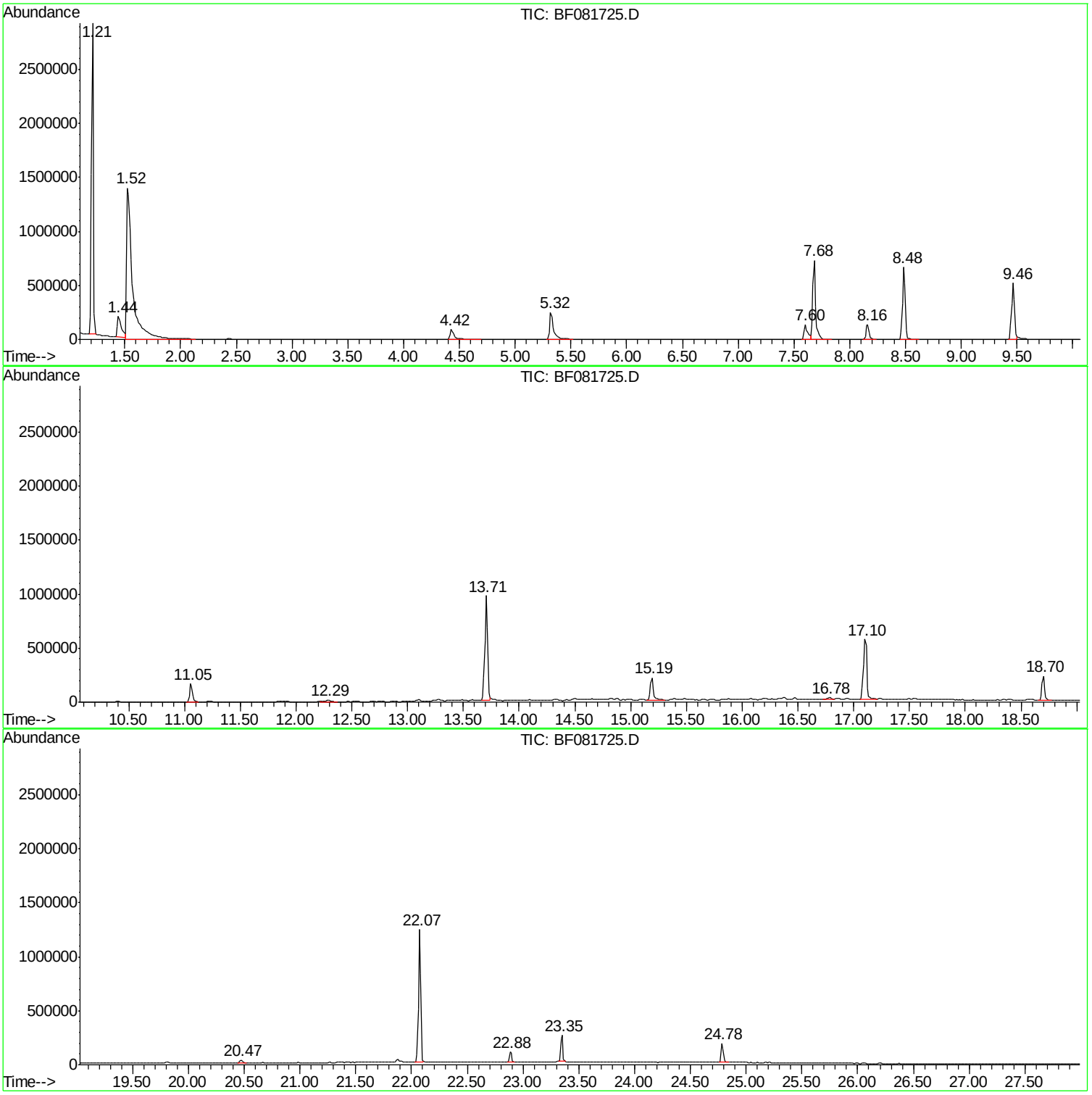
Operator : UM/IZ
Sample : G3717-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PZ-6-9-17-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081725.D
Acq On : 21 Sep 2015 21:31
Operator : UM/IZ
Sample : G3717-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-9-17-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

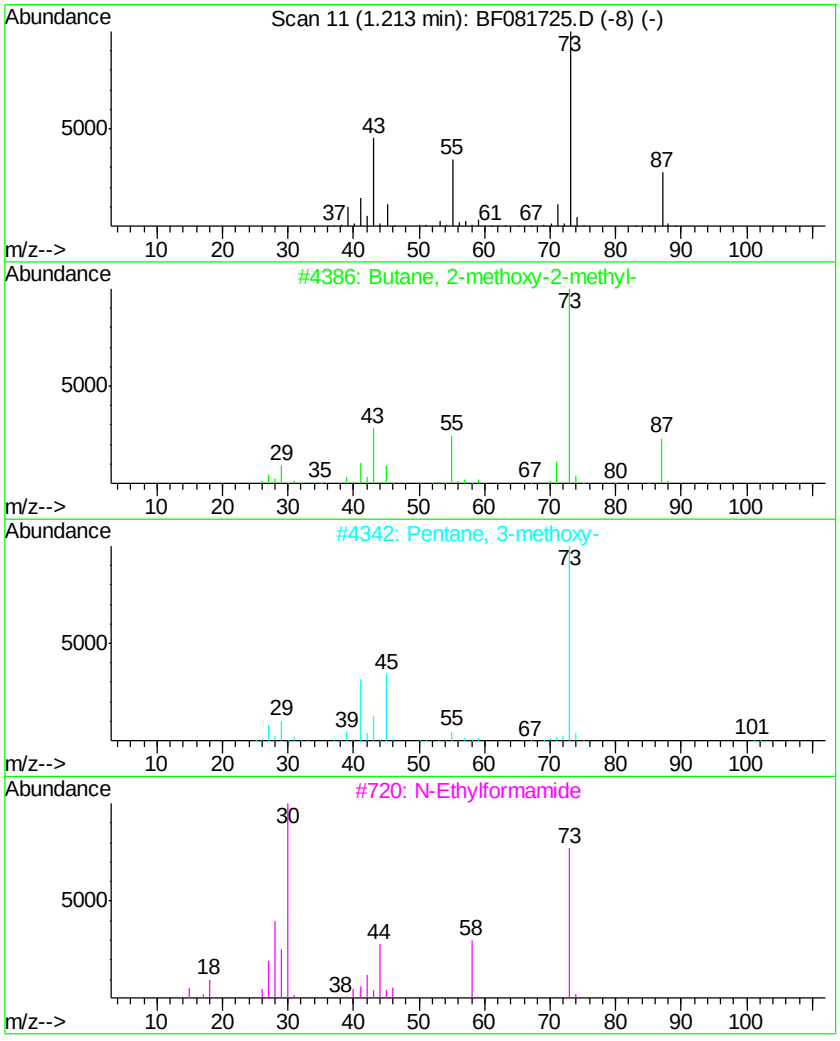
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

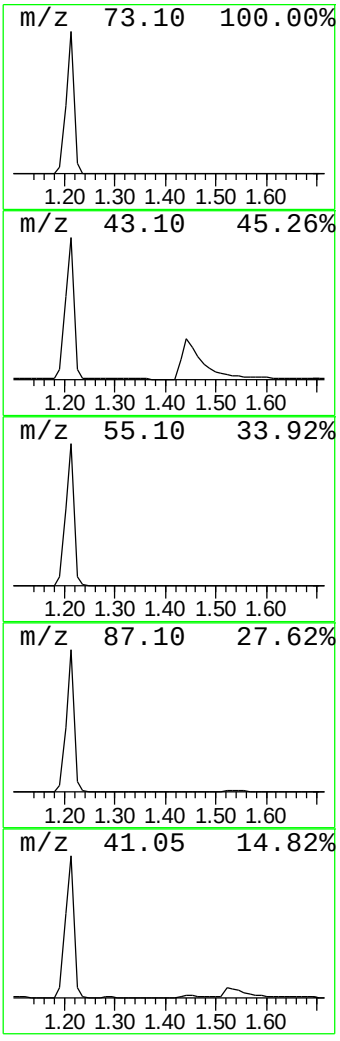
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.21	251.78 ng	3228440	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081725.D
Acq On : 21 Sep 2015 21:31
Operator : UM/IZ
Sample : G3717-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-9-17-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

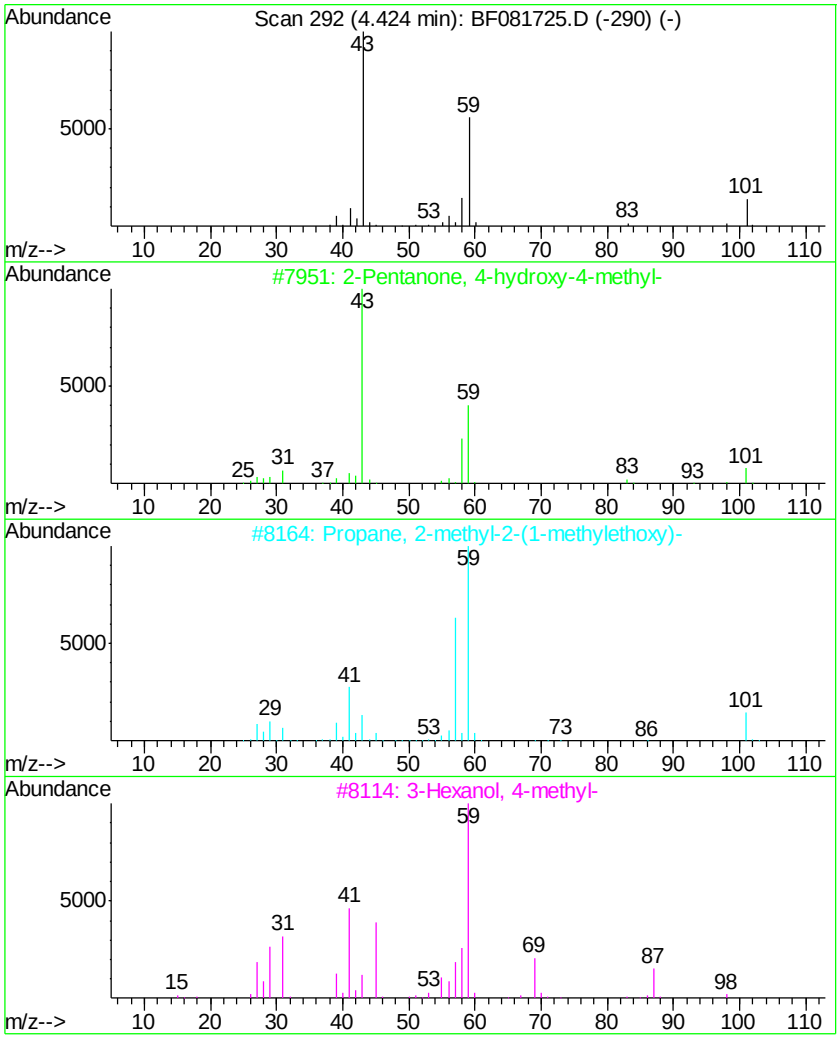
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

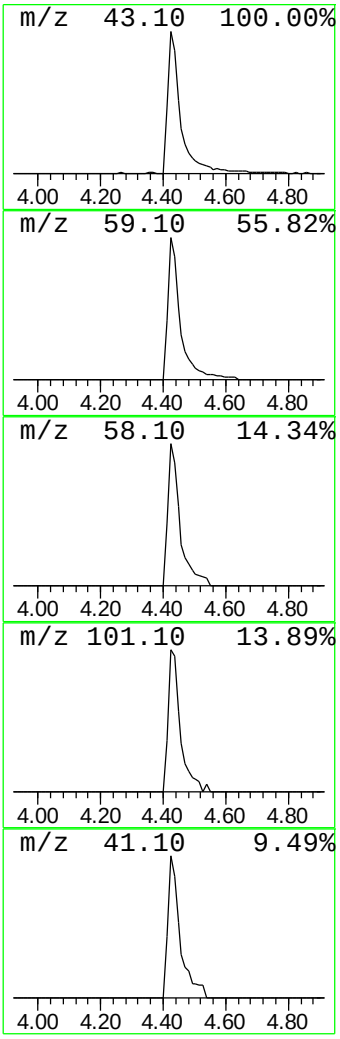
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.42	19.26 ng	246960	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081725.D
Acq On : 21 Sep 2015 21:31
Operator : UM/IZ
Sample : G3717-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-9-17-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

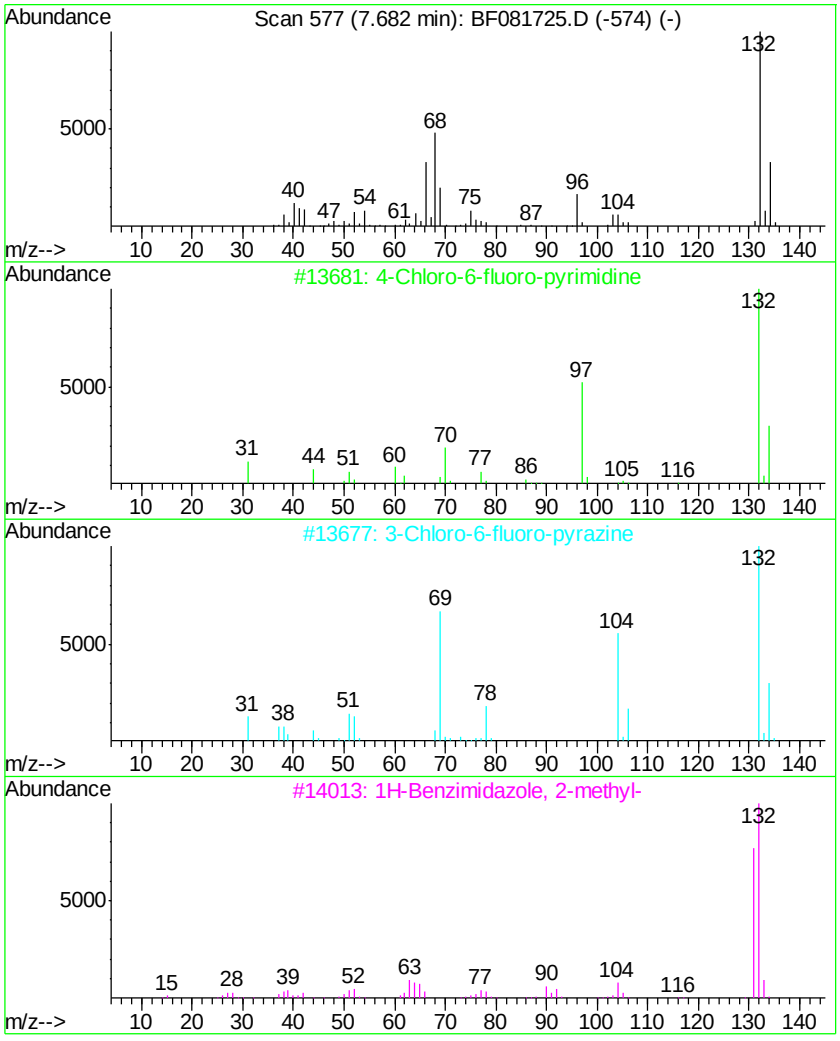
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

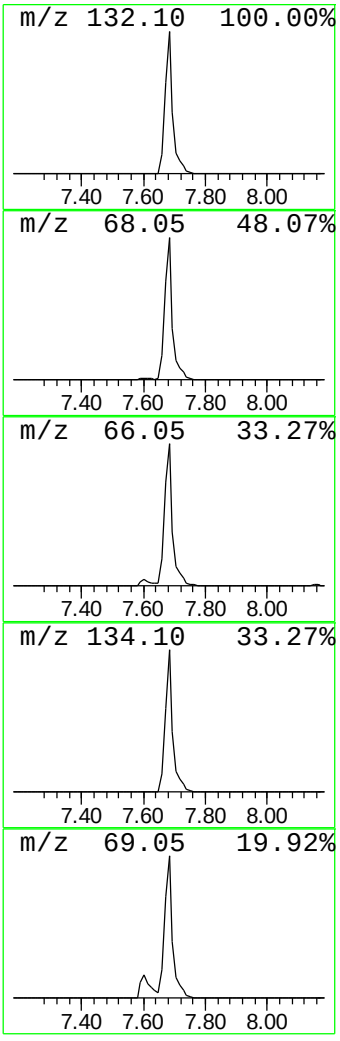
****

Peak Number 5 unknown7.68 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	103.15 ng	1322680	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081725.D
Acq On : 21 Sep 2015 21:31
Operator : UM/IZ
Sample : G3717-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-9-17-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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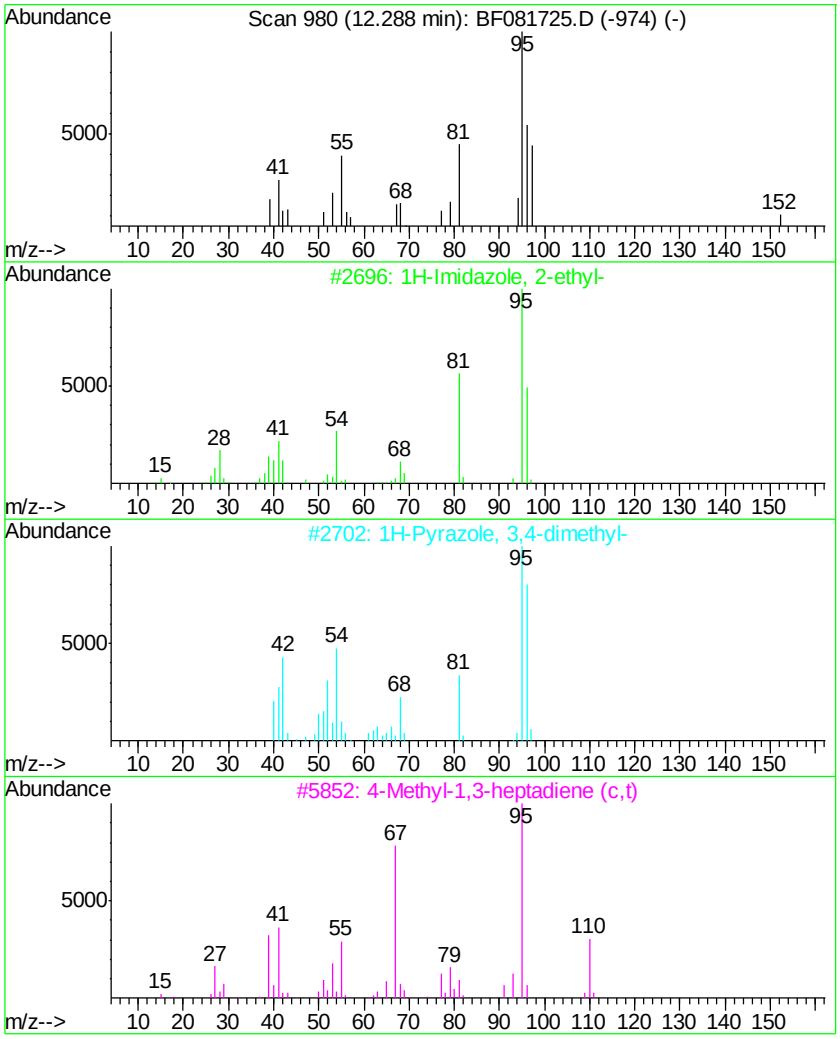
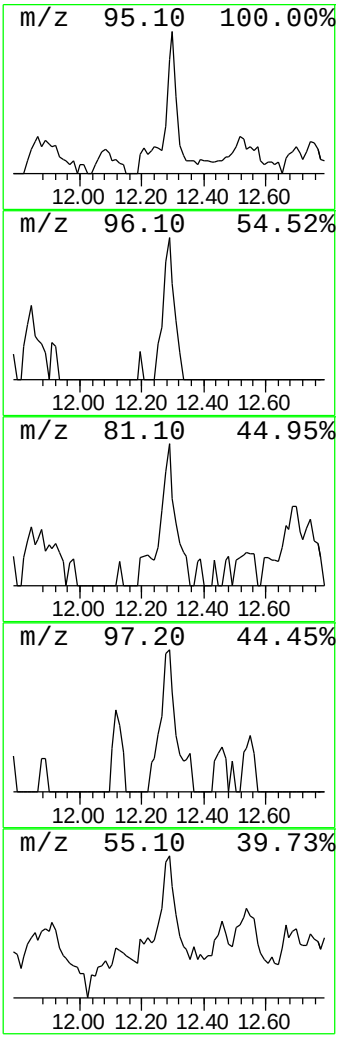
Peak Number 7 unknown12.29 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	3.46 ng	54485	Naphthalene-d8	11.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Imidazole, 2-ethyl-	96	C5H8N2	001072-62-4	49
2	1H-Pyrazole, 3,4-dimethyl-	96	C5H8N2	002820-37-3	47
3	4-Methyl-1,3-heptadiene (c,t)	110	C8H14	017603-57-5	25
4	Cyclohexene, 3-(bromomethyl)-	174	C7H11Br	034825-93-9	25
5	Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	091884-67-2	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
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Operator : UM/IZ
Sample : G3717-11
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-9-17-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

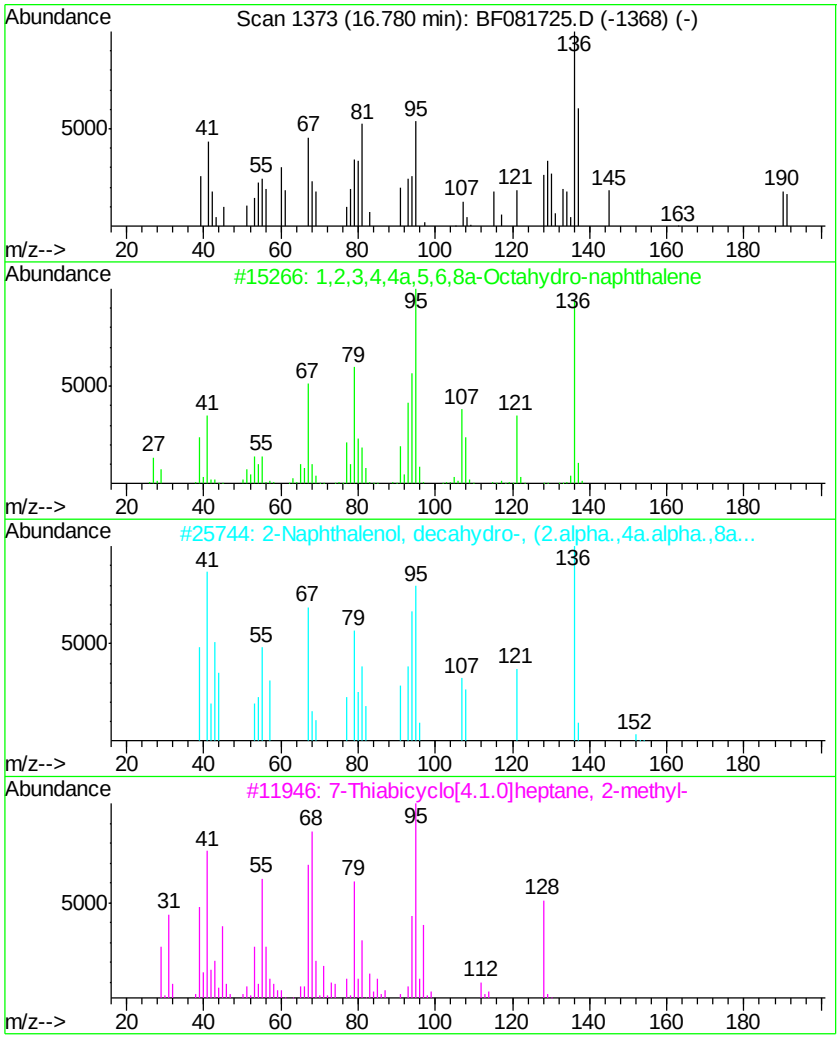
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

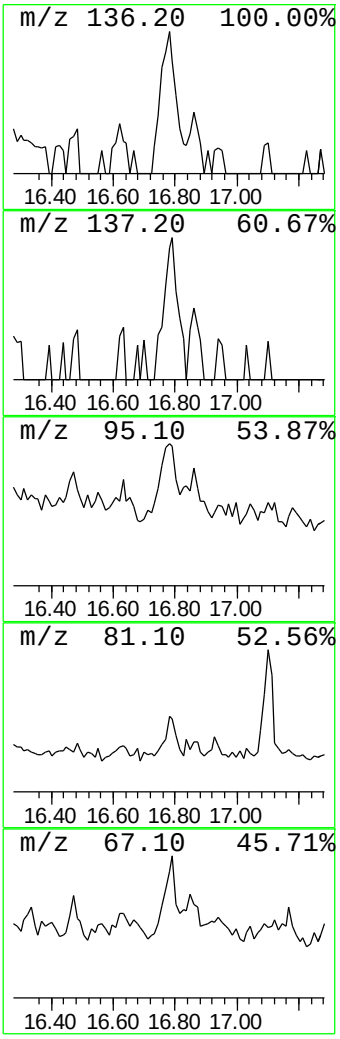
****

Peak Number 8 unknown16.78 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.78	3.25 ng	66250	Acenaphthene-d10	15.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,3,4,4a,5,6,8a-Octahydro-naph...	136	C10H16	031244-58-3	46
2	2-Naphthalenol, decahydro-, (2.a...	154	C10H18O	002529-06-8	43
3	7-Thiabicyclo[4.1.0]heptane, 2-m...	128	C7H12S	054773-76-1	38
4	Adamantane	136	C10H16	000281-23-2	38
5	2.alpha., 4a.beta., 8a.beta.-Dec...	154	C10H18O	001424-37-9	37





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Instrument : BNA_F
ClientSampleId : PZ-6-9-17-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

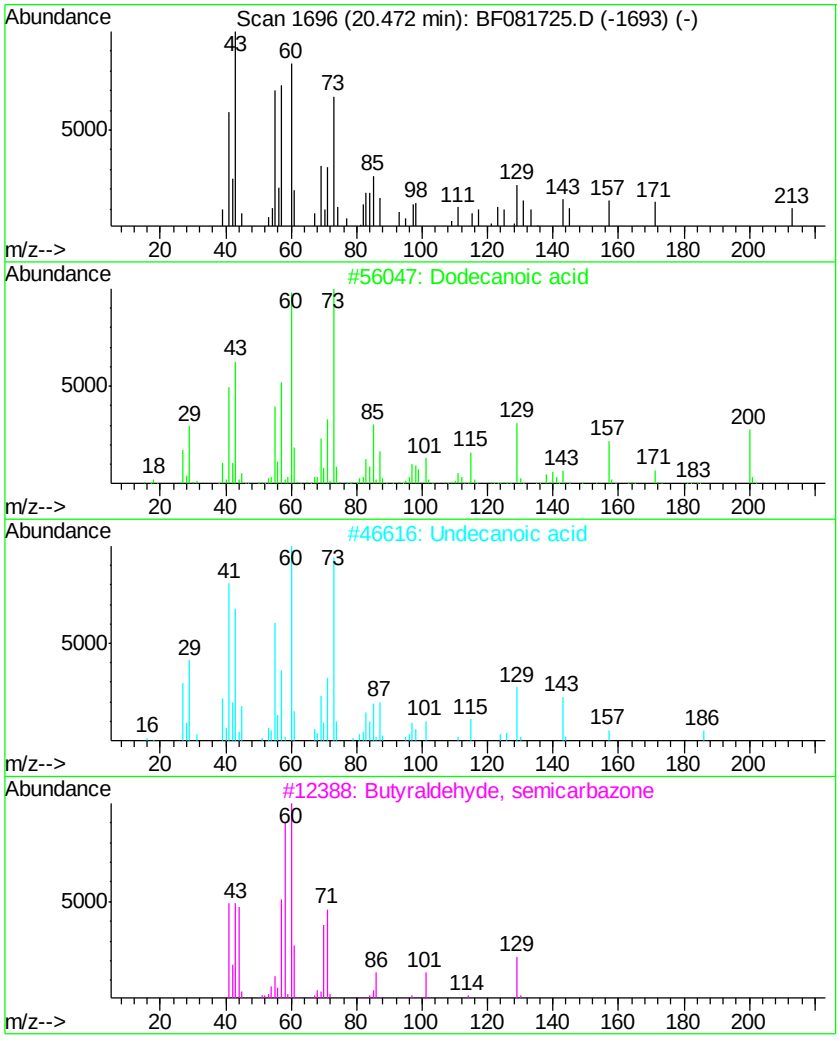
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

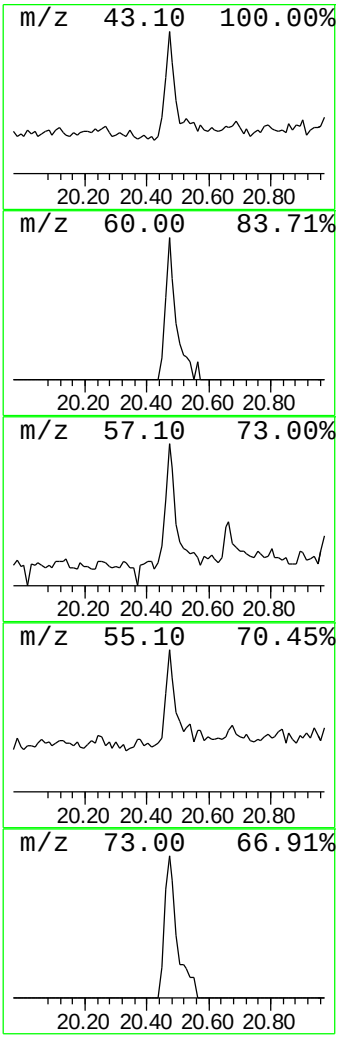
****

Peak Number 9 Dodecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.47	3.39 ng	65684	Phenanthrene-d10	18.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	64
2	Undecanoic acid	186	C11H22O2	000112-37-8	50
3	Butyraldehyde, semicarbazone	129	C5H11N3O	013183-21-6	47
4	n-Decanoic acid	172	C10H20O2	000334-48-5	43
5	Octanoic Acid	144	C8H16O2	000124-07-2	43





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

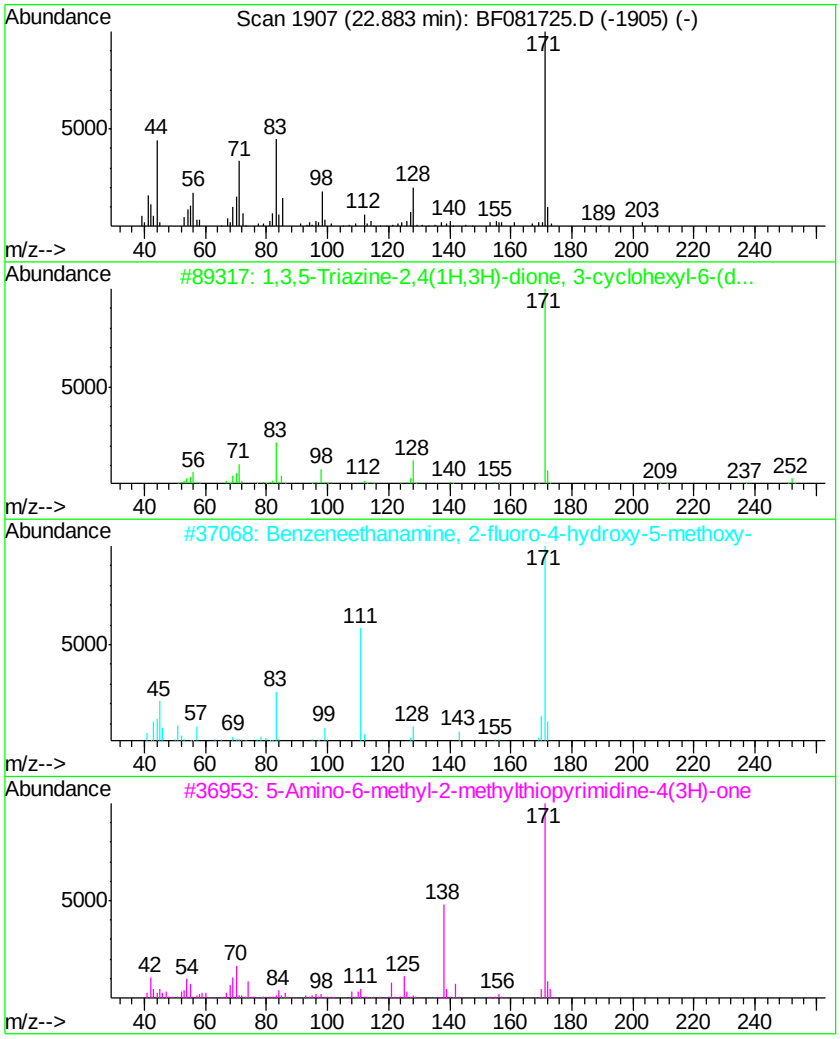
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

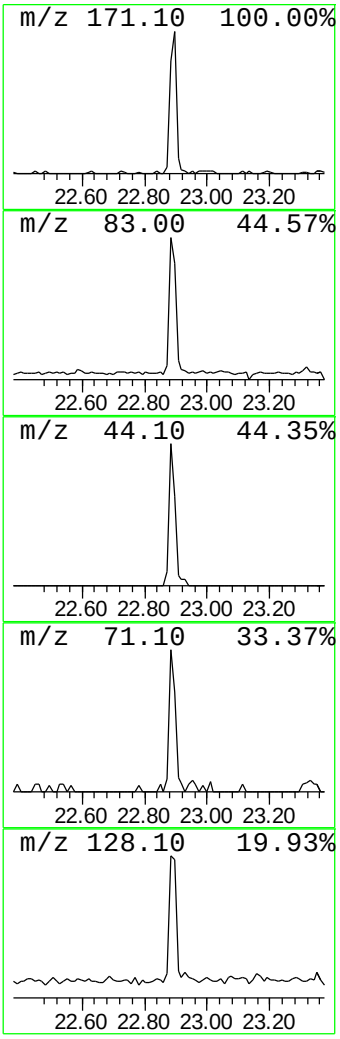
****

Peak Number 10 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.88	8.35 ng	136351	Chrysene-d12	23.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4(1H,3H)-dione,...	252	C12H20N4O2	051235-04-2	91
2	Benzeneethanamine, 2-fluoro-4-hy...	171	C8H10FNO2	1000116-43-3	35
3	5-Amino-6-methyl-2-methylthiopyr...	171	C6H9N3OS	342402-52-2	27
4	Phenylethan-1,2-diol, 2-fluoro-4...	202	C9H11FO4	141523-14-0	27
5	4-Pyrrolylbenzaldehyde	171	C11H9NO	023351-05-5	27





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...	1.21	251.8	ng	3228440	1	8.16	256447	20.0
2-Pentanone, 4-hy...	4.42	19.3	ng	246960	1	8.16	256447	20.0
unknown7.68	7.68	103.2	ng	1322680	1	8.16	256447	20.0
unknown12.29	12.29	3.5	ng	54485	2	11.05	314546	20.0
unknown16.78	16.78	3.3	ng	66250	3	15.19	408031	20.0
Dodecanoic acid	20.47	3.4	ng	65684	4	18.70	387429	20.0
1,3,5-Triazine-2,...	22.88	8.3	ng	136351	5	23.35	326591	20.0