LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086489.D
Acq On : 29 Apr 2016 13:50
Operator : UM/SJ
Sample : H2741-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

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-BF042716.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	2.521	35	38	40	rBV	131049	201483	4.96%	0.586%
2	2.555	40	41	48	rVB	116344	140575	3.46%	0.409%
3	3.287	102	105	113	rBV	250162	482688	11.87%	1.404%
4	4.293	190	193	196	rBV	1502596	1859699	45.74%	5.409%
5	4.521	210	213	217	rVB	30629	50983	1.25%	0.148%
6	4.590	217	219	222	rBV	36355	48422	1.19%	0.141%
7	4.967	250	252	259	rBV2	135965	246955	6.07%	0.718%
8	5.378	285	288	290	rBV	3253809	3278854	80.64%	9.537%
9	6.407	376	378	381	rBV2	1890992	2546549	62.63%	7.407%
10	6.544	387	390	392	rBV	3568295	3506412	86.24%	10.199%
11	6.773	408	410	417	rBV	966190	1020075	25.09%	2.967%
12	6.933	421	424	426	rVV	2909784	2791932	68.67%	8.120%
13	6.990	428	429	432	rVV	51058	73373	1.80%	0.213%
14	7.070	434	436	439	rVV2	119824	205783	5.06%	0.599%
15	7.127	439	441	445	rVB	29989	42973	1.06%	0.125%
16	7.344	457	460	462	rBV	2042392	2422217	59.57%	7.045%
17	8.064	520	523	525	rBV	1110467	1307109	32.15%	3.802%
18	8.853	590	592	602	rVB2	30120	42086	1.04%	0.122%
19	9.139	614	617	620	rBV	3570690	3741661	92.03%	10.883%
20	9.813	673	676	679	rBV	1105724	1079011	26.54%	3.138%
21	10.602	742	745	747	rBV	2504733	2678542	65.88%	7.791%
22	11.299	803	806	808	rBV	1039828	1372174	33.75%	3.991%
23	12.888	942	945	947	rBV	2714791	4065889	100.00%	11.826%
24	13.928	1033	1036	1049	rBV	569118	937006	23.05%	2.725%
25	15.334	1156	1159	1169	rVB3	72943	175939	4.33%	0.512%
26	15.677	1182	1189	1194	rBV3	13334	63161	1.55%	0.184%

Sum of corrected areas: 34381551

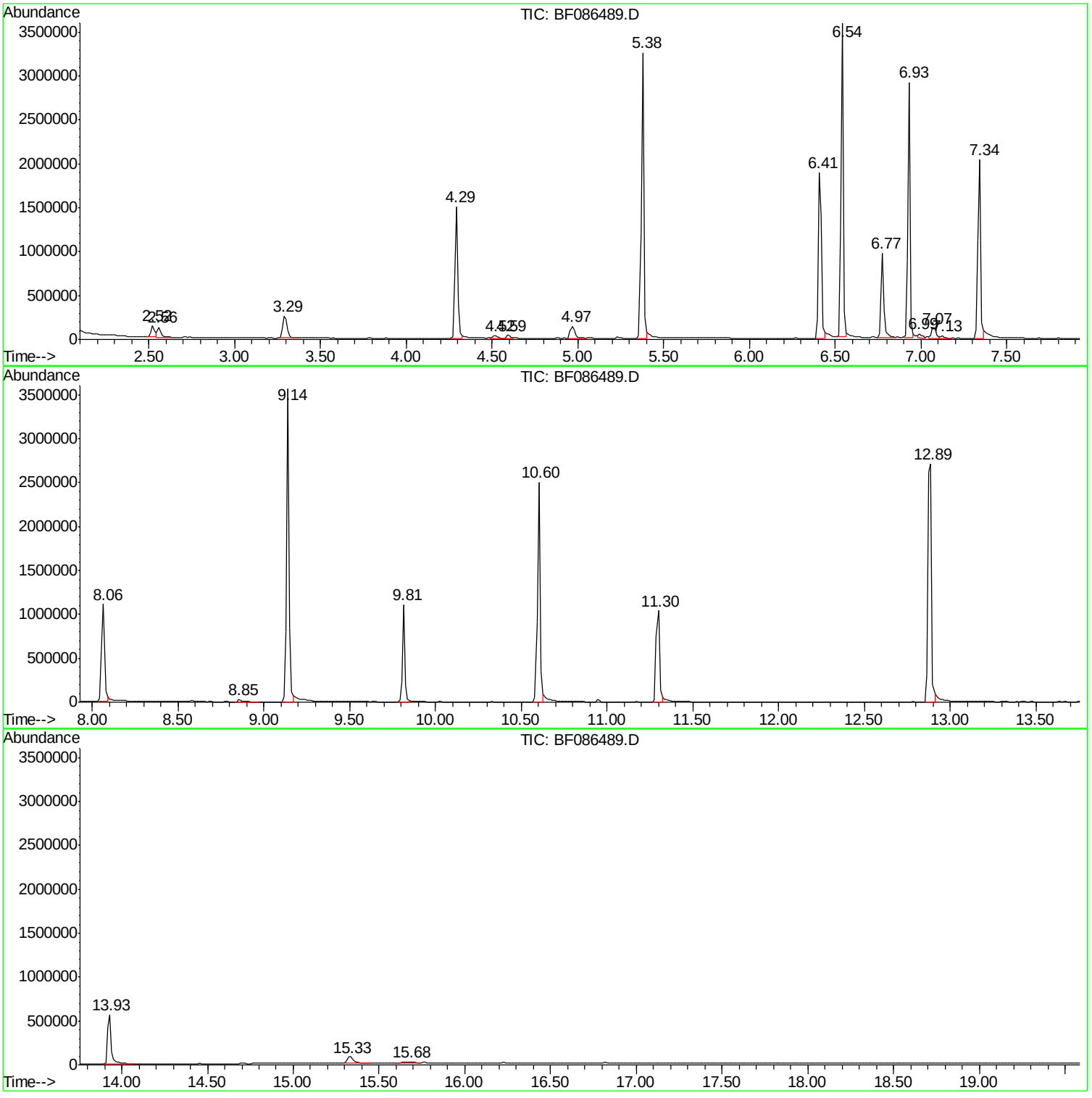
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086489.D
Acq On : 29 Apr 2016 13:50
Operator : UM/SJ
Sample : H2741-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086489.D
Acq On : 29 Apr 2016 13:50
Operator : UM/SJ
Sample : H2741-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

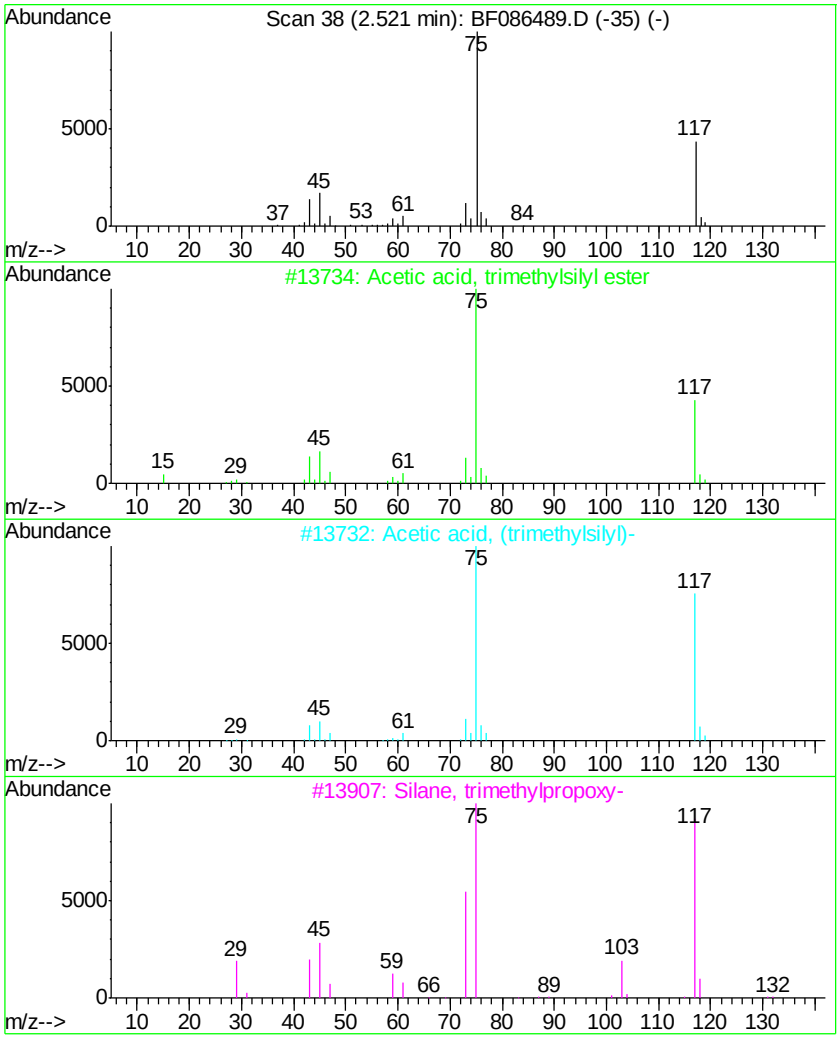
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

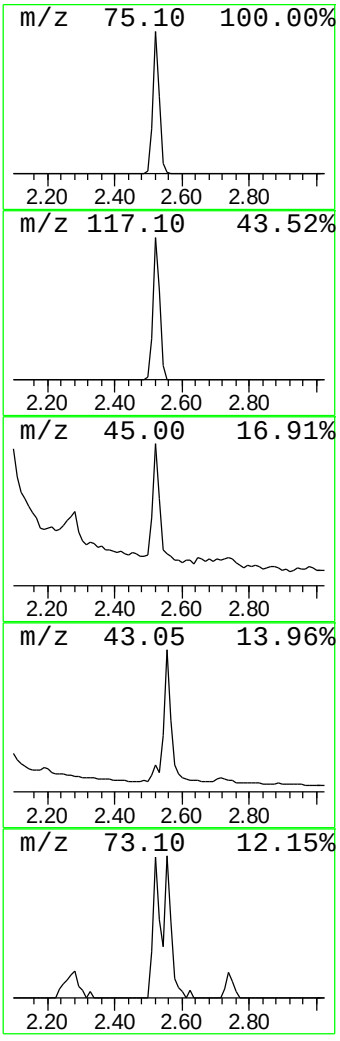
****

Peak Number 1 Acetic acid, trimethylsilyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.52	3.95 ng	201483	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, trimethylsilyl ester	132	C5H12O2Si	018147-36-9	90
2	Acetic acid, (trimethylsilyl)-	132	C5H12O2Si	002345-38-2	83
3	Silane, trimethylpropoxy-	132	C6H16OSi	001825-63-4	56
4	3-(Methylthio)-2-butanone	118	C5H10OS	053475-15-3	50
5	Silane, trimethyl(1-methylethoxy)-	132	C6H16OSi	001825-64-5	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086489.D
Acq On : 29 Apr 2016 13:50
Operator : UM/SJ
Sample : H2741-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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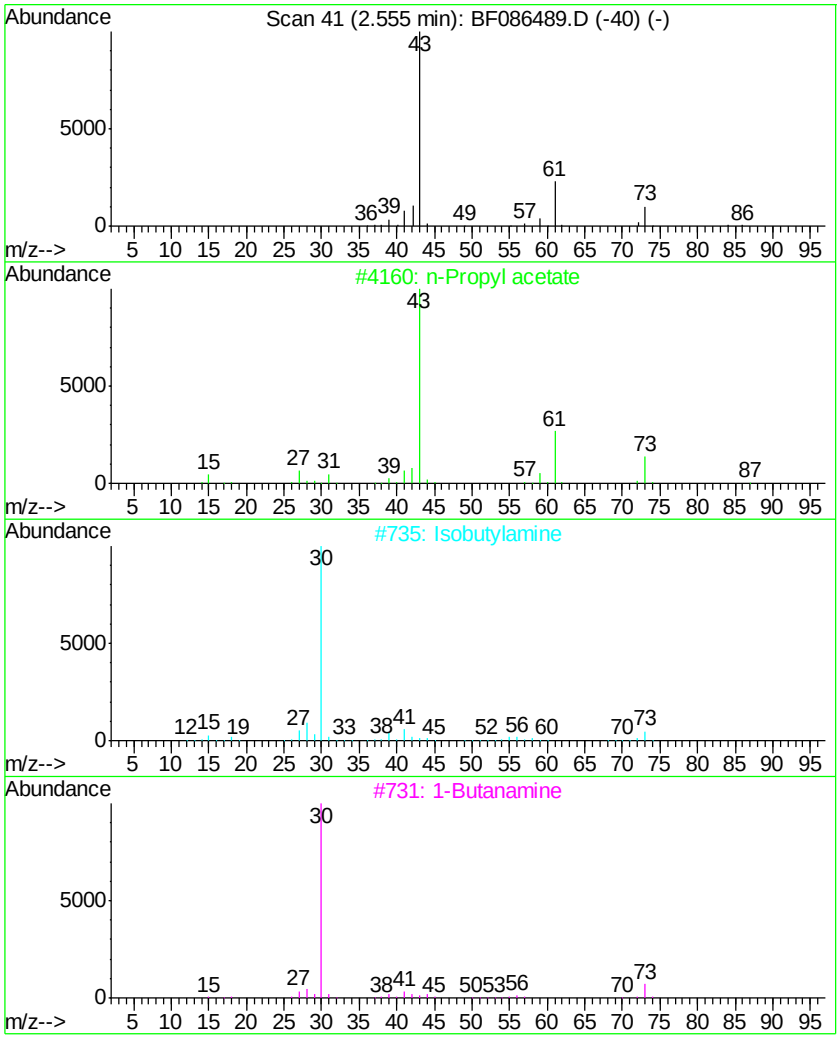
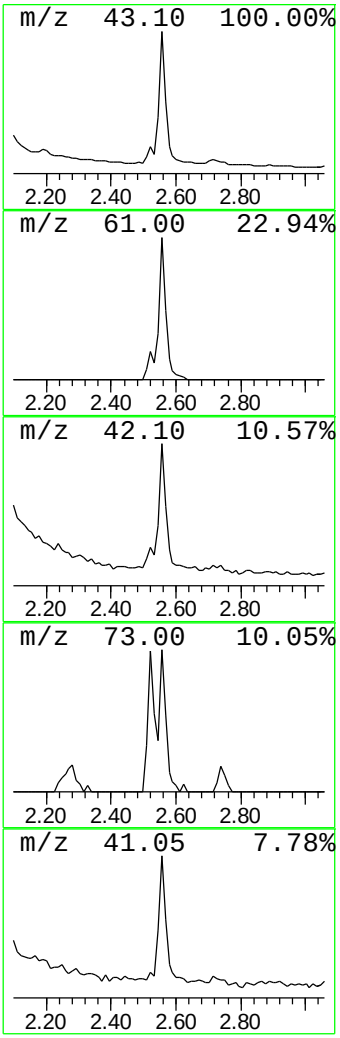
Peak Number 2 n-Propyl acetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.56	2.76 ng	140575	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	Isobutylamine	73	C4H11N	000078-81-9	7
3	1-Butanamine	73	C4H11N	000109-73-9	4
4	Pentane	72	C5H12	000109-66-0	4
5	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	4





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086489.D
Acq On : 29 Apr 2016 13:50
Operator : UM/SJ
Sample : H2741-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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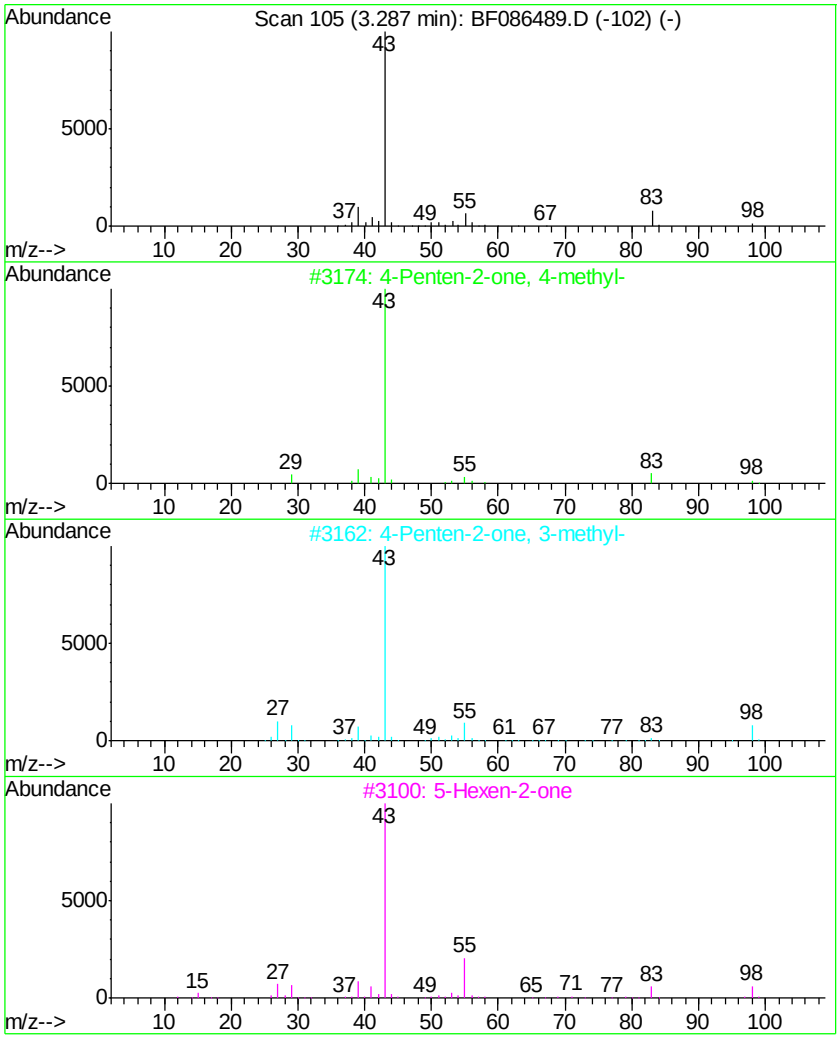
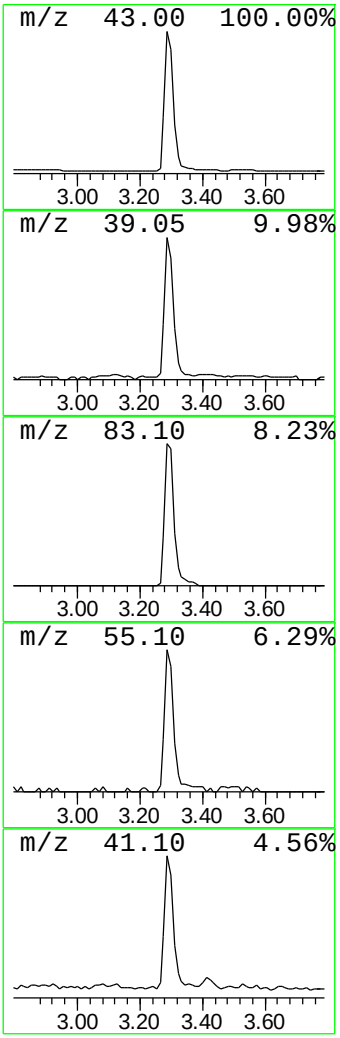
Peak Number 3 4-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.29	9.46 ng	482688	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	64
2	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	42
3	5-Hexen-2-one	98	C6H10O	000109-49-9	42
4	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
5	4-Hexen-2-one	98	C6H10O	025659-22-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086489.D
Acq On : 29 Apr 2016 13:50
Operator : UM/SJ
Sample : H2741-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

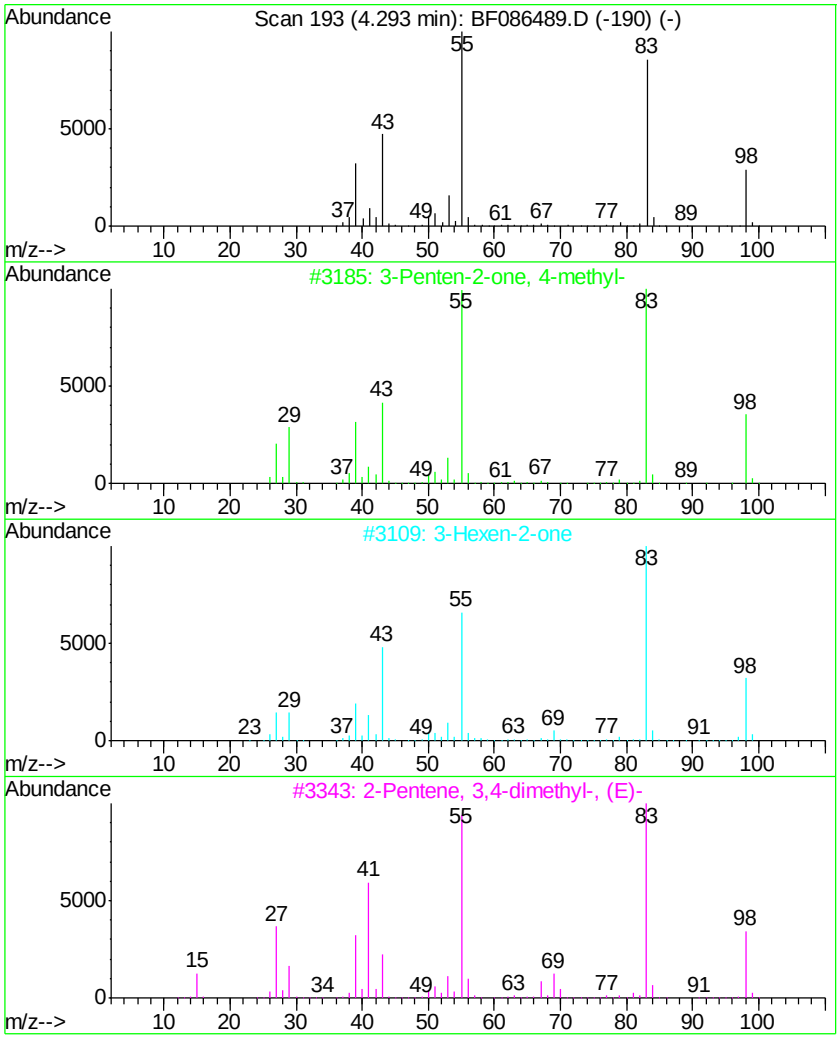
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

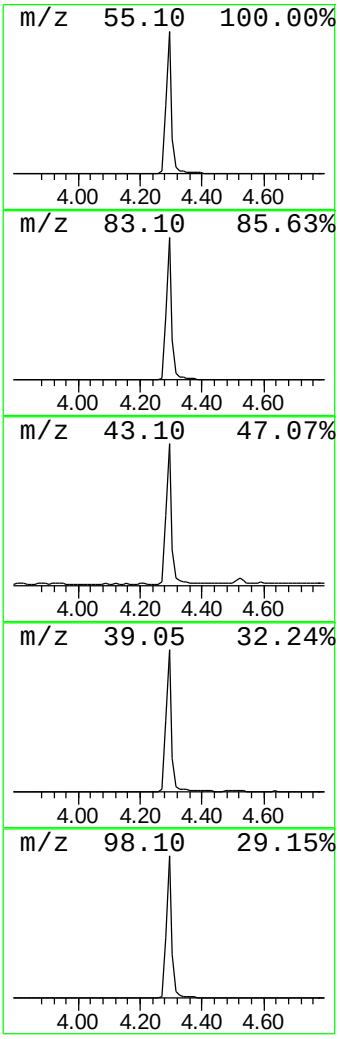
****

Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.29	36.46 ng	1859700	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	87
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086489.D
Acq On : 29 Apr 2016 13:50
Operator : UM/SJ
Sample : H2741-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

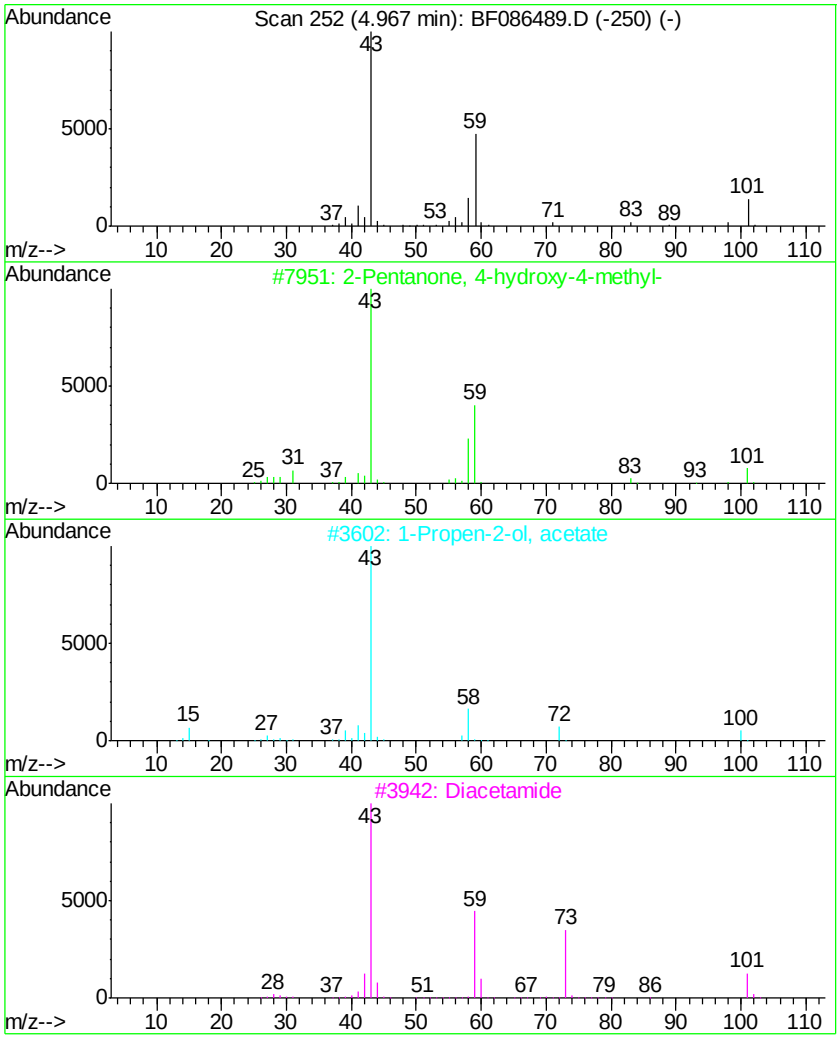
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

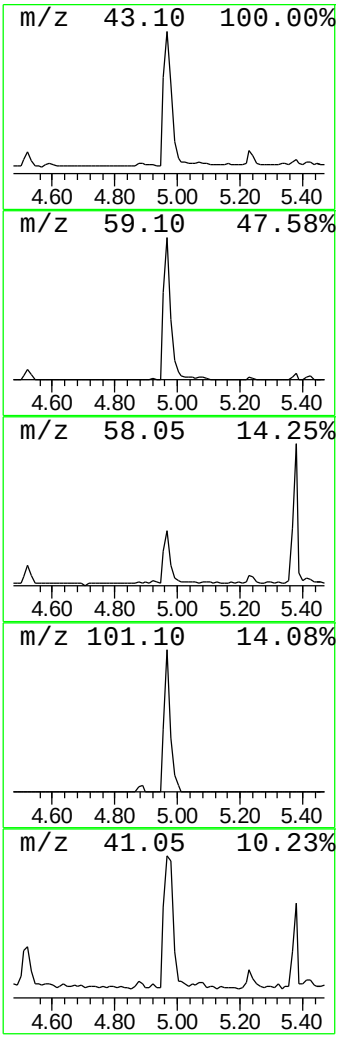
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	4.84 ng	246955	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Cyclobutylamine	71	C4H9N	002516-34-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086489.D
Acq On : 29 Apr 2016 13:50
Operator : UM/SJ
Sample : H2741-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

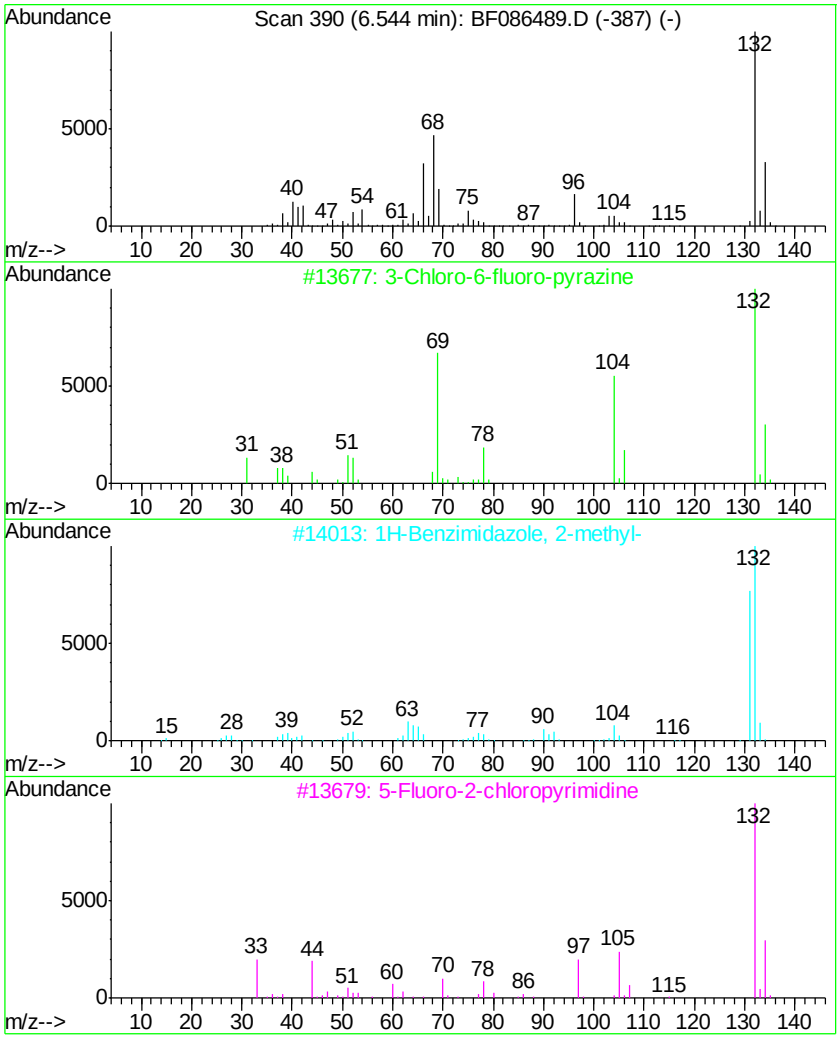
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

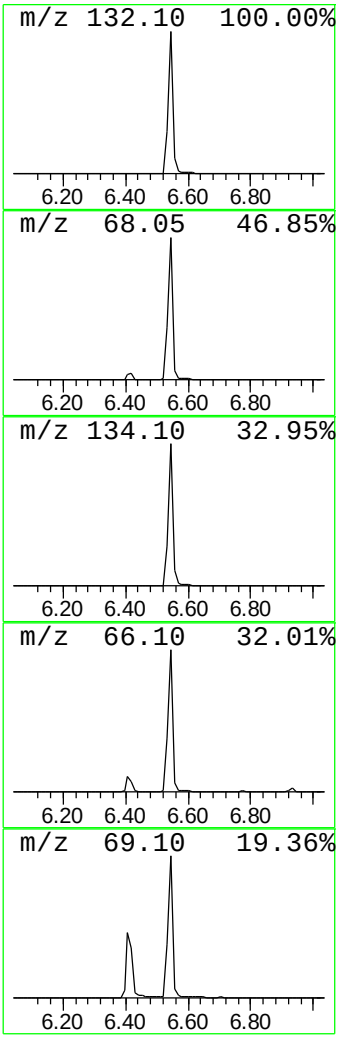
****

Peak Number 6 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	68.75 ng	3506410	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086489.D
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Operator : UM/SJ
Sample : H2741-03
Misc :
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Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

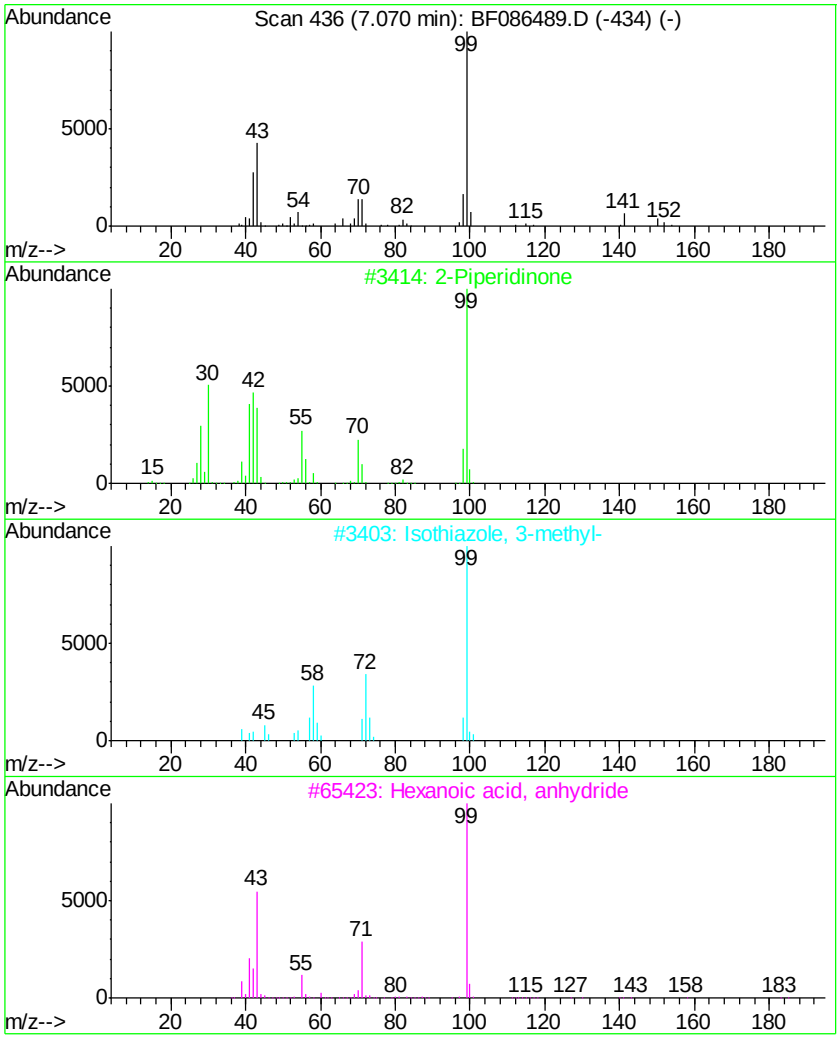
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

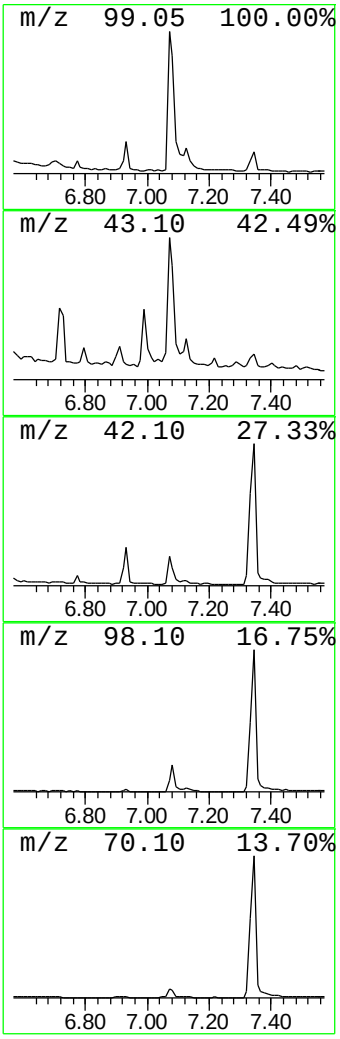
****

Peak Number 8 2-Piperidinone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	4.03 ng	205783	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Piperidinone	99	C5H9NO	000675-20-7	64
2	Isothiazole, 3-methyl-	99	C4H5NS	000693-92-5	50
3	Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	42
4	2-Furancarboxylic acid, tetrahyd...	144	C6H8O4	022073-04-7	40
5	2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	40





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042916\
Data File : BF086489.D
Acq On : 29 Apr 2016 13:50
Operator : UM/SJ
Sample : H2741-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

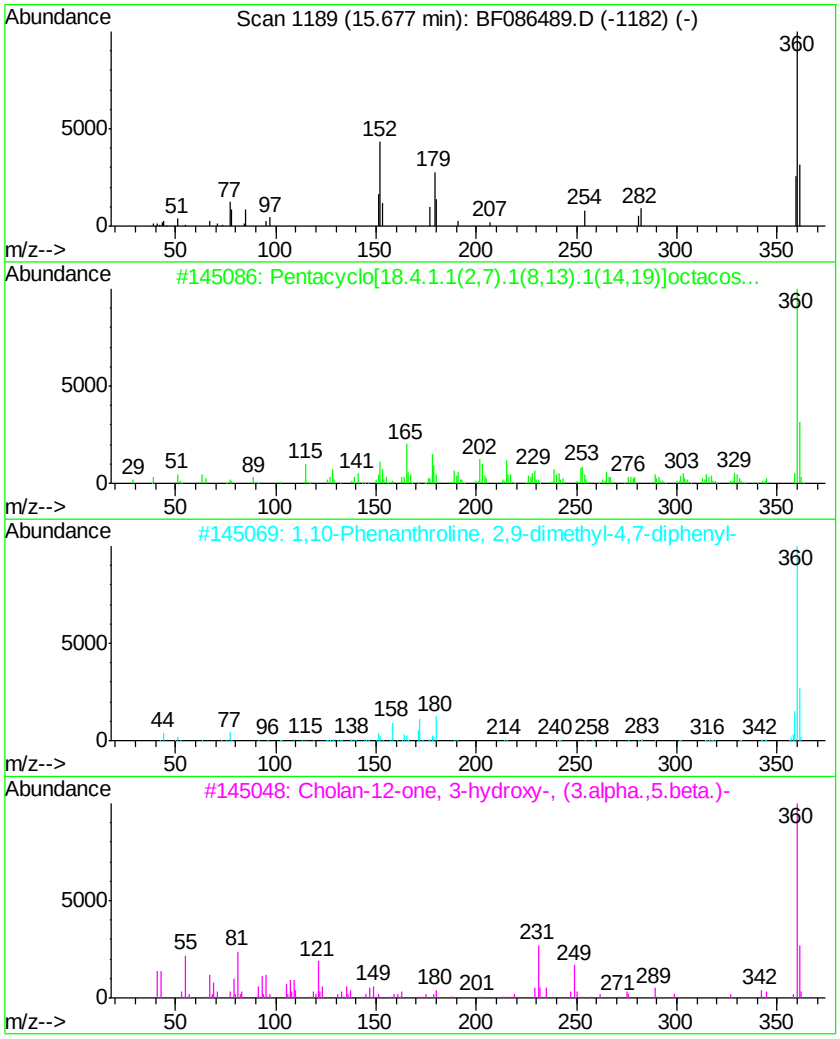
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

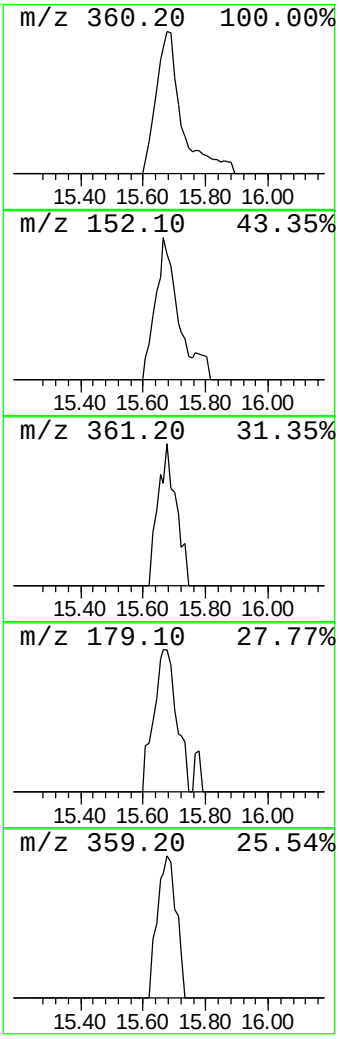
****

Peak Number 9 unknown15.68 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.68	7.18 ng	63161	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacyclo[18.4.1.1(2,7).1(8,13)...	360	C28H24	101077-60-5	9
2	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	9
3	Cholan-12-one, 3-hydroxy-, (3.al...	360	C24H40O2	054411-58-4	5
4	2-Cyclohexylamino-3-methyl(phenv...	360	C23H24N2O2	134614-17-8	5
5	Vanadium, bis(.eta.-5-cyclopenta...	360	C20H18V2	1000155-21-4	5





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042916\
Data File : BF086489.D
Acq On : 29 Apr 2016 13:50
Operator : UM/SJ
Sample : H2741-03
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetic acid, trim...	2.52	4.0	ng	201483	1	6.77	1020080	20.0
n-Propyl acetate	2.56	2.8	ng	140575	1	6.77	1020080	20.0
4-Penten-2-one, 4...	3.29	9.5	ng	482688	1	6.77	1020080	20.0
3-Penten-2-one, 4...	4.29	36.5	ng	1859700	1	6.77	1020080	20.0
2-Pentanone, 4-hy...	4.97	4.8	ng	246955	1	6.77	1020080	20.0
unknown6.54	6.54	68.8	ng	3506410	1	6.77	1020080	20.0
2-Piperidinone	7.07	4.0	ng	205783	1	6.77	1020080	20.0
unknown15.68	15.68	7.2	ng	63161	6	15.32	175939	20.0