LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041015\
Data File : BF078431.D
Acq On : 11 Apr 2015 8:54
Operator : TP/IZ
Sample : G1744-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TD-2

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-BF040115.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	1.024	9	12	14	rBV	1777102	1830181	100.00%	20.274%
2	1.127	18	21	24	rVB	70742	101977	5.57%	1.130%
3	1.275	31	34	36	rVB	40891	55852	3.05%	0.619%
4	1.527	55	56	63	rVV	19141	30779	1.68%	0.341%
5	1.618	63	64	81	rVB	335676	557893	30.48%	6.180%
6	3.561	230	234	243	rVB	11259	28579	1.56%	0.317%
7	4.521	317	318	326	rBV	47937	81496	4.45%	0.903%
8	5.116	368	370	375	rBV	396676	503454	27.51%	5.577%
9	6.464	486	488	490	rBV	416683	501196	27.39%	5.552%
10	6.579	495	498	500	rBV	442646	551465	30.13%	6.109%
11	6.864	520	523	525	rBV	153988	172566	9.43%	1.912%
12	7.047	536	539	541	rBV	468179	441608	24.13%	4.892%
13	7.562	582	584	586	rBV	367943	325687	17.80%	3.608%
14	8.442	658	661	663	rBV	246662	241769	13.21%	2.678%
15	9.790	776	779	781	rBV	500609	682000	37.26%	7.555%
16	10.293	821	823	826	rBV	28090	28770	1.57%	0.319%
17	10.591	847	849	852	rBV	237786	291909	15.95%	3.234%
18	11.573	932	935	937	rBV	404378	431342	23.57%	4.778%
19	12.419	1007	1009	1012	rBV	326546	311742	17.03%	3.453%
20	14.408	1181	1183	1186	rBV	622861	850614	46.48%	9.423%
21	15.597	1285	1287	1292	rBV	69958	127223	6.95%	1.409%
22	15.688	1292	1295	1297	rVV	281508	394747	21.57%	4.373%
23	15.768	1299	1302	1304	rBV	12532	21485	1.17%	0.238%
24	16.008	1320	1323	1328	rBV3	8004	22382	1.22%	0.248%
25	16.865	1395	1398	1401	rBV	16035	29811	1.63%	0.330%
26	17.380	1441	1443	1446	rBV	269636	410615	22.44%	4.549%

Sum of corrected areas: 9027142

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Misc :
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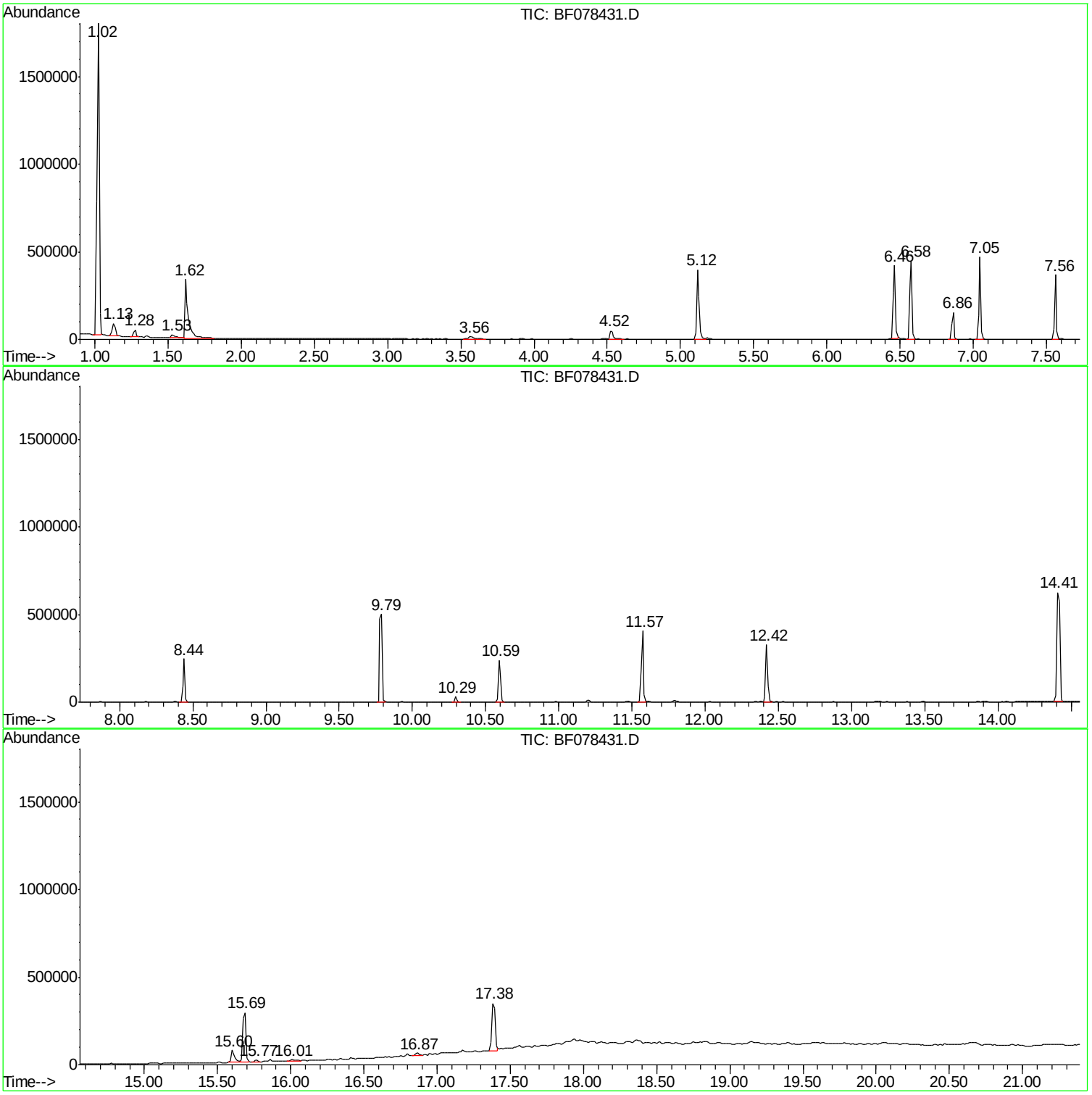
Instrument : BNA_F
ClientSampleId : TD-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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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Data File : BF078431.D
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Operator : TP/IZ
Sample : G1744-06
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ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

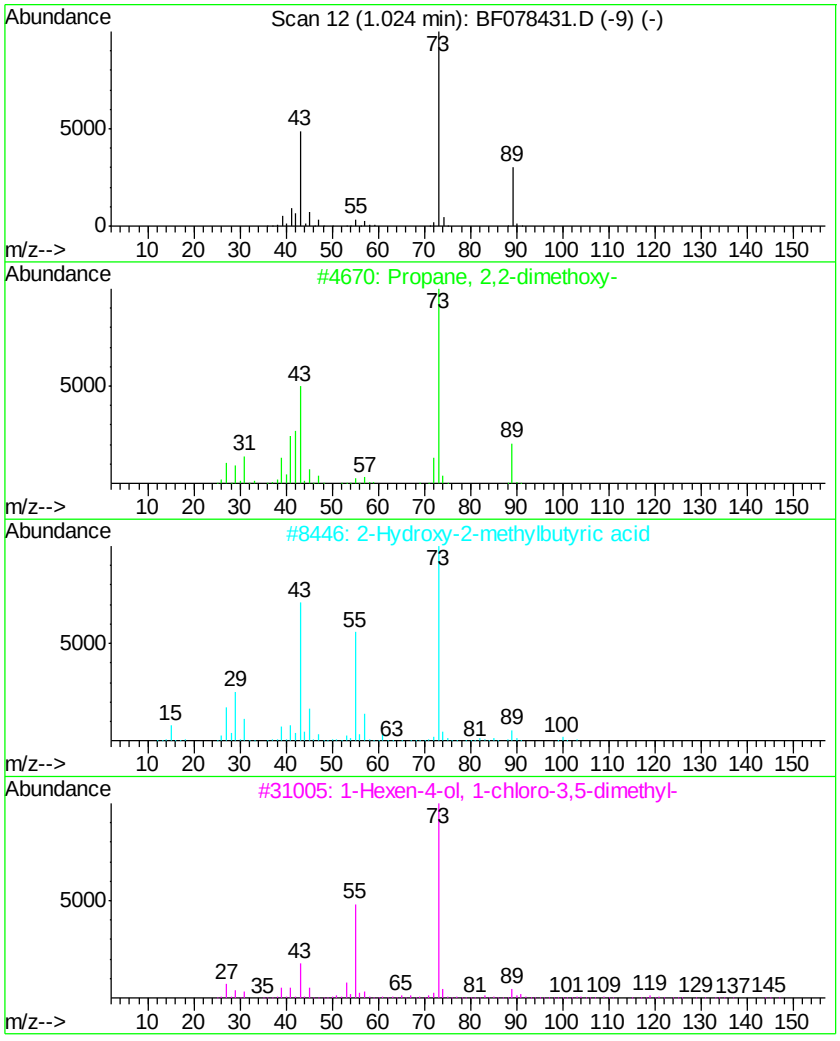
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

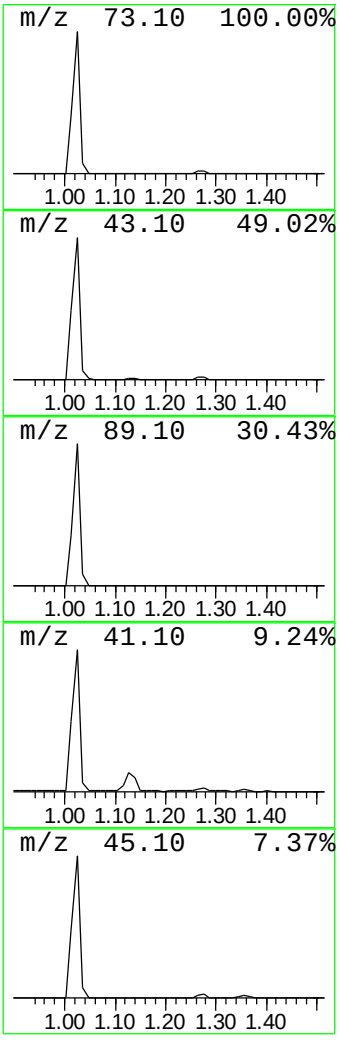
****

Peak Number 1 unknown1.02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.02	212.11 ng	1830180	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
3	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	5





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041015\
Data File : BF078431.D
Acq On : 11 Apr 2015 8:54
Operator : TP/IZ
Sample : G1744-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TD-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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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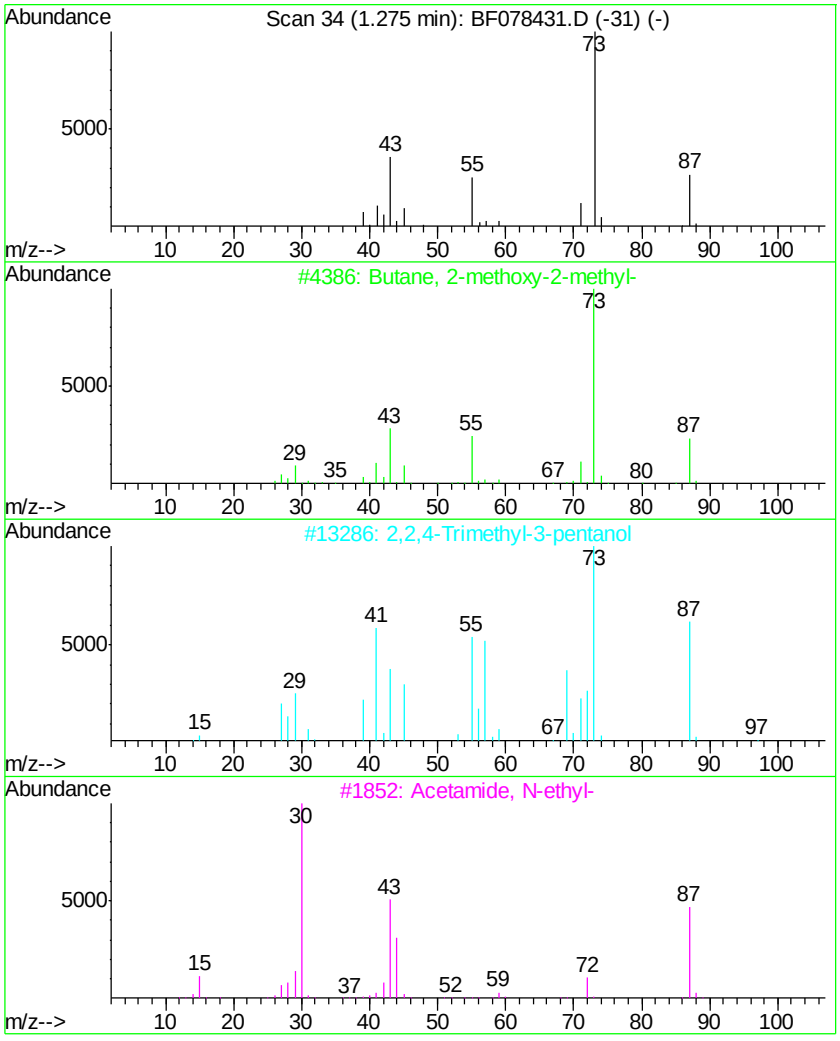
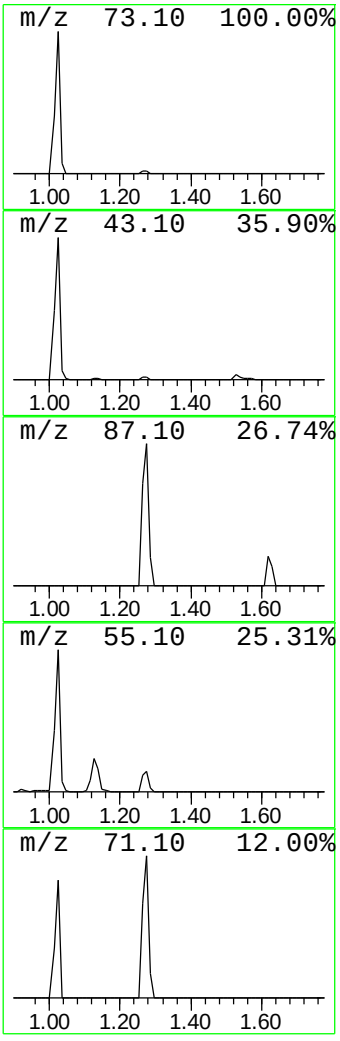
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	6.47 ng	55852	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041015\
Data File : BF078431.D
Acq On : 11 Apr 2015 8:54
Operator : TP/IZ
Sample : G1744-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TD-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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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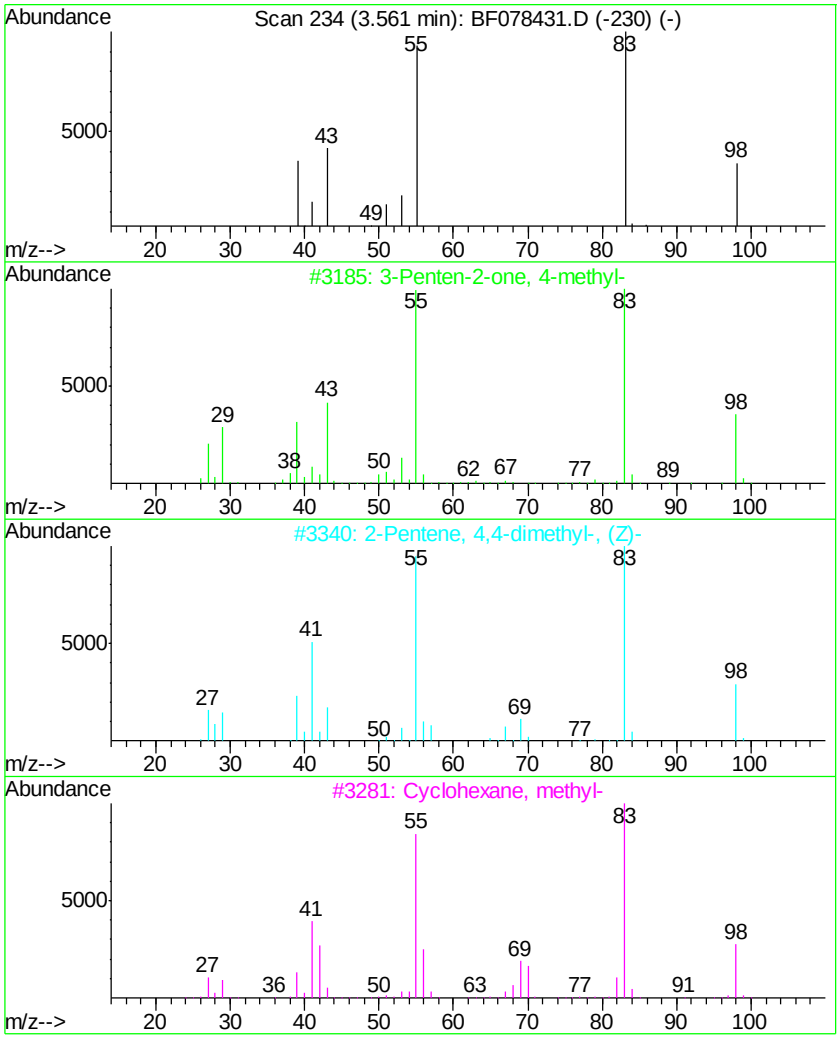
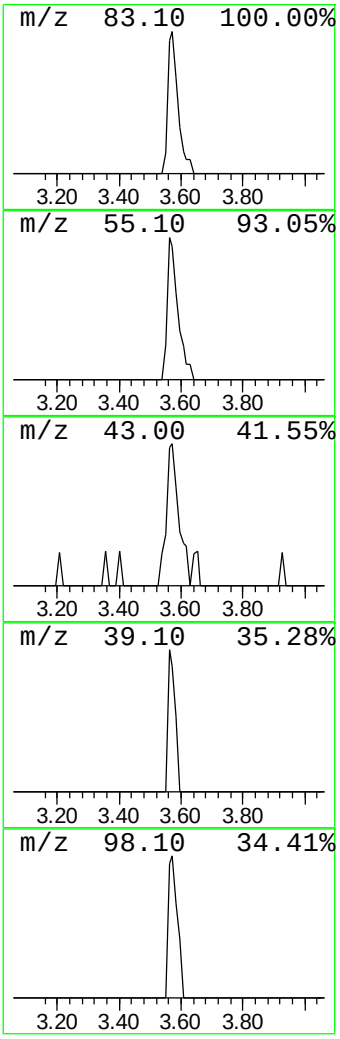
Peak Number 6 3-Penten-2-one, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.56	3.31 ng	28579	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
2	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	56
3	Cyclohexane, methyl-	98	C7H14	000108-87-2	50
4	3-Hexen-2-one	98	C6H10O	000763-93-9	50
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	40





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041015\
Data File : BF078431.D
Acq On : 11 Apr 2015 8:54
Operator : TP/IZ
Sample : G1744-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TD-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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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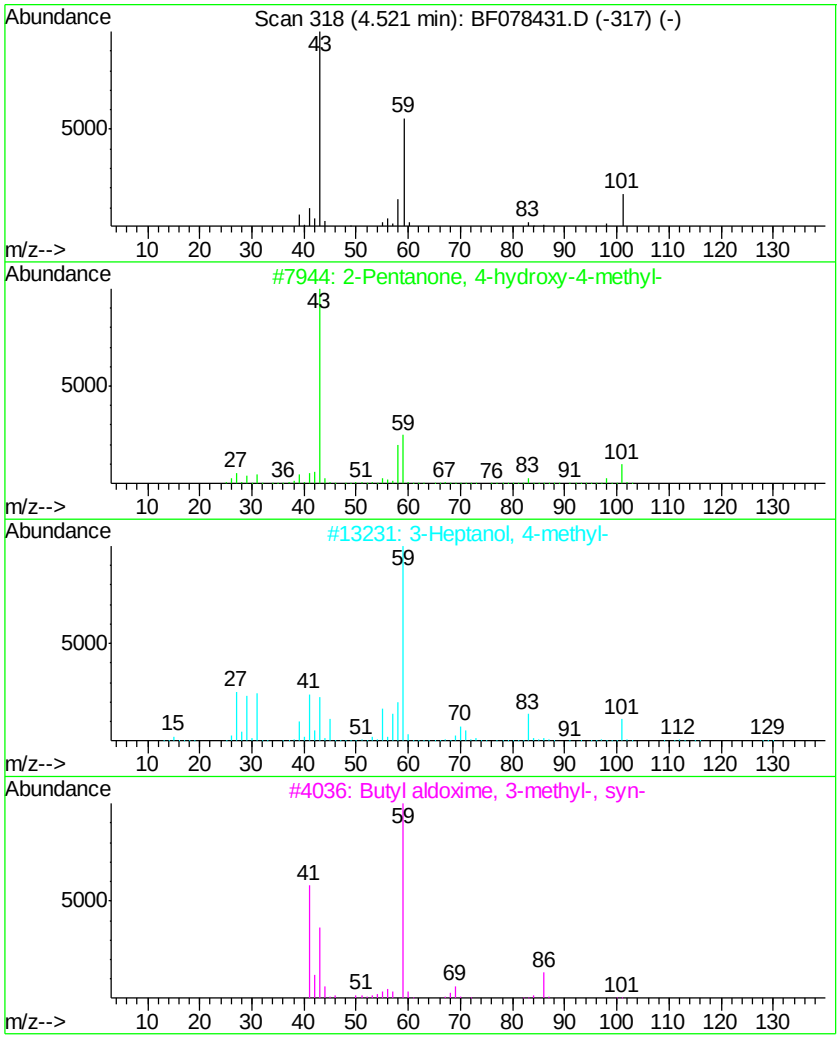
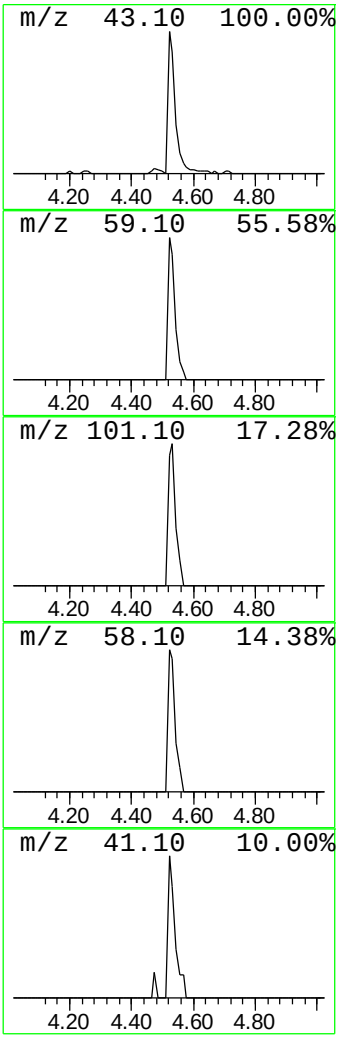
Peak Number 7 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	9.45 ng	81496	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	33
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32
4	3-Heptanol	116	C7H16O	000589-82-2	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041015\
Data File : BF078431.D
Acq On : 11 Apr 2015 8:54
Operator : TP/IZ
Sample : G1744-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TD-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

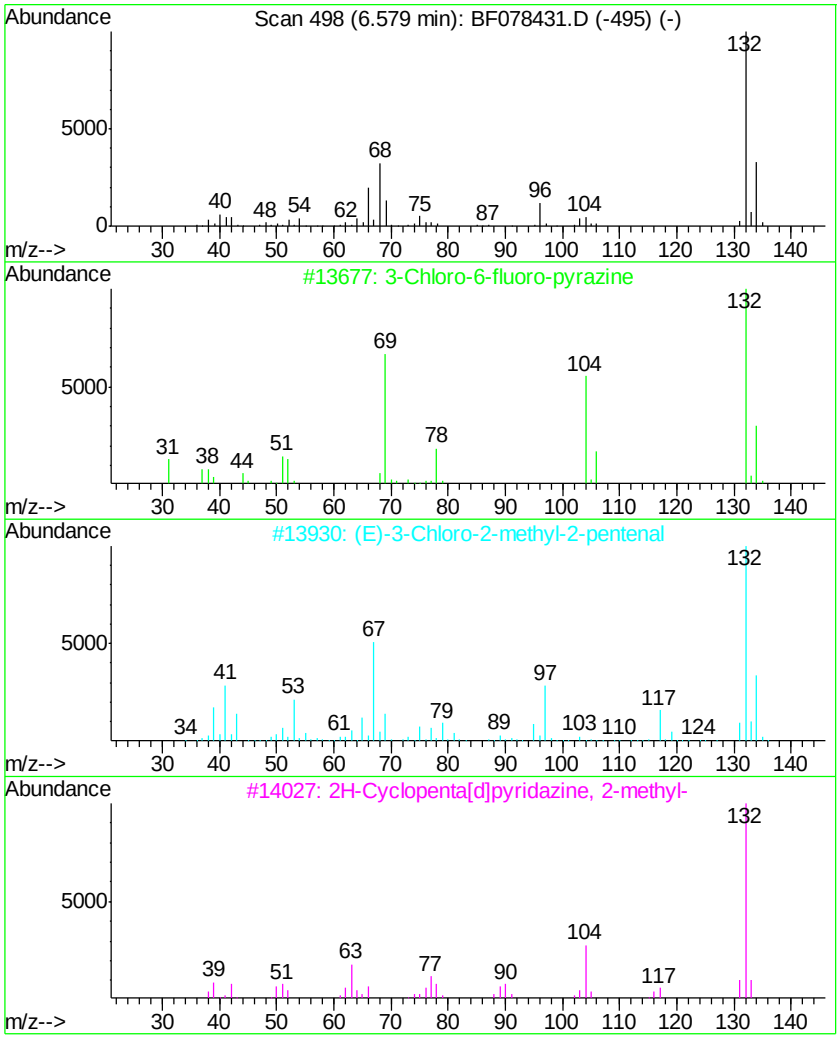
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

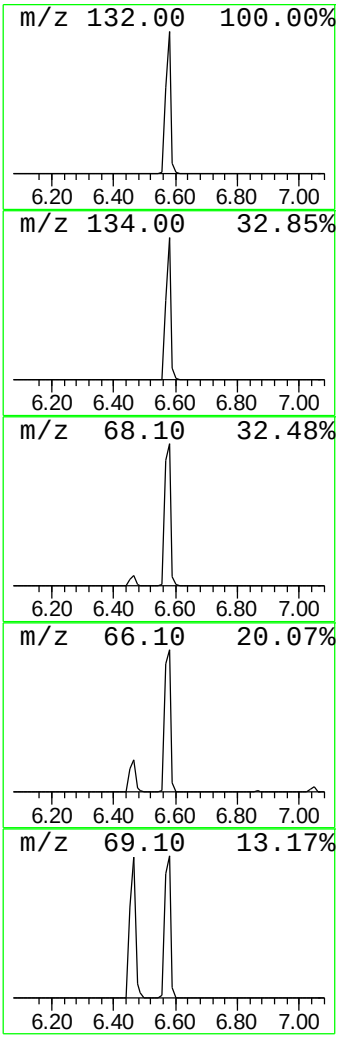
****

Peak Number 8 unknown6.58 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	63.91 ng	551465	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Sample : G1744-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TD-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

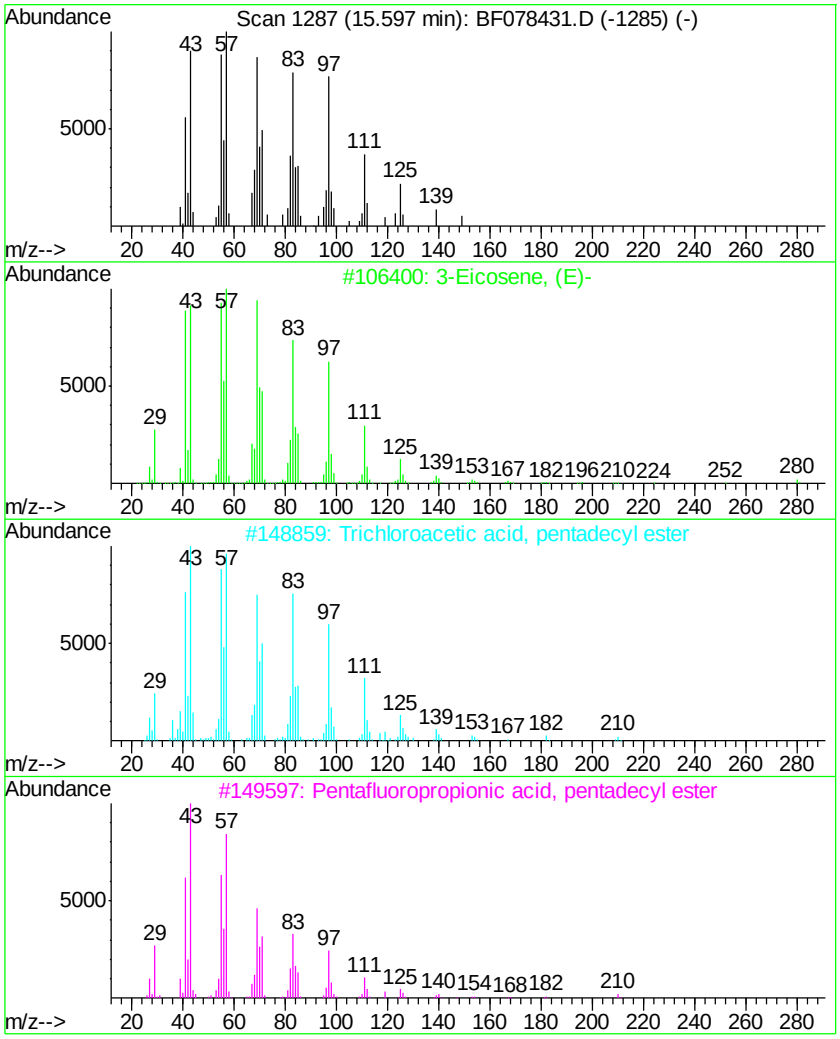
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

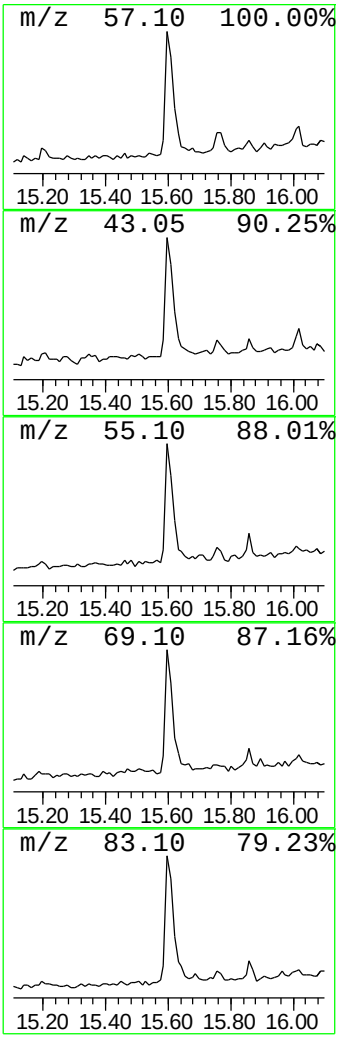
****

Peak Number 10 3-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	6.45 ng	127223	Chrysene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	91
4	1-Heptadecanol	256	C17H36O	001454-85-9	90
5	1-Hexadecanol	242	C16H34O	036653-82-4	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041015\
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Instrument : BNA_F
ClientSampleId : TD-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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
unknown1.02	1.02	212.1	ng	1830180	1	6.86	172566	20.0
Butane, 2-methoxy...	1.28	6.5	ng	55852	1	6.86	172566	20.0
3-Penten-2-one, 4...	3.56	3.3	ng	28579	1	6.86	172566	20.0
2-Pentanone, 4-hy...	4.52	9.4	ng	81496	1	6.86	172566	20.0
unknown6.58	6.58	63.9	ng	551465	1	6.86	172566	20.0
3-Eicosene, (E)-	15.60	6.5	ng	127223	5	15.69	394747	20.0