Supporting Information

Acid-Catalyzed Reactions of 3-Hydroxy-2-oxindoles with Electron-rich Substrates: Synthesis of 2-Oxindoles with All-Carbon Quaternary Center

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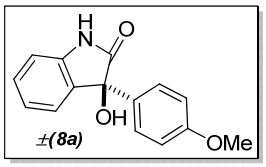
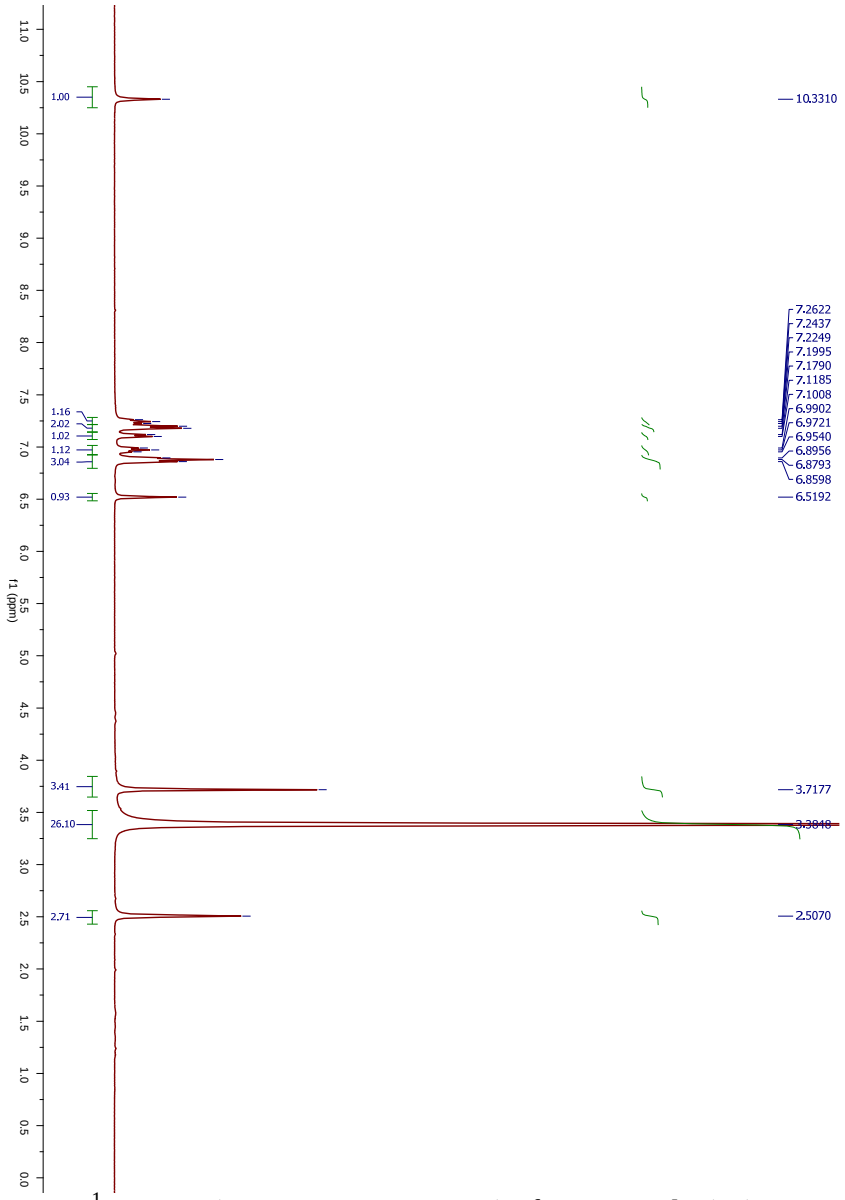
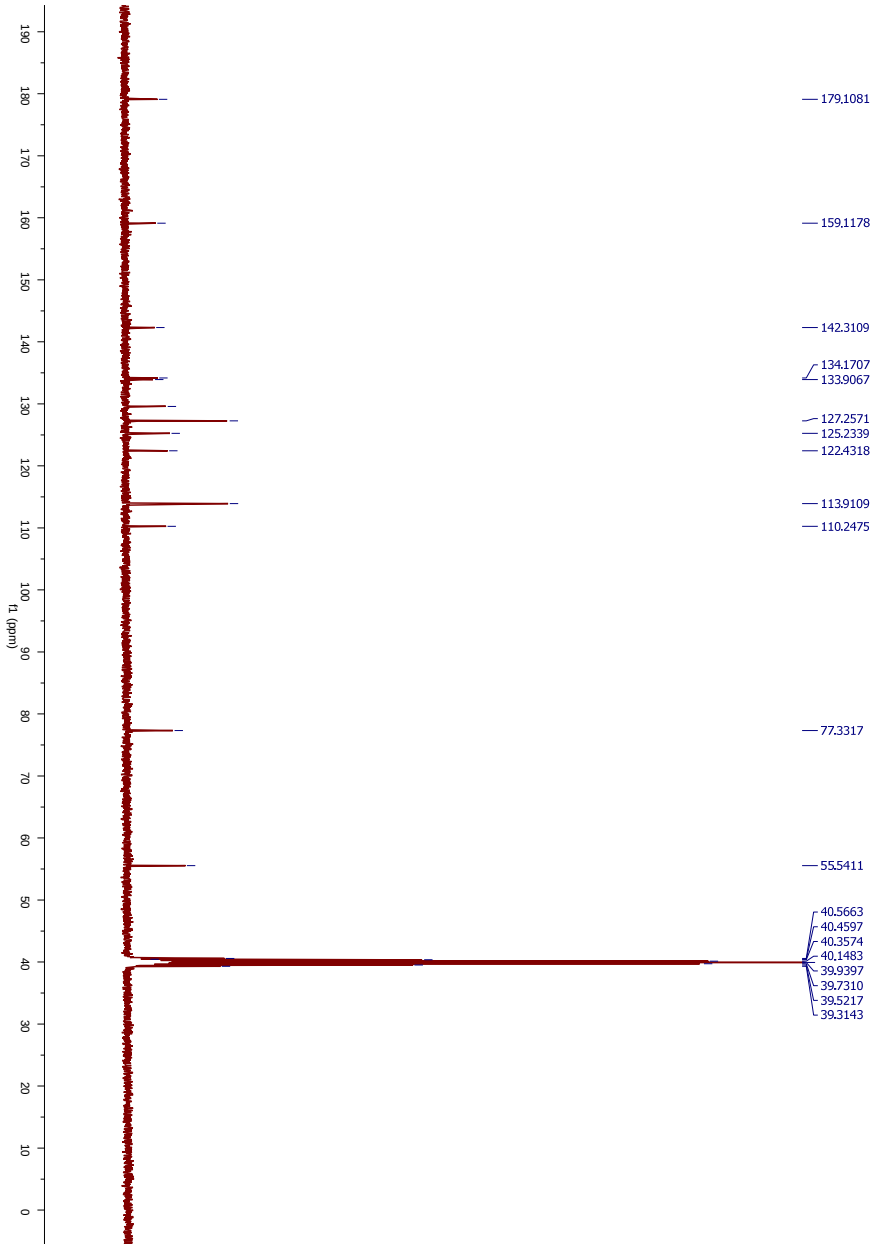
^{1}H-NMR, ^{13}C-NMR, and Scanned copies of Mass spectrum

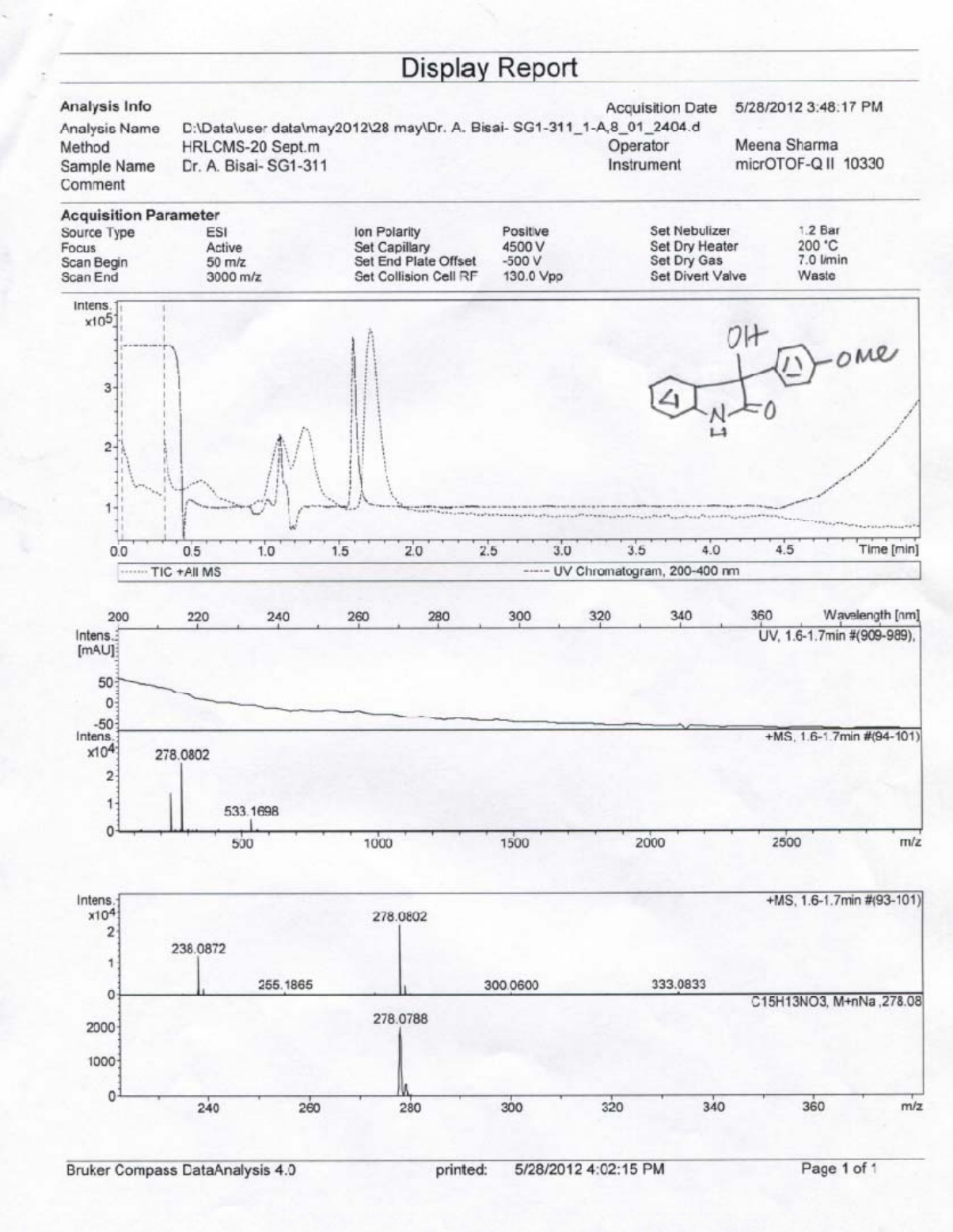




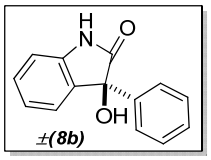
^{1}H NMR (400 MHz, DMSO-D_6,) of compound ±(**8a**)

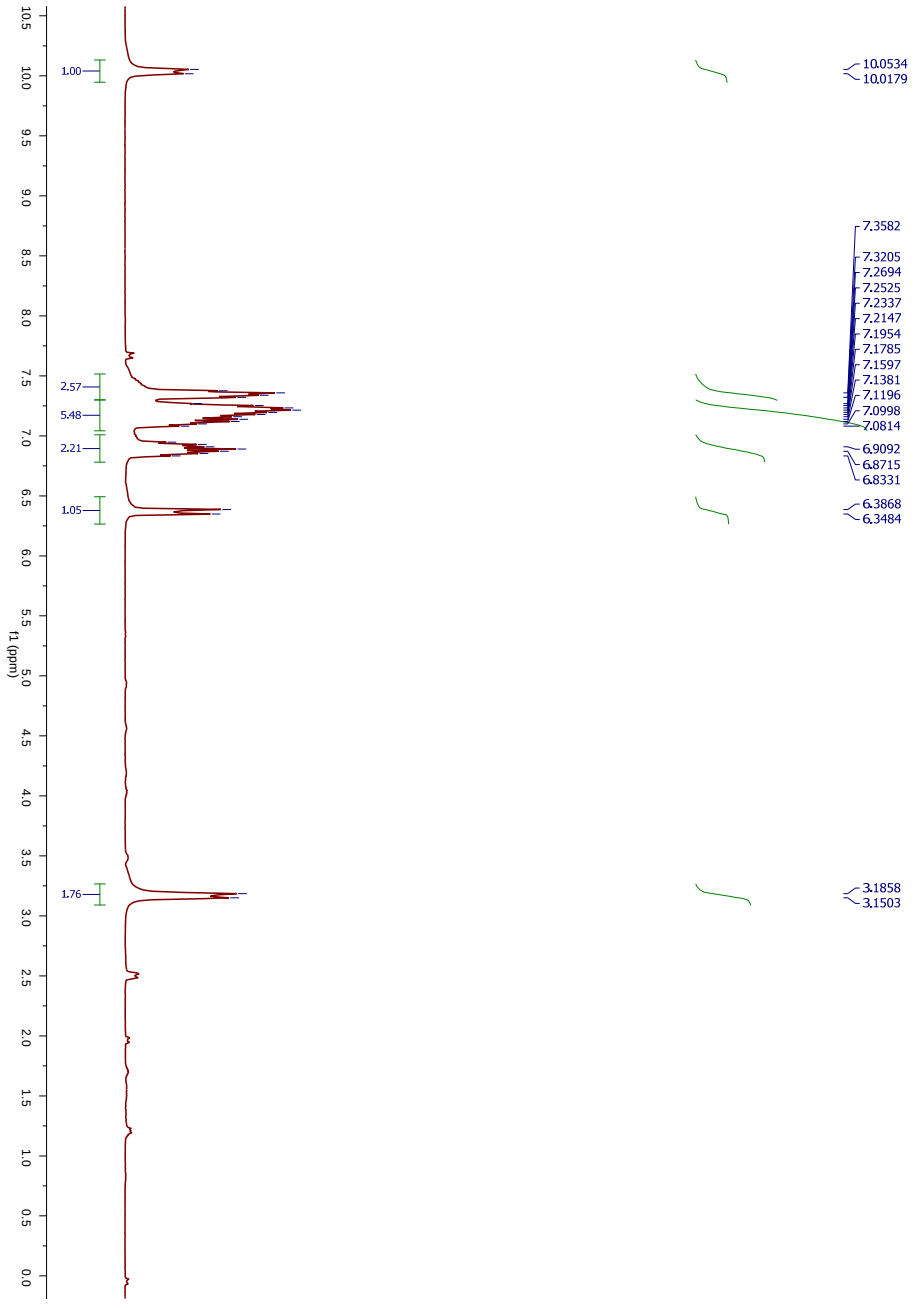


^{13}C NMR (100 MHz, DMSO-D_6,) of compound ±(**8a**)

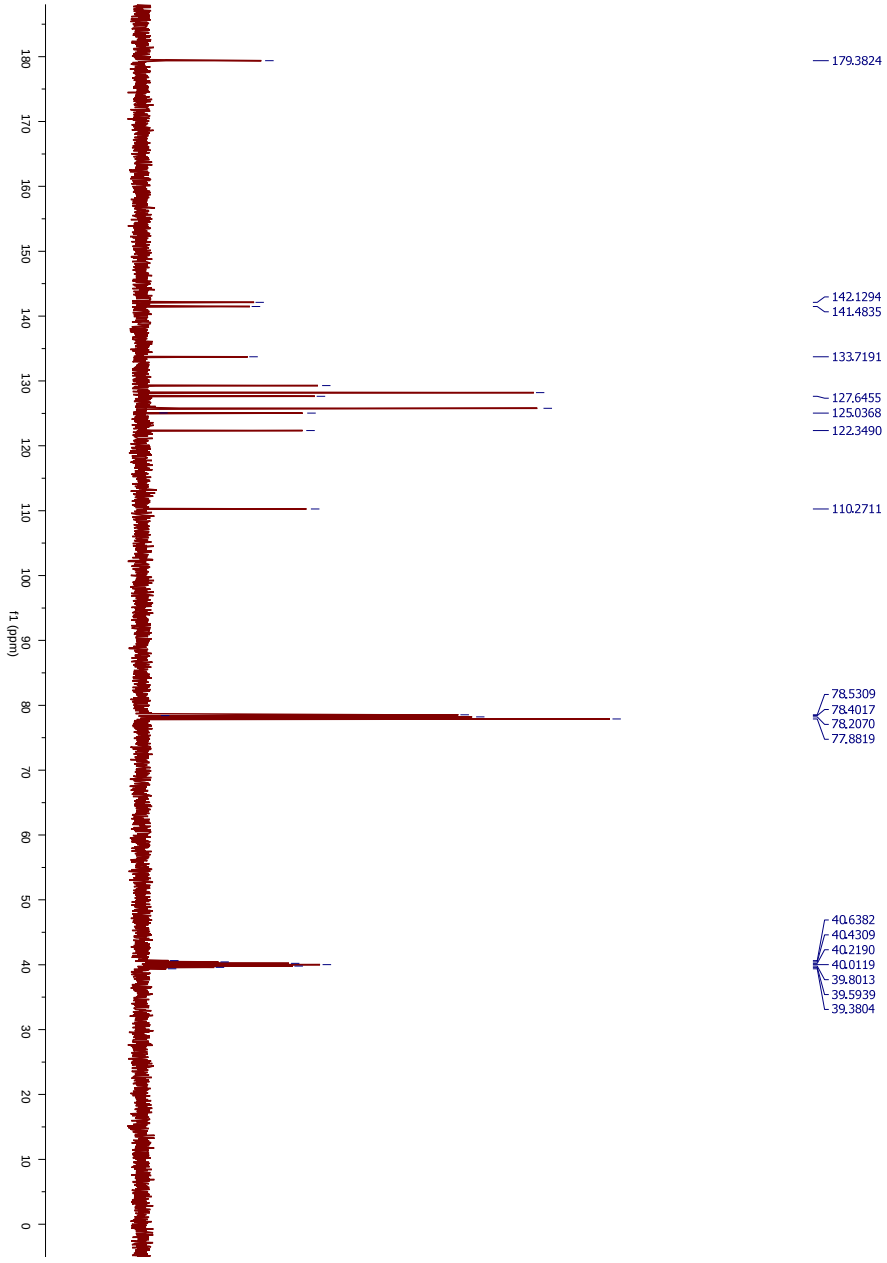


Scanned copy of mass spectrum (HRMS) of ±(**8a**)





^{1}H NMR (400 MHz, 0.1ml of DMSO-D_6, 0.5ml of $CDCl_3$) of compound ±(**8b**)



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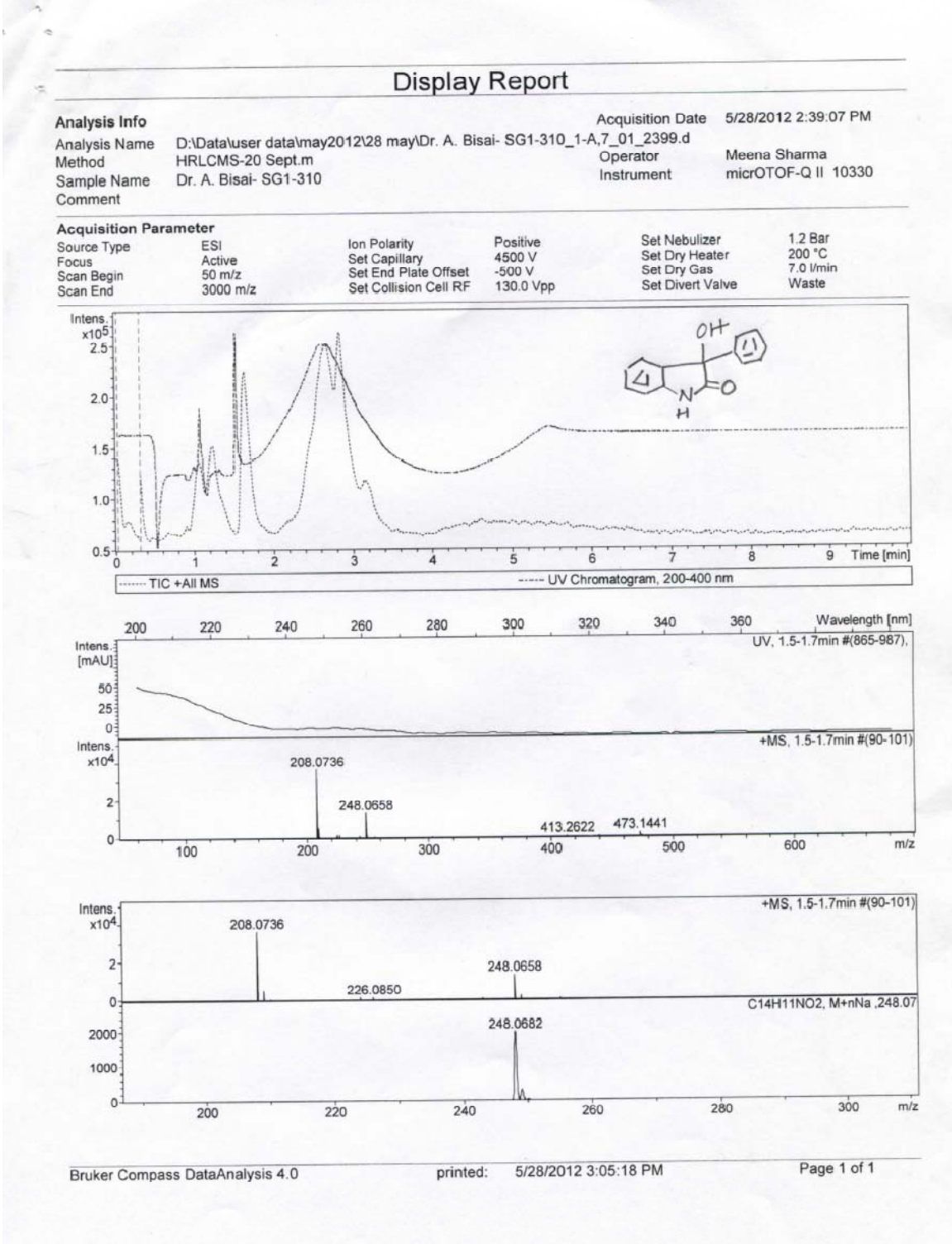
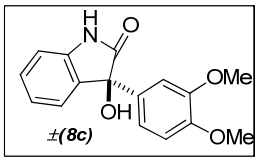
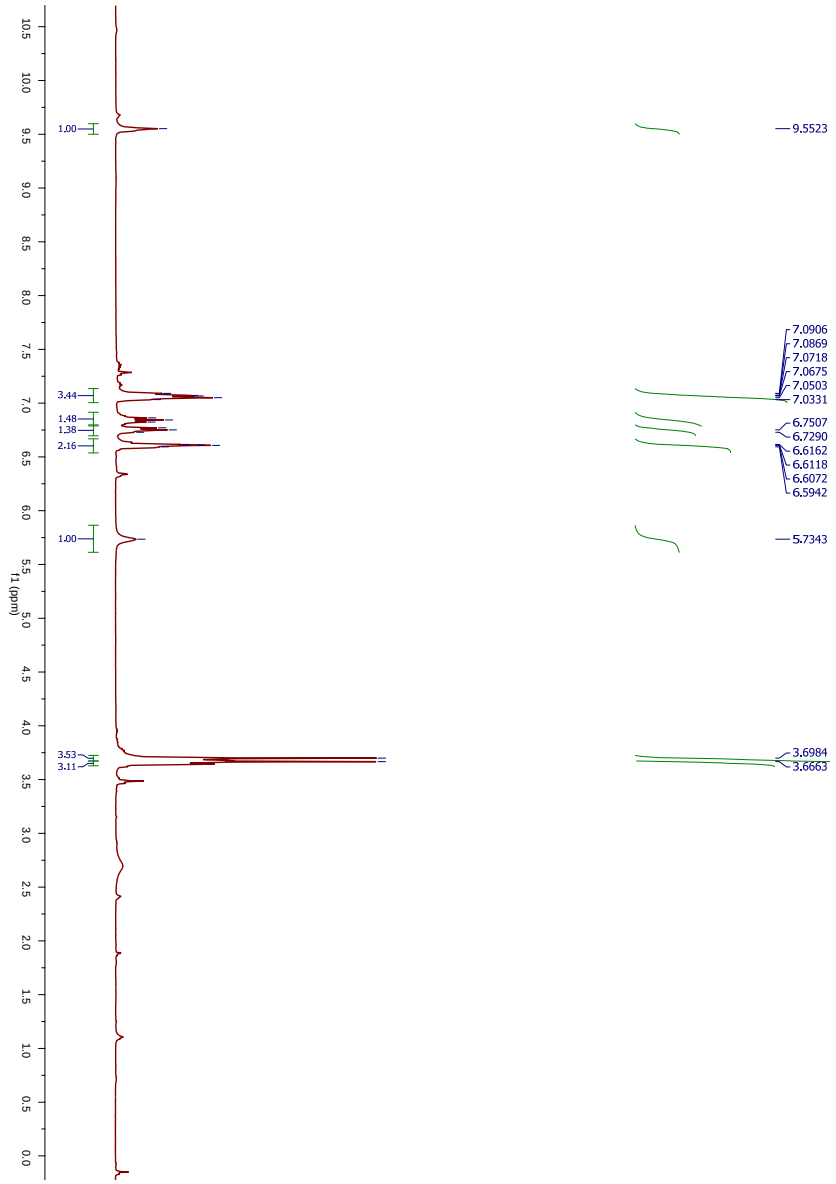
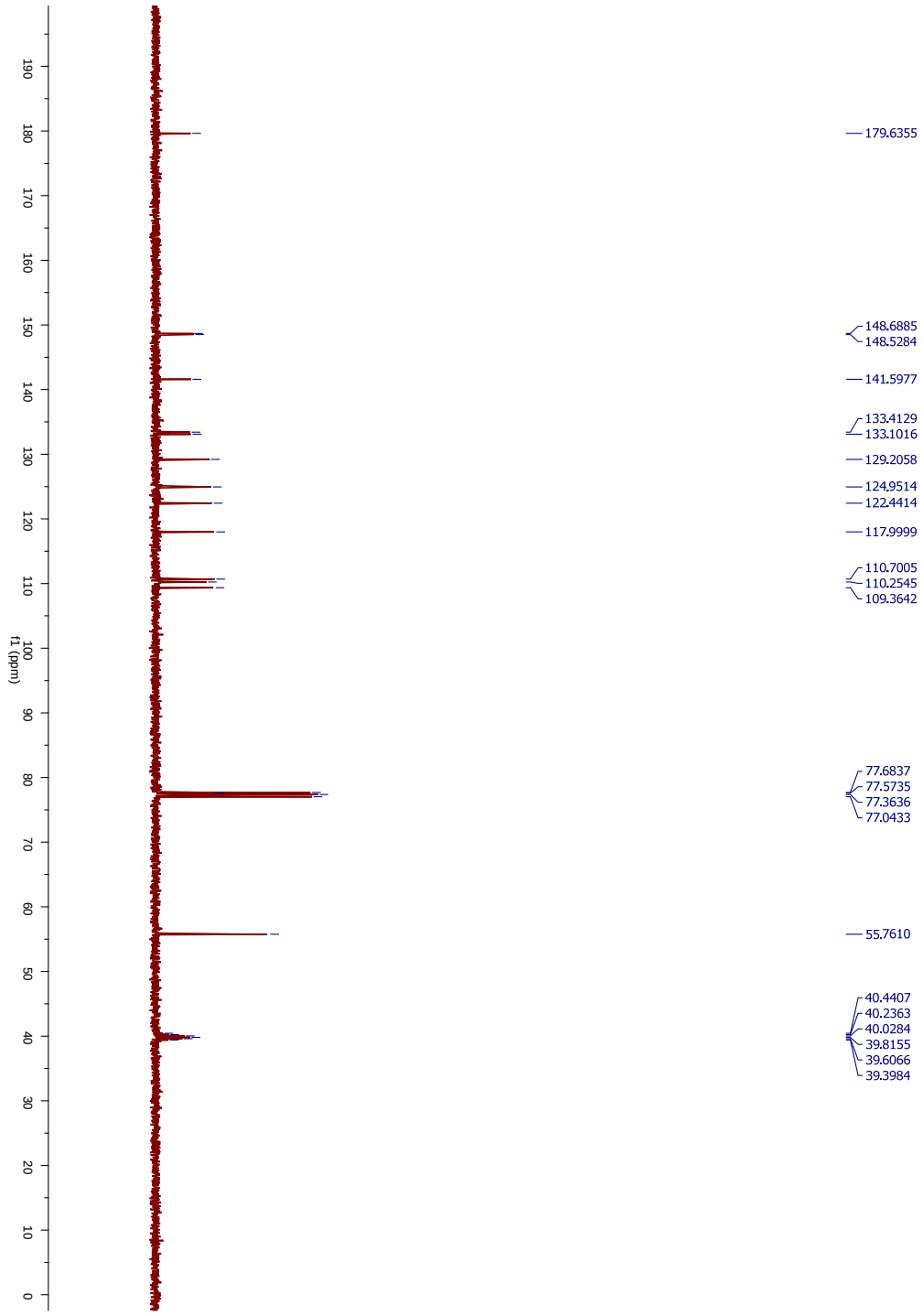


Scanned copy of mass spectrum of compound ±(**8b**)





^{1}H NMR (400 MHz, 0.1ml of DMSO-D_6, 0.5ml of $CDCl_3$) of compound ±(**8c**)



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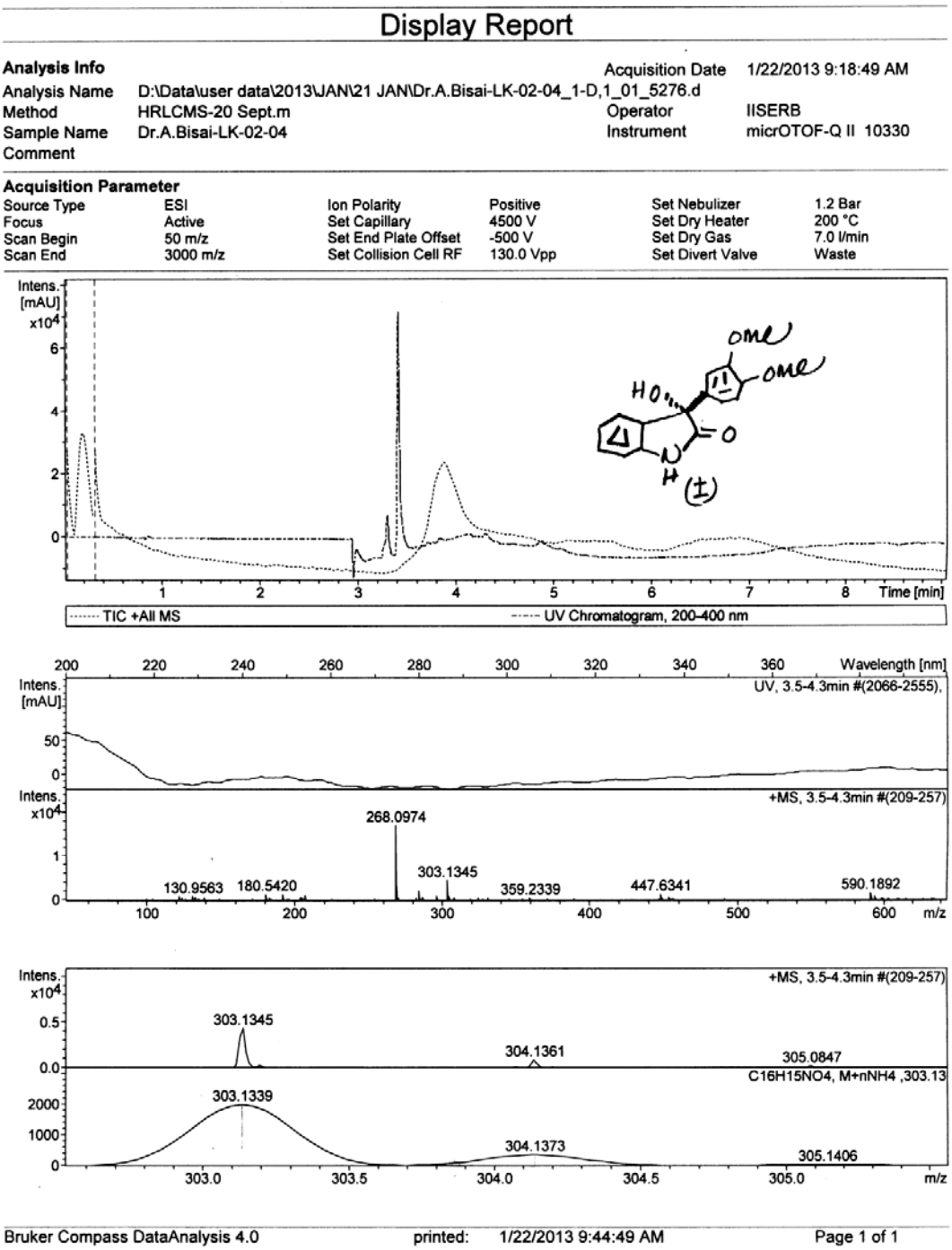

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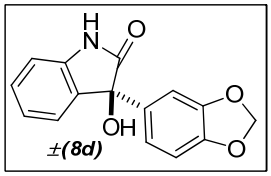
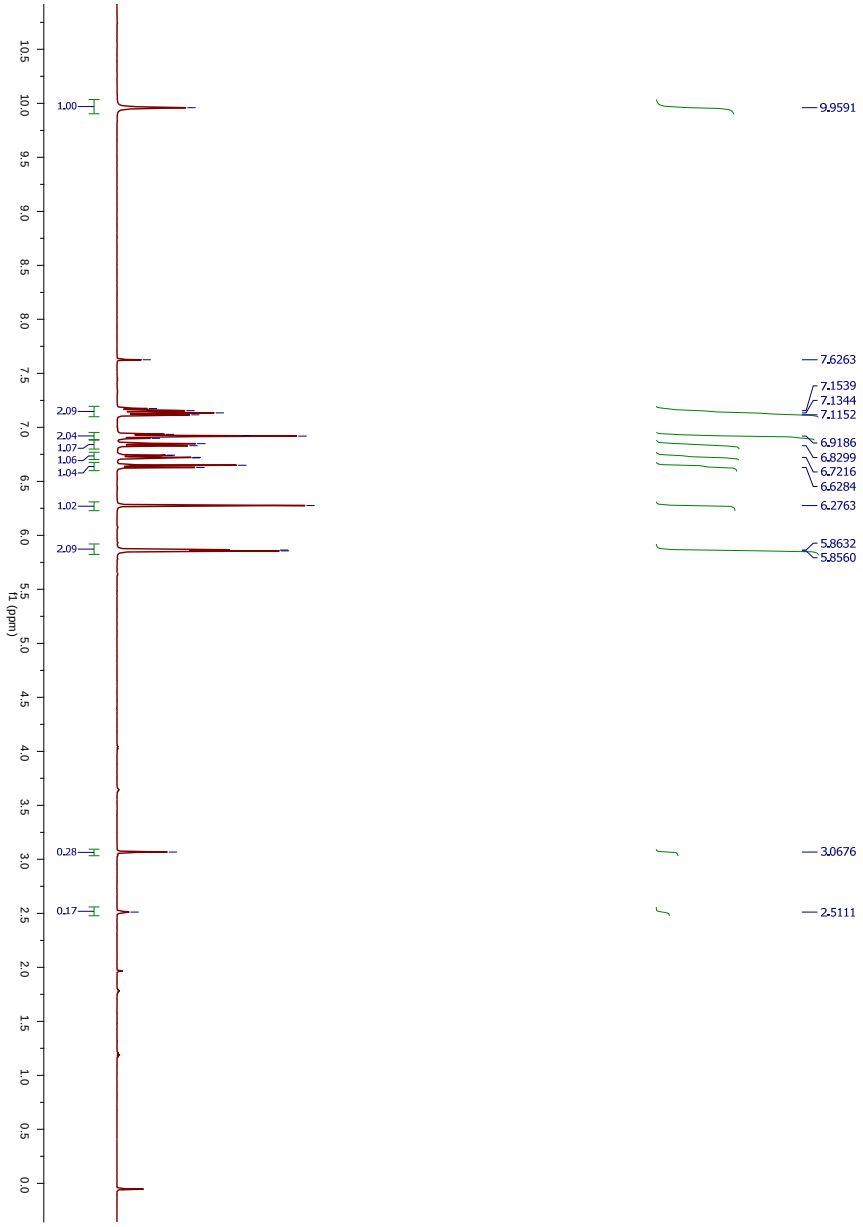
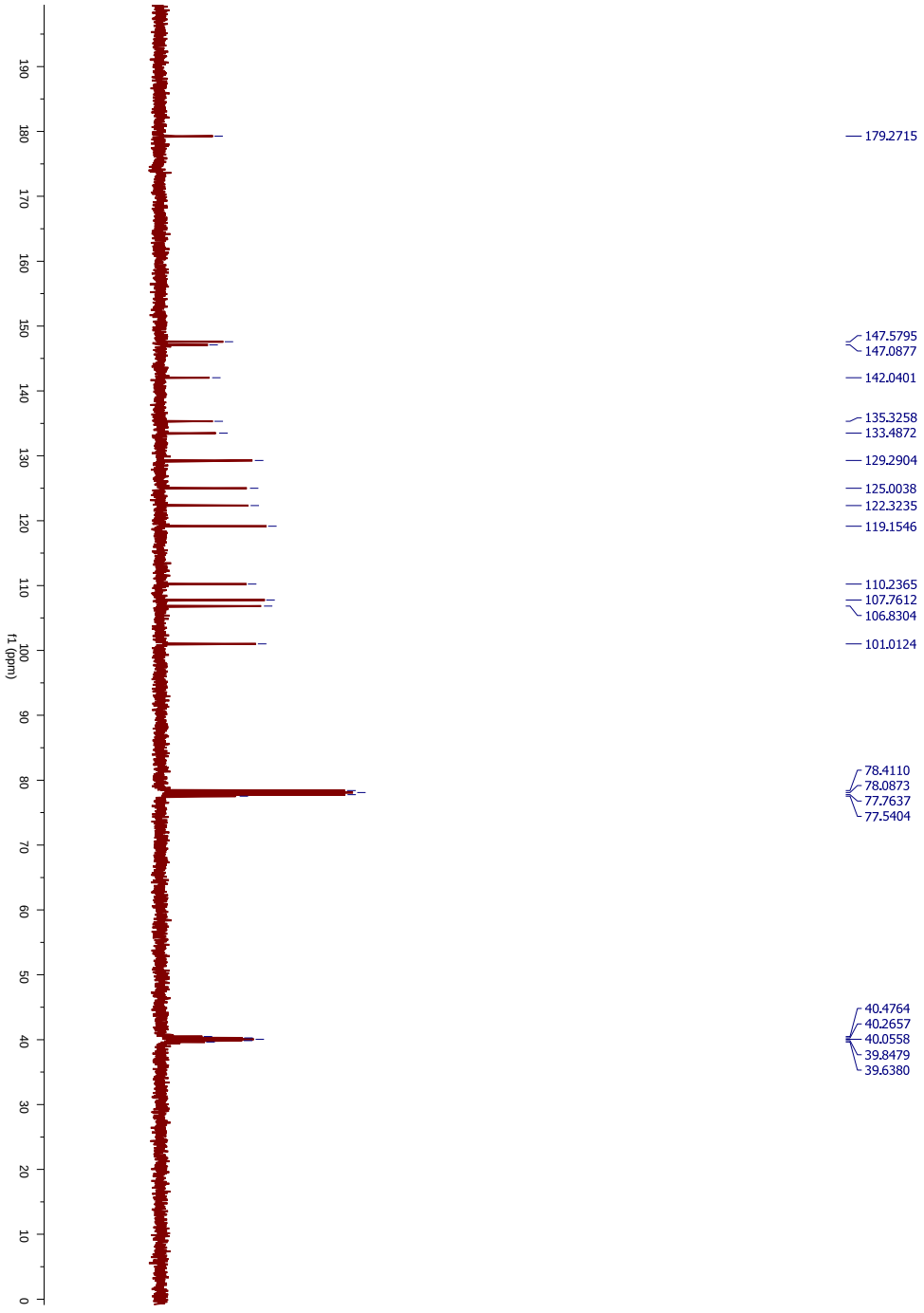




^{1}H NMR (400 MHz, 0.1ml of DMSO-D_6, 0.5ml of $CDCl_3$) of compound ±(**8d**)



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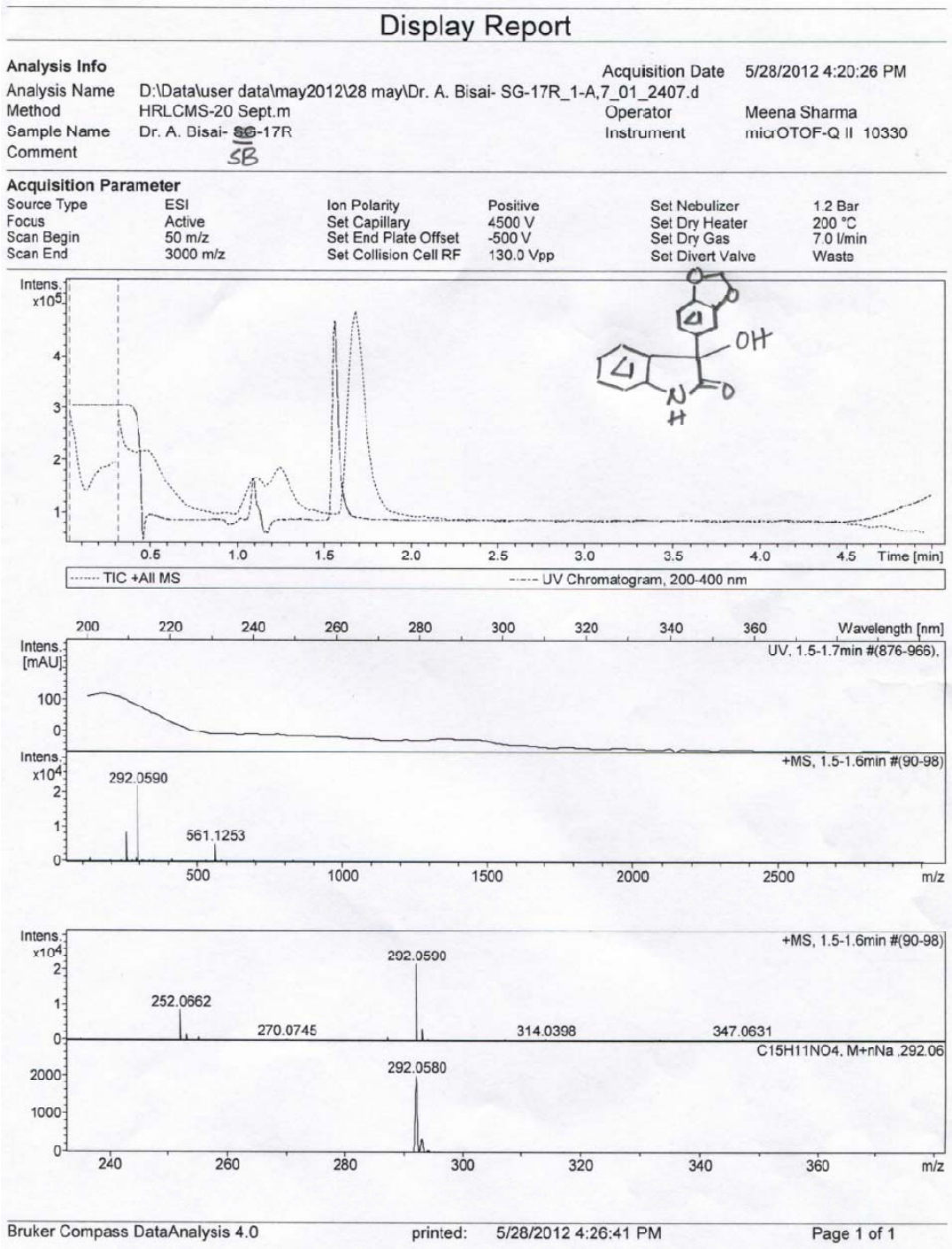

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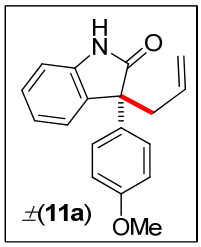
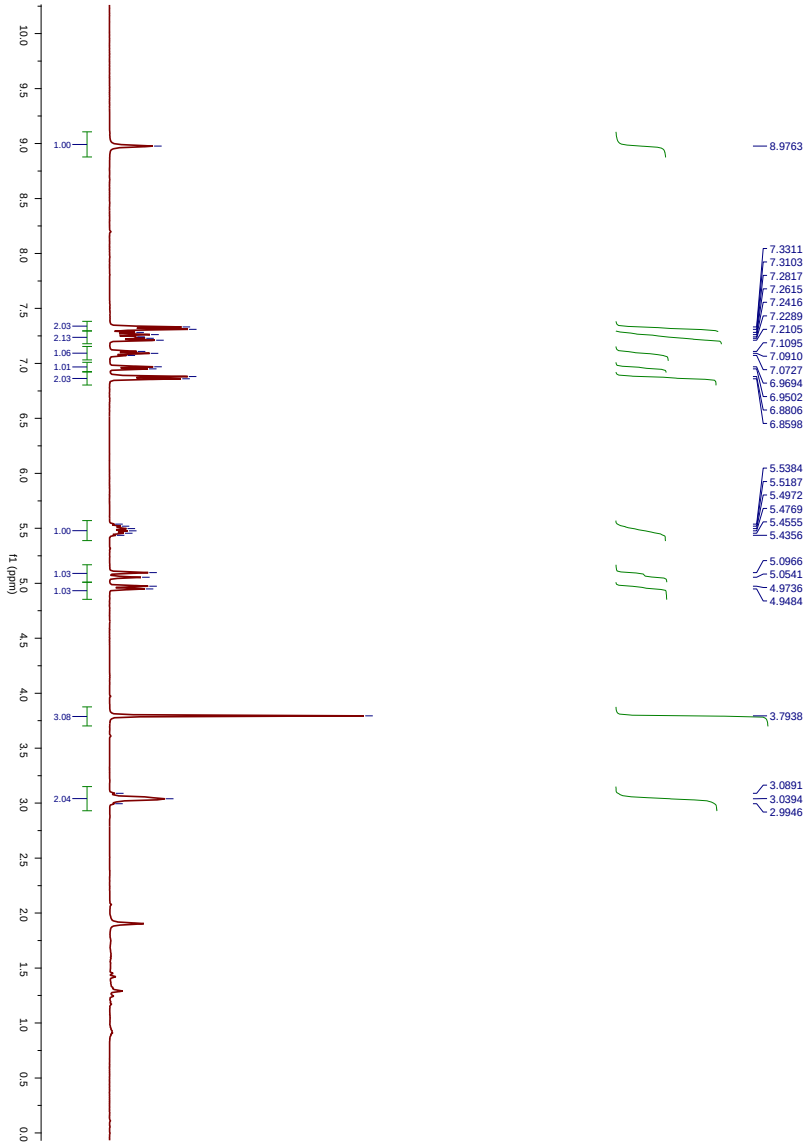
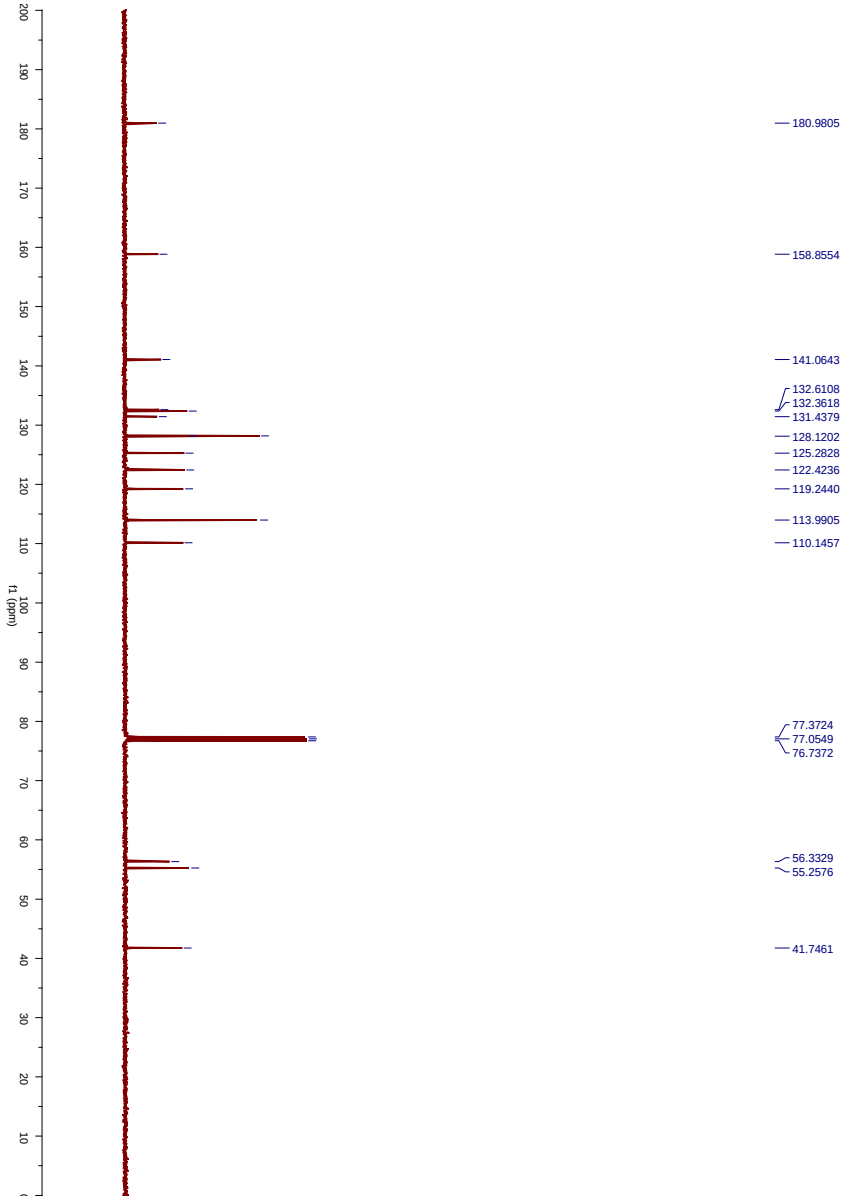




^{1}H NMR (400 MHz, $CDCl_3$) of compound ±(**11a**)



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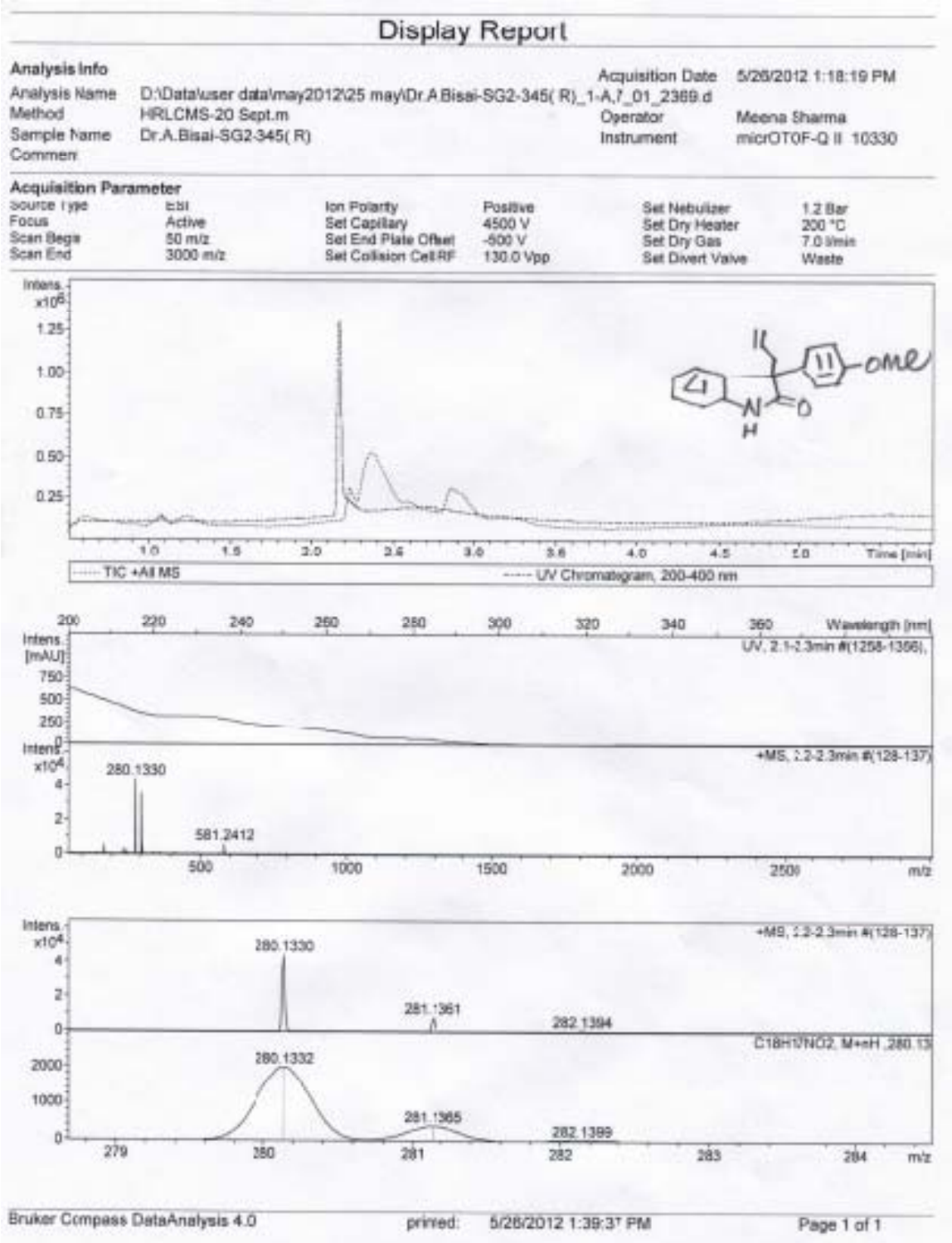
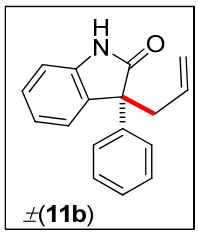
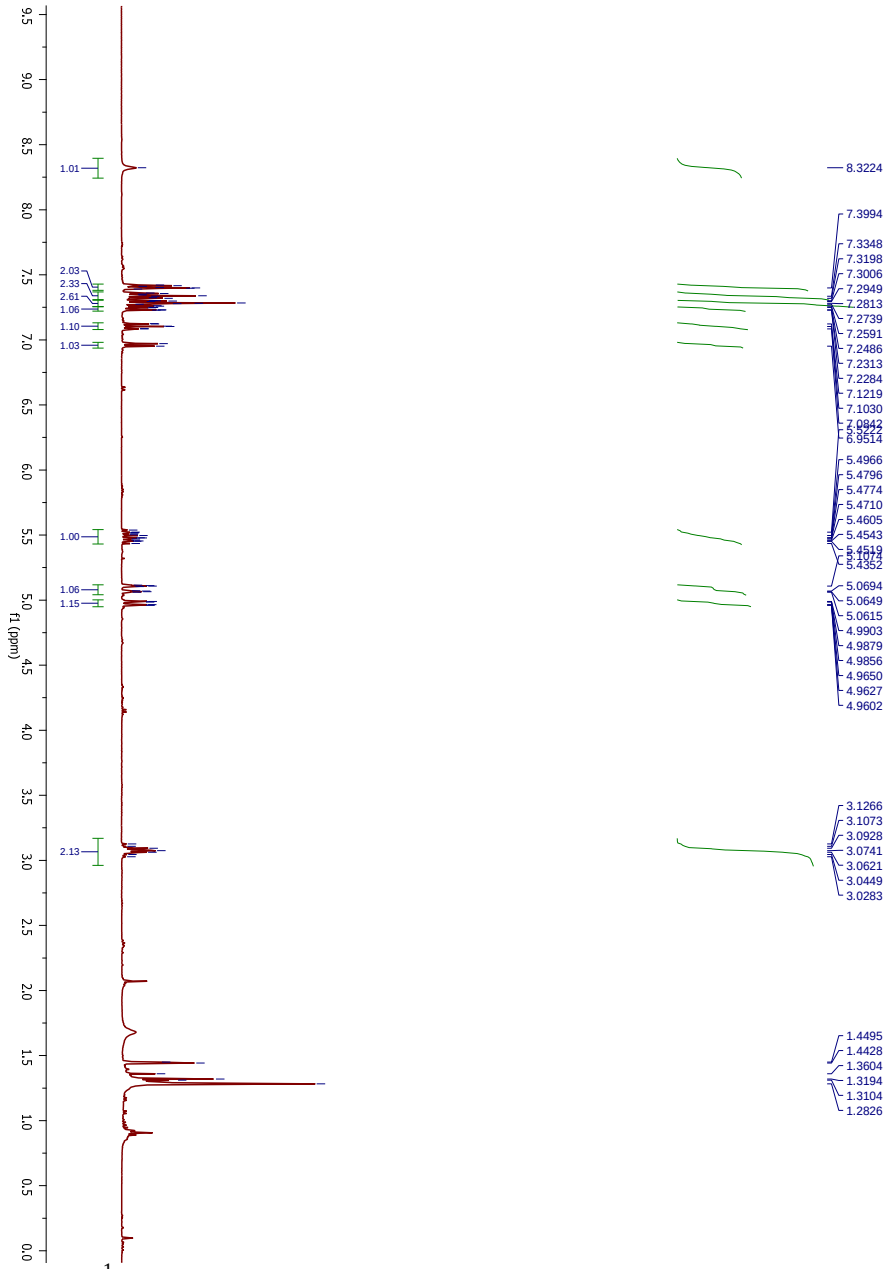


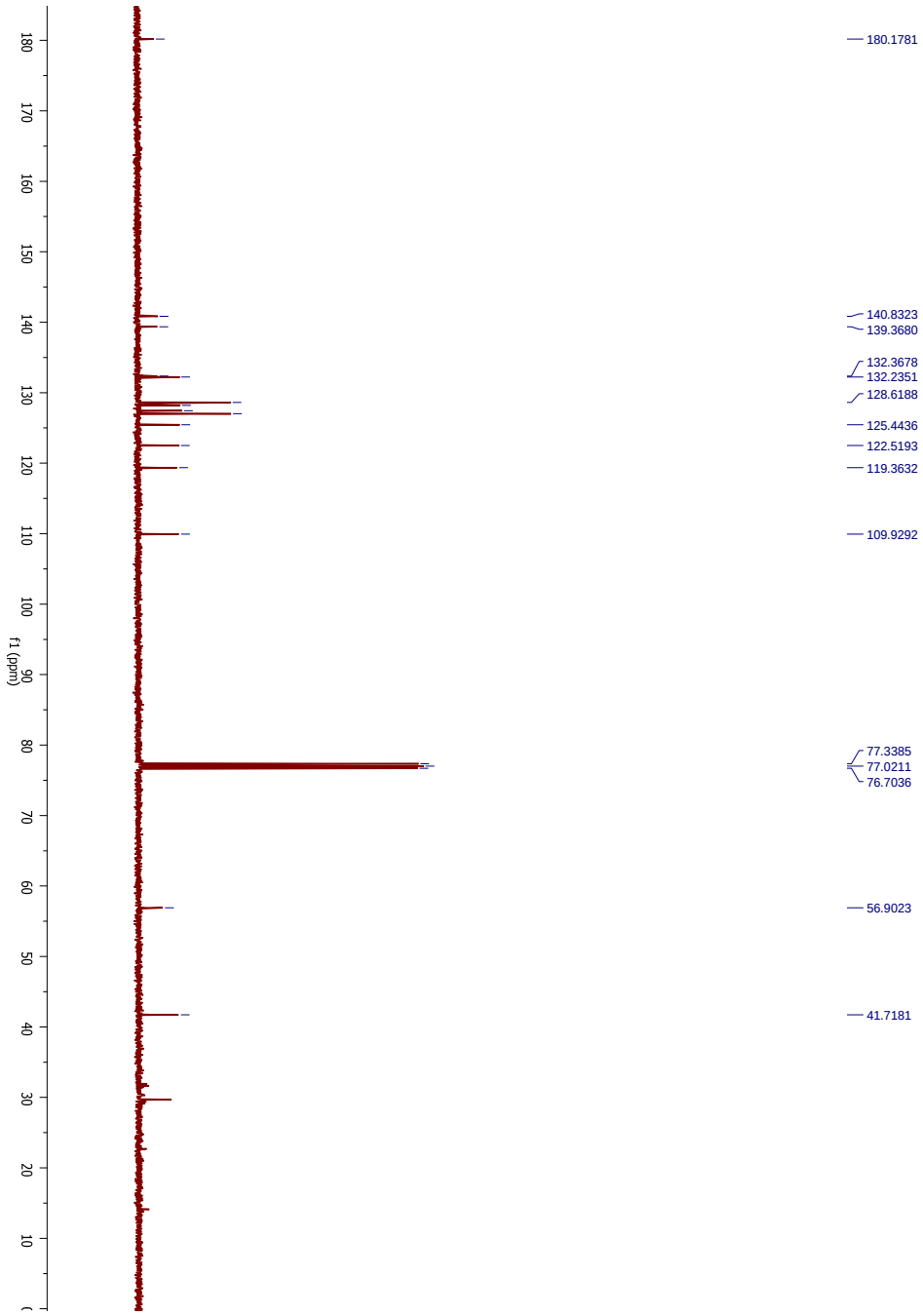
Scanned copy of mass spectrum of compound ±(**11a**)



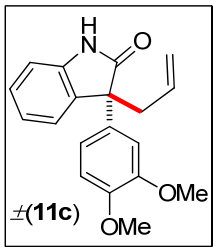
±(**11b**)



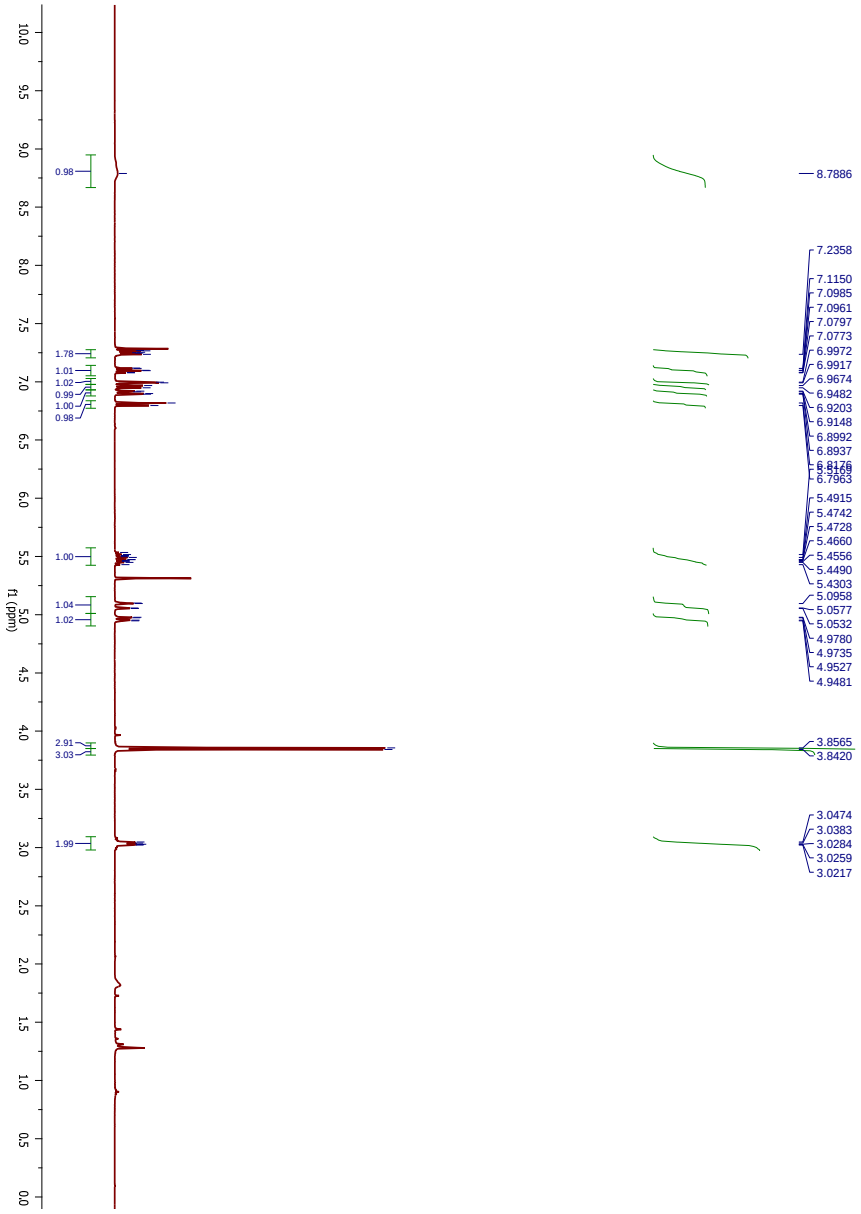
^{1}H NMR **(**400 MHz, $CDCl_3$) of compound ±(**11b**)



^{13}C NMR **(**100 MHz, $CDCl_3$) of compound ±(**11b**)



±(**11c**)



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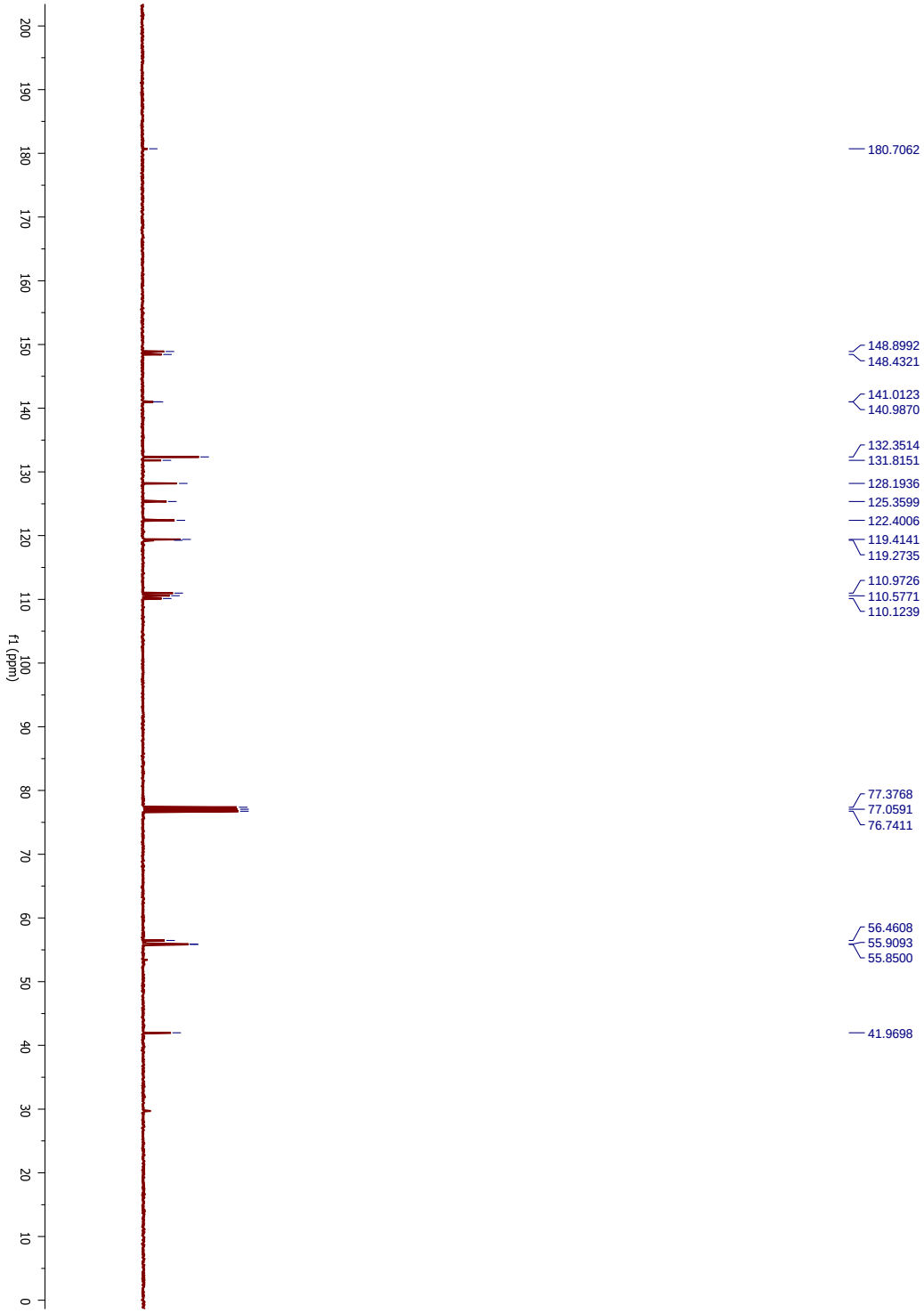

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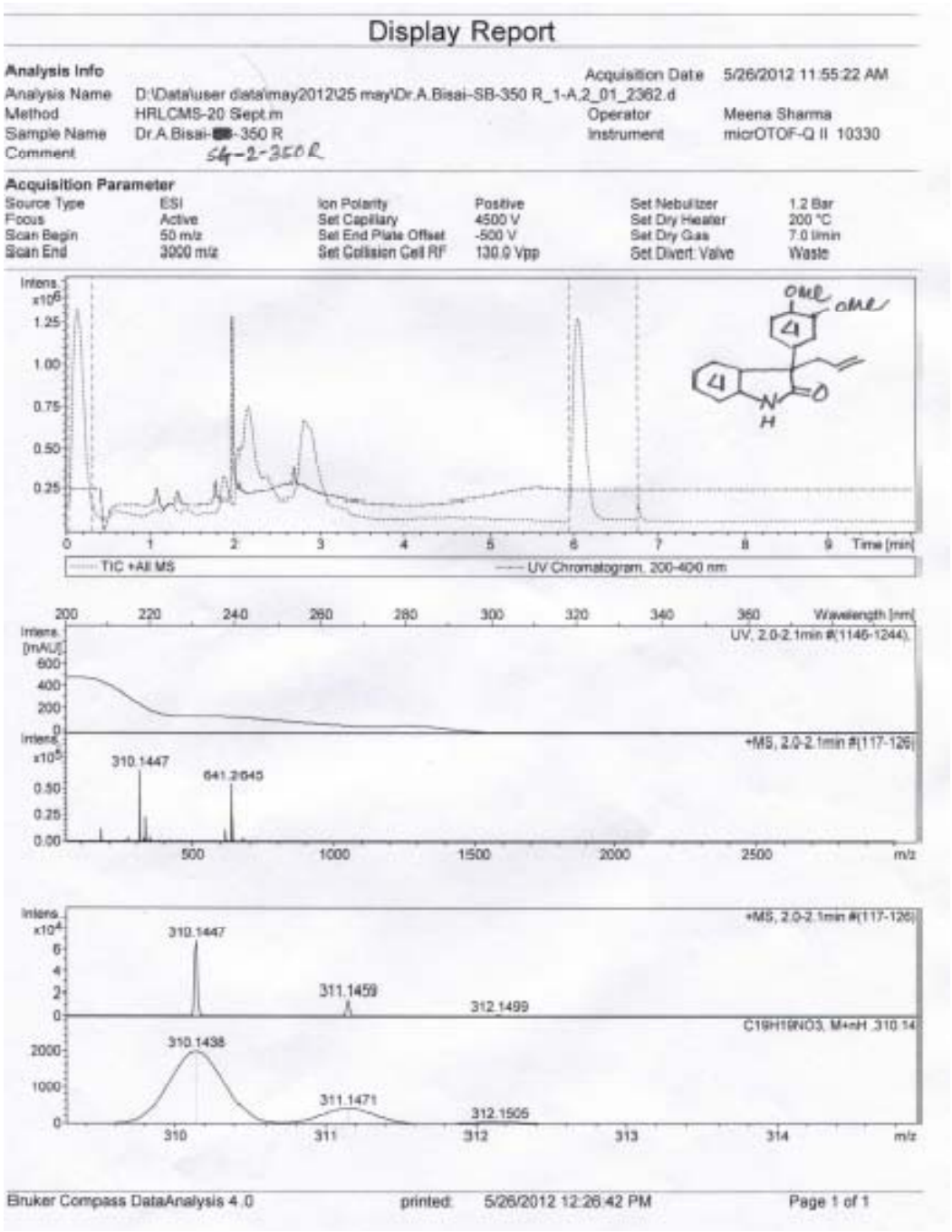
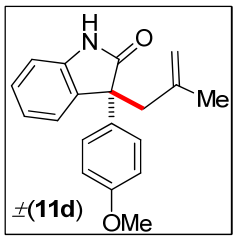
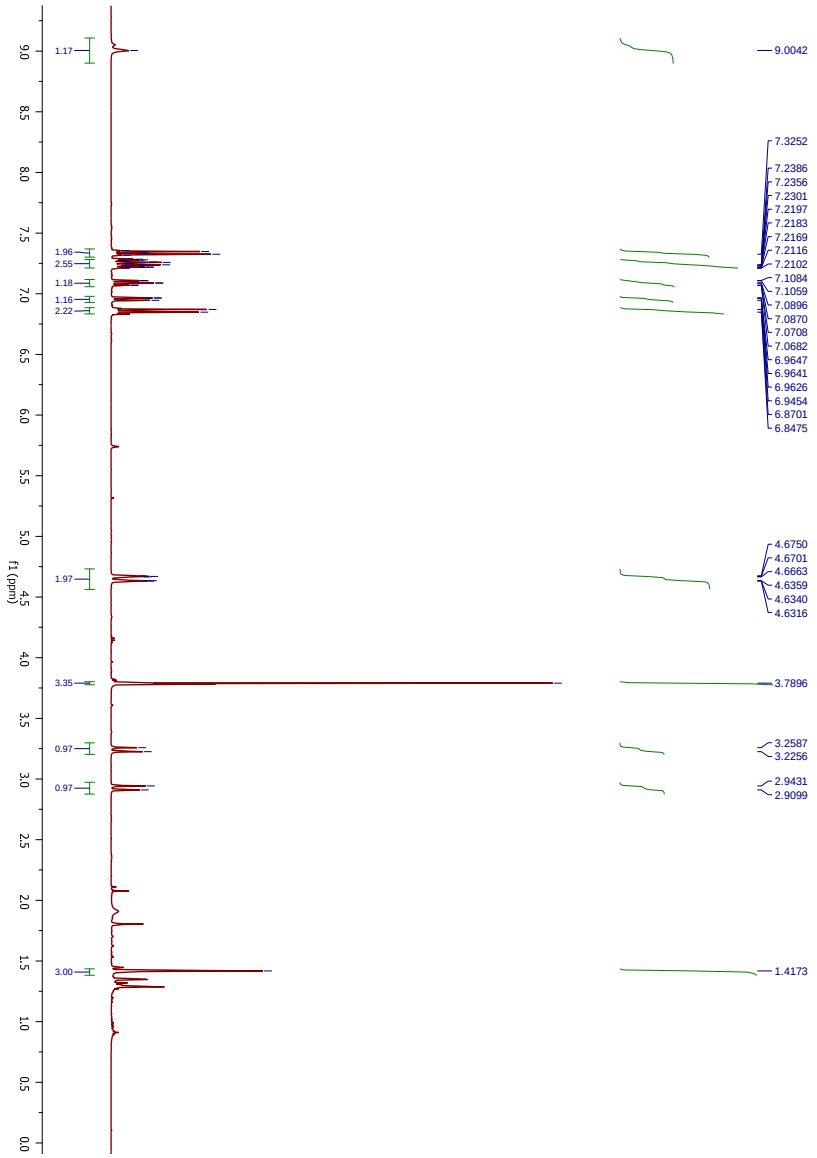
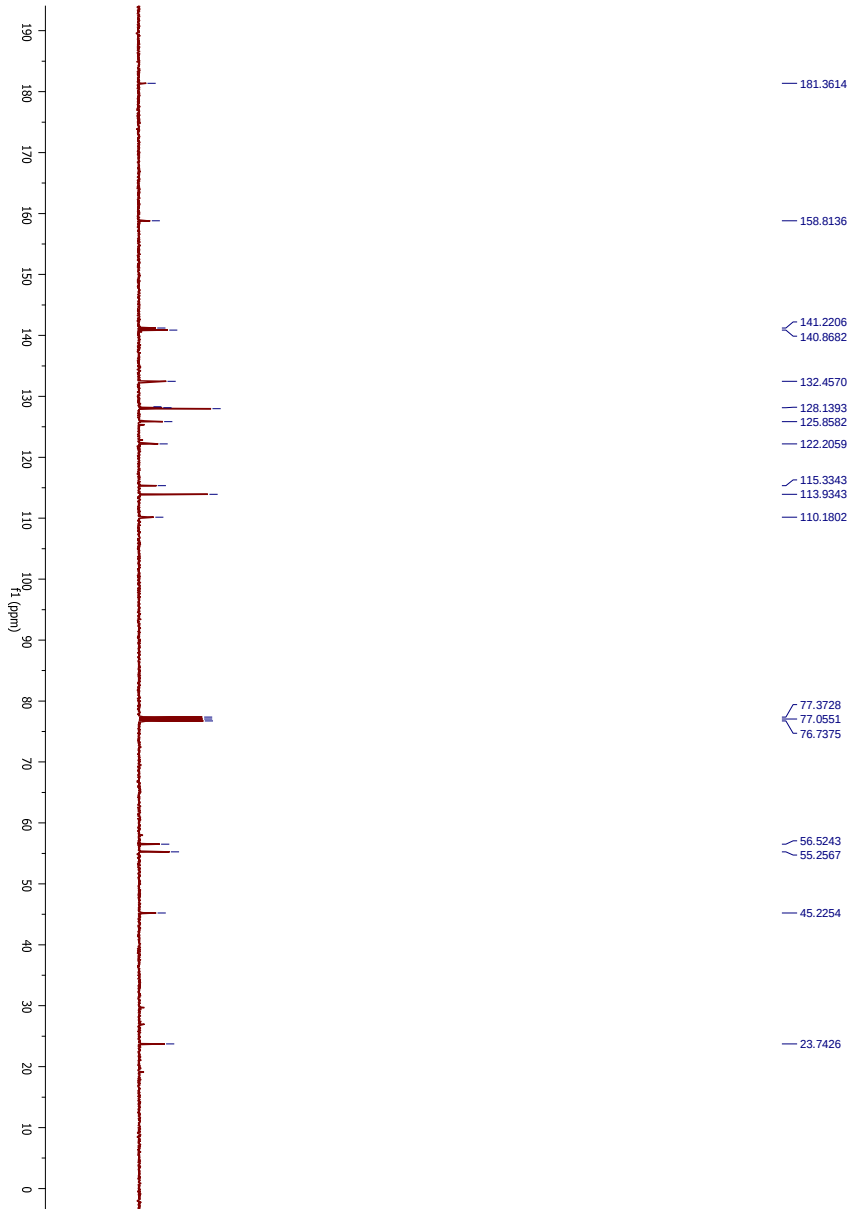


Scanned copy of mass spectrum of compound ±(**11c**)





^{1}H NMR **(**400 MHz, $CDCl_3$) of compound ±(**11d**)



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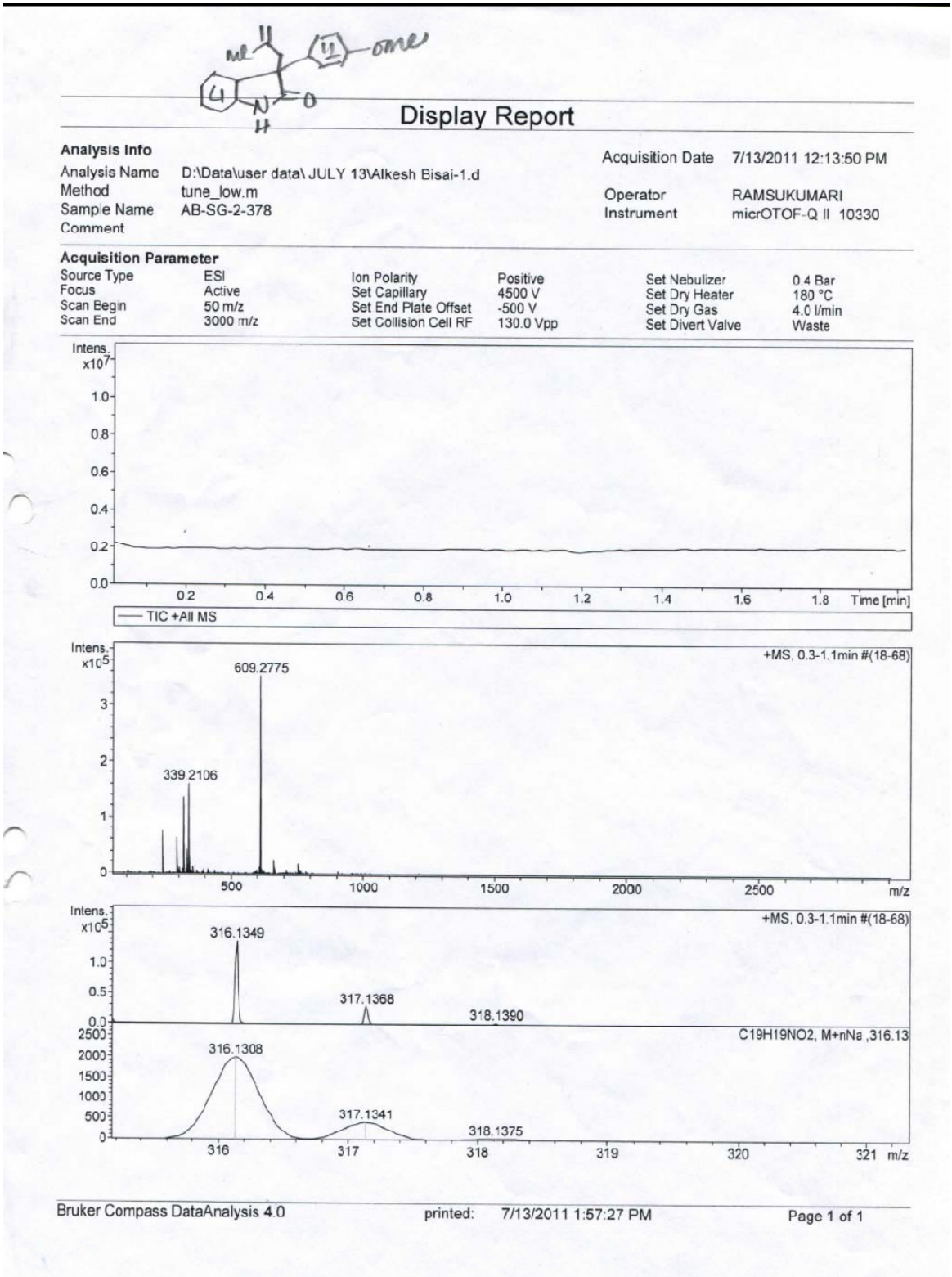
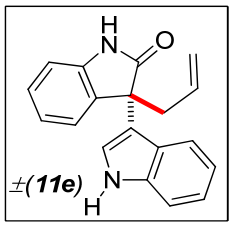
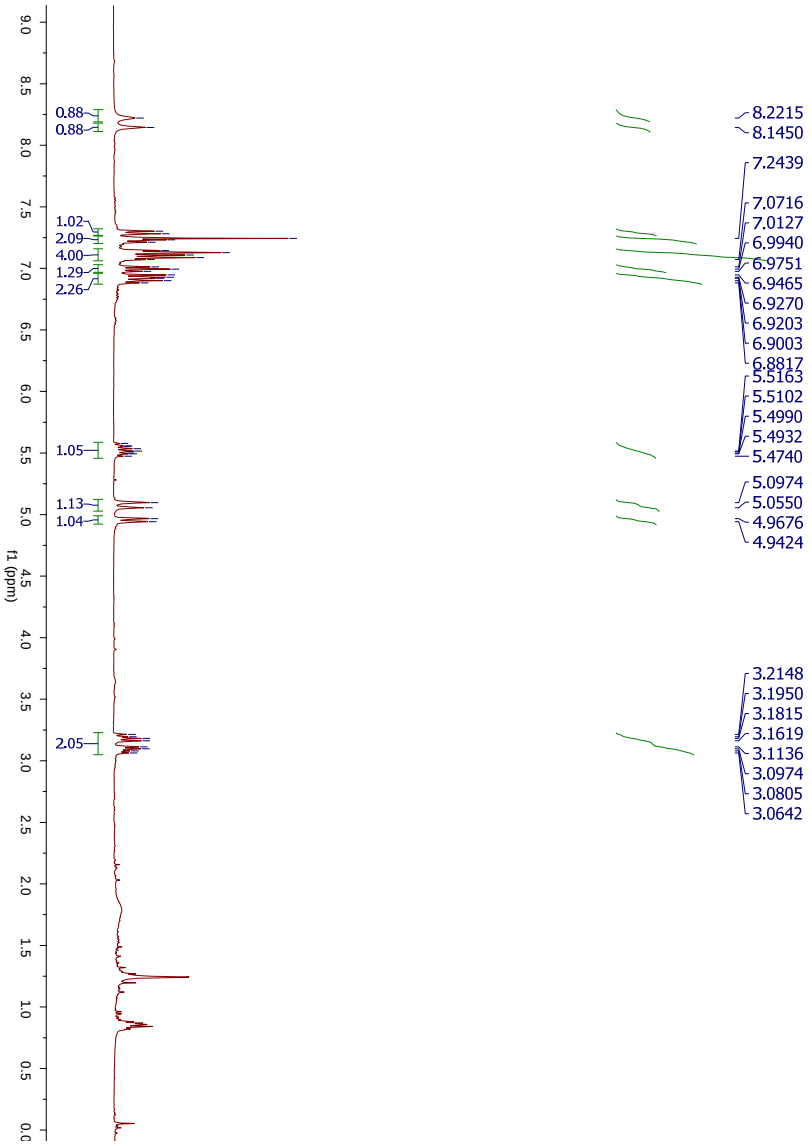
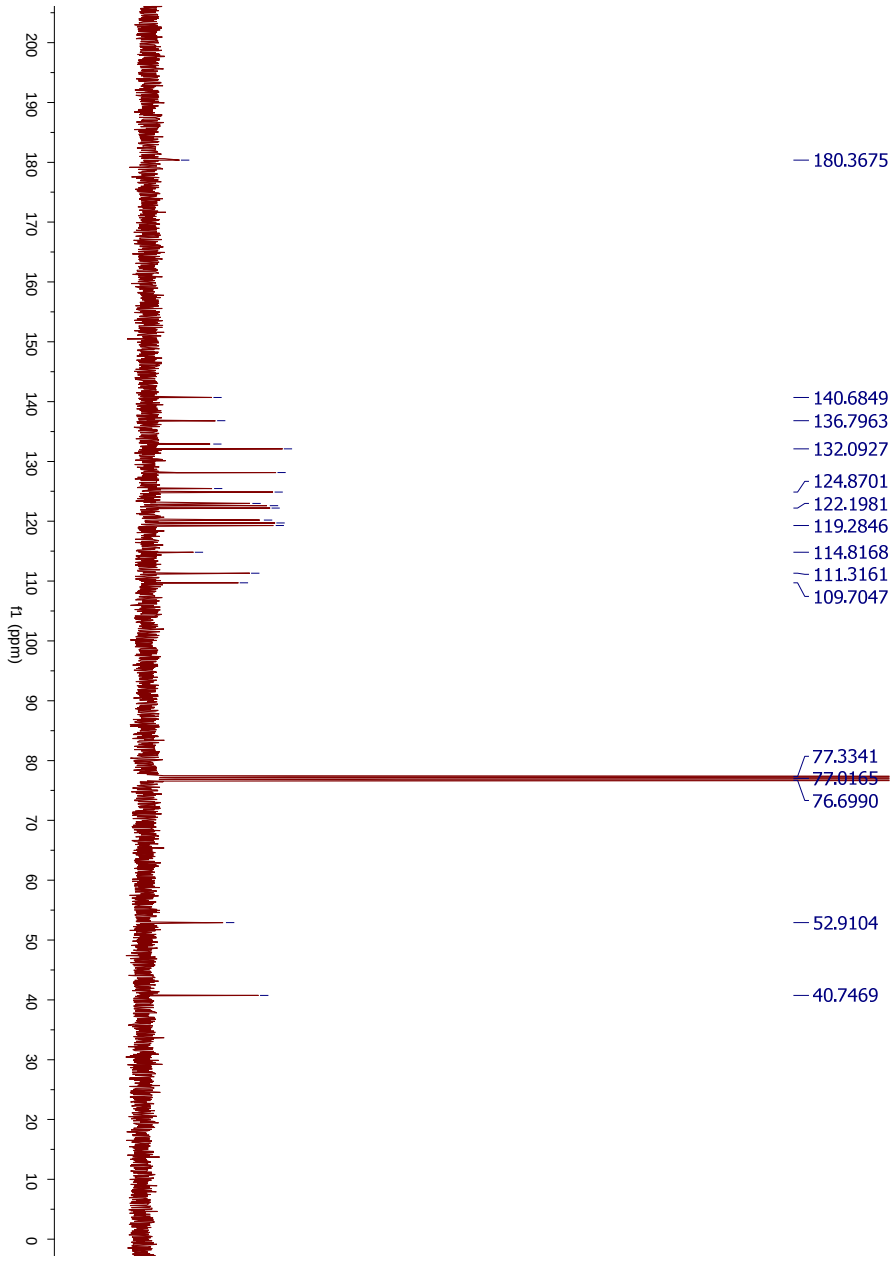


Scanned copy of mass spectrum (HRMS) of ±(**11d**)





^{1}H NMR (400 MHz, $CDCl_3$) of compound ±(**11e**)



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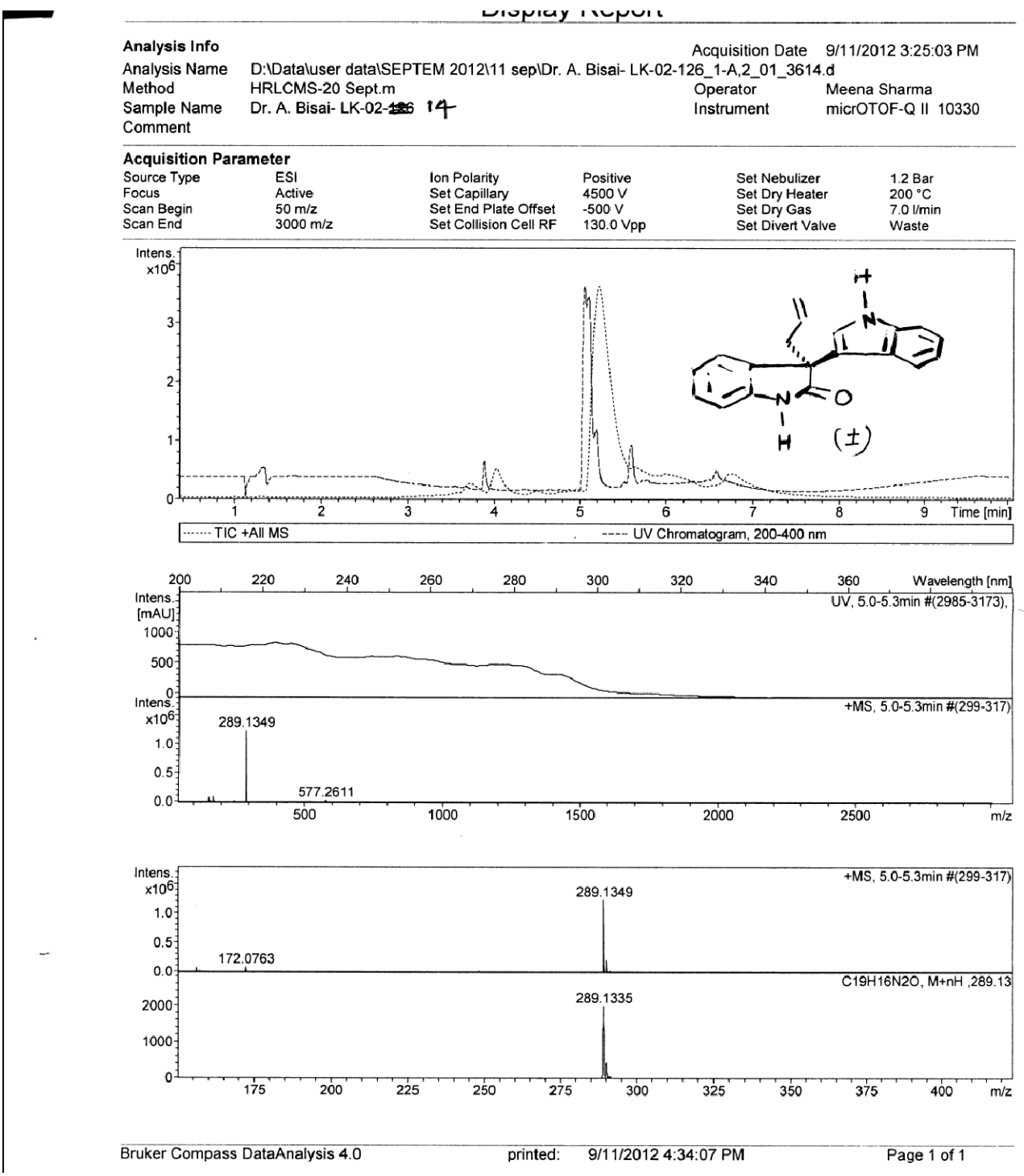
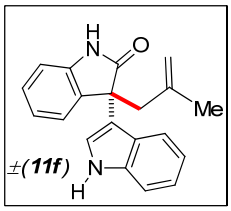
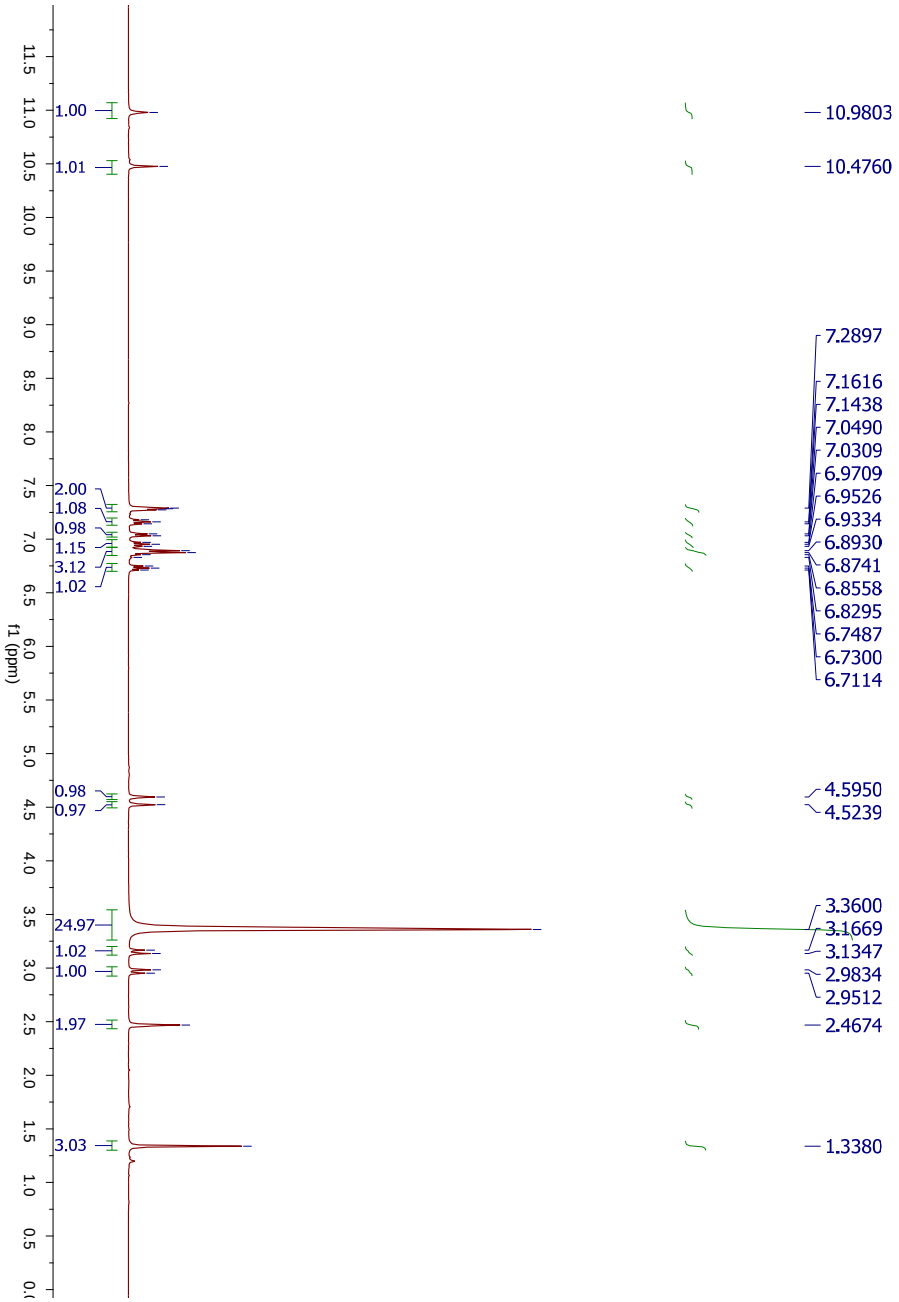
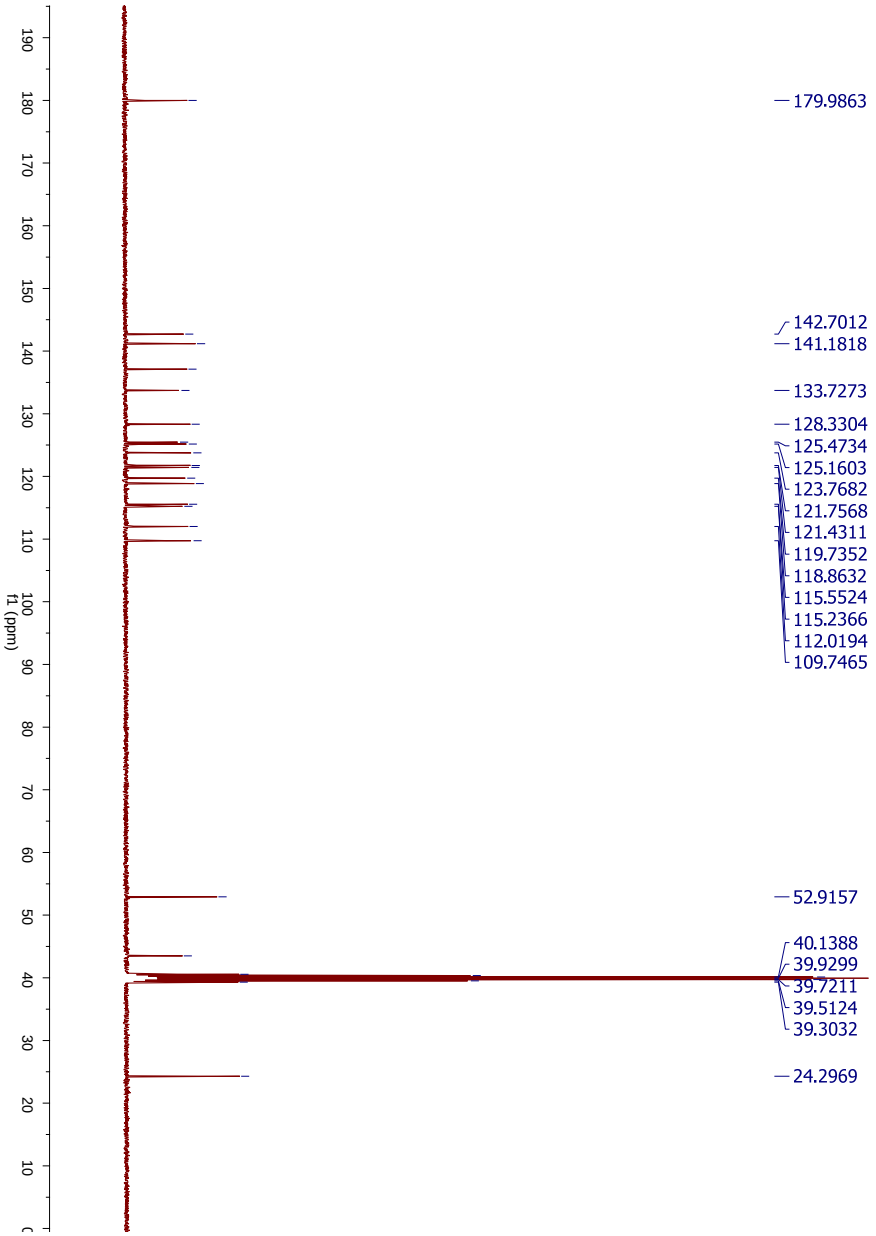


Scanned copy of mass spectrum of compound ±(**11e**)

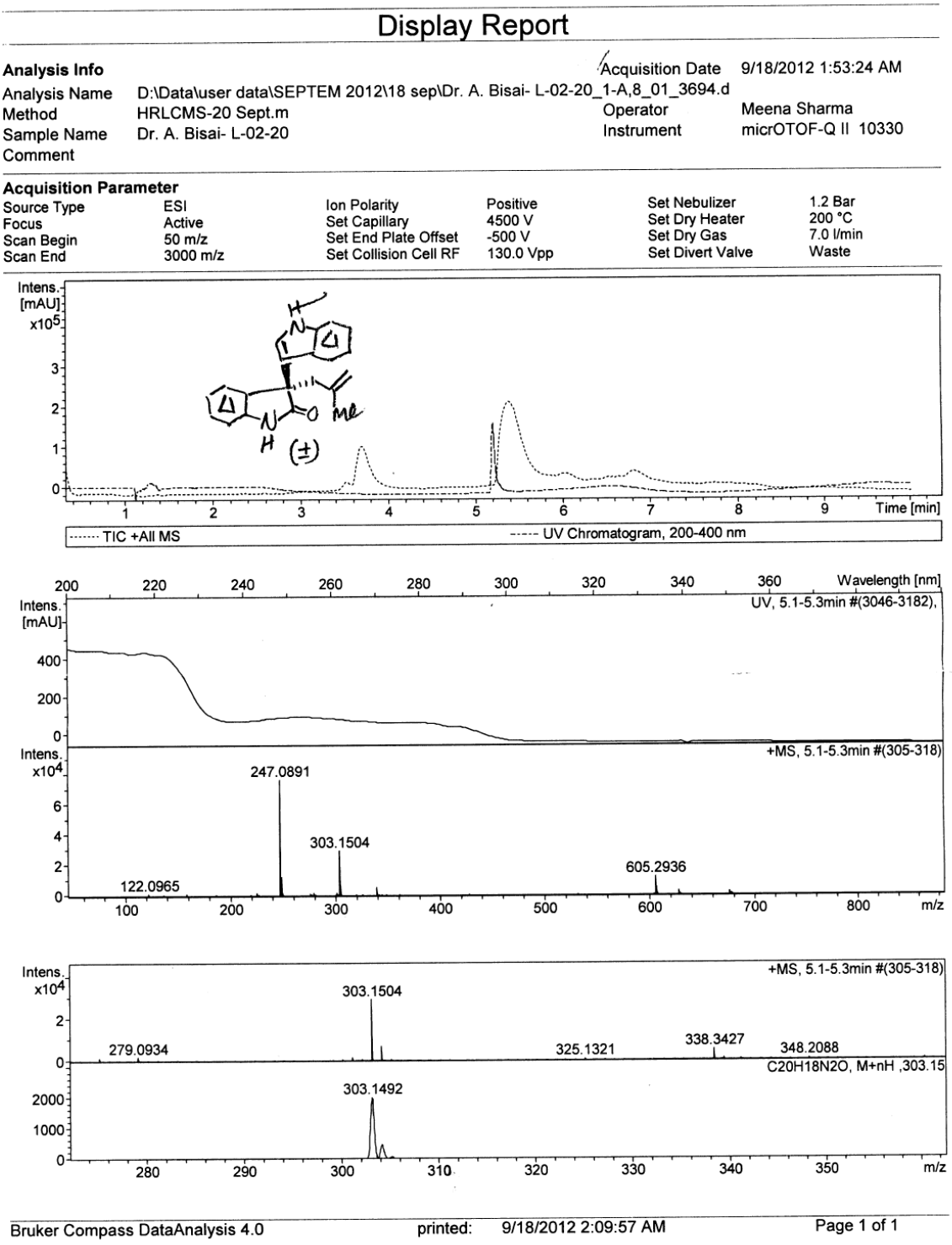




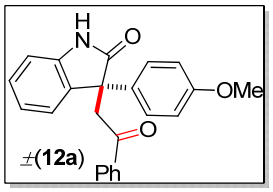
^{1}H NMR (400 MHz, DMSO-D6) of compound ±(**11f**)

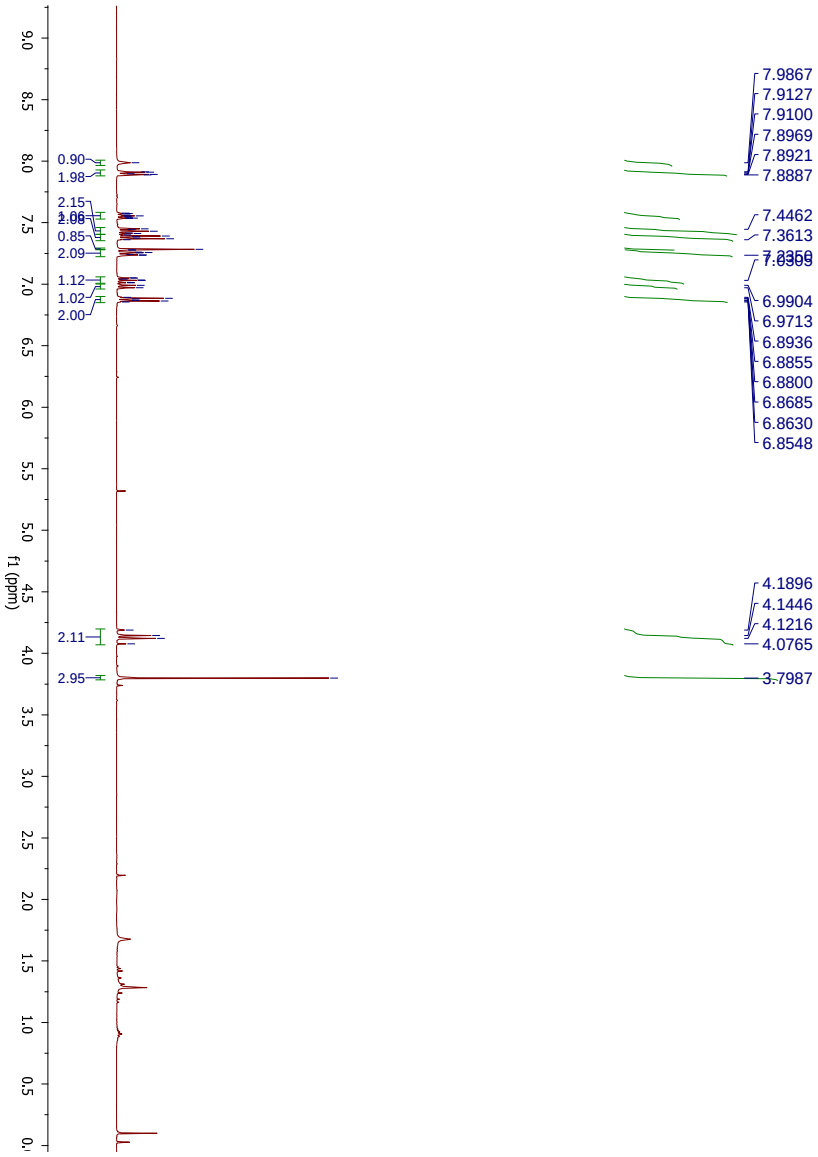


^{13}C NMR (100 MHz, DMSO-D6) of compound ±(**11f**)

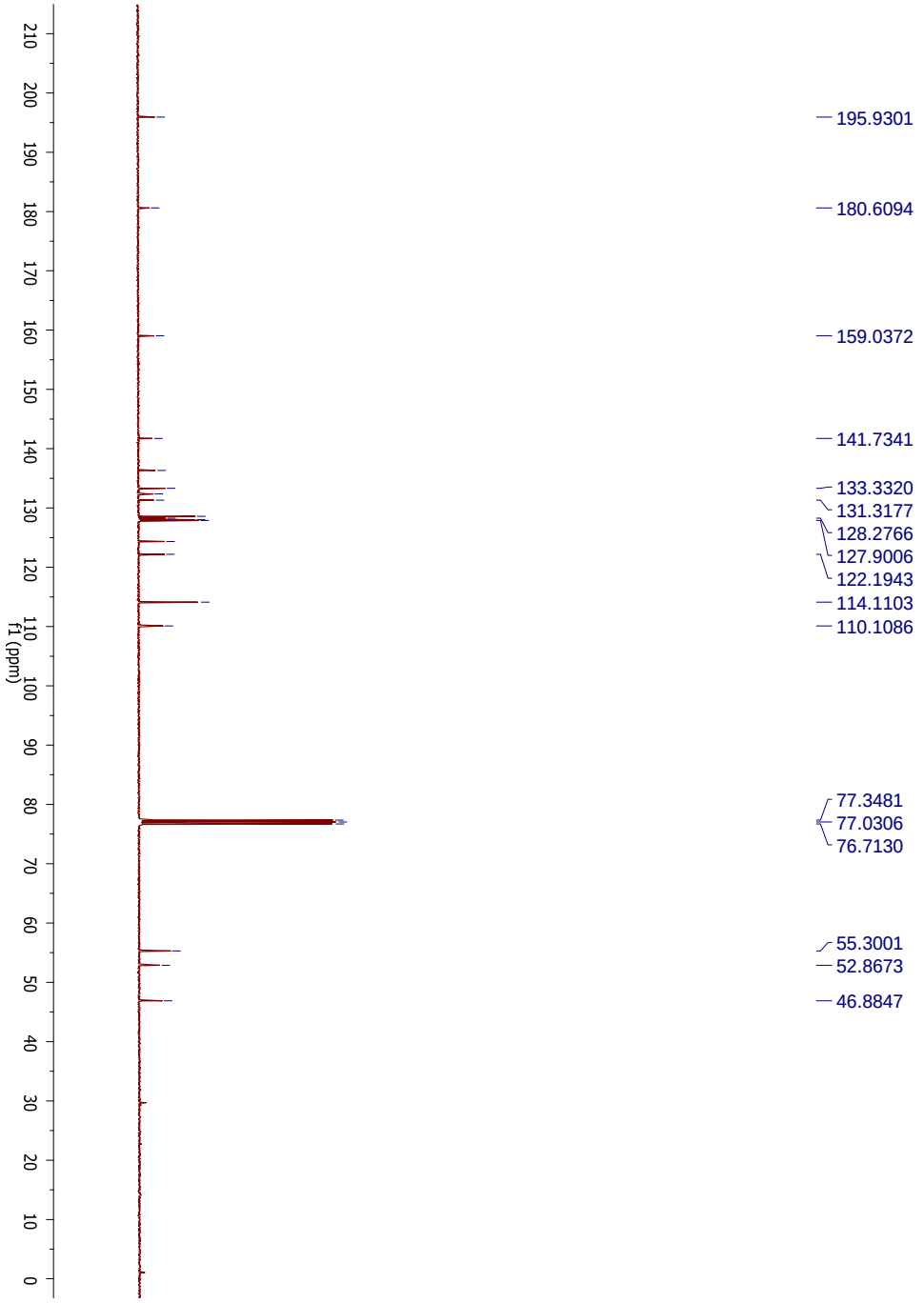


Scanned copy of mass spectrum of compound ±(**11f**)





^{1}H NMR **(**400 MHz, $CDCl_3$) of compound ±(**12a**)



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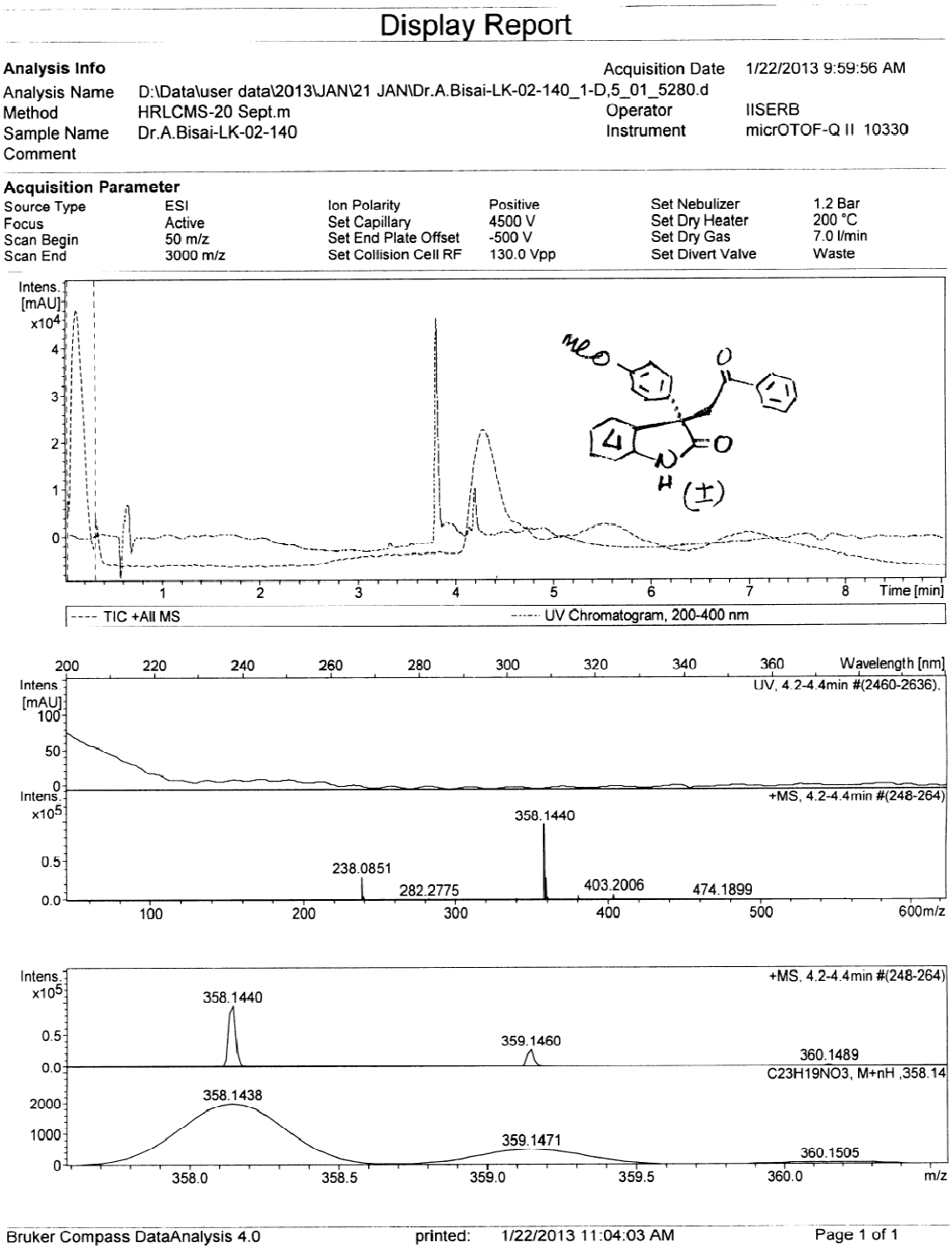
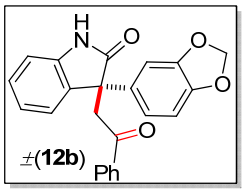
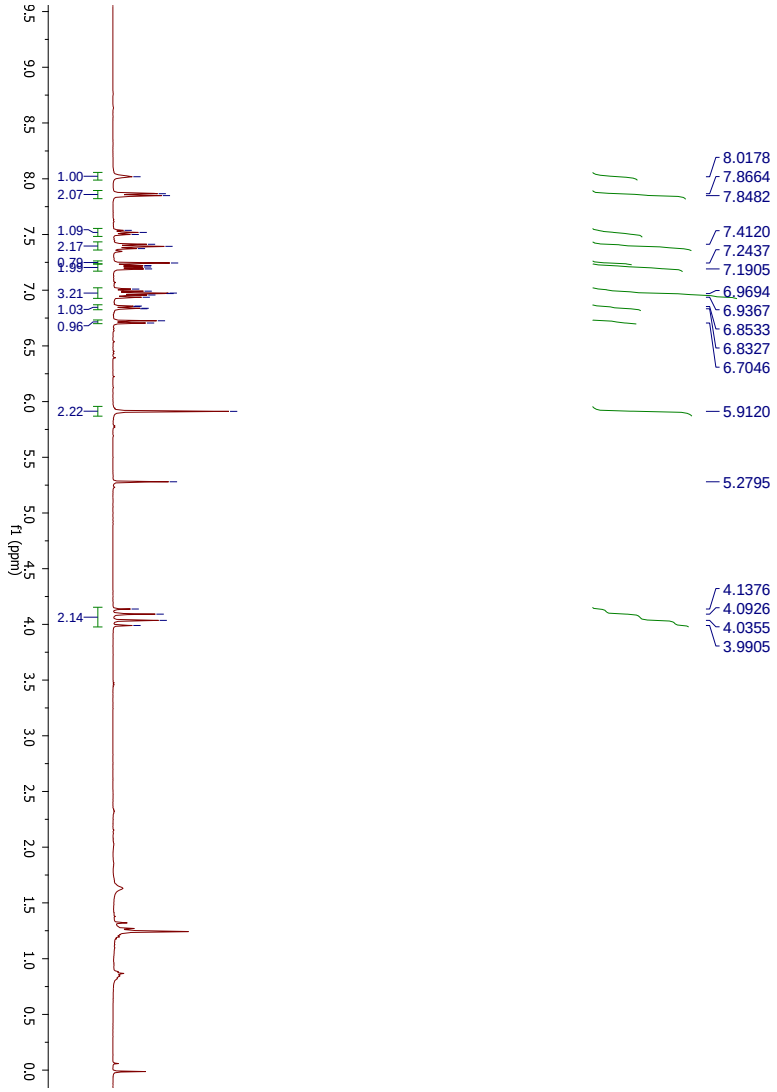
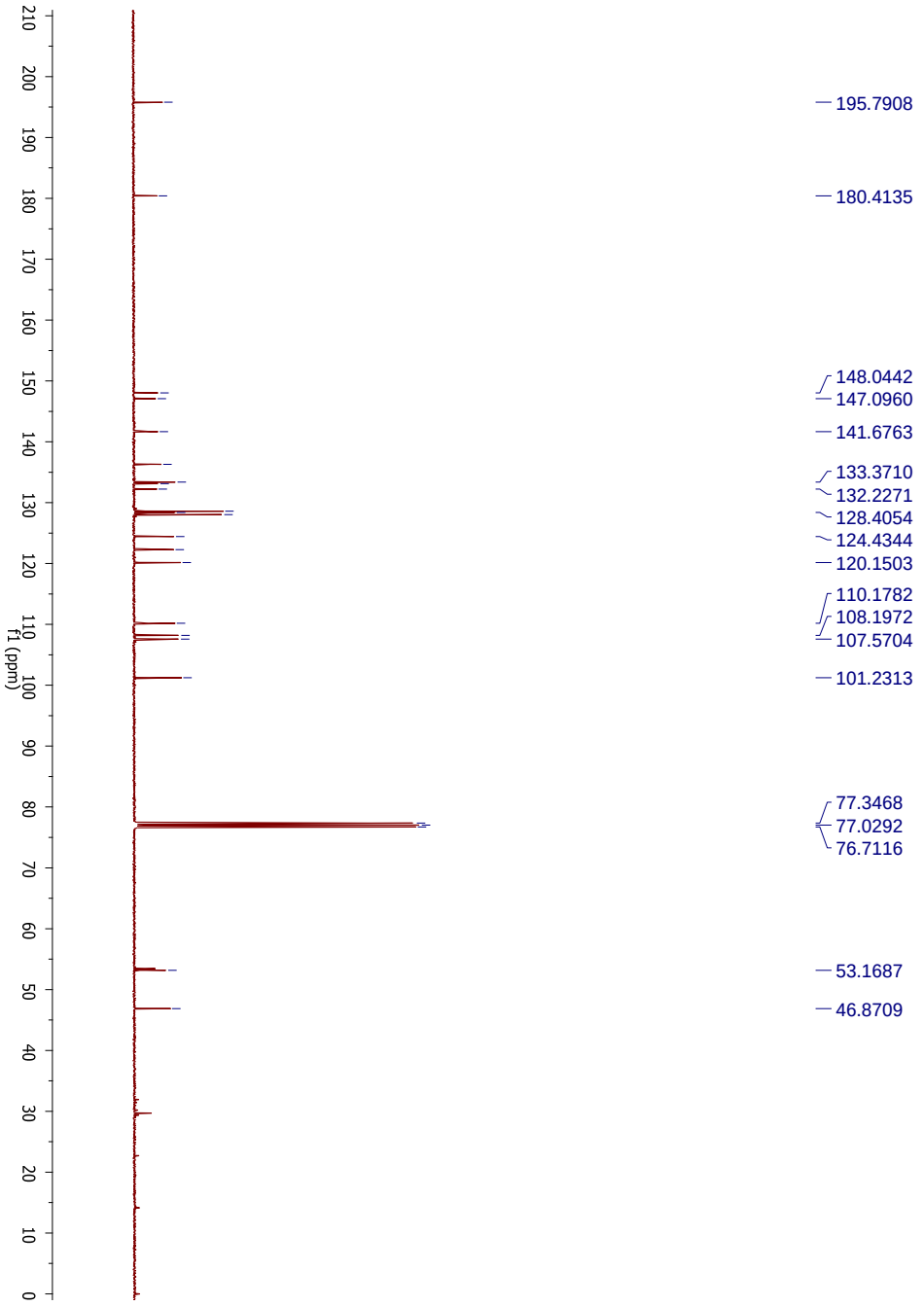


Scanned copy of mass spectrum (HRMS) of ±(**12a**)





^{1}H NMR **(**400 MHz, $CDCl_3$) of compound ±(**12b**)



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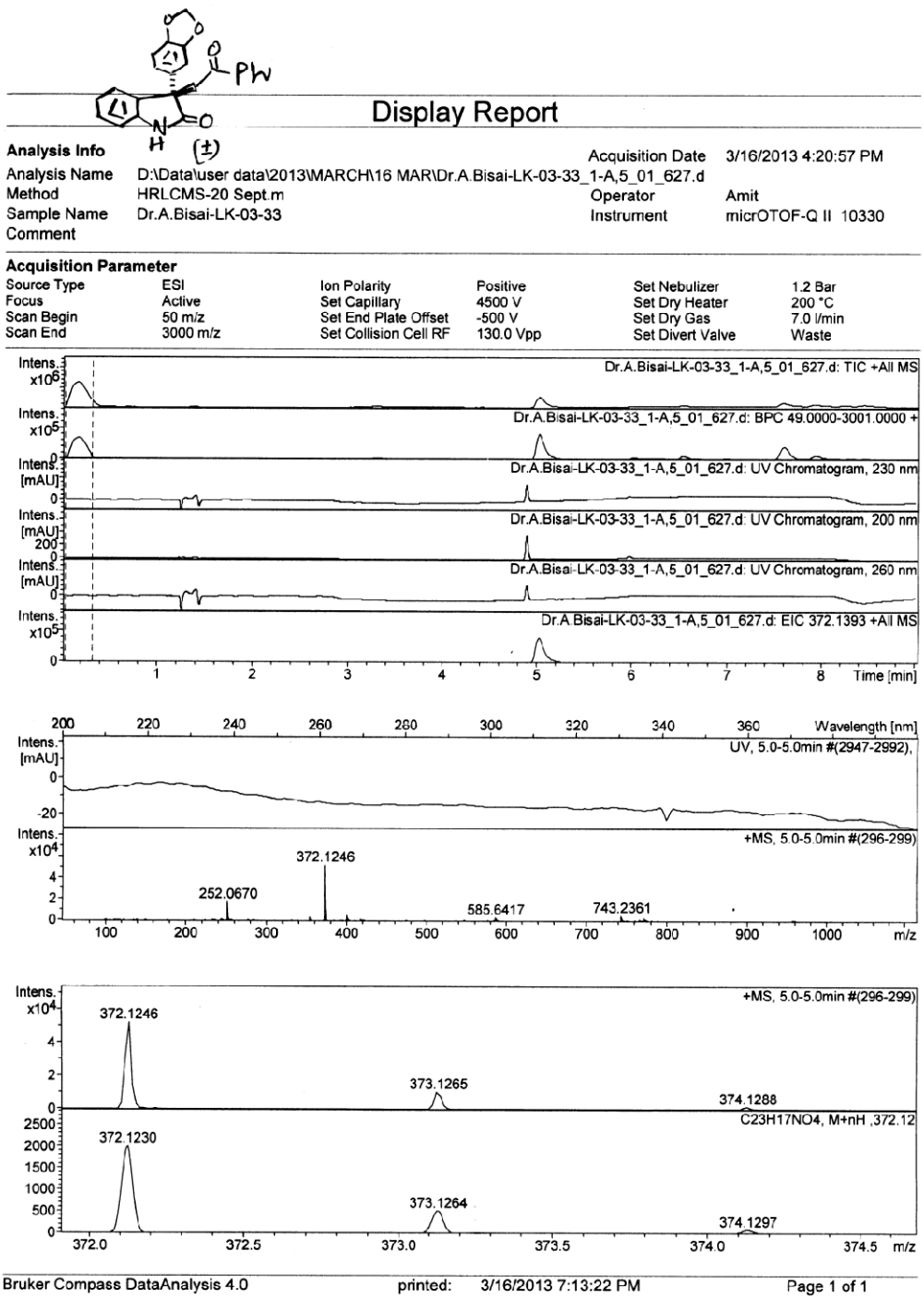
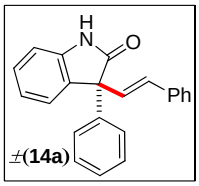
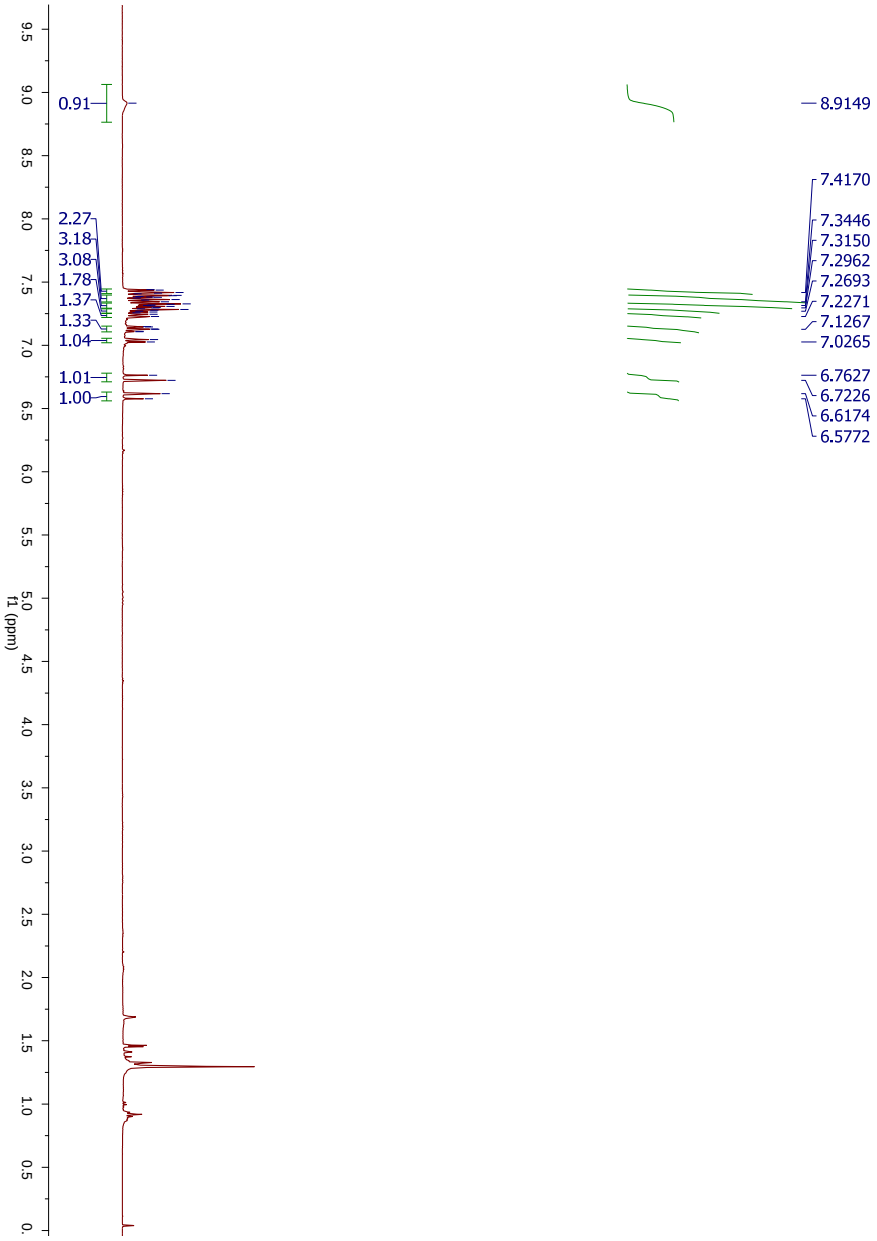
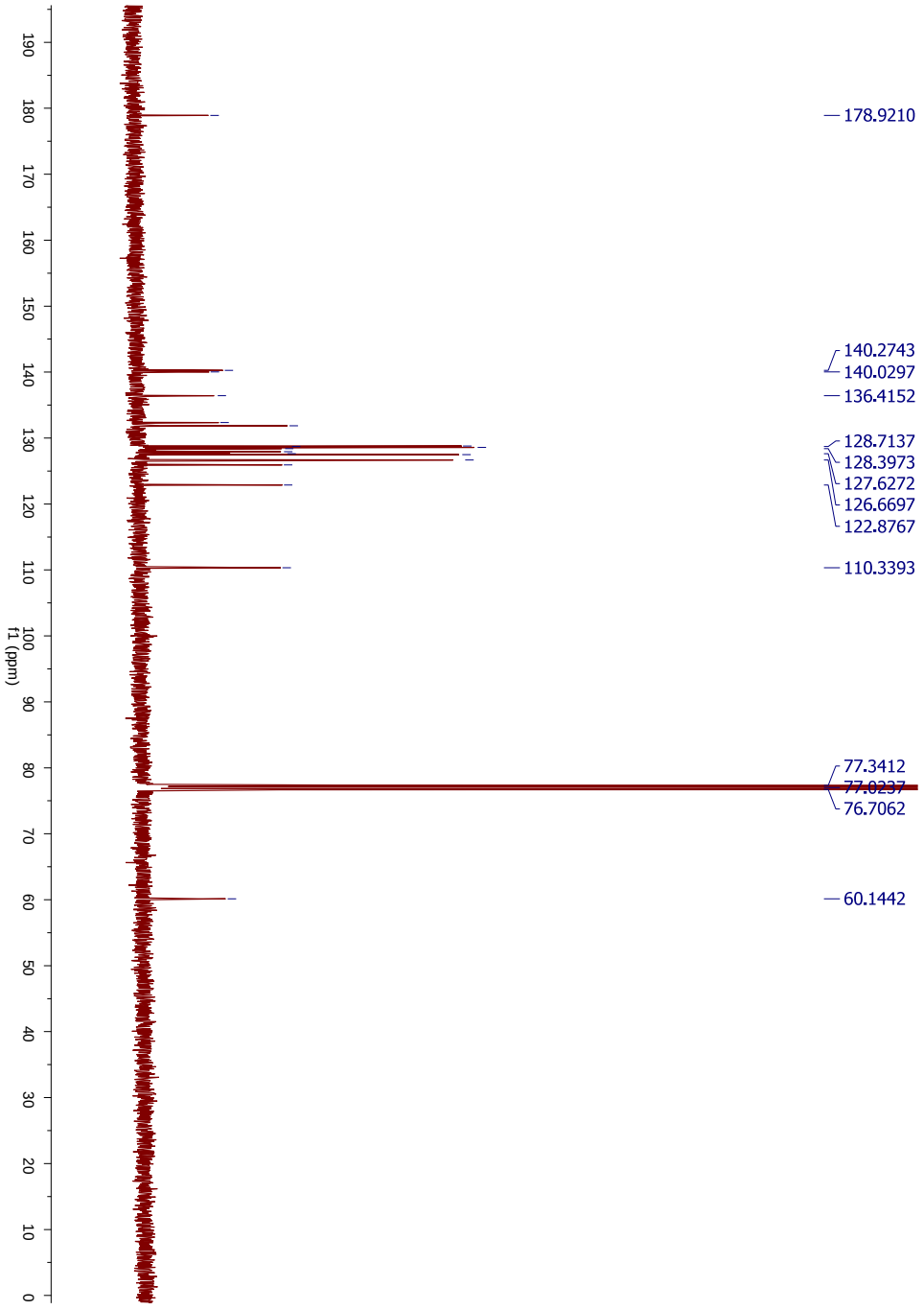


Scanned copy of mass spectrum (HRMS) of ±(**12b**)

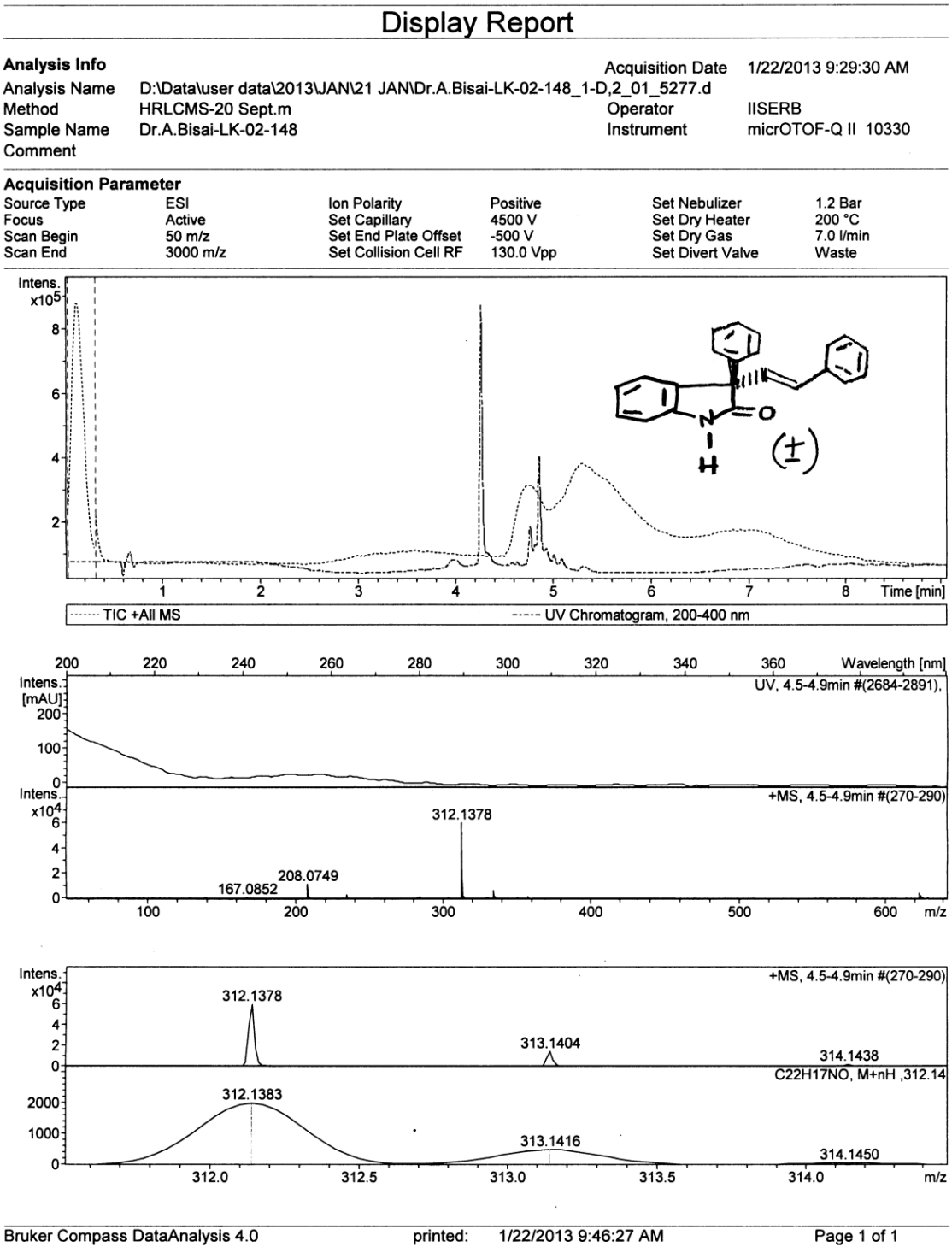




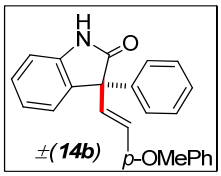
^{1}H NMR (400 MHz, $CDCl_3$) of compound ±(**14a**)

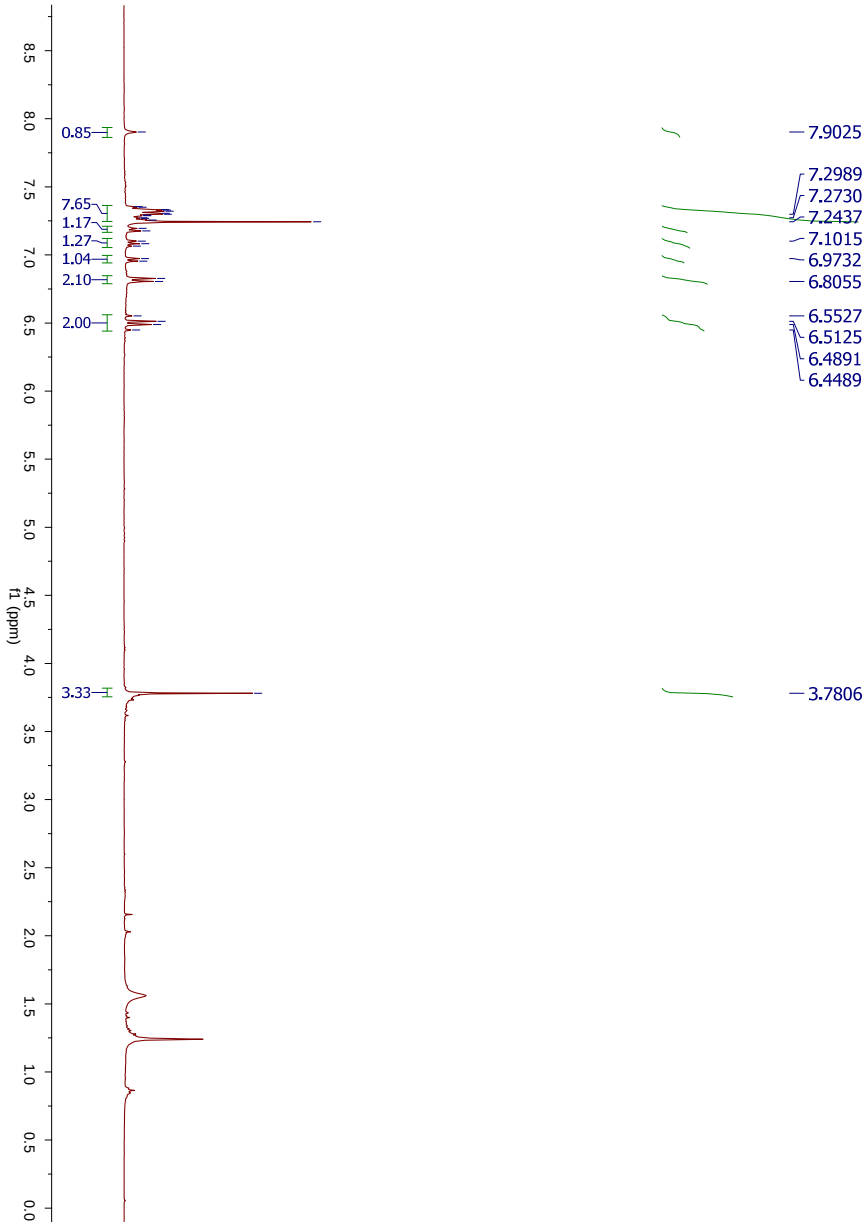


^{13}C NMR (100 MHz, $CDCl_3$) of compound ±(**14a**)

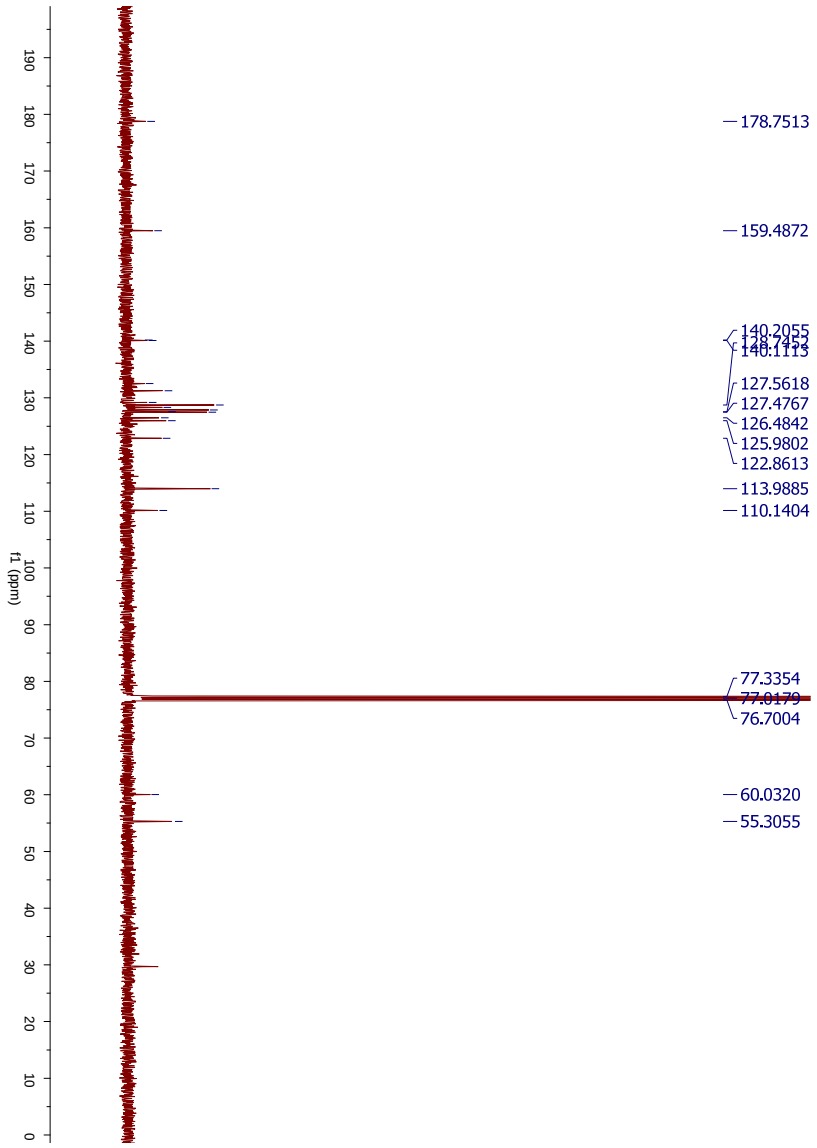


Scanned copy of mass spectrum (LRMS) of ±(**14a**)

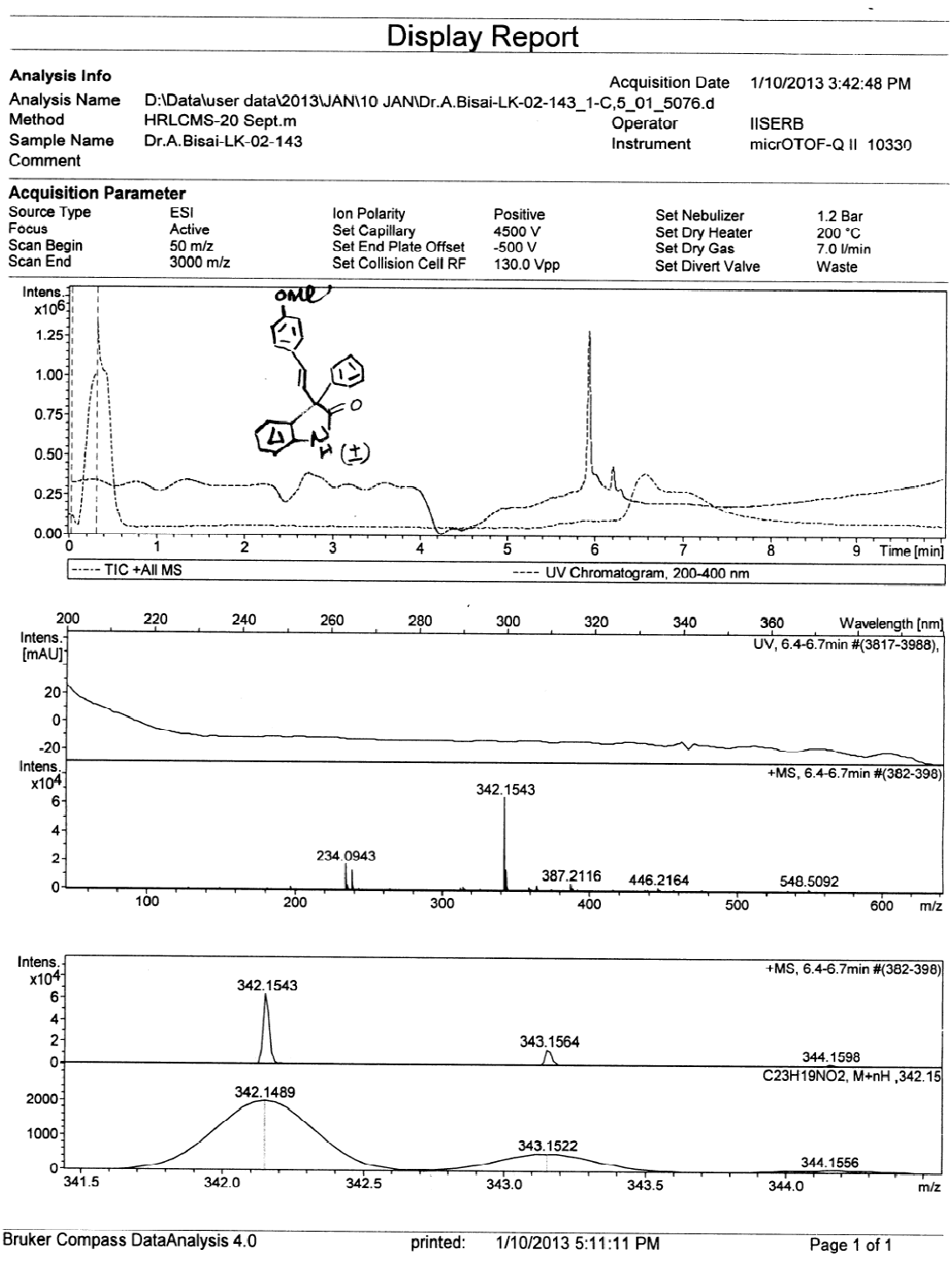




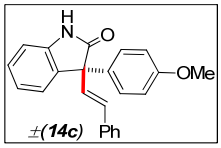
^{1}H NMR (400 MHz, $CDCl_3$) of compound ±(**14b**)

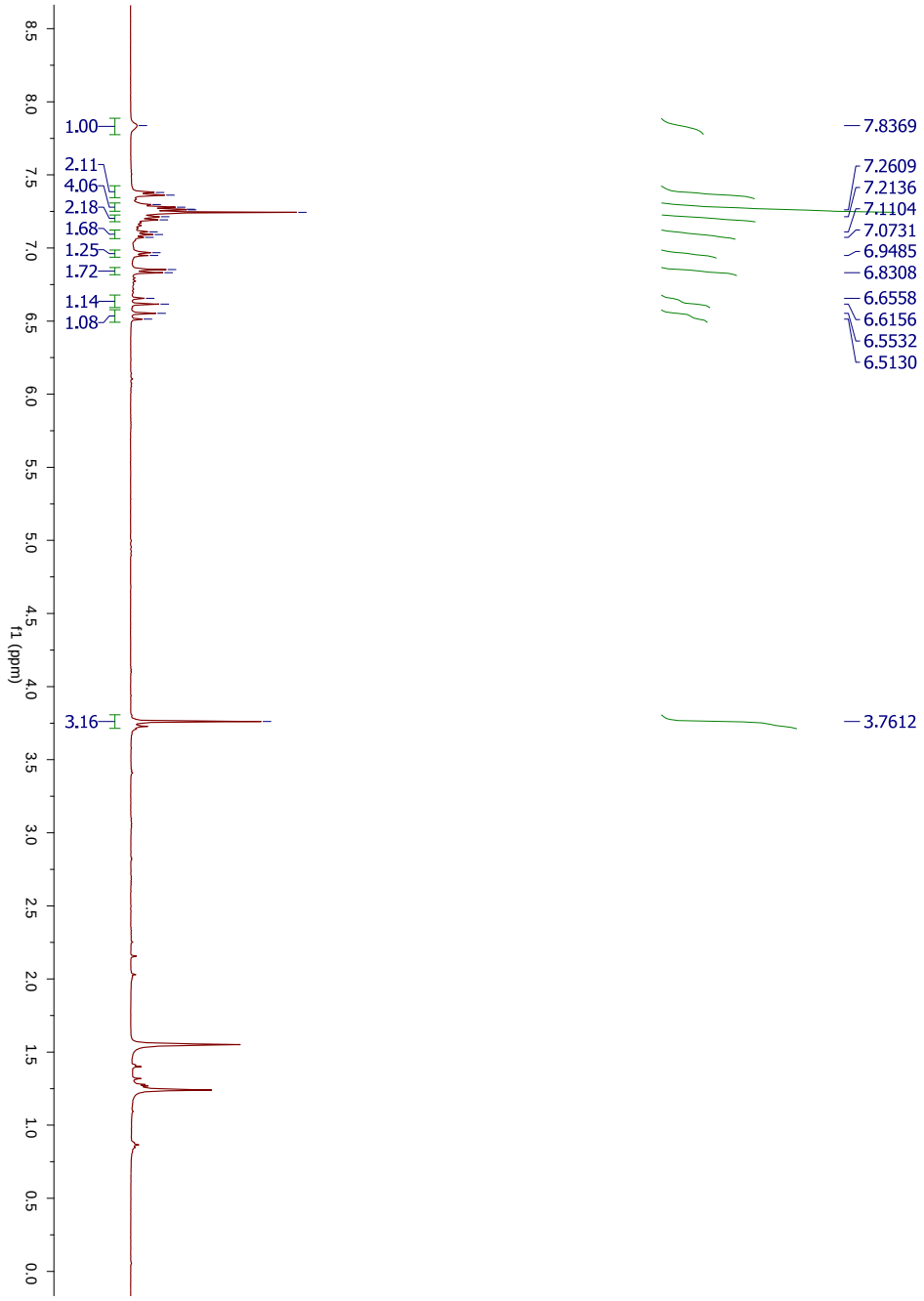


^{13}C NMR (100 MHz, $CDCl_3$) of compound ±(**14b**)

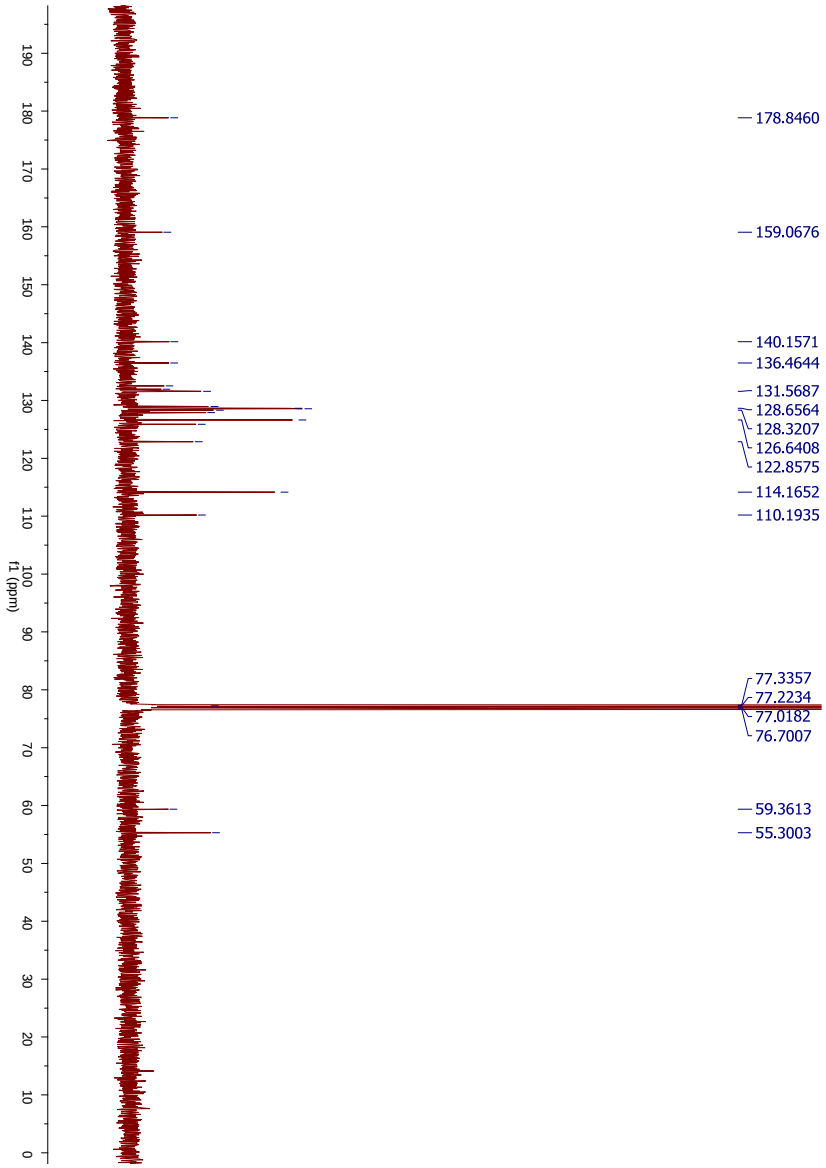


Scanned copy of mass spectrum (LRMS) of ±(**14b**)

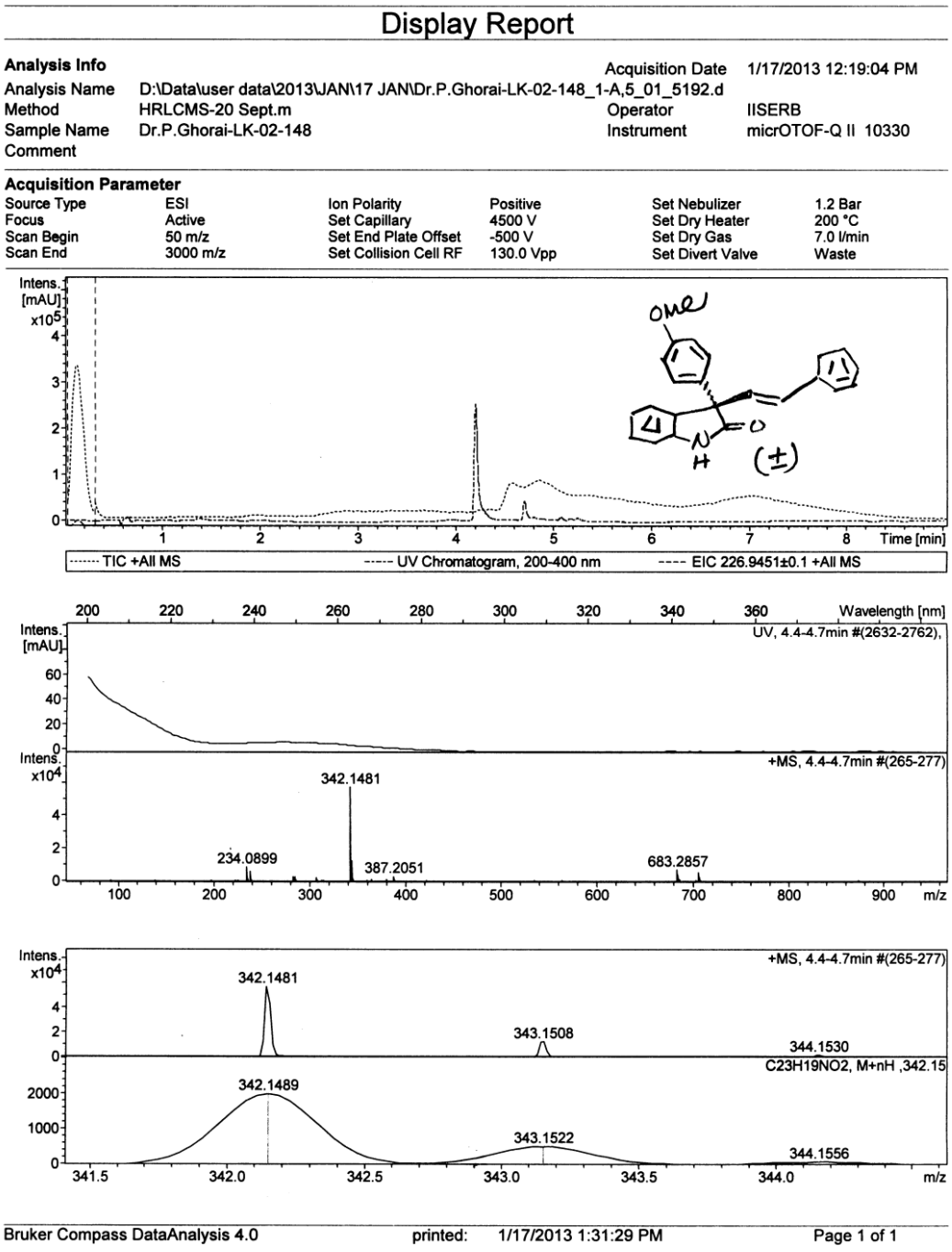




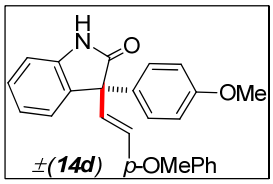
^{1}H NMR (400 MHz, $CDCl_3$) of compound ±(**14c**)

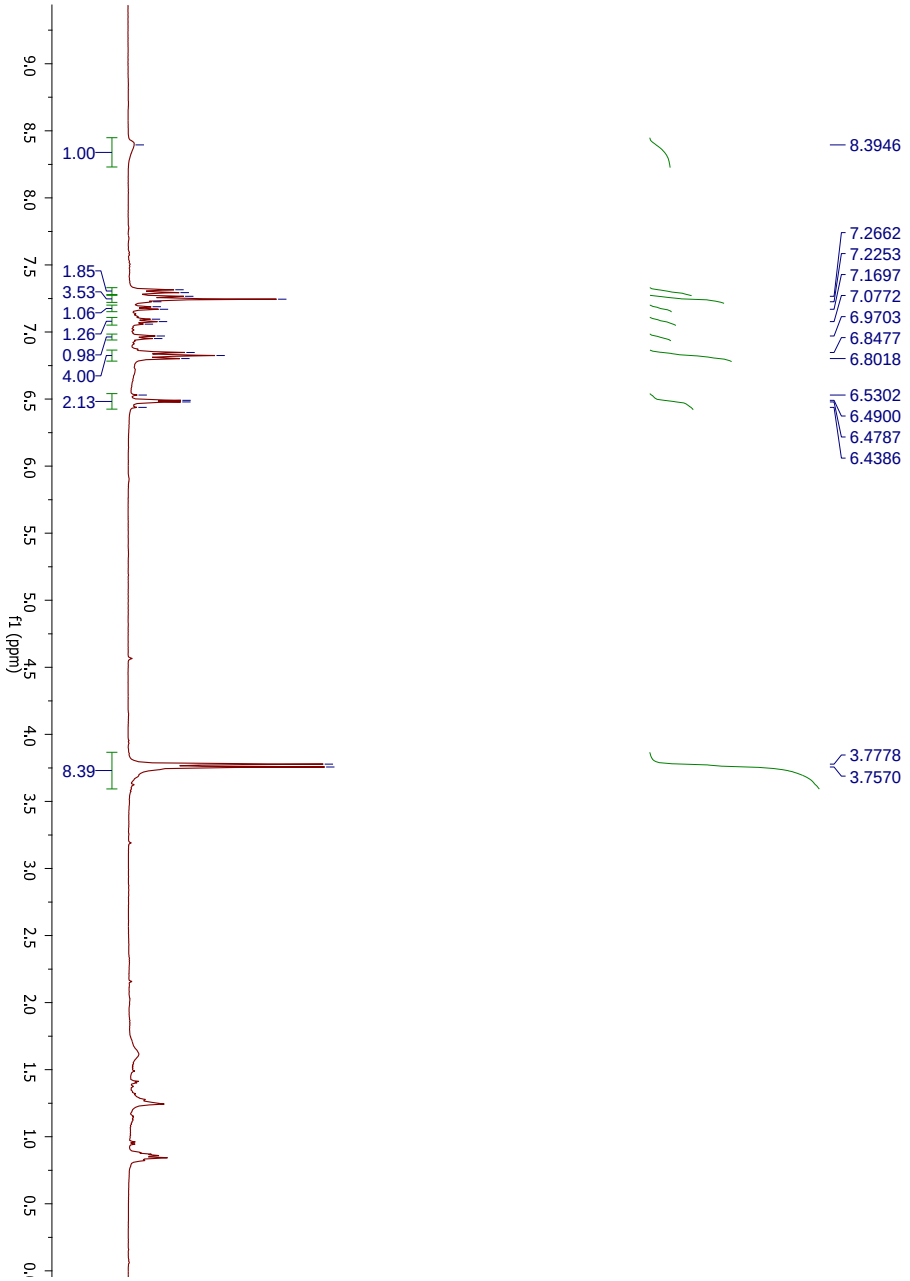


^{13}C NMR (100 MHz, $CDCl_3$) of compound ±(**14c**)

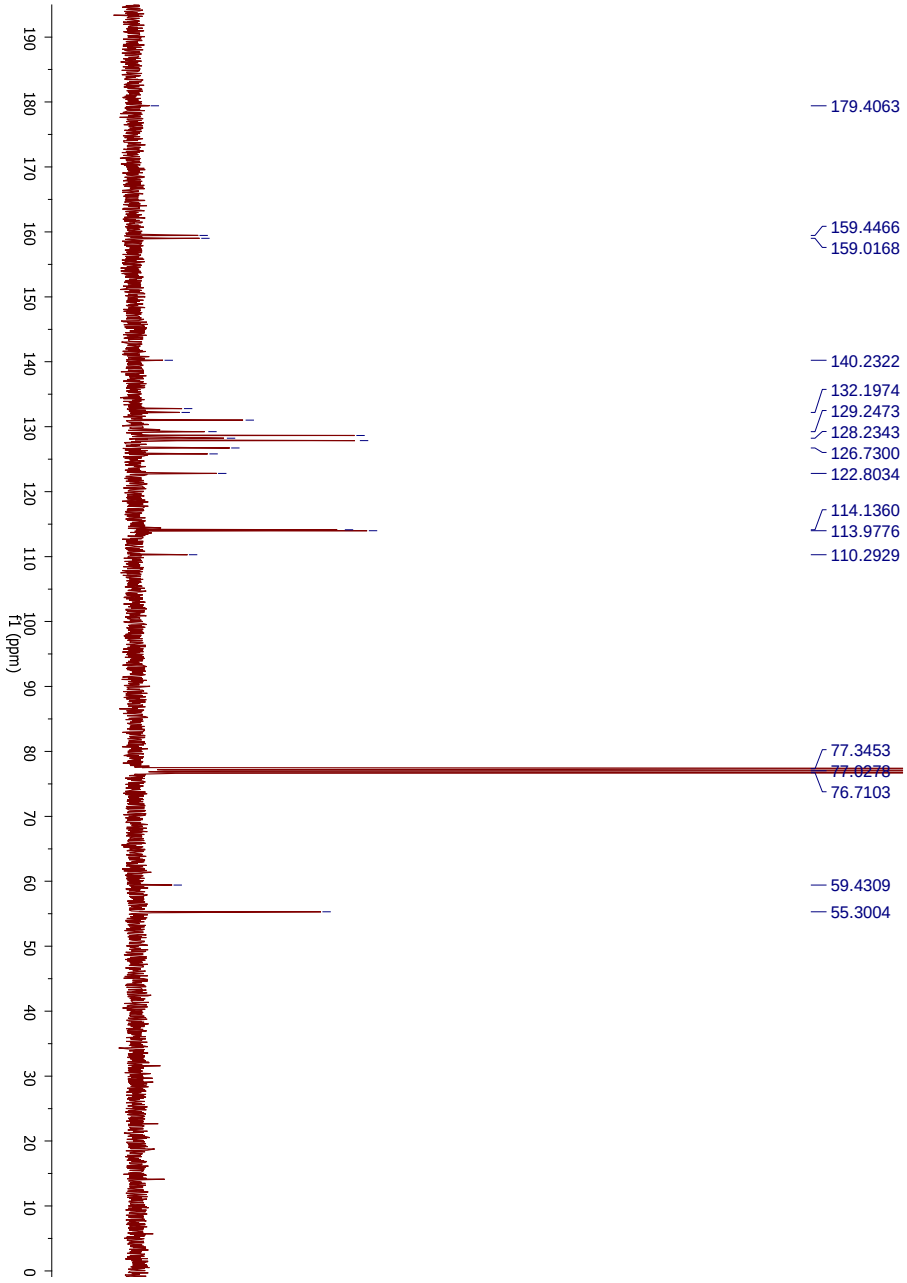


Scanned copy of mass spectrum (HRMS) of ±(**14c**)

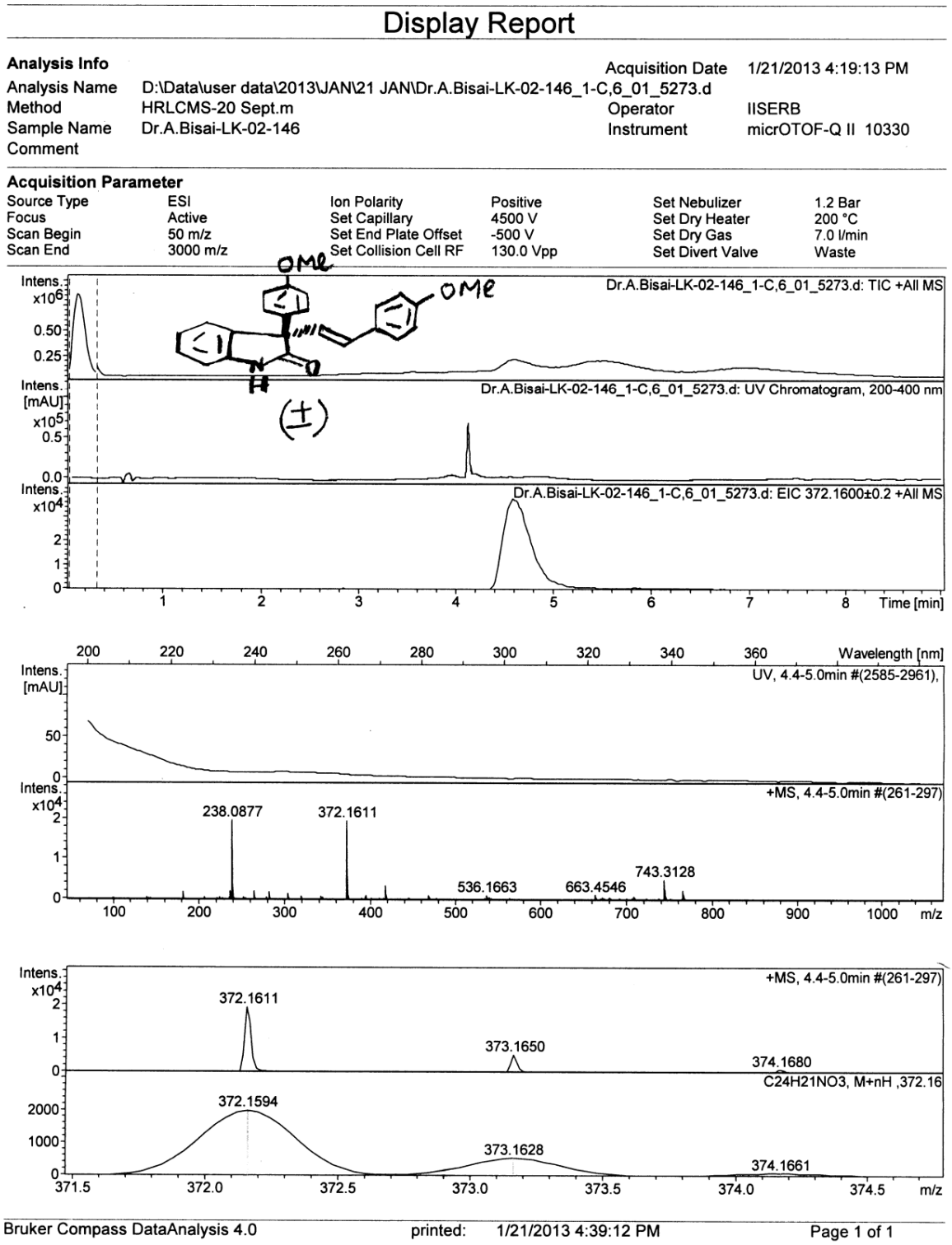




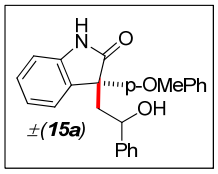
^{1}H NMR (400 MHz, $CDCl_3$) of compound ±(**14d**)

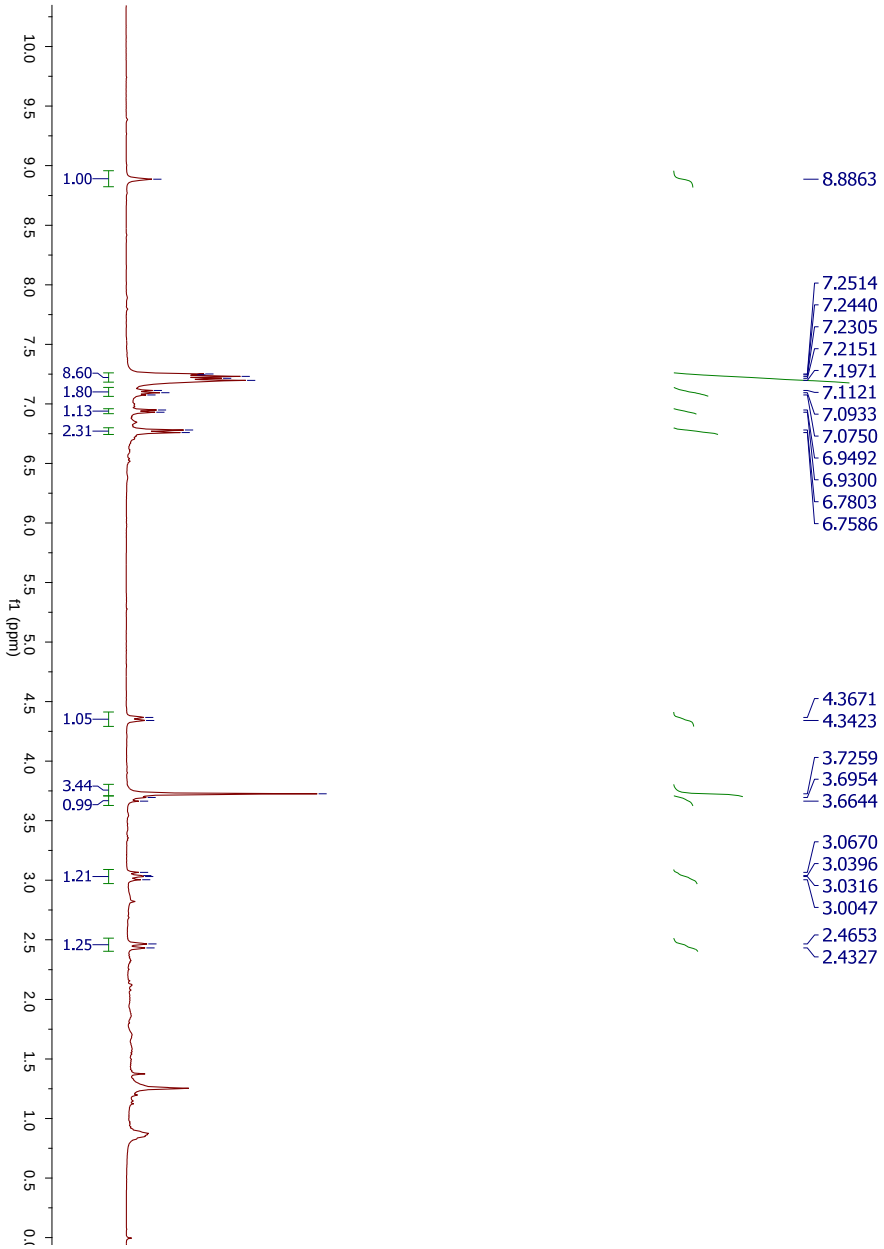


^{13}C NMR (100 MHz, $CDCl_3$) of compound ±(**14d**)

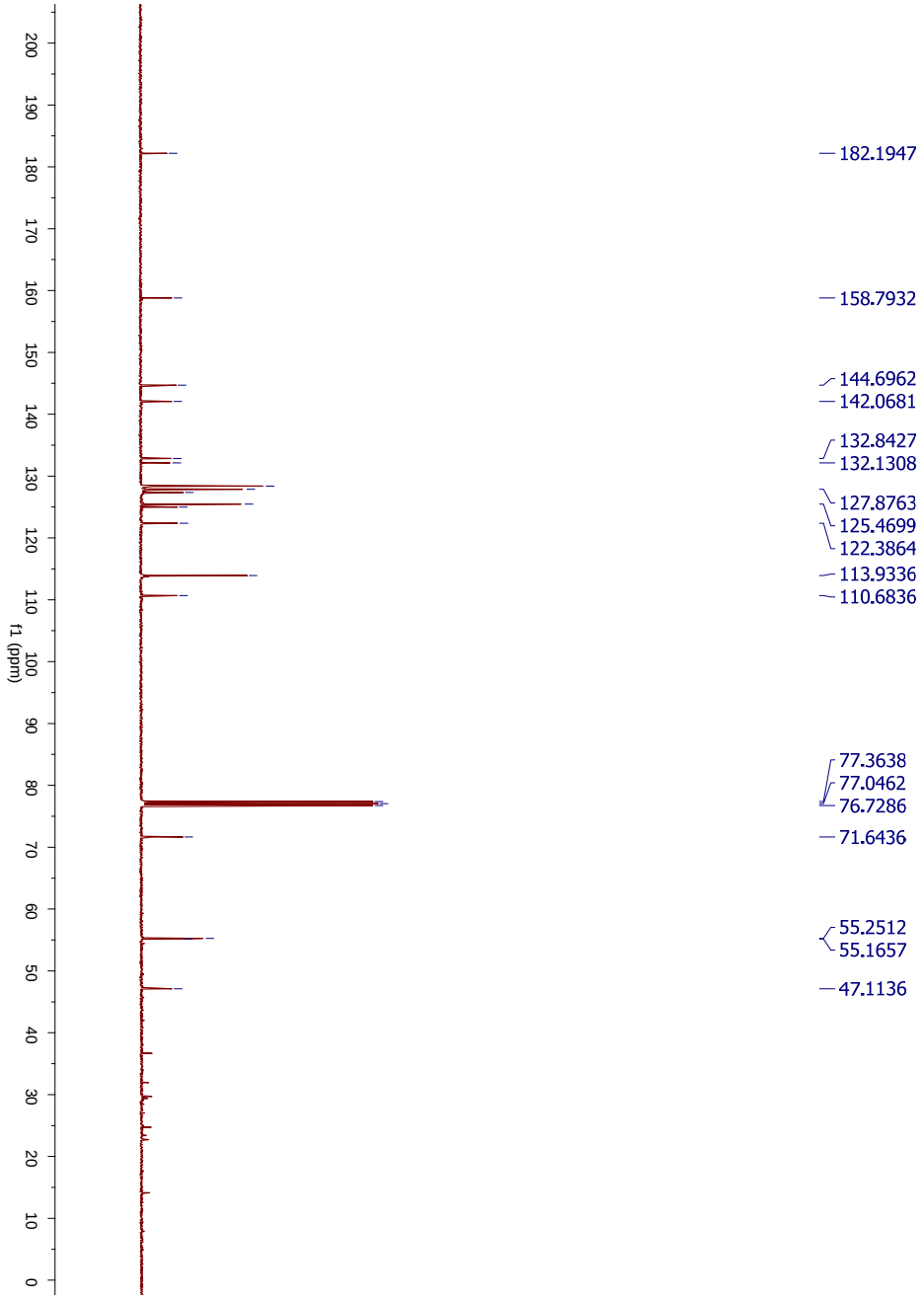


Scanned copy of mass spectrum (HRMS) of ±(**14d**)

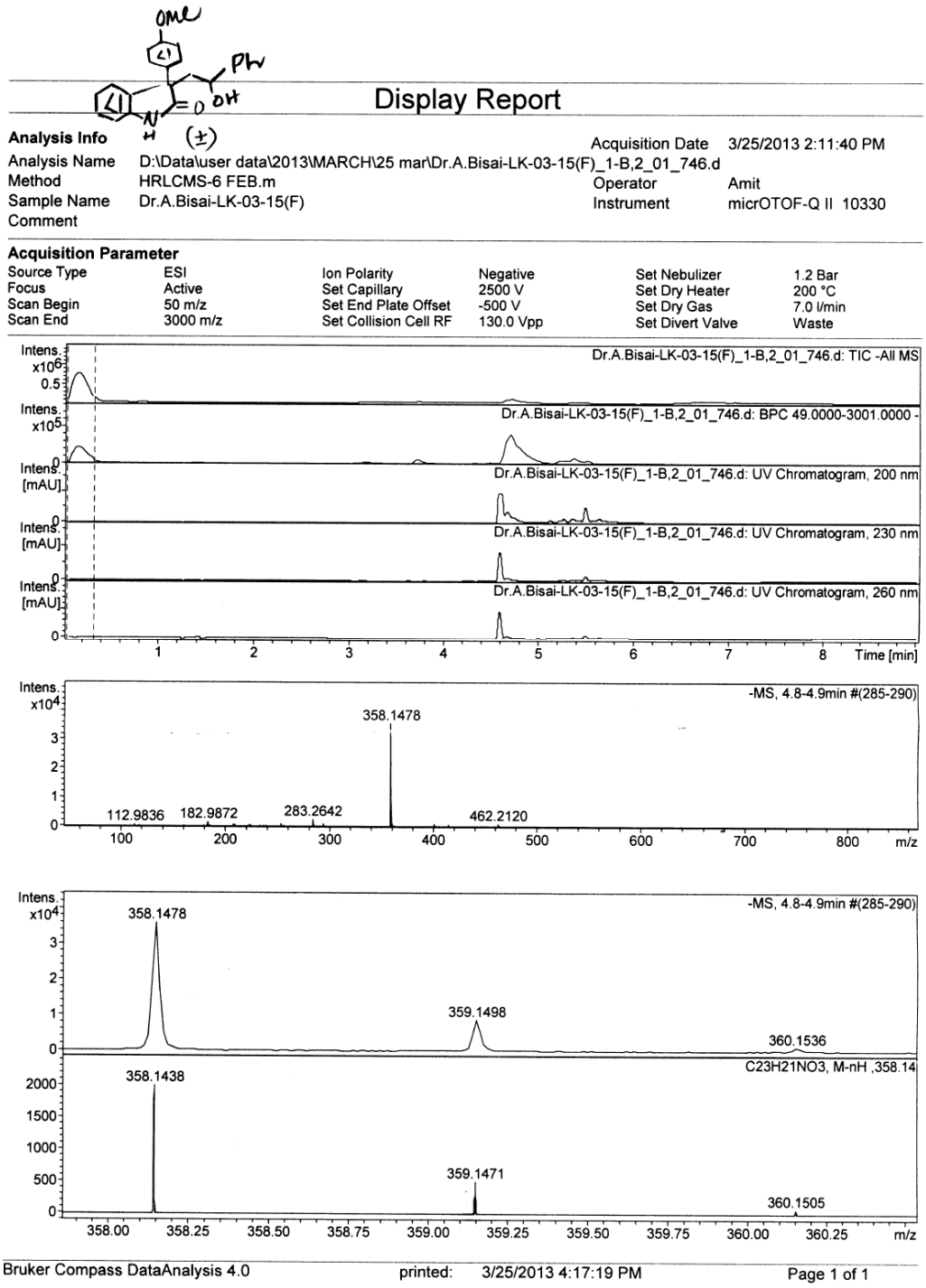




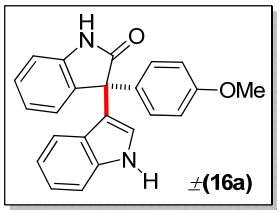
^{1}H NMR (400 MHz, $CDCl_3$) of compound ±(**15a**)

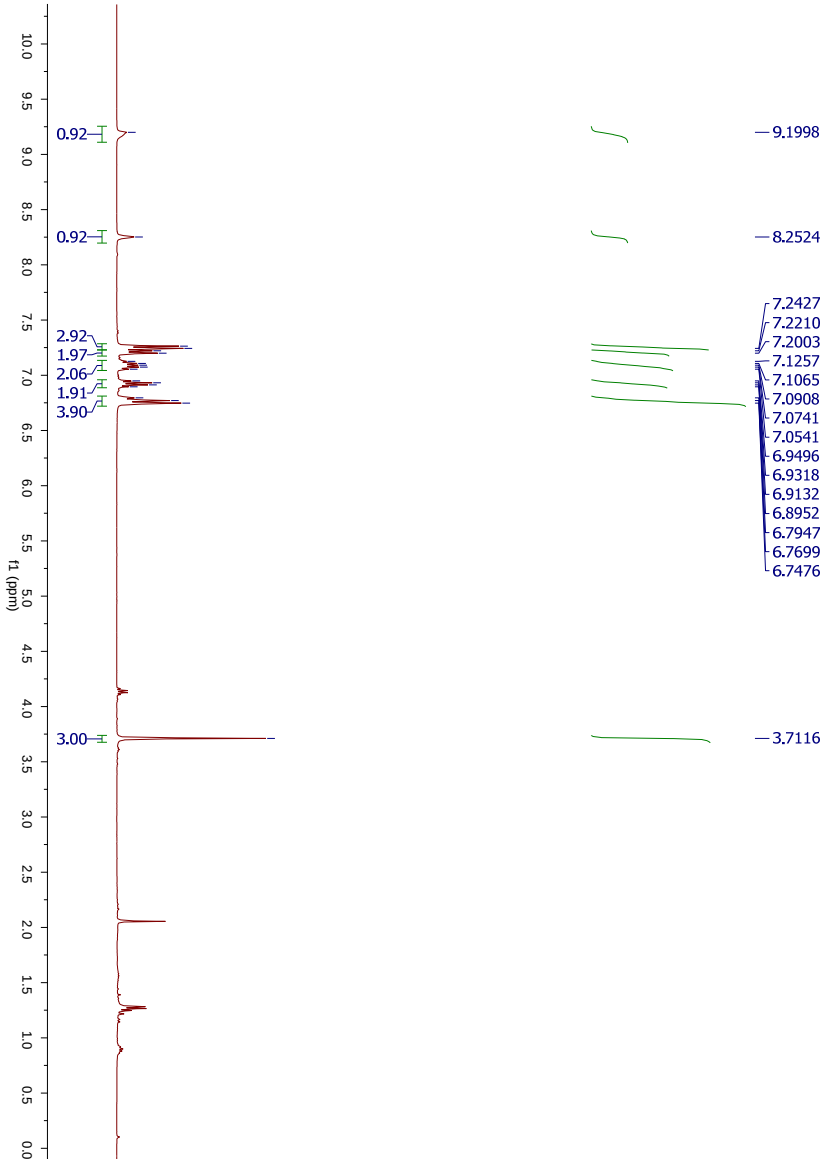


^{13}C NMR (100 MHz, $CDCl_3$) of compound ±(**15a**)

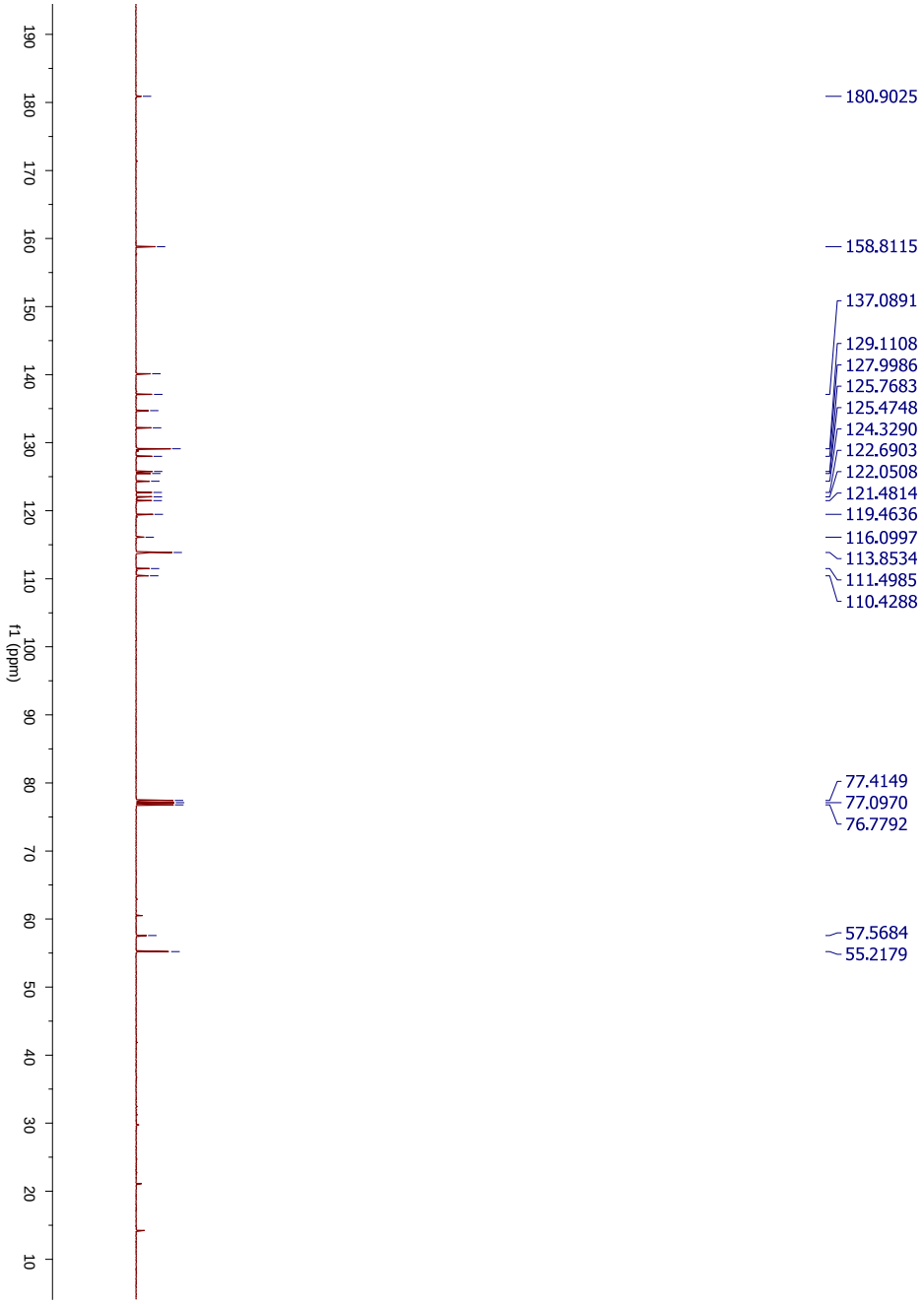


Scanned copy of mass spectrum (HRMS) of ±(**15a**)

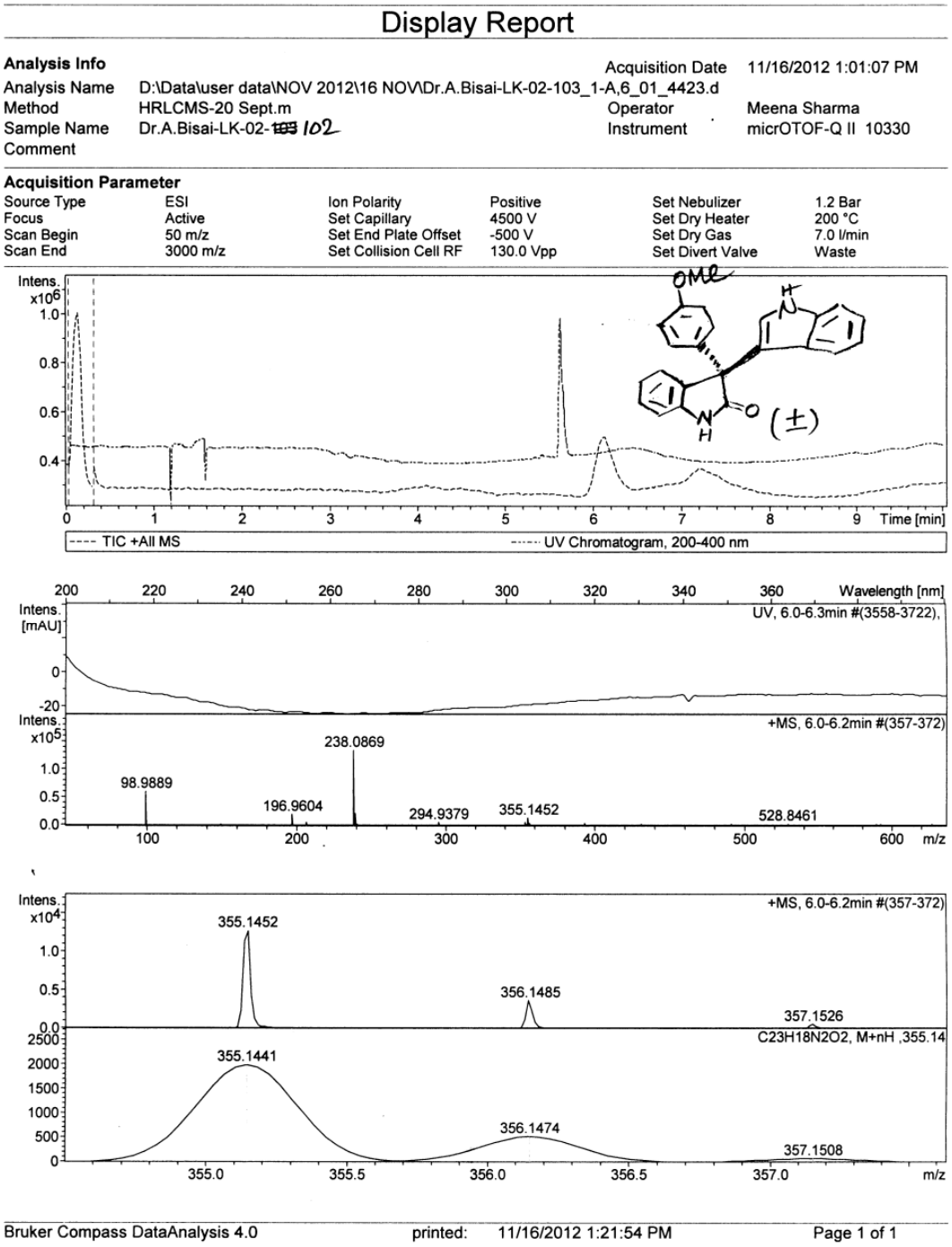




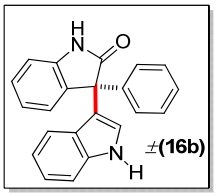
^{1}H NMR (400 MHz, $CDCl_3$) of compound ±(**16a**)

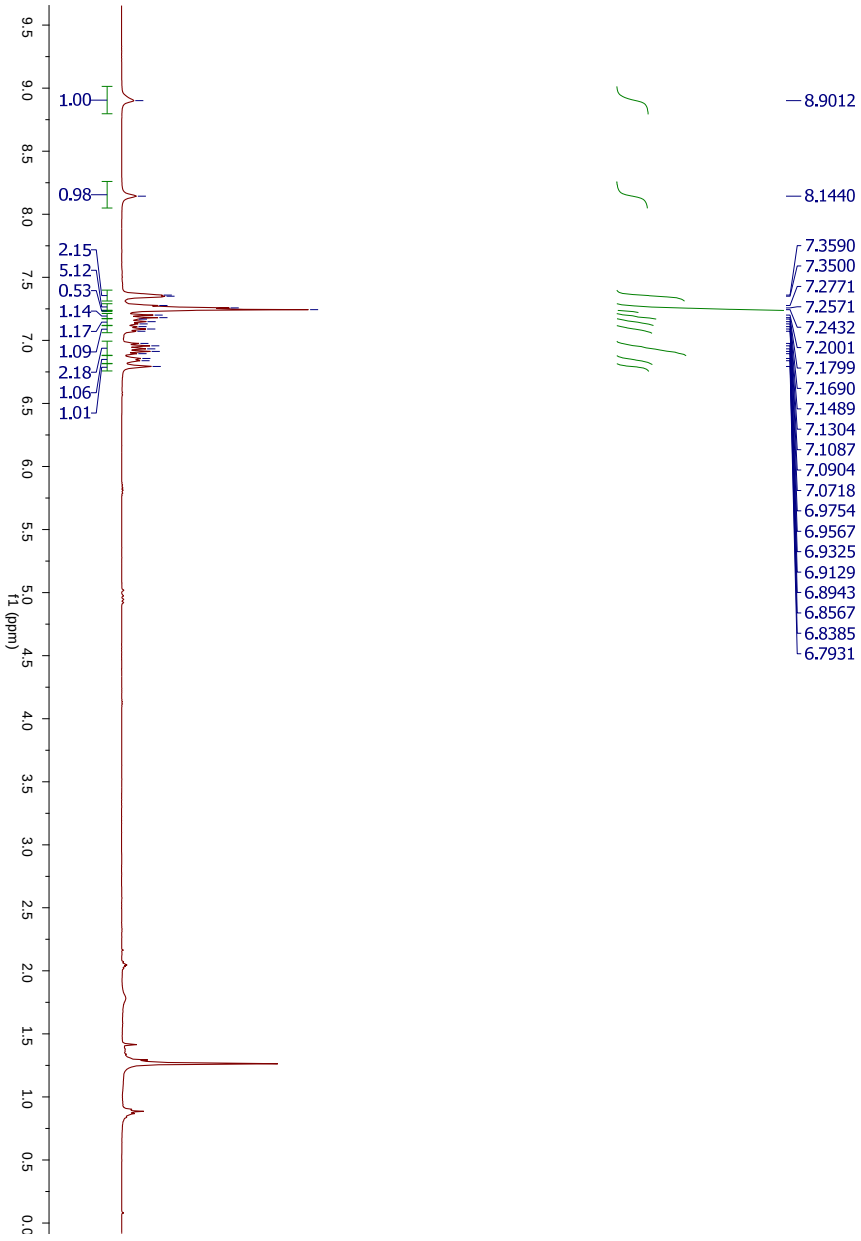


^{13}C NMR (100 MHz, $CDCl_3$) of compound ±(**16a**)

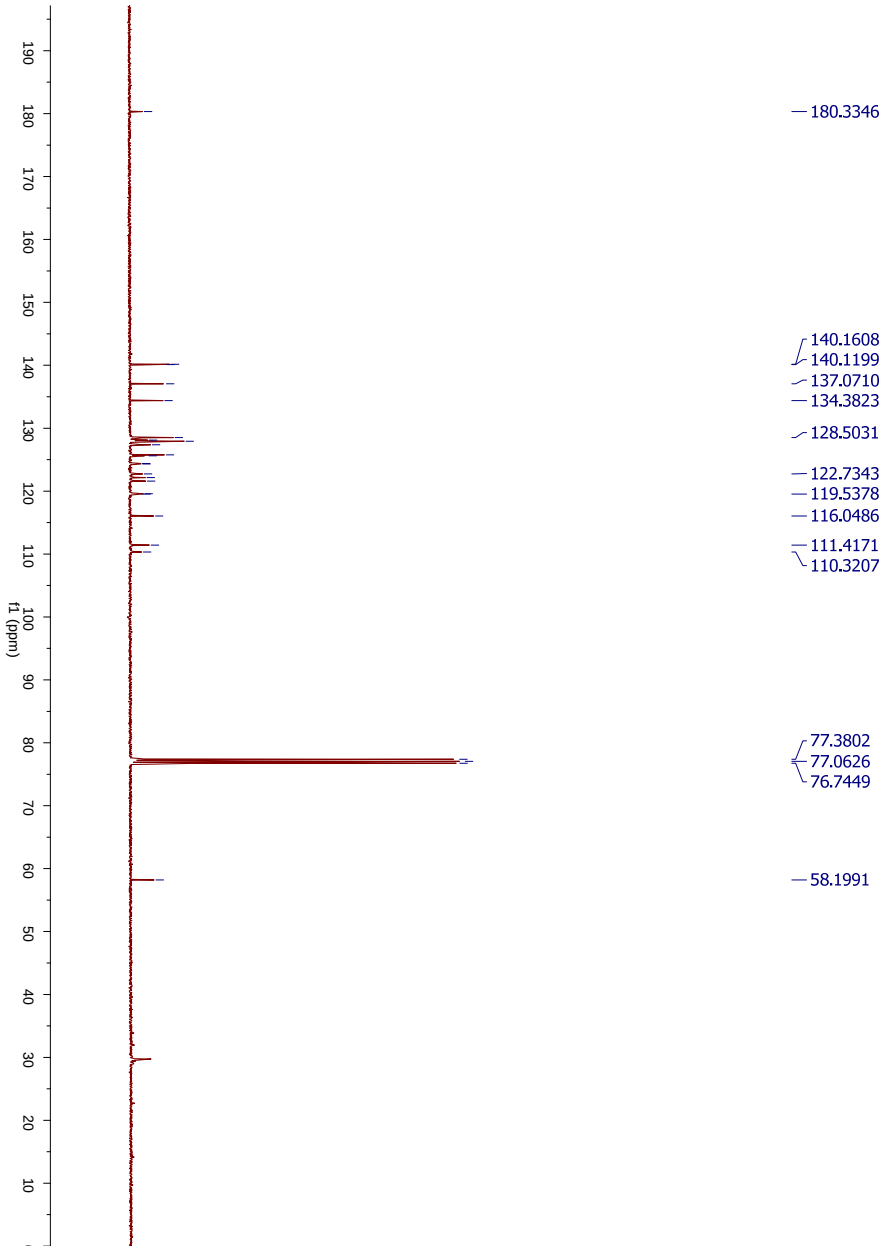


Scanned copy of mass spectrum (HRMS) of ±(**16a**)

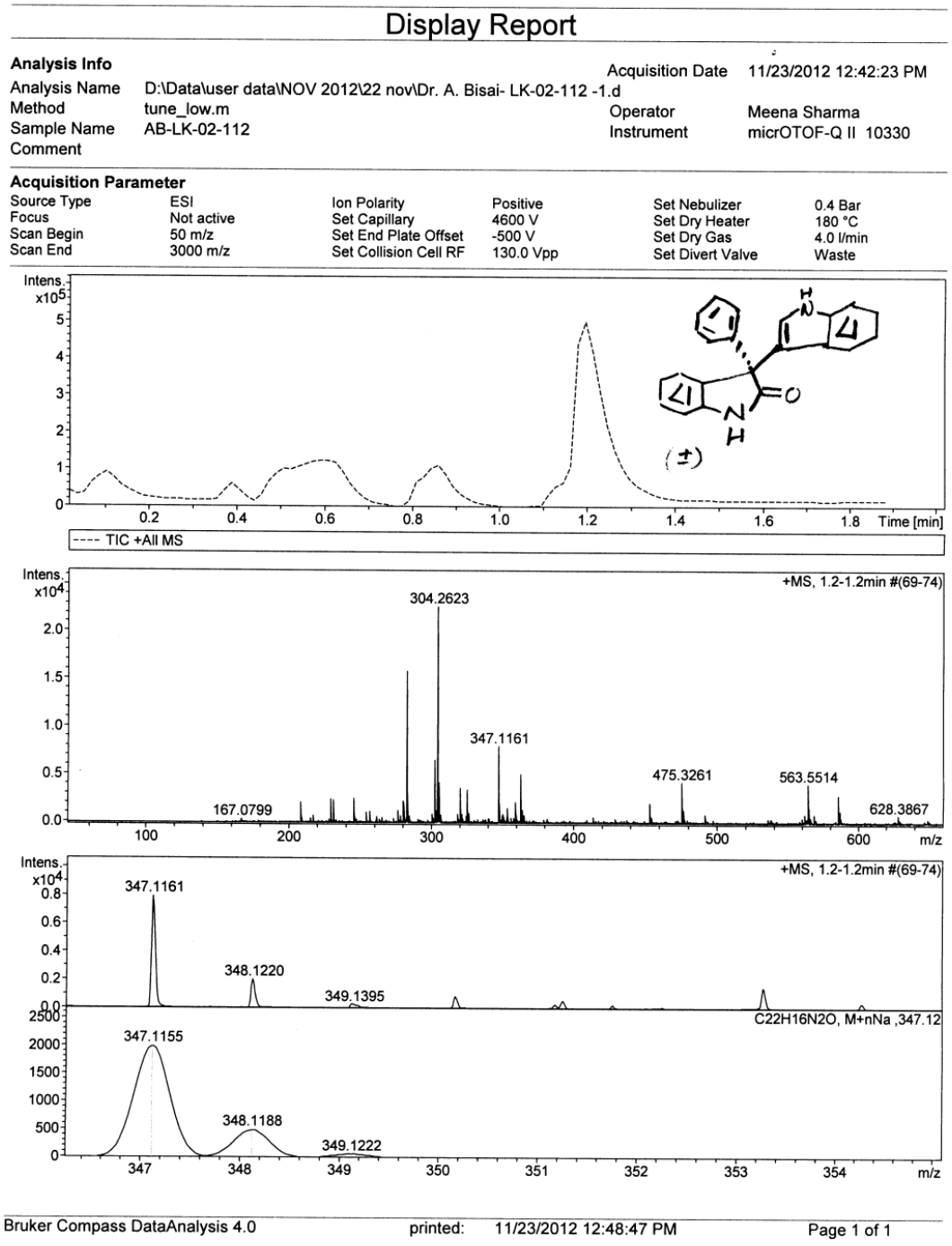




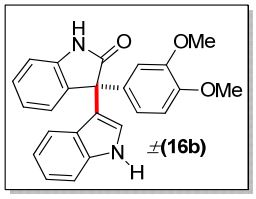
^{1}H NMR (400 MHz, $CDCl_3$) of compound ±(**16b**)

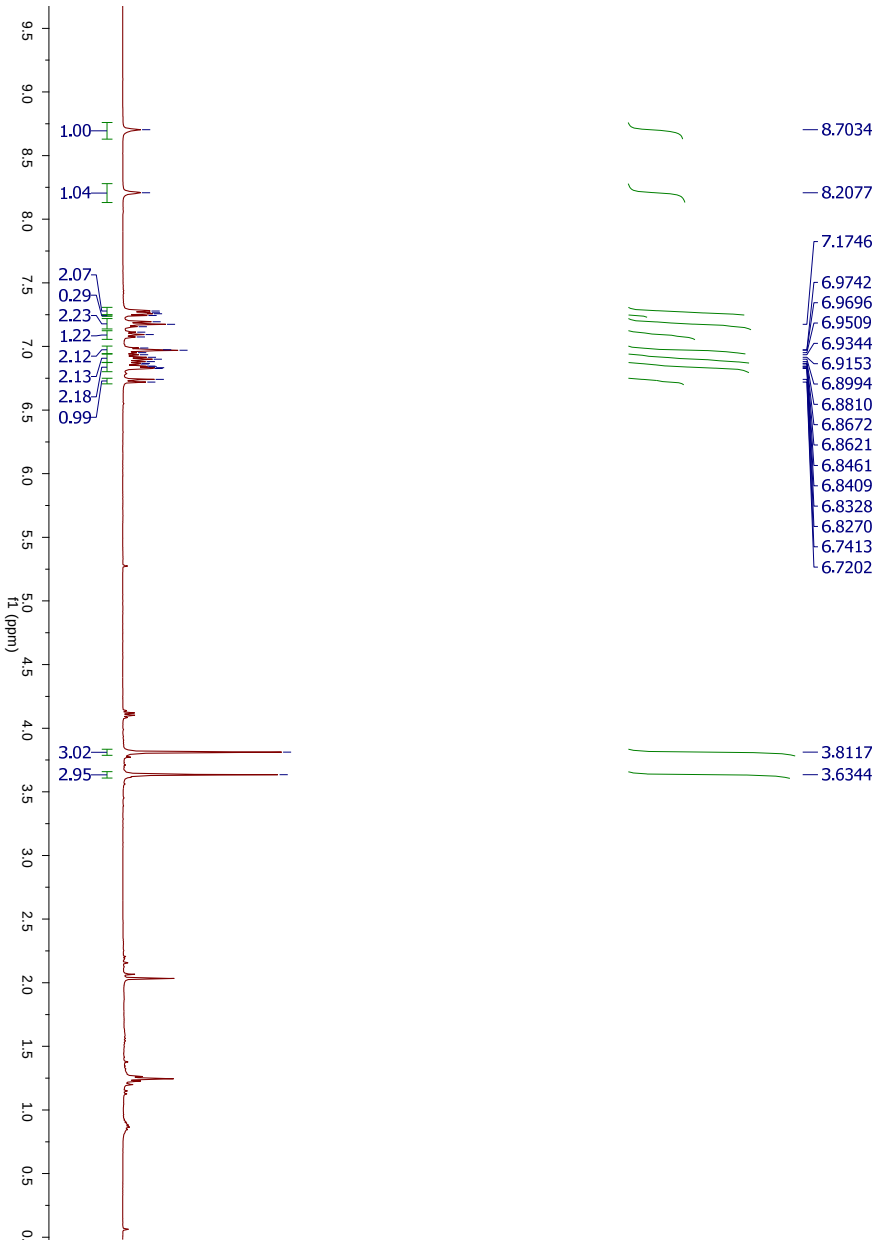


^{13}C NMR (100 MHz, $CDCl_3$) of compound ±(**16b**)

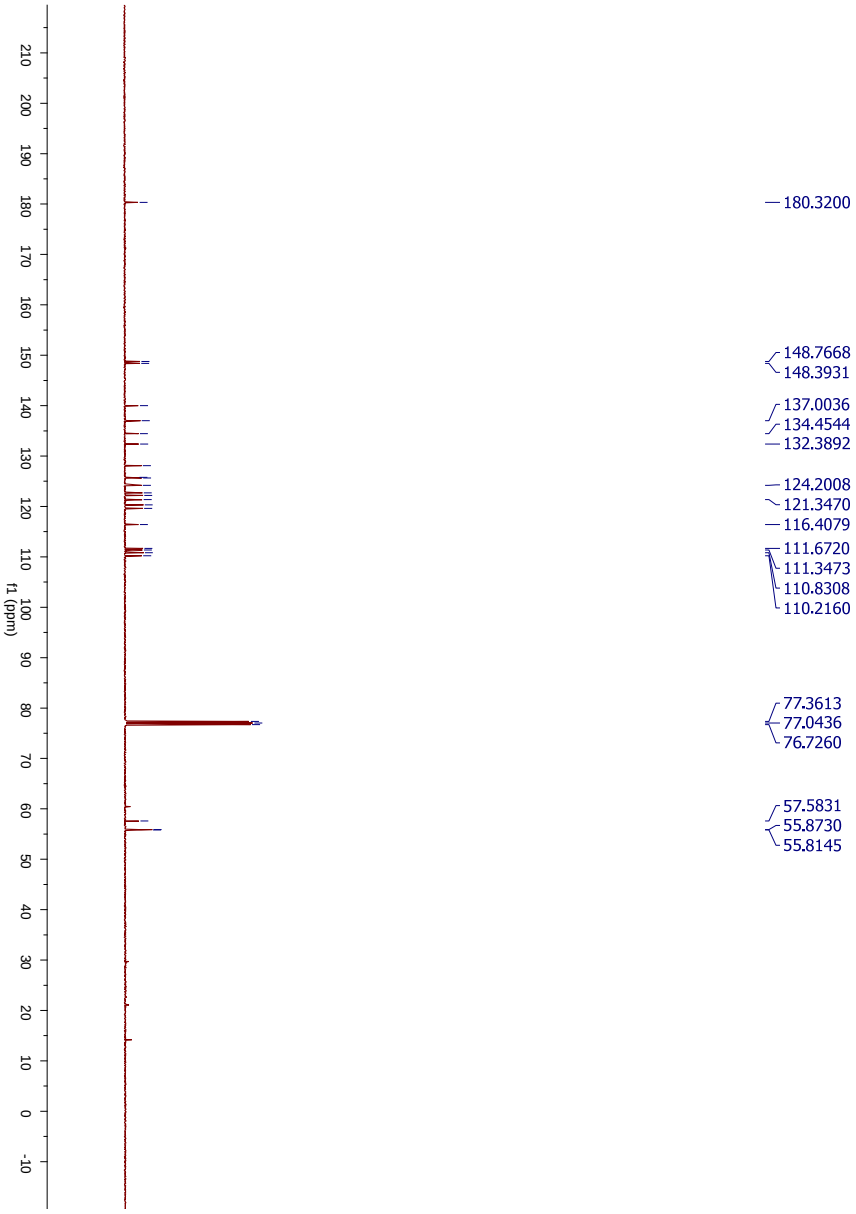


Scanned copy of mass spectrum (HRMS) of ±(**16b**)

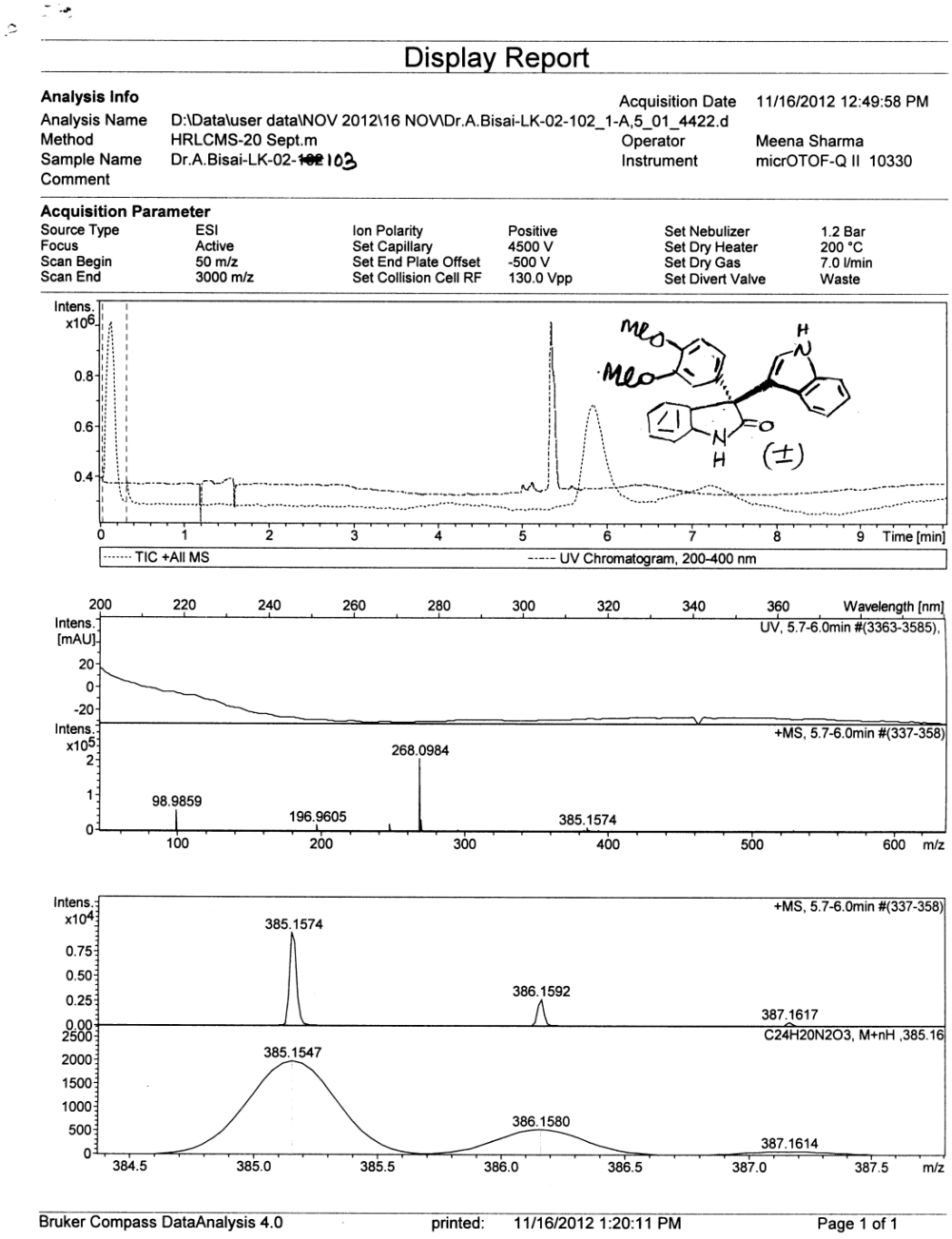




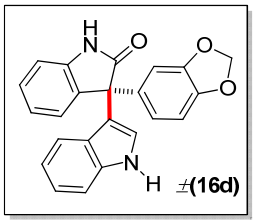
^{1}H NMR (400 MHz, $CDCl_3$) of compound ±(**16c**)

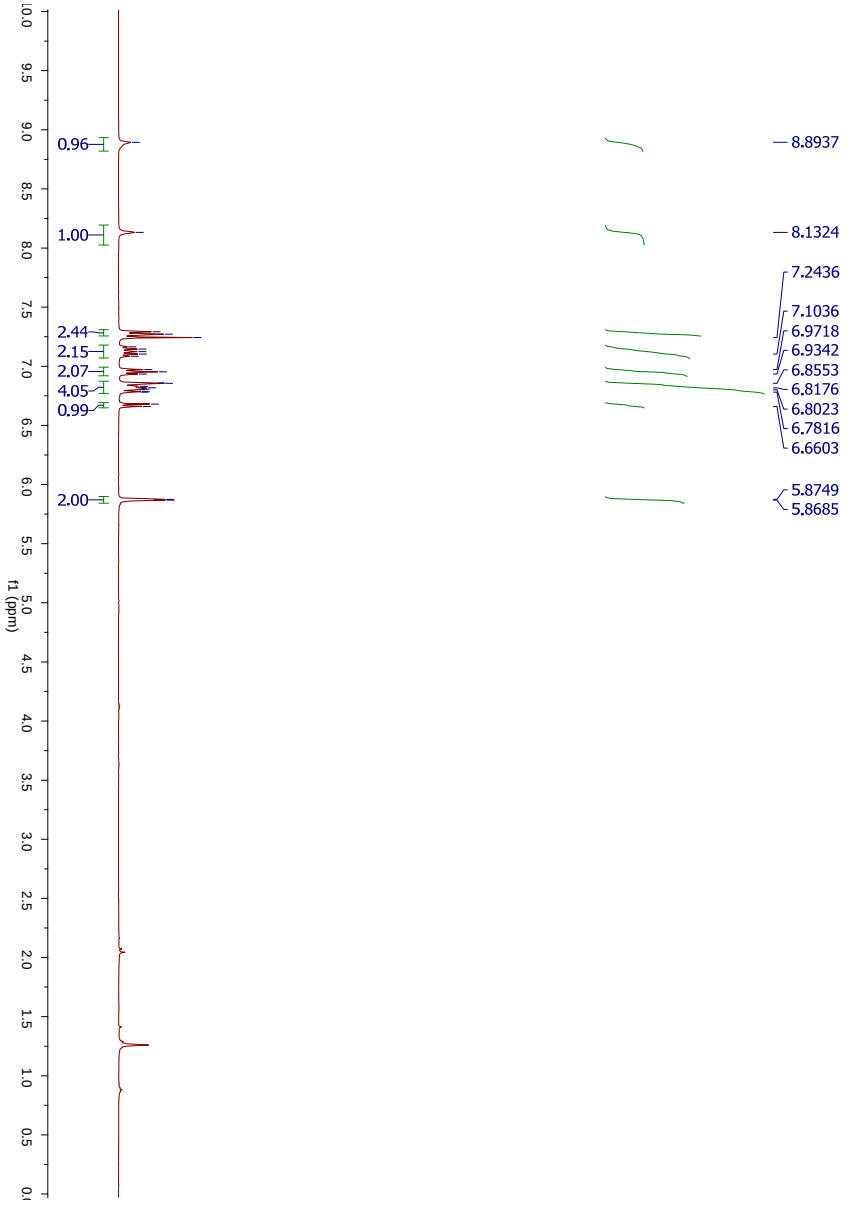


^{13}C NMR (100 MHz, $CDCl_3$) of compound ±(**16c**)

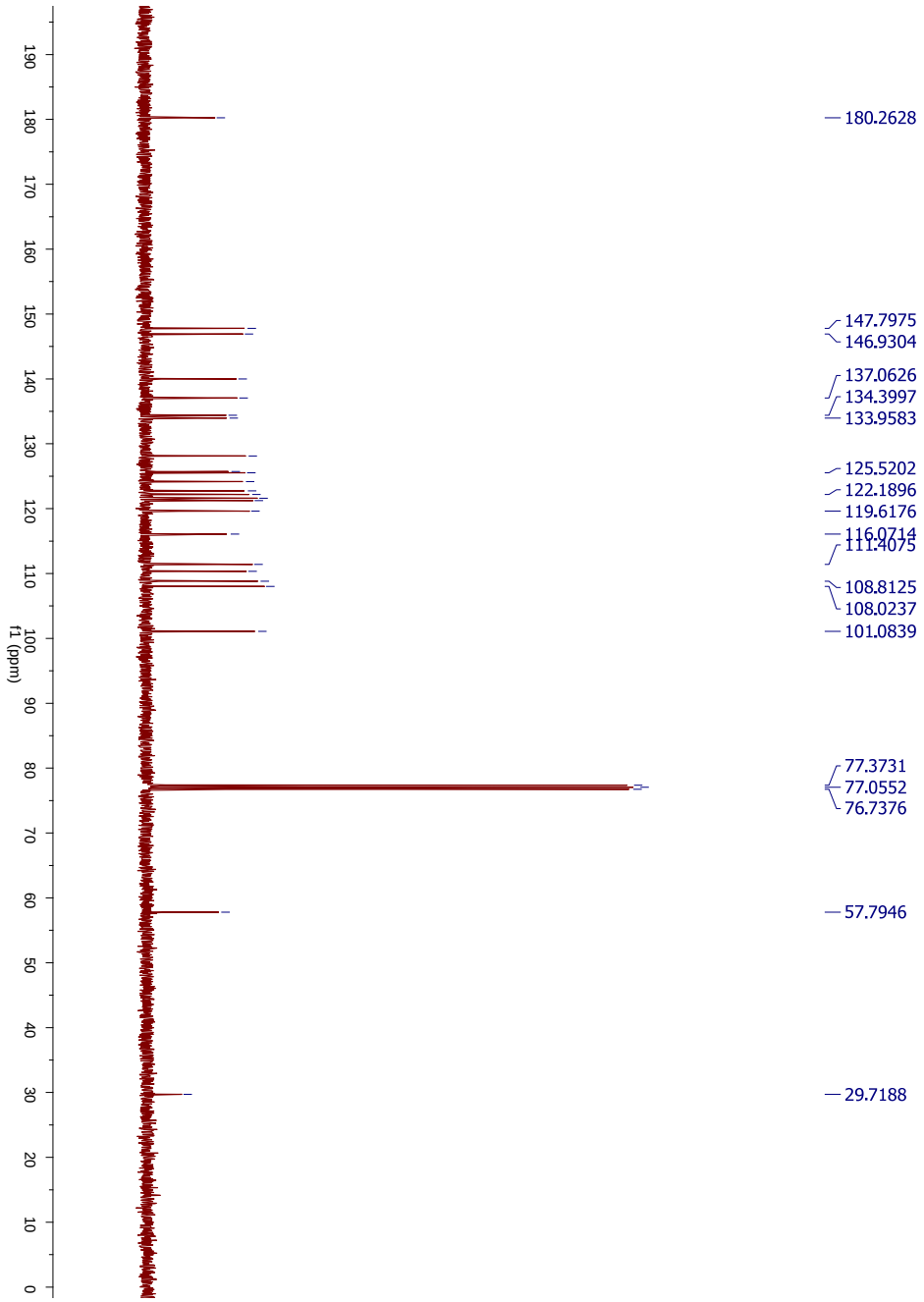


Scanned copy of mass spectrum (HRMS) of ±(**16c**)

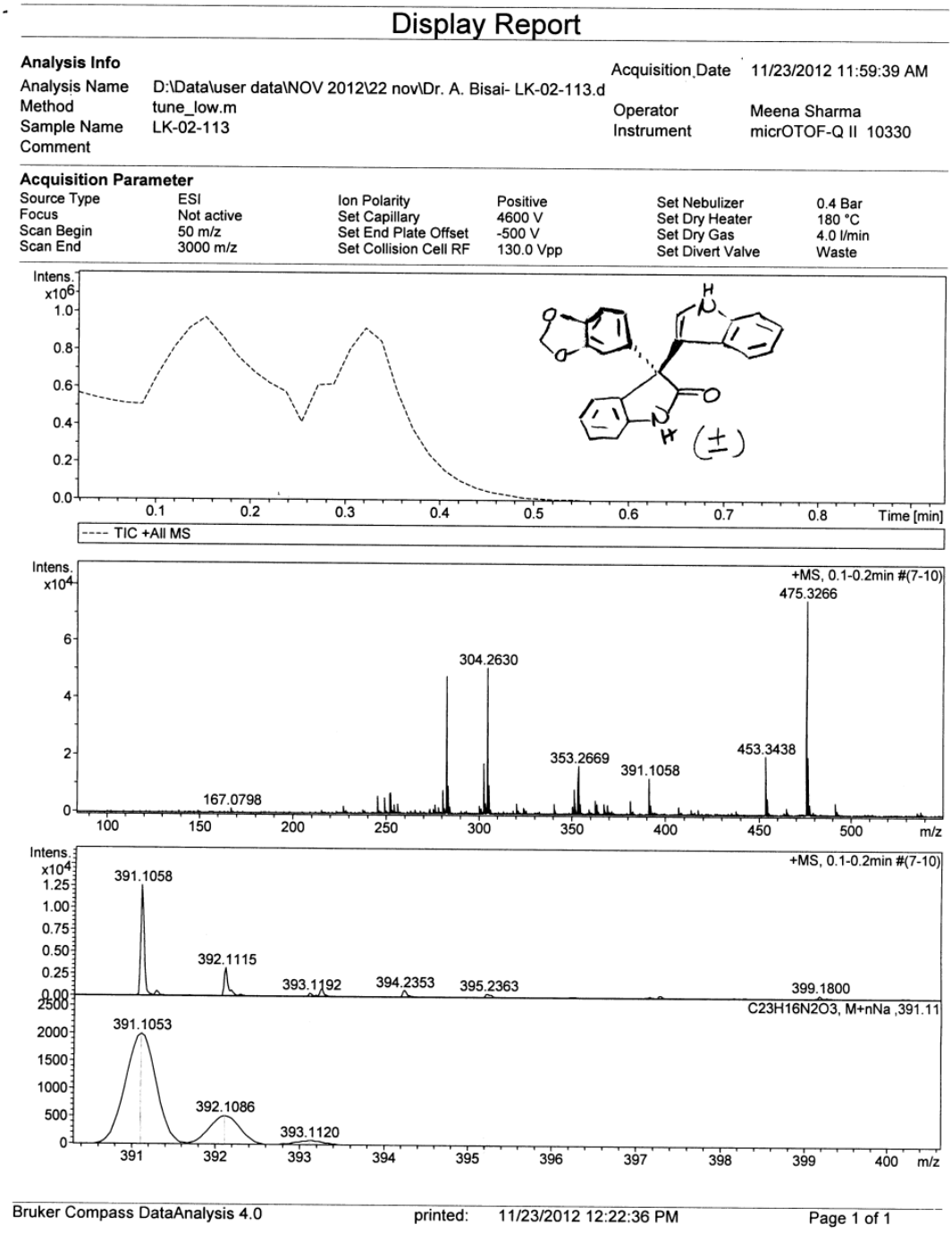




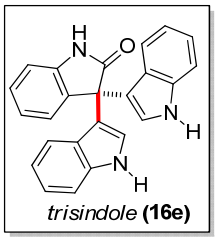
^{1}H NMR (400 MHz, $CDCl_3$) of compound ±(**16d**)

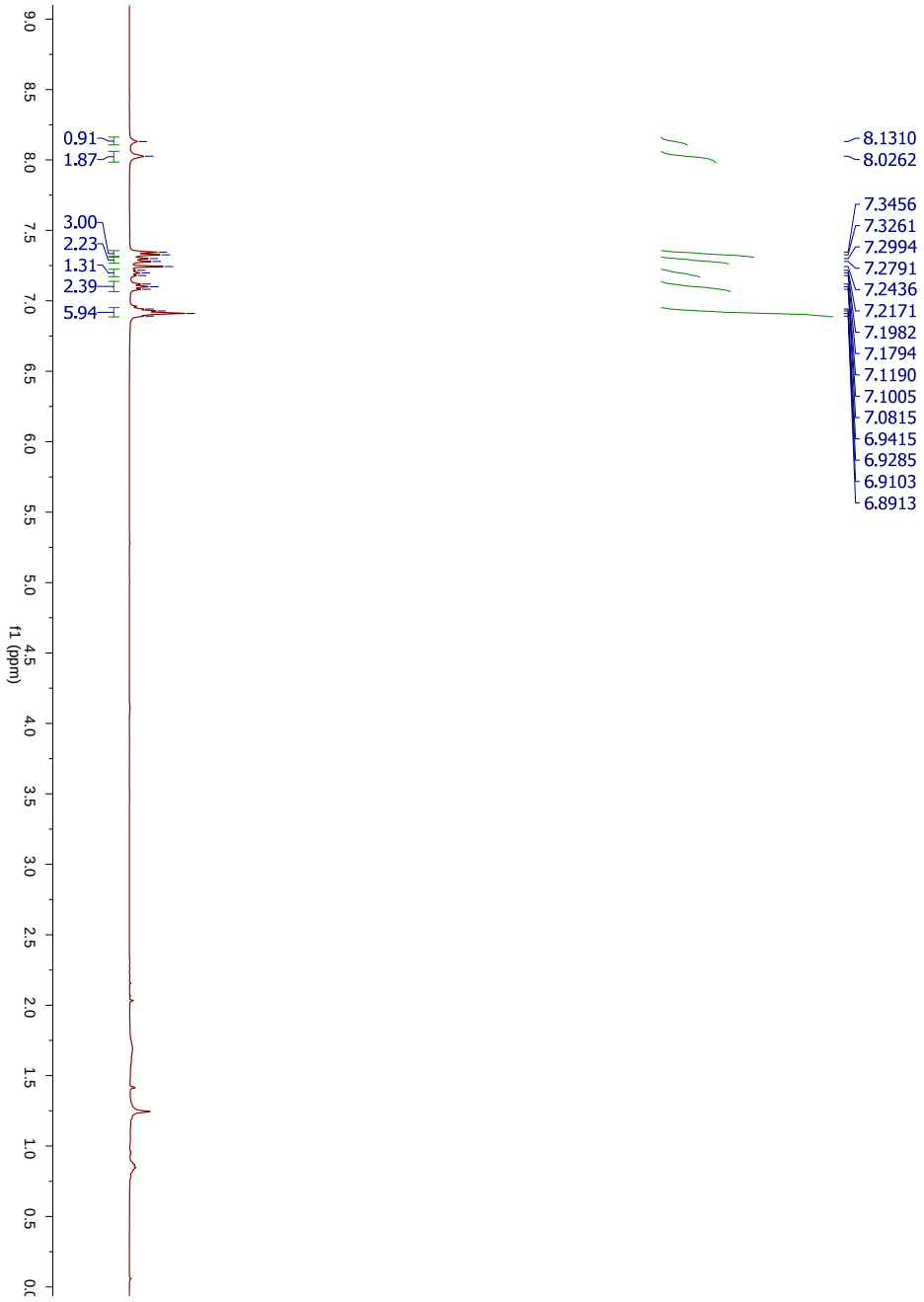


^{13}C NMR (100 MHz, $CDCl_3$) of compound ±(**16d**)

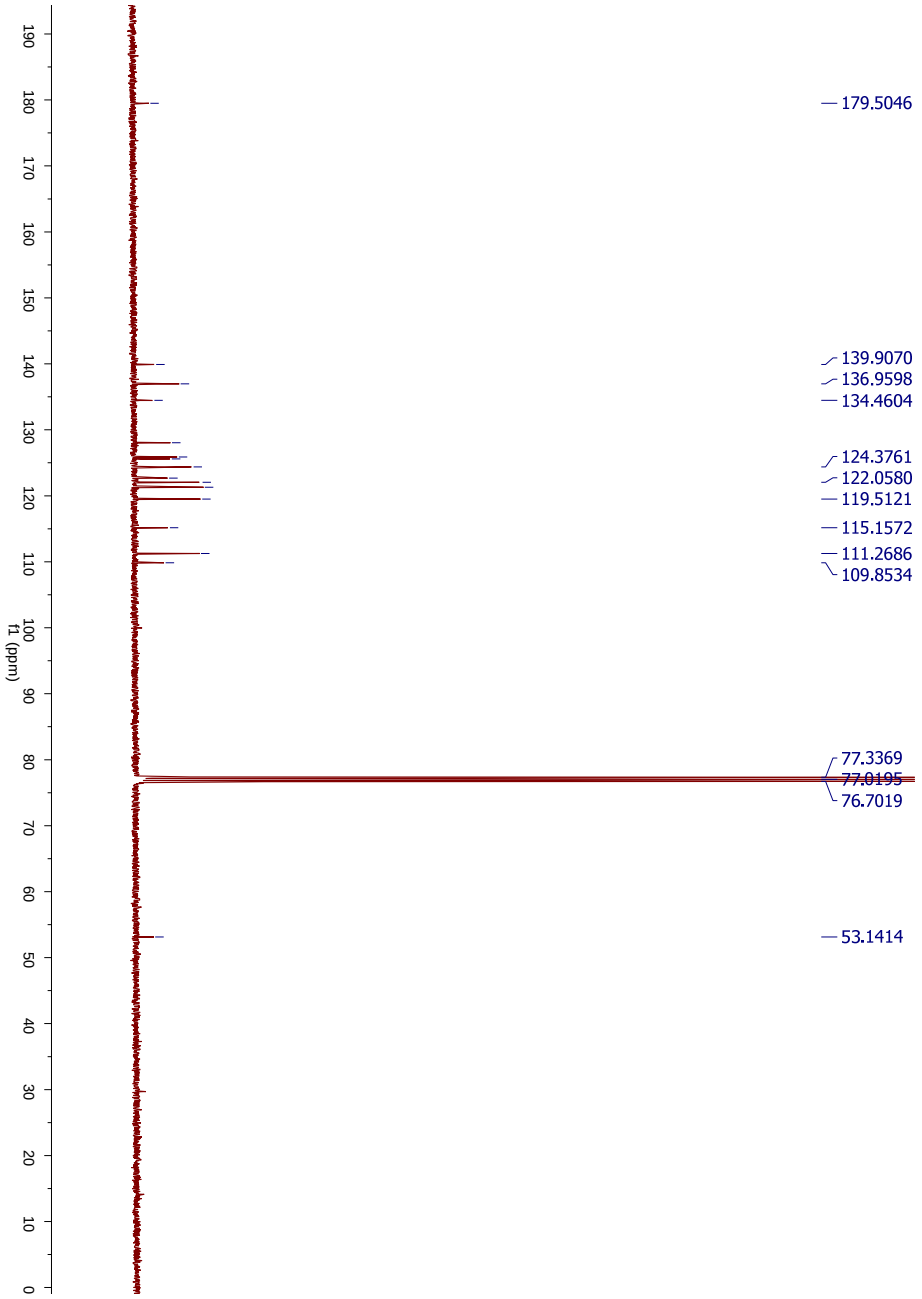


Scanned copy of mass spectrum (HRMS) of ±(**16d**)

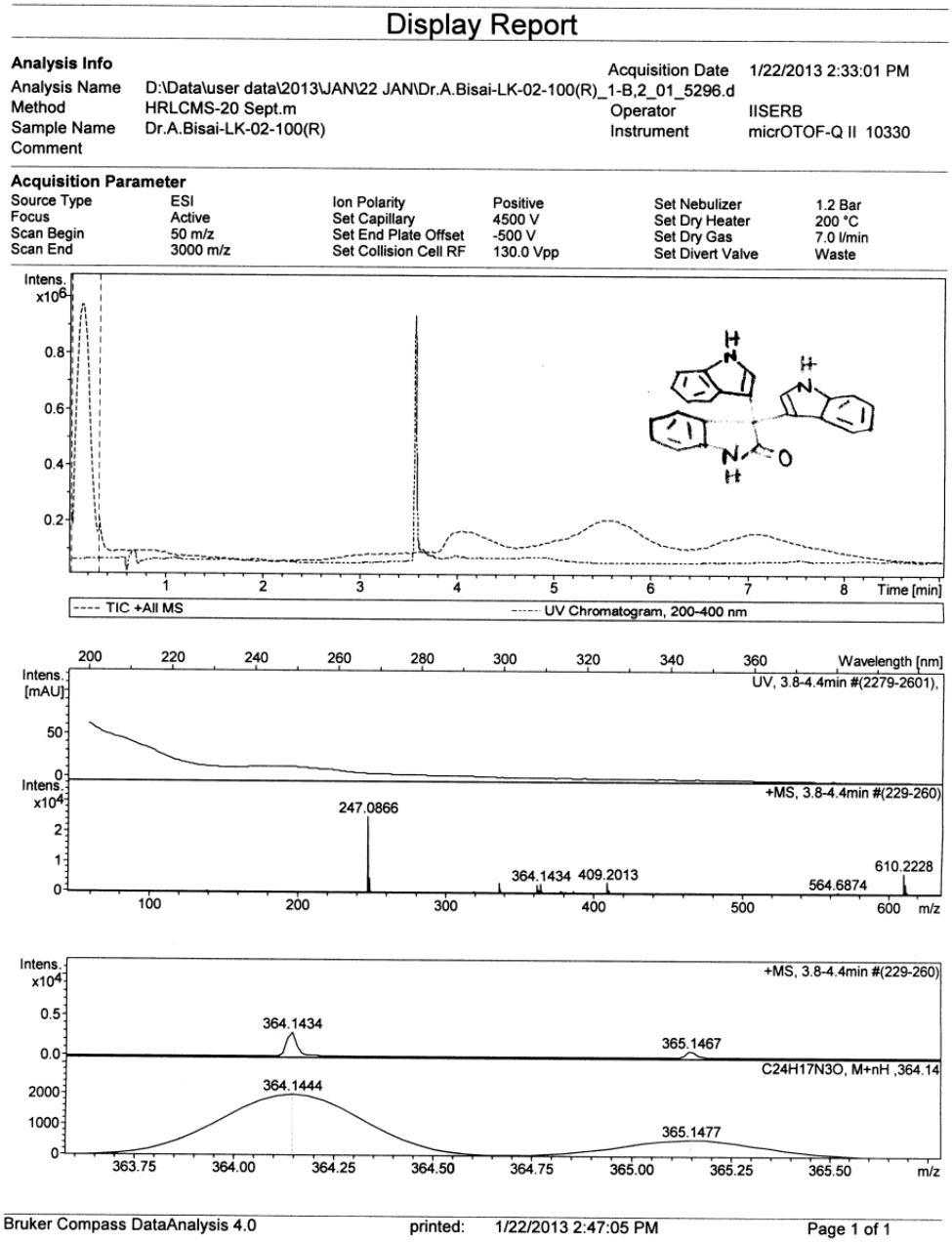




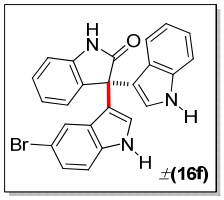
^{1}H NMR (400 MHz, $CDCl_3$) of compound (**16e**)

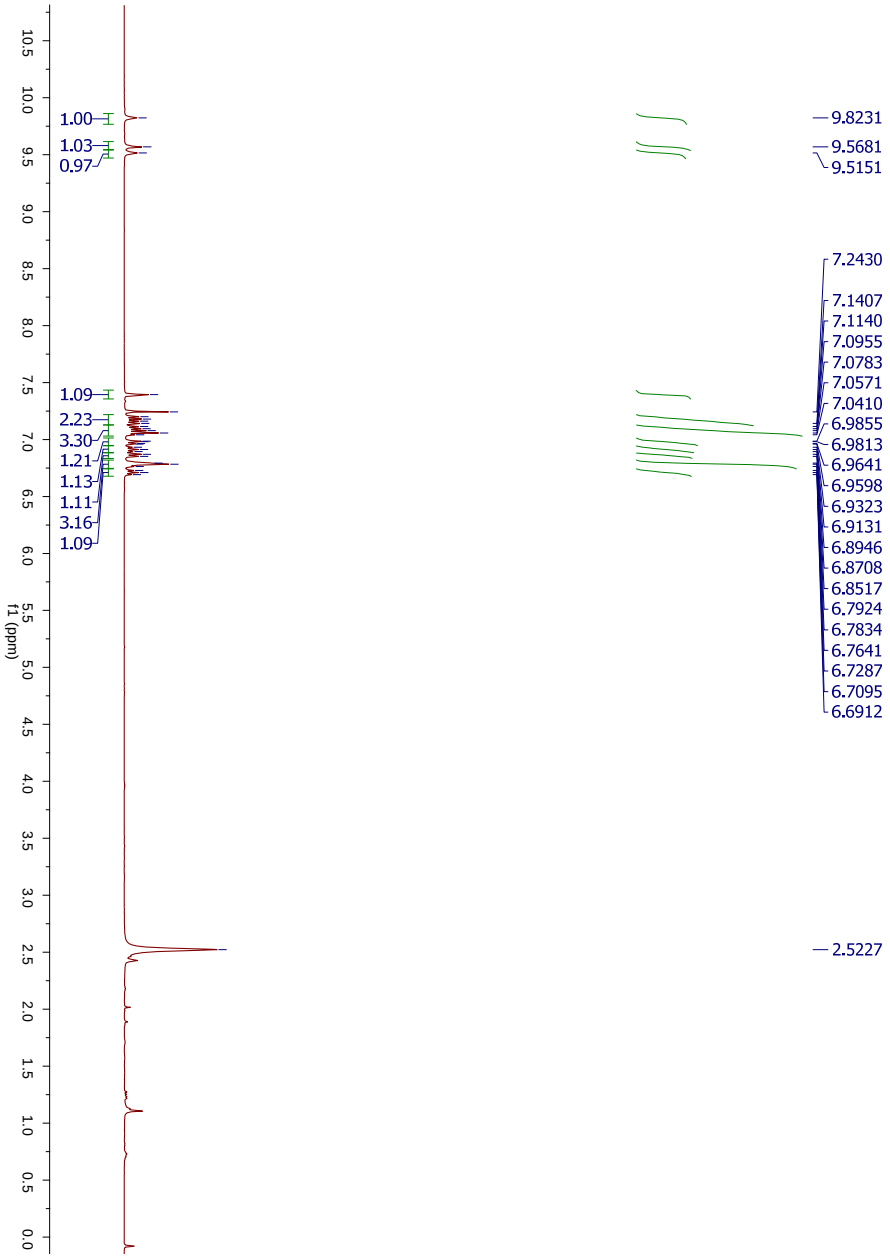


^{13}C NMR (100 MHz, $CDCl_3$) of compound (**16e**)

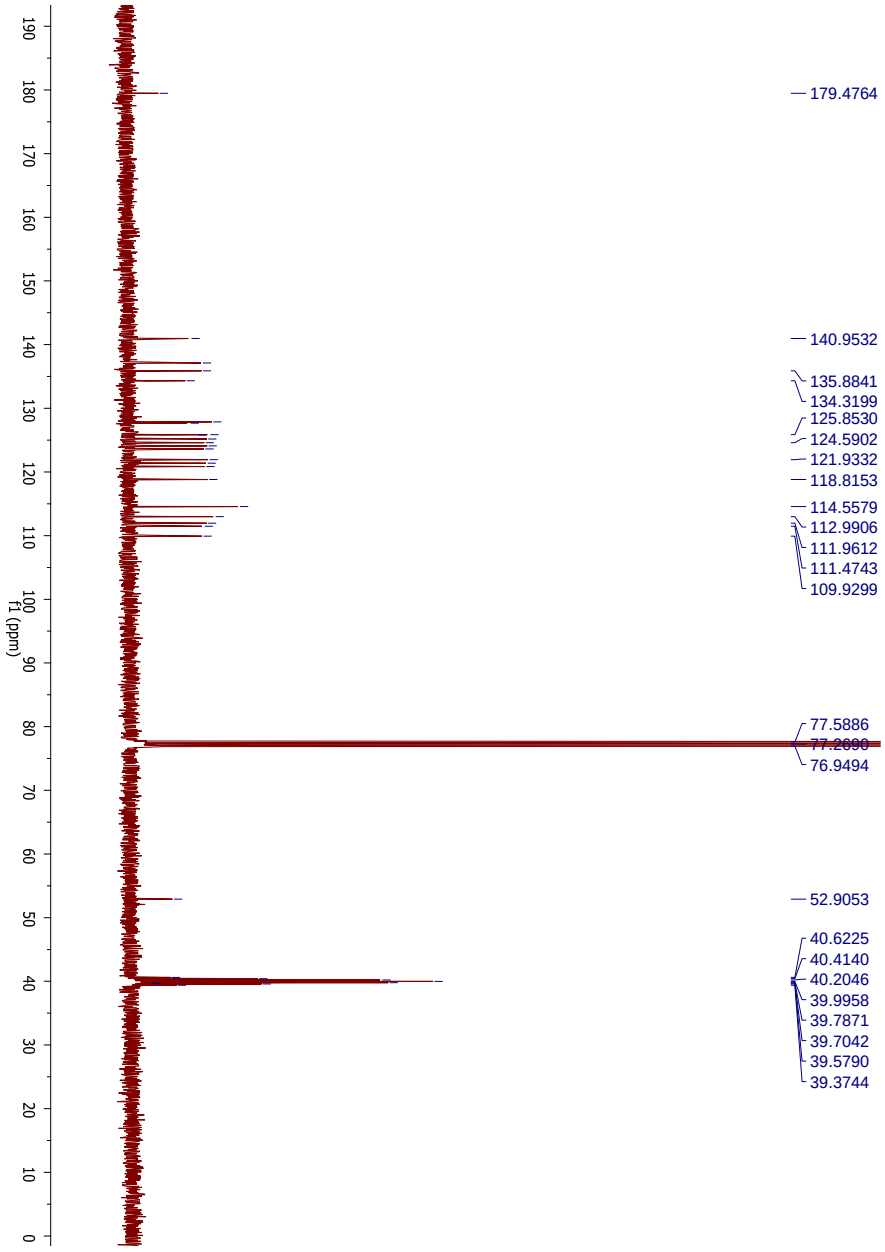


Scanned copy of mass spectrum (HRMS) of (**16e**)

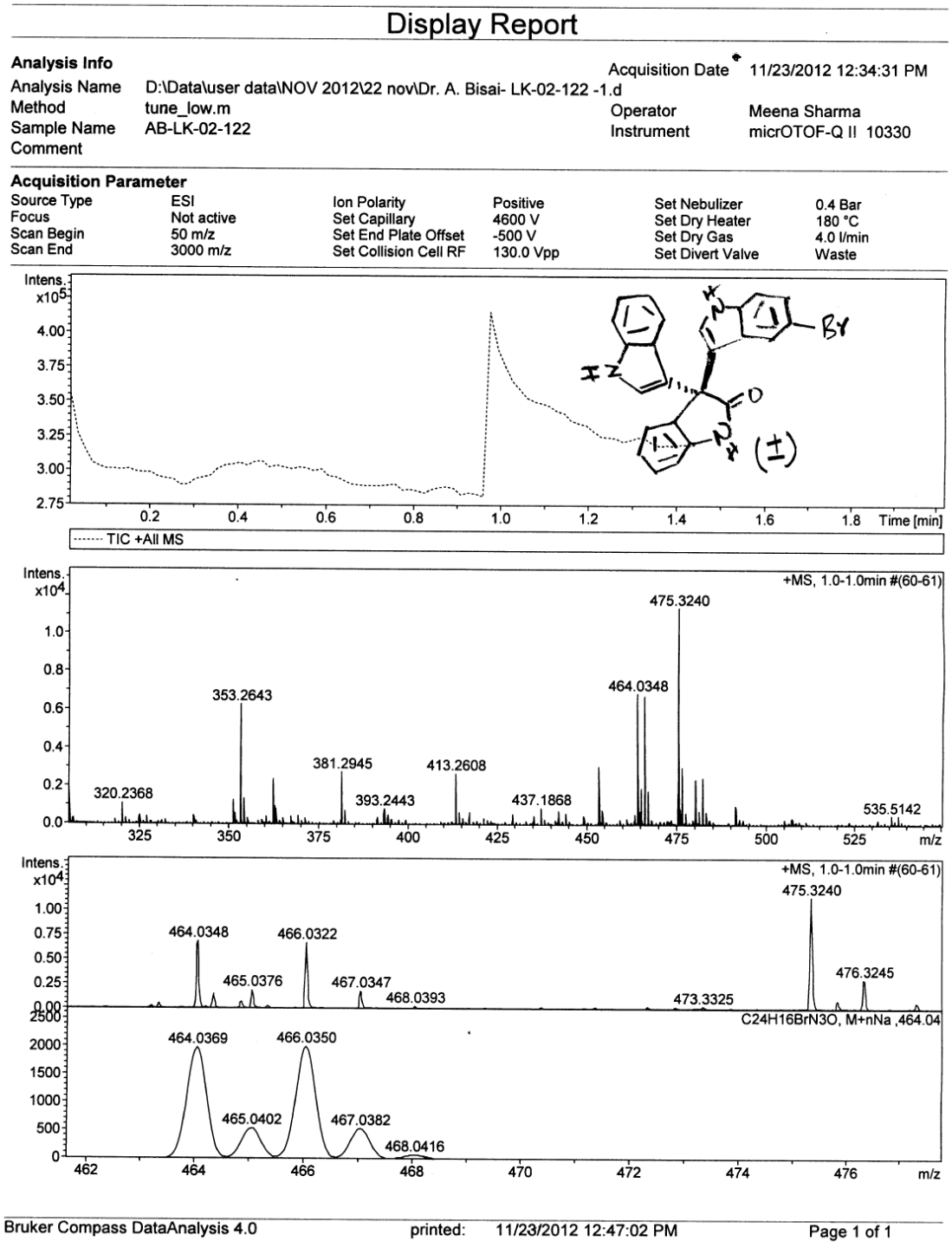




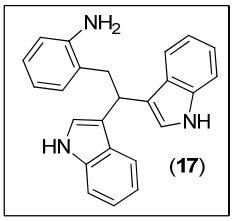
^{1}H NMR (400 MHz,0.4mL $CDCl_3$,0.1mL DMSO-D_6) of compound ±(**16f**)

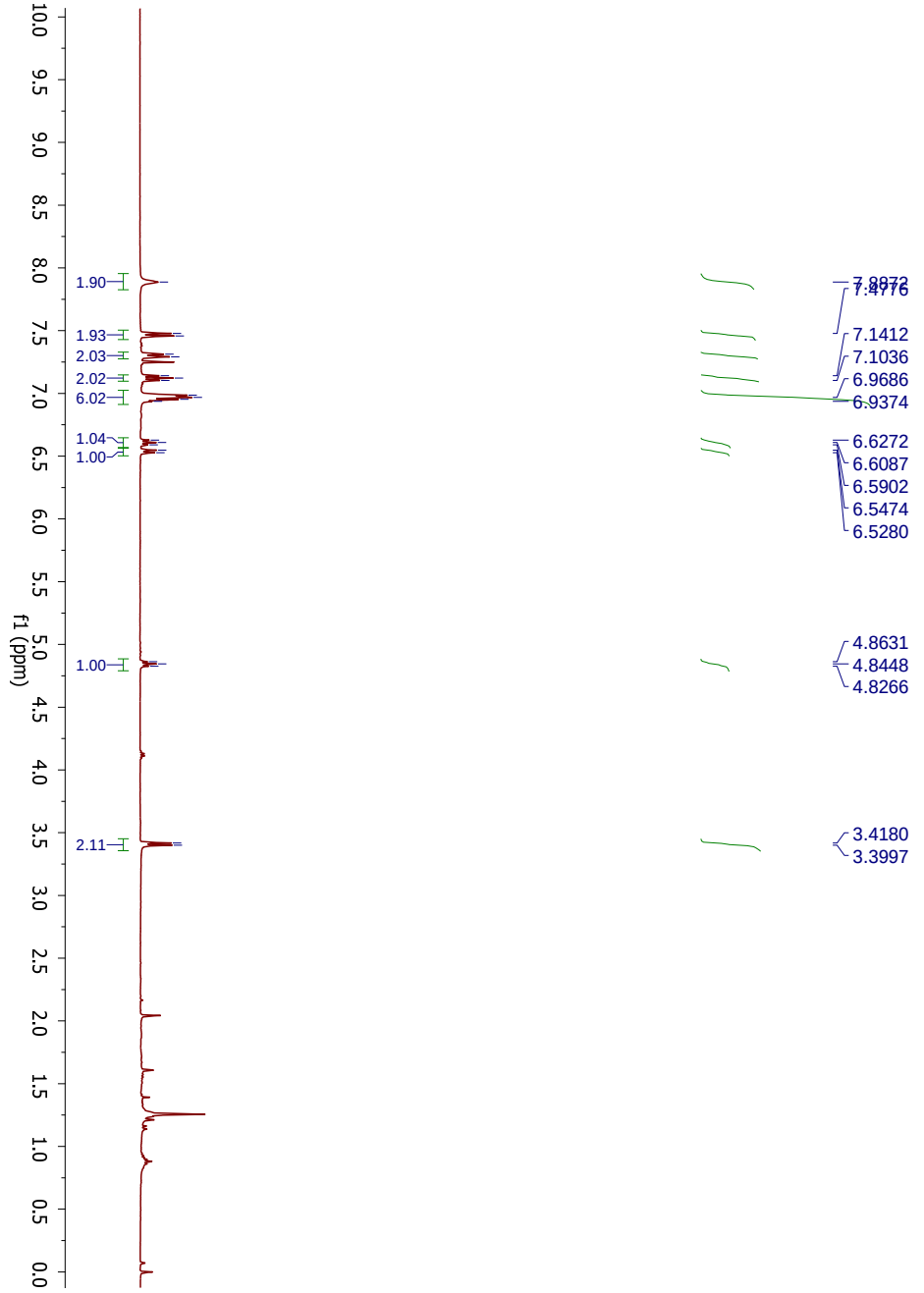


^{13}C NMR (100 MHz,0.4 mL $CDCl_3$, 0.1mL DMSO-D_6) of compound ± (**16f**)

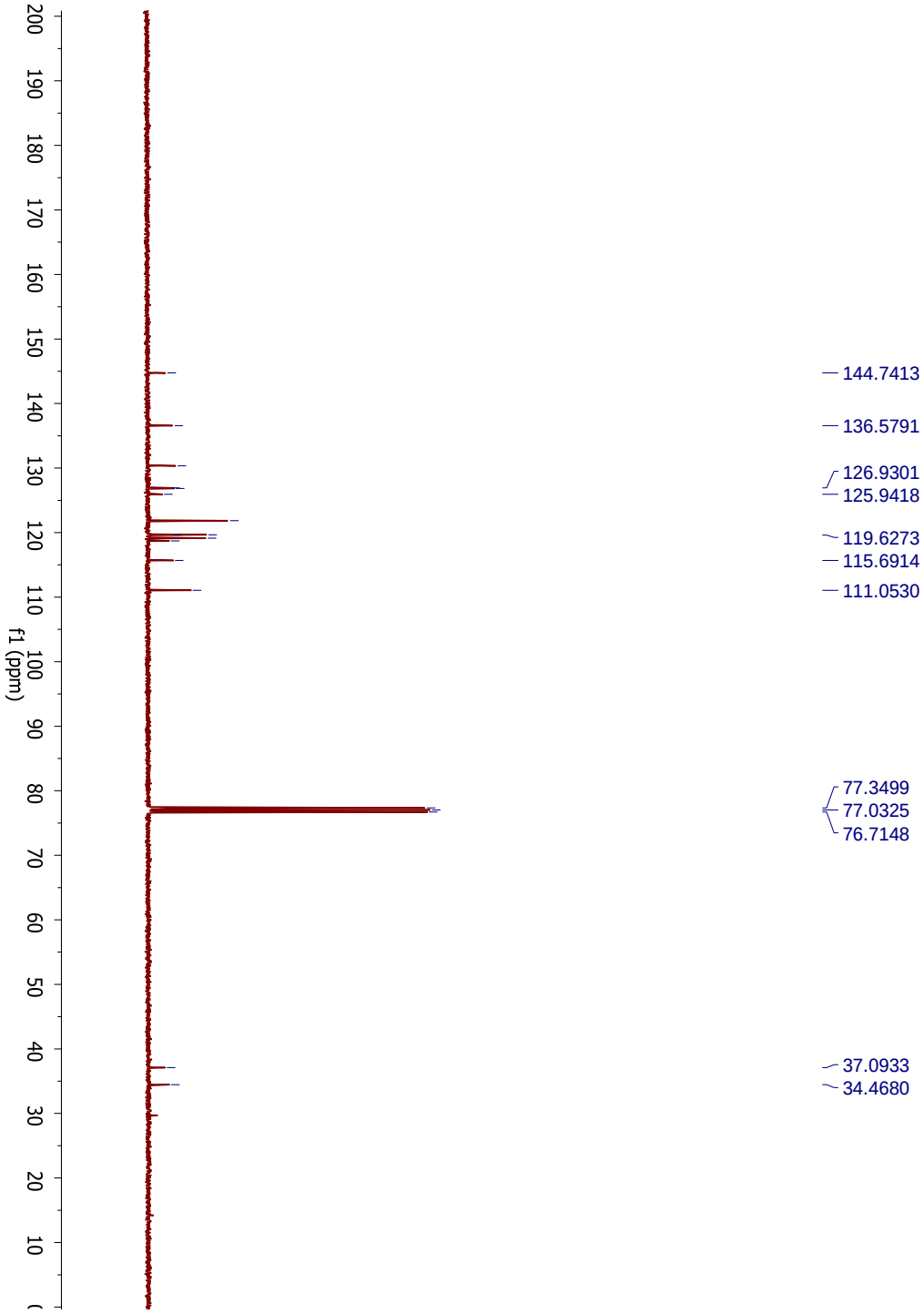


Scanned copy of mass spectrum (HRMS) of ±(**16f**)

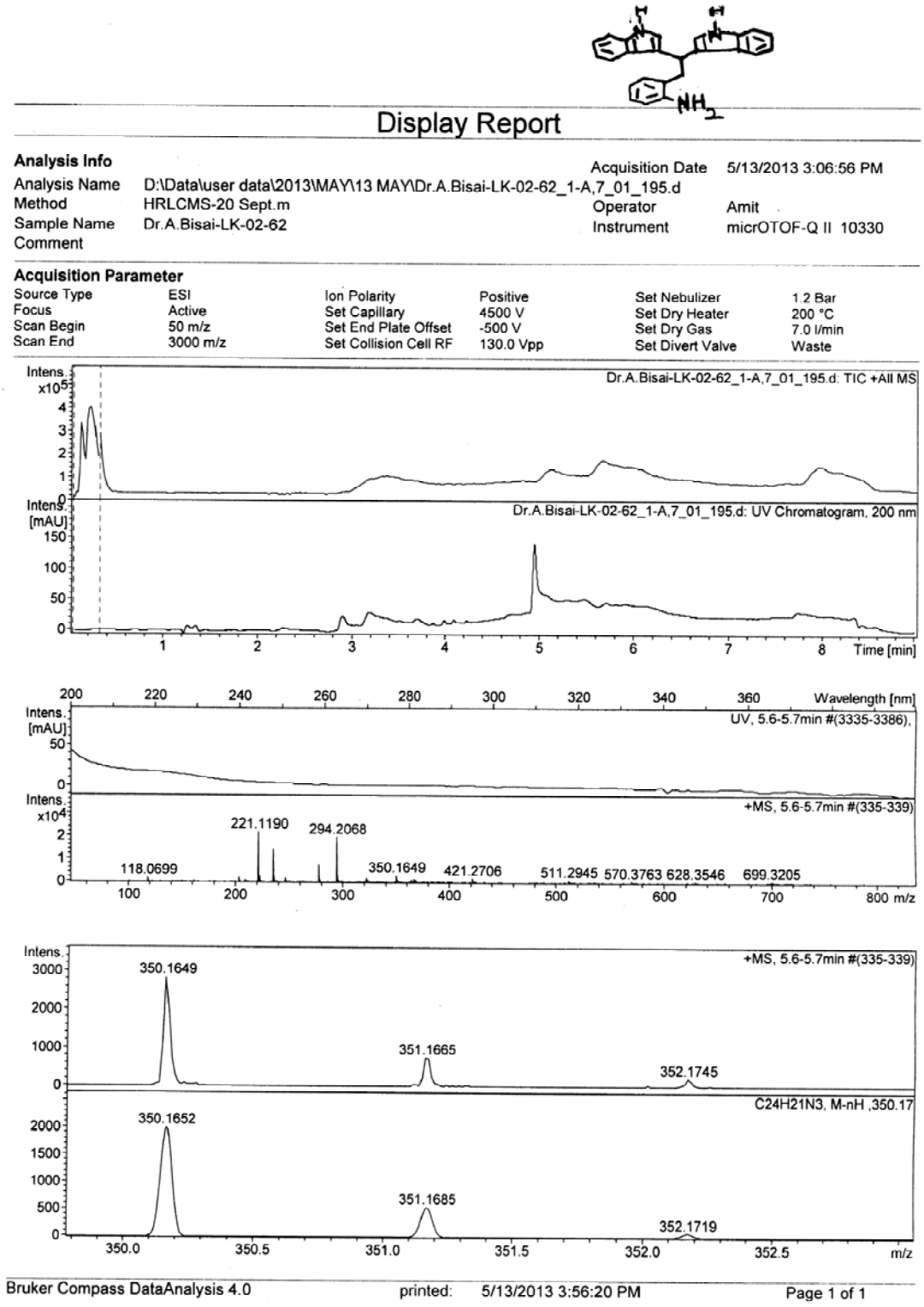




^{1}H NMR (400 MHz, $CDCl_3$) of compound (**17**)



^{13}C NMR (100 MHz, $CDCl_3$) of compound (**17**)



Scanned copy of mass spectrum of (**17**)

checkCIF/PLATON (standard)

Datablock: 12a

```
Bond precision:     C-C = 0.0033 A              Wavelength=0.71073
Cell:         a=11.245(2)    b=12.063(3)    c=13.951(3)
              alpha=90       beta=97.496(10) gamma=90
Temperature: 298 K
                    Calculated                      Reported
Volume              1876.3(7)                       1876.4(7)
Space group         P 21/n                          P 21/n
Hall group          -P 2yn                          -P 2yn
Moiety formula      C23 H19 N O3                    ?
Sum formula         C23 H19 N O3                    C23 H19 N O3
Mr                  357.39                          357.39
Dx,g cm-3           1.265                           1.265
Z                   4                               4
Mu (mm-1)           0.084                           0.084
F000                752.0                           752.0
F000'               752.35
h,k,lmax            14,15,18                        14,15,18
Nref                4514                            4382
Tmin,Tmax           0.983,0.992                     0.983,0.992
Tmin'               0.983
Correction method= MULTI-SCAN
Data completeness= 0.971       Theta(max)= 27.970
R(reflections)= 0.0460( 1743)     wR2(reflections)= 0.1303( 4382)
S = 0.839             Npar= 246
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.175
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low .... 40 Perc.
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.971
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C12
PLAT334_ALERT_2_C Small Average Benzene C-C Dist. C9 -C14 1.37 Ang.

Alert level G

PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms 1

PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c P21/n
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum .... ?
PLAT793_ALERT_4_G The Model has Chirality at C7 (Verify) .... S

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

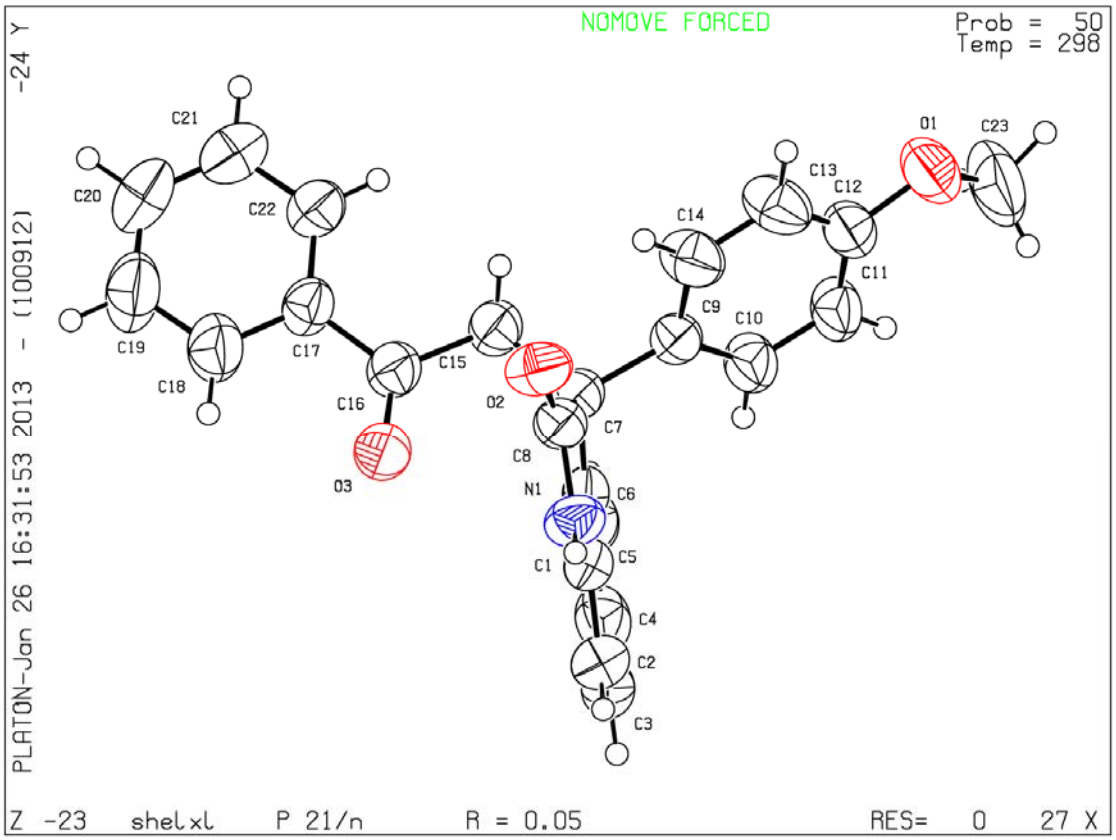
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*,*Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure thatfull publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock shelxl - ellipsoid plot (**12a**)



4/3/13 checkCIF/PLATON (standard)

checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) LAX

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: LAX

Bond precision: C-C = 0.0026 A Wavelength=0.71073

Cell: a=10.8852(16) b=12.4799(18) c=13.7493(18)
alpha=90 beta=103.481(5) gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	1816.3(4)	1816.3(4)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C23 H17 N O4	?
Sum formula	C23 H17 N O4	C23 H17 N O4
Mr	371.38	371.38
Dx,g cm-3	1.358	1.358
Z	4	4
Mu (mm-1)	0.094	0.094
F000	776.0	776.0
F000'	776.39	
h,k,lmax	14,16,18	14,16,18
Nref	4692	4679
Tmin,Tmax	0.991,0.991	0.991,0.991
Tmin'	0.991	

Correction method= MULTI-SCAN

Data completeness= 0.997 Theta(max)= 28.700

R(reflections)= 0.0513(3091) wR2(reflections)= 0.1388(4679)

S = 1.038 Npar= 253

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for O1
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 3.267
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) 2
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 4

Alert level G

PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms 1
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c P21/n
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum .... ?
PLAT793_ALERT_4_G The Model has Chirality at C5 (Verify) .... S
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 7

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1 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additionall measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the

vm02b.iucr.org/cgi-bin/checkcif_hkl.pl 1/3

Datablock shelxl - ellipsoid plot (**12b**)

individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

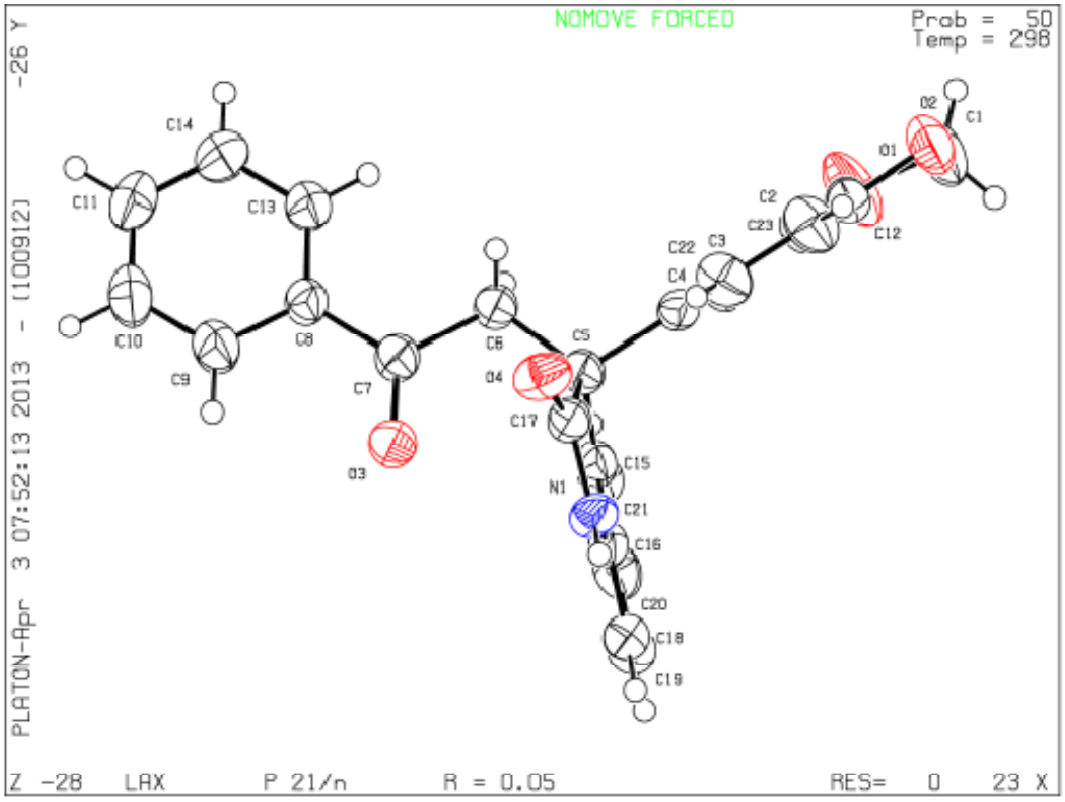
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock LAX - ellipsoid plot



CheckCIF data of 17

Datablock: 17

```
Bond precision:     C-C = 0.0050 A              Wavelength=0.71073
Cell:       a=6.7467(4)    b=12.8110(7)   c=21.6174(13)
            alpha=90       beta=90        gamma=90
Temperature: 298 K
                  Calculated                      Reported
Volume            1868.43(19)                     1868.43(19)
Space group       P 21 21 21                      P 21 21 21
Hall group        P 2ac 2ab                       P 2ac 2ab
Moiety formula    C24 H21 N3                      ?
Sum formula       C24 H21 N3                      C24 H21 N3
Mr                351.44                          351.44
Dx,g cm-3         1.249                           1.249
Z                 4                               4
Mu (mm-1)         0.074                           0.074
F000              744.0                           744.0
F000'             744.24
h,k,lmax          9,17,29                         9,17,29
Nref              5022[ 2872]                     5021
Tmin,Tmax         0.996,0.996                     0.993,0.996
Tmin'             0.993
Correction method= MULTI-SCAN
Data completeness= 1.75/1.00   Theta(max)= 29.130
R(reflections)= 0.0706( 2663)     wR2(reflections)= 0.1849( 5021)
S = 1.025             Npar= 244
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT230_ALERT_2_B Hirshfeld Test Diff for N2 -- C16 .. 7.5 su

Alert level C

And 3 other PLAT230 Alerts
More ...
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C22
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C19
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0050 Ang
PLAT420_ALERT_2_C D-H Without Acceptor N1 - H1 ... ?
And 2 other PLAT420 Alerts
More ...

Alert level G

PLAT007_ALERT_5_G Note: Number of Unrefined Donor-H Atoms 4

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or
oversight
   1 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or
deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

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Publication of your CIF in other journals

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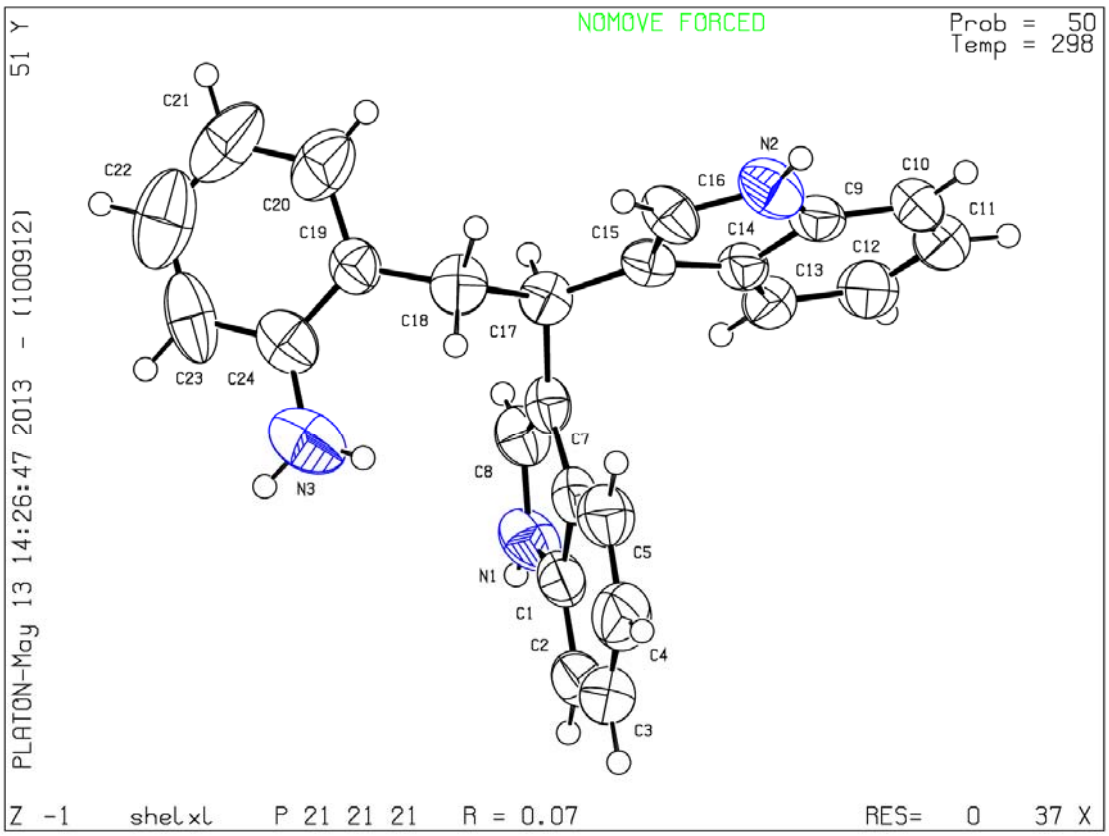
PLATON version of 24/04/2013; check.def file version of 23/04/2013
Datablock 18 - ellipsoid plot


NOMOVE FORCED
Prob = 50
Temp = 298
51 Y
PLATON-May 13 14:26:47 2013 - (100912)
C21
C22
C20
C19
C18
C17
C16
N2
C10
C9
C11
C15
C14
C12
C13
C23
C24
N3
C7
C8
N1
C5
C1
C2
C4
C3
Z -1
shelxl
P 21 21 21
R = 0.07
RES= 0 37 X