

Supporting information for

Synthesis of Imidazoles via Cascade Reaction of Nitroallylic Acetates with Amidines and Studies on Their Trypanocidal Activity

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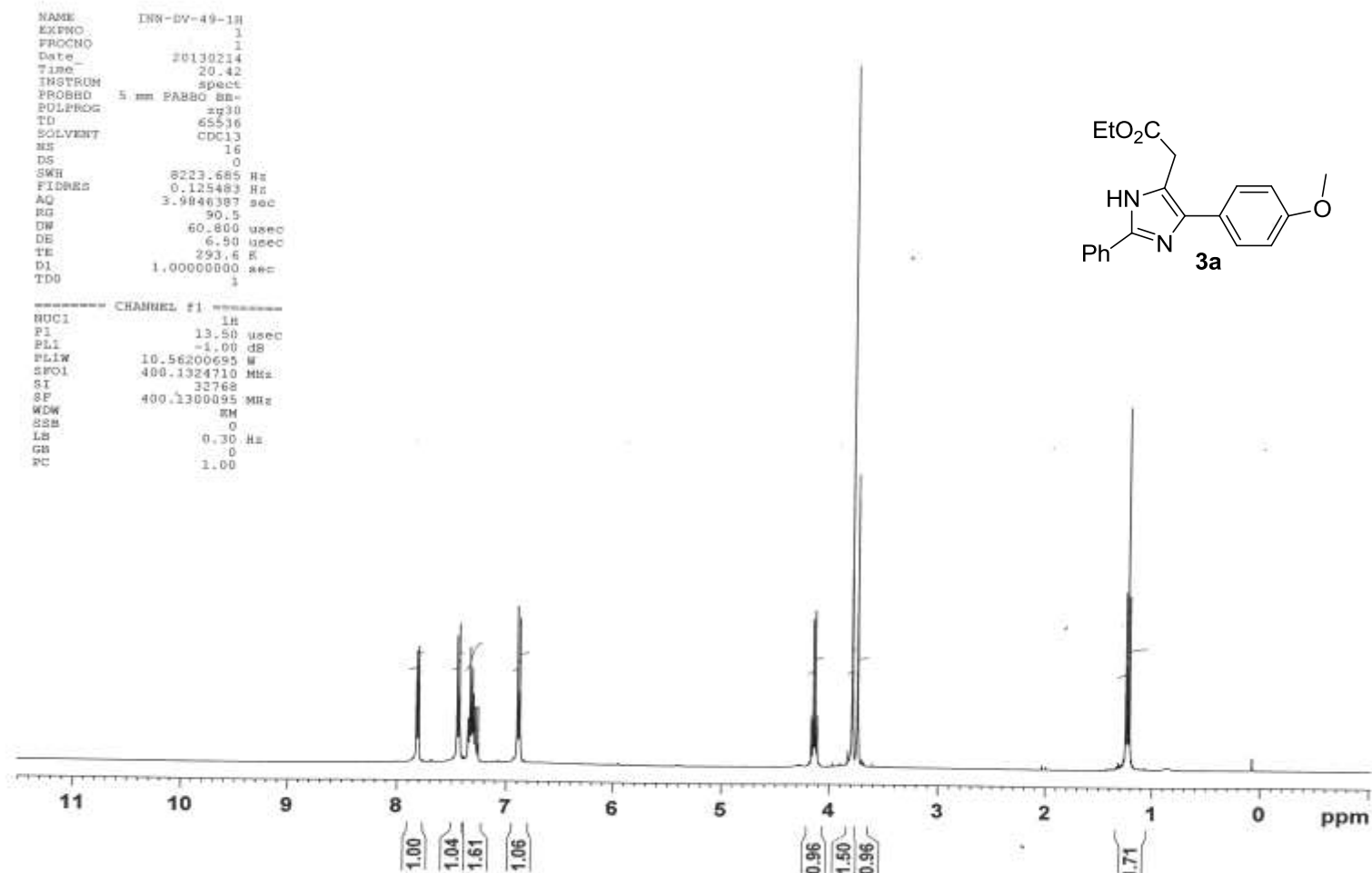


Figure S1. ^1H NMR spectrum of **3a**

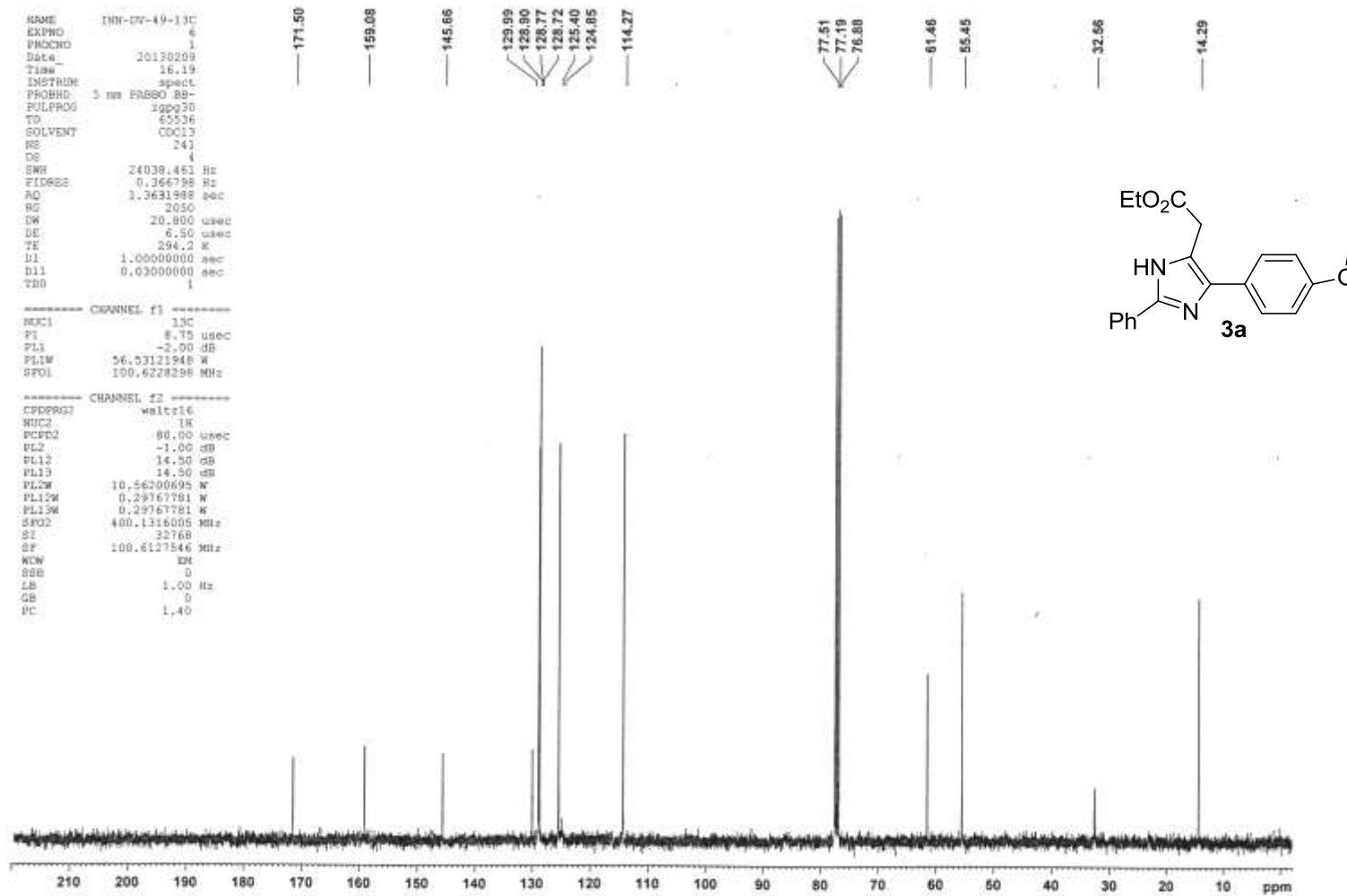


Figure S2. ^{13}C NMR spectrum of **3a**

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Analysis Info

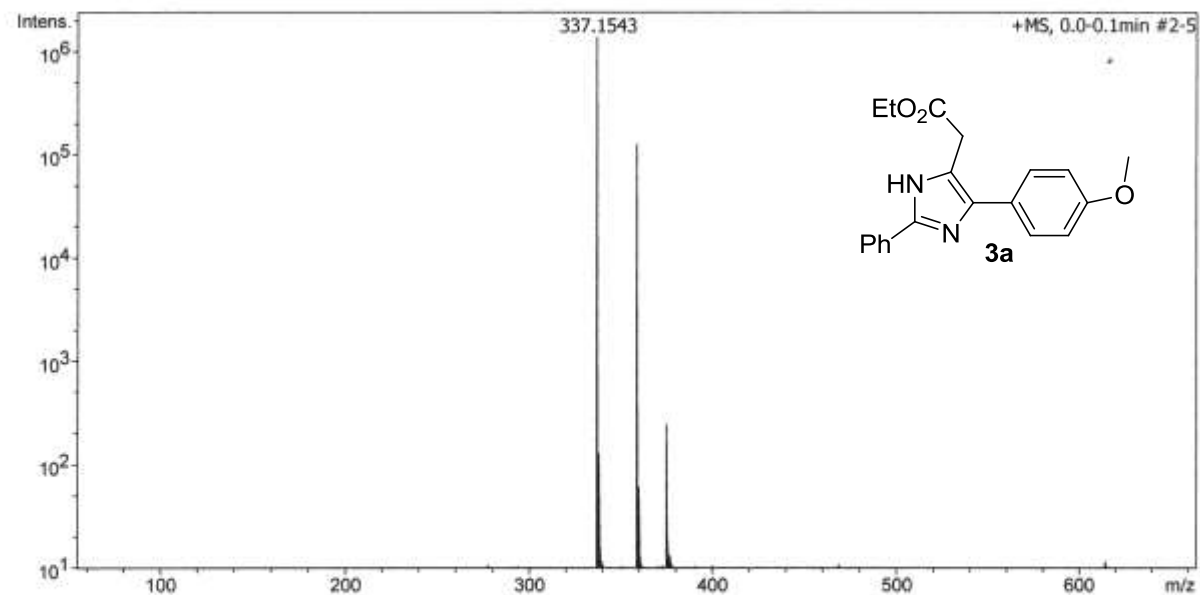
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Operator IIT-B
 Instrument maXis impact 282001.00081

Acquisition Parameter

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Scan End	1000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
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Figure S3. HRMS spectrum of **3a**

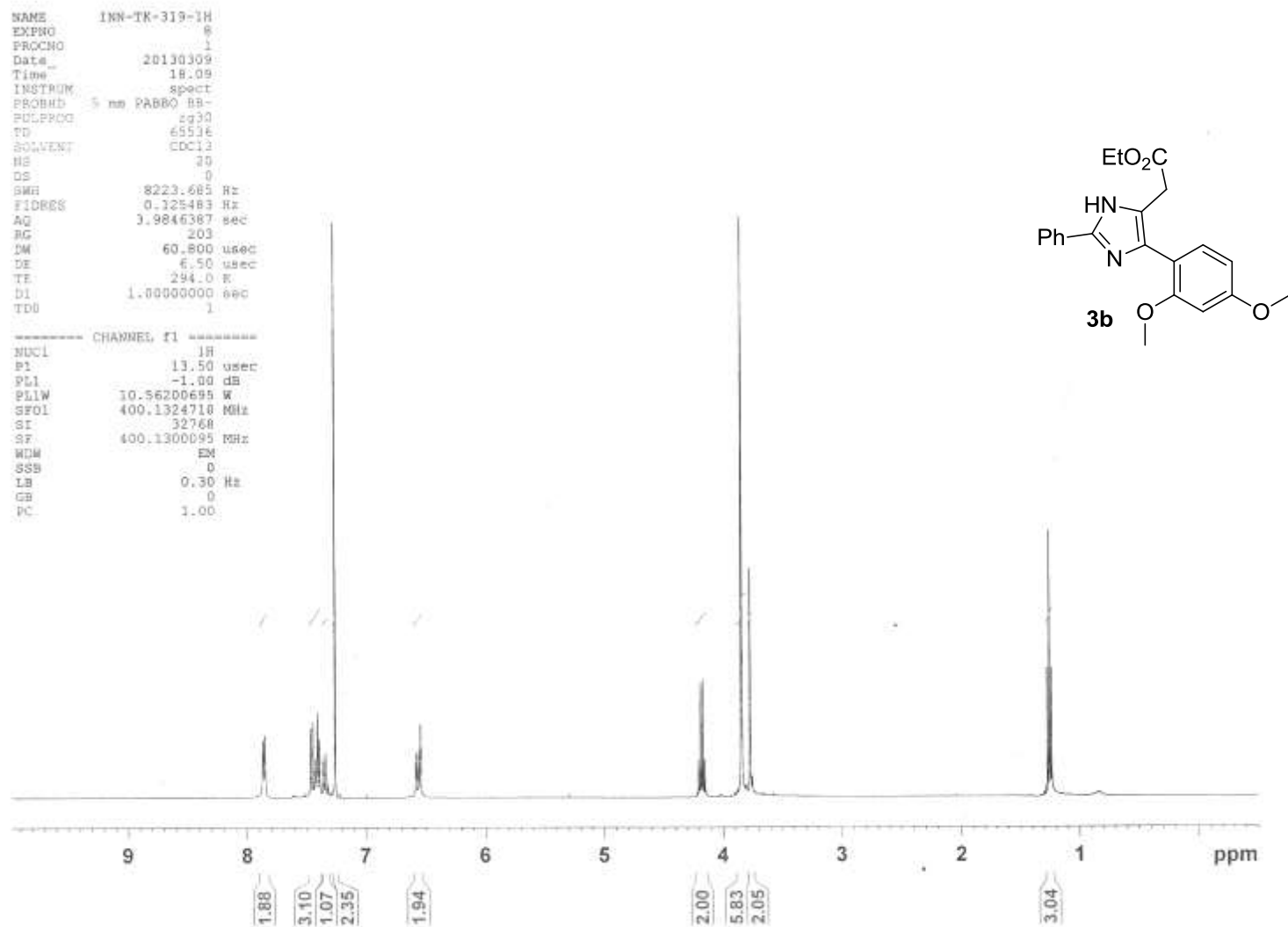


Figure S4. ^1H NMR spectrum of **3b**

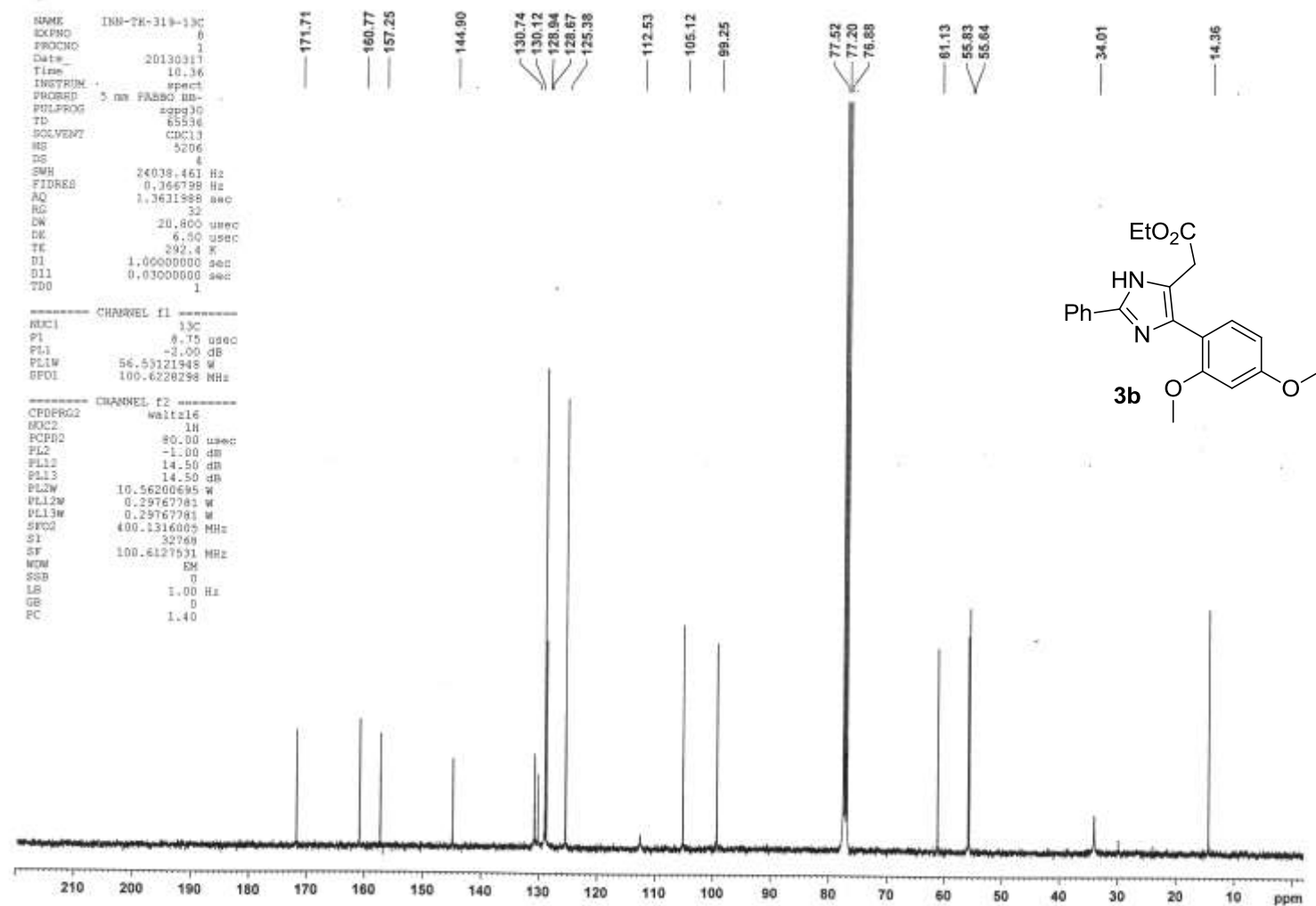


Figure S5. ¹³C NMR spectrum of **3b**

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Analysis Info

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Acquisition Date 3/15/2013 3:44:51 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

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Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source

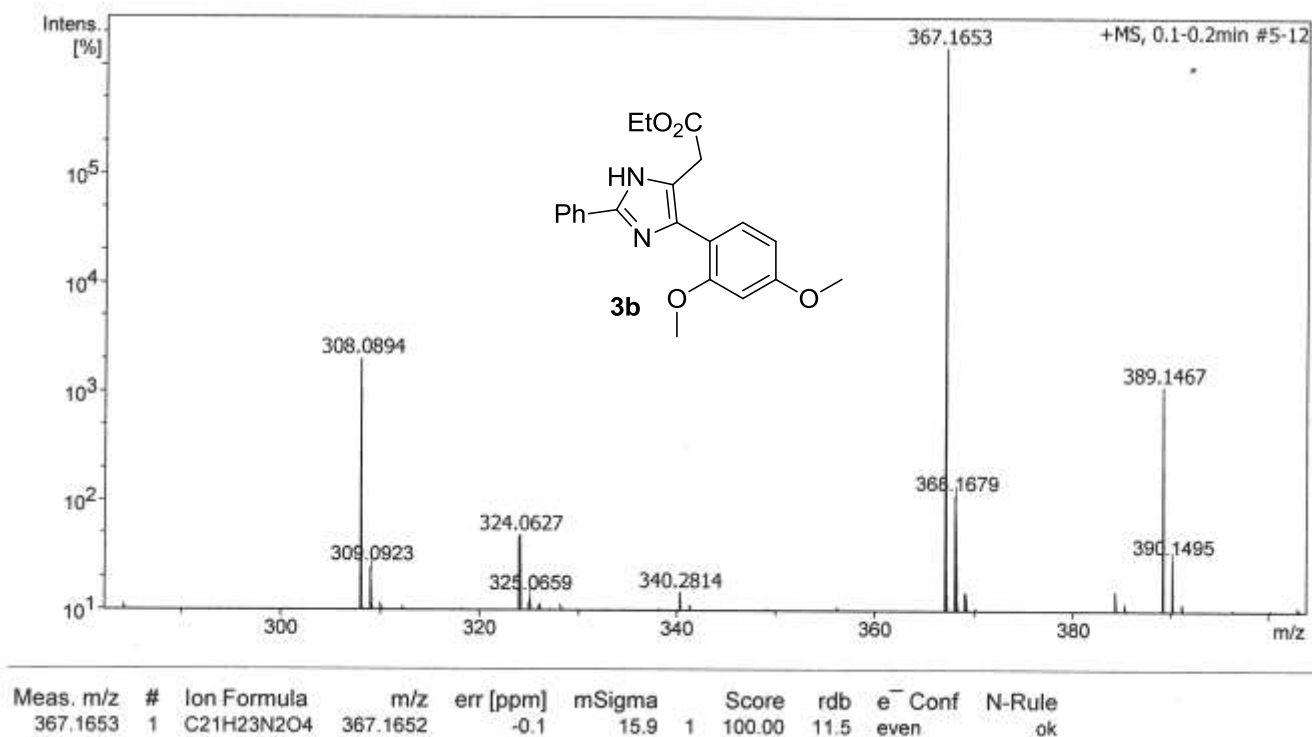


Figure S6. HRMS spectrum of **3b**

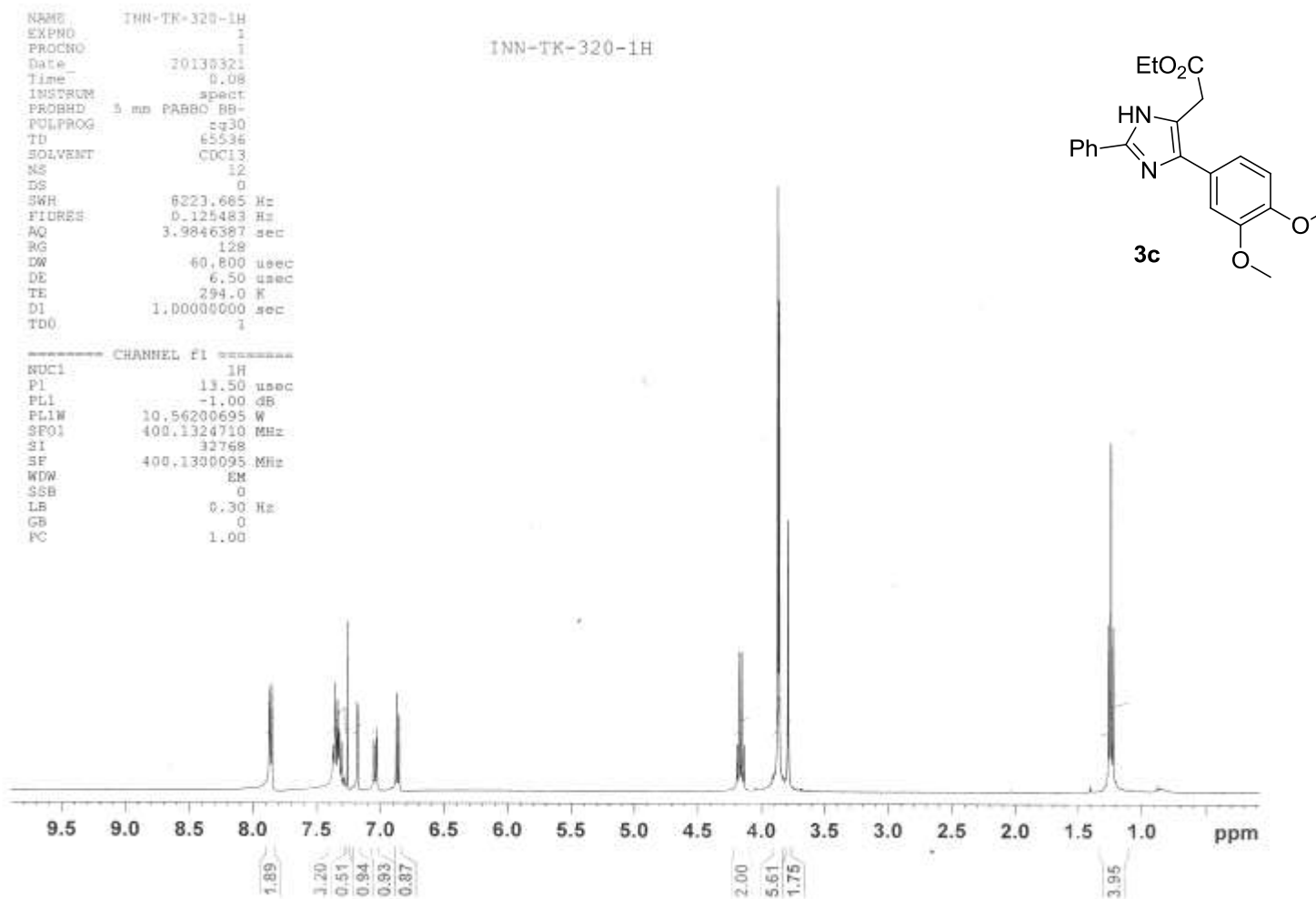


Figure S7. ^1H NMR spectrum of **3c**

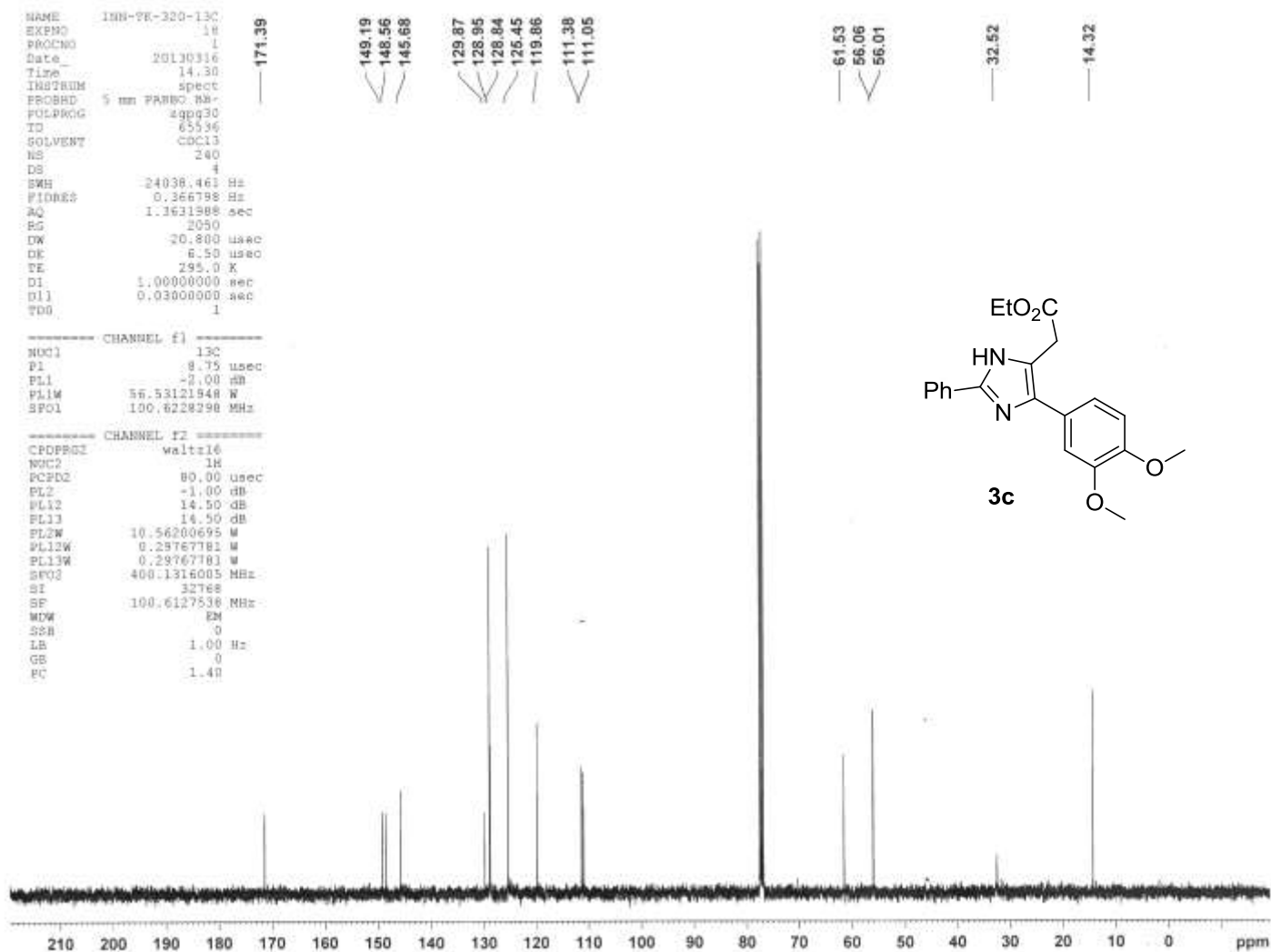


Figure S8. ¹³C NMR spectrum of **3c**

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Analysis Info

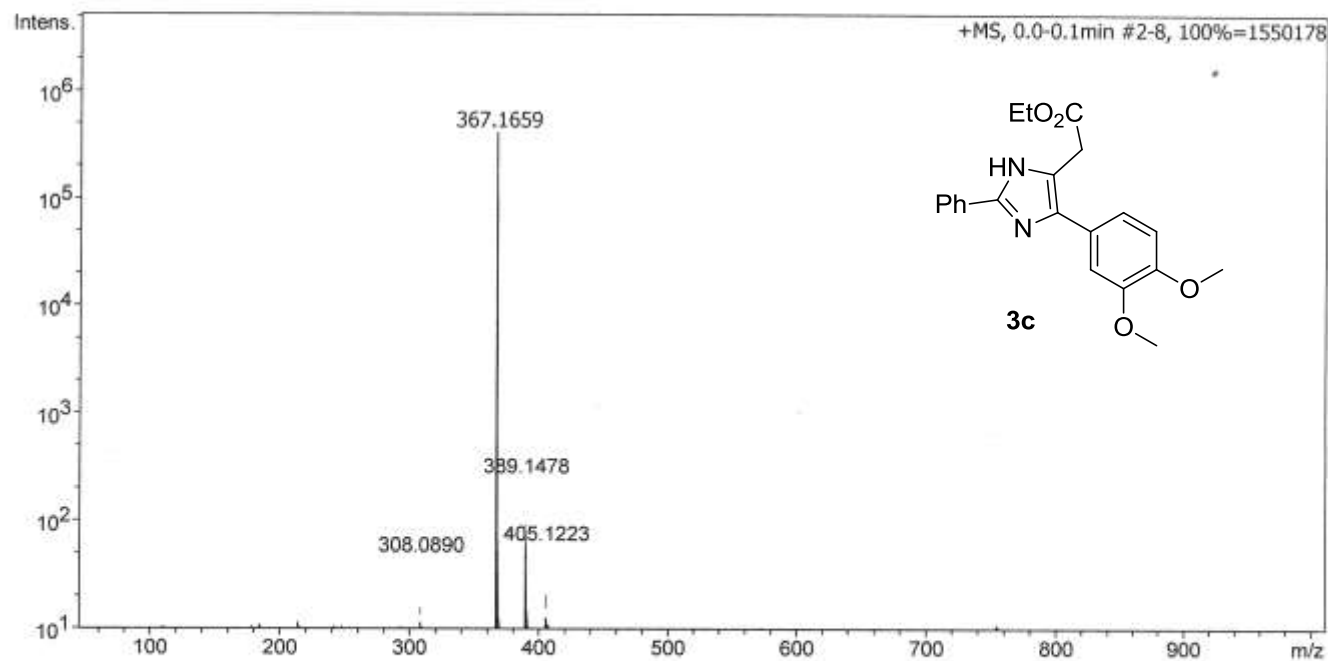
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Acquisition Date 6/10/2013 6:03:19 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

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Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
367.1659	1	C21H23N2O4	367.1652	-1.9	30.3	1	100.00	11.5	even	ok

Figure S9. HRMS spectrum of **3c**

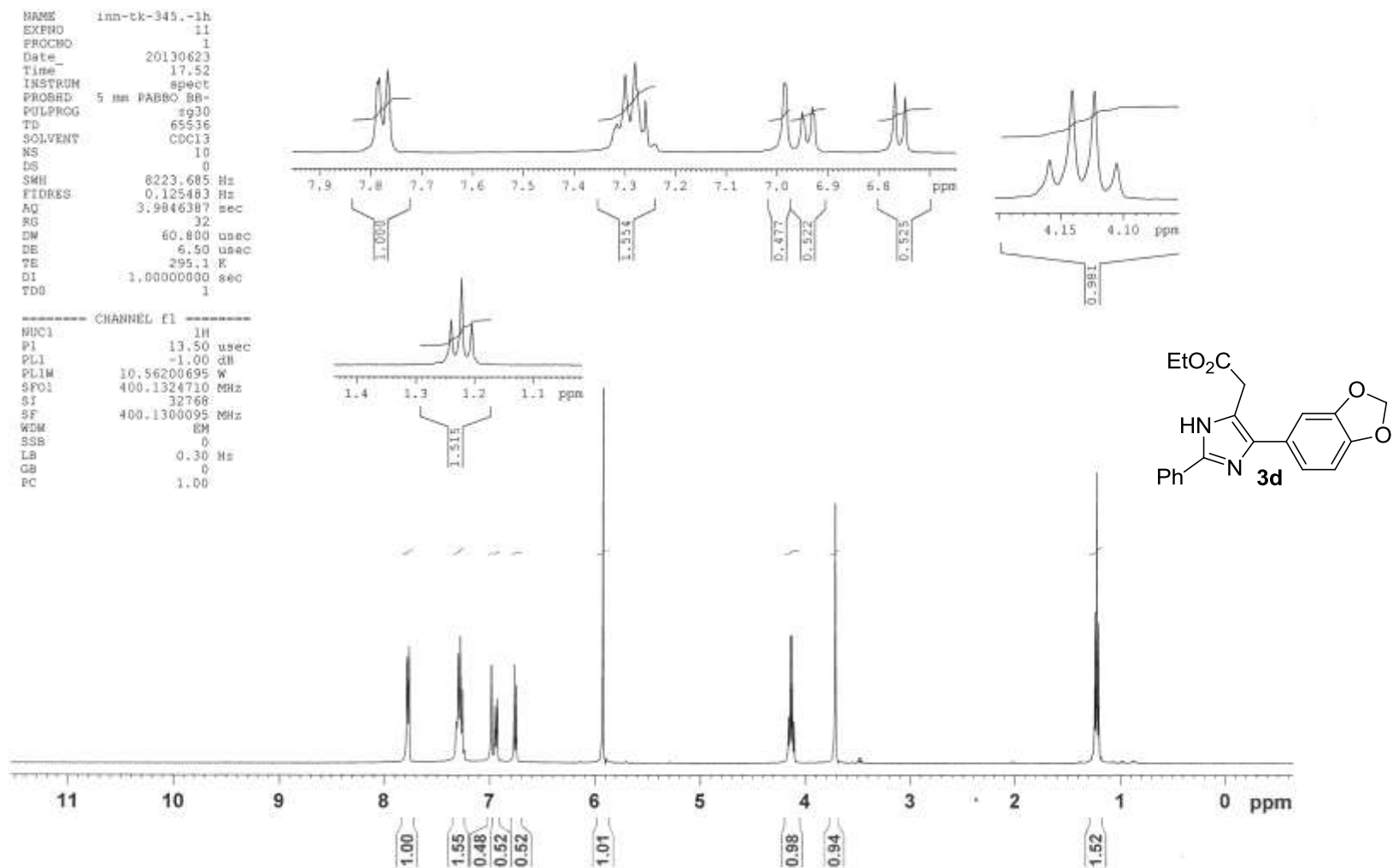


Figure S10. ¹H NMR spectrum of **3d**

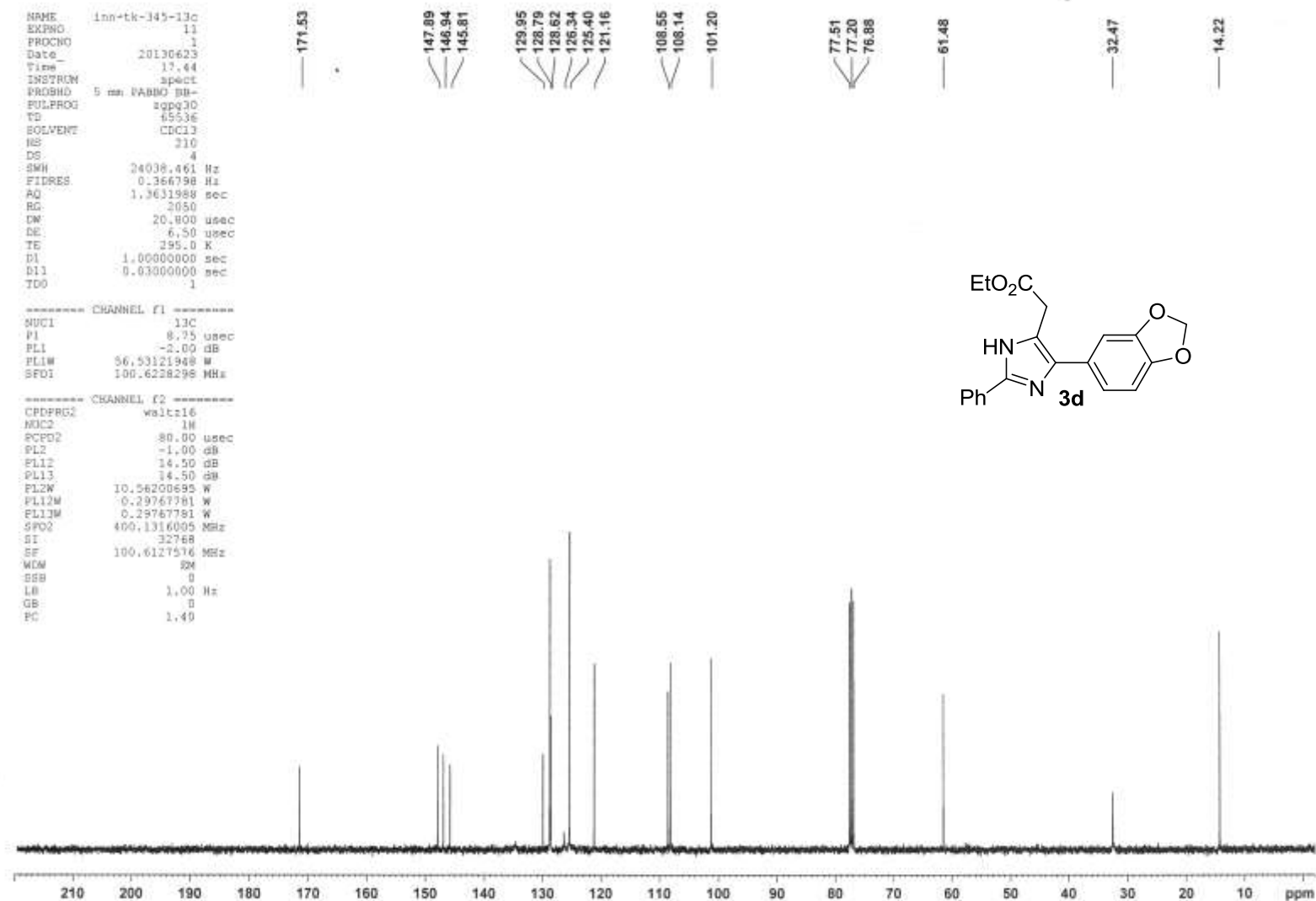


Figure S11. ¹³C NMR spectrum of **3d**

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Analysis Info

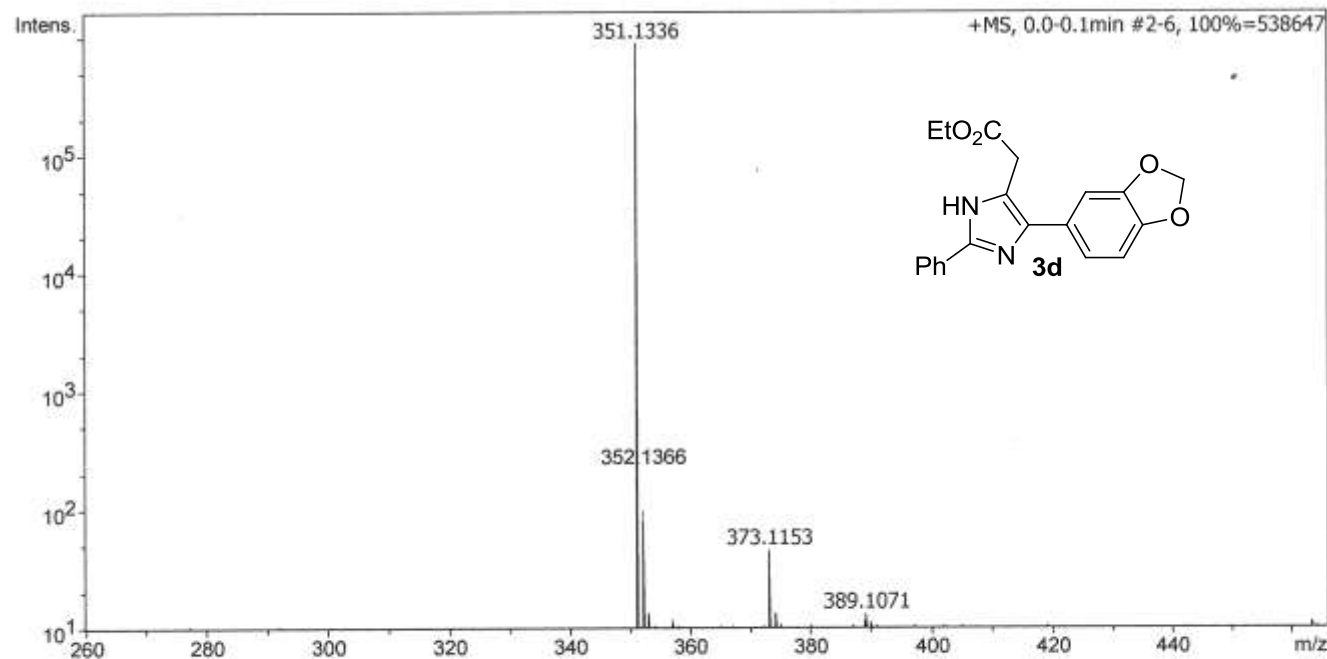
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 Comment C20H18N2O4

Acquisition Date 6/10/2013 6:27:32 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

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Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
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Figure S12. HRMS spectrum of **3d**

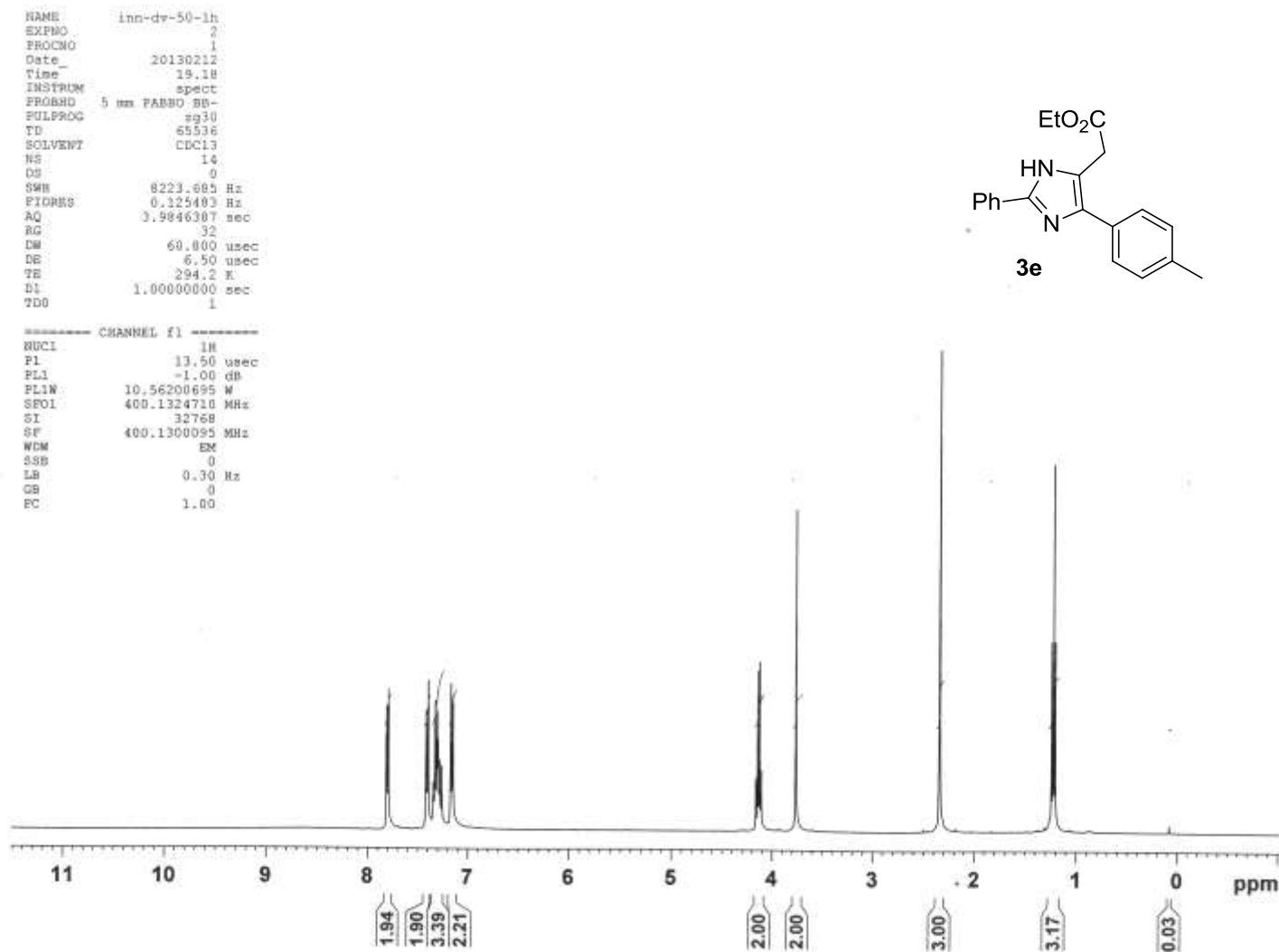


Figure S13. ^1H NMR spectrum of **3e**

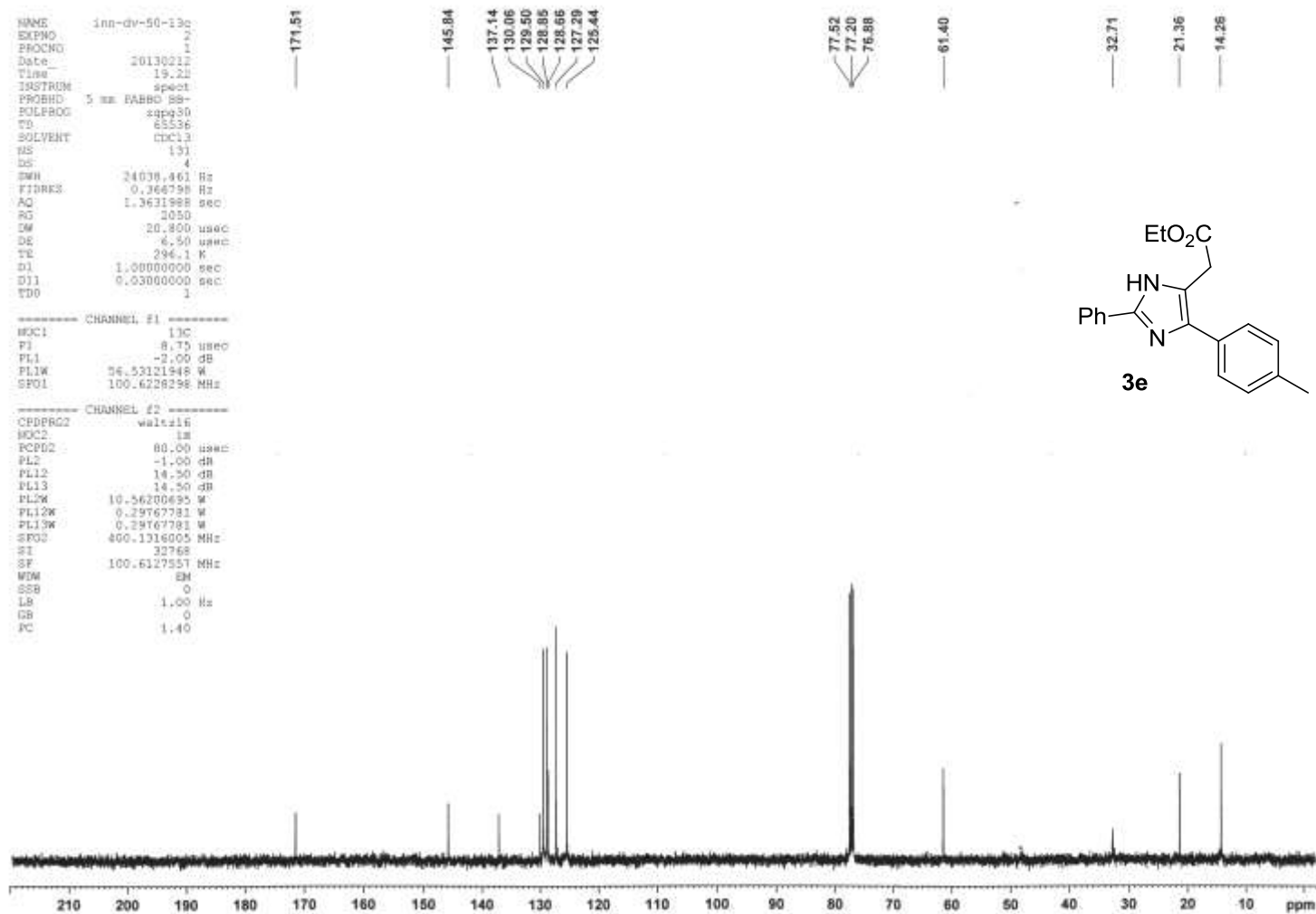


Figure S14. ¹³C NMR spectrum of **3e**

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Analysis Info

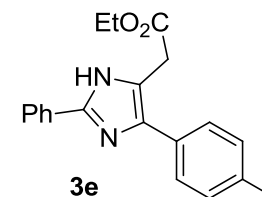
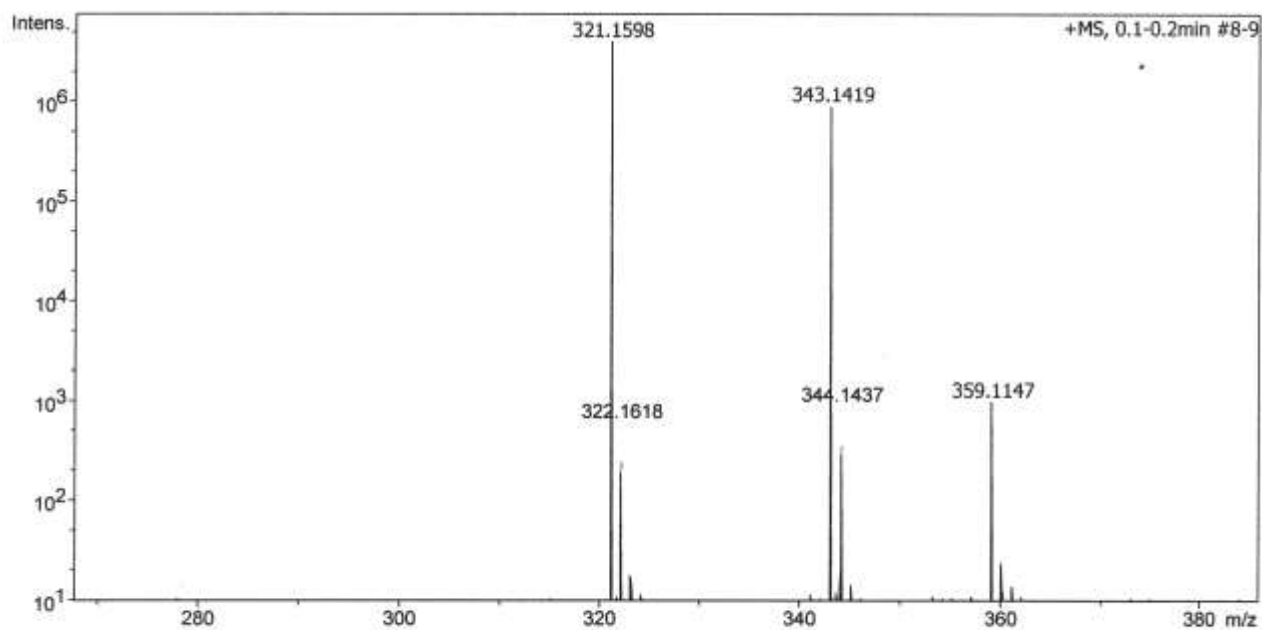
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Operator IIT-B
 Instrument maXis impact 282001.00081

Acquisition Parameter

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Scan End	1000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
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Figure S15. HRMS spectrum of **3e**

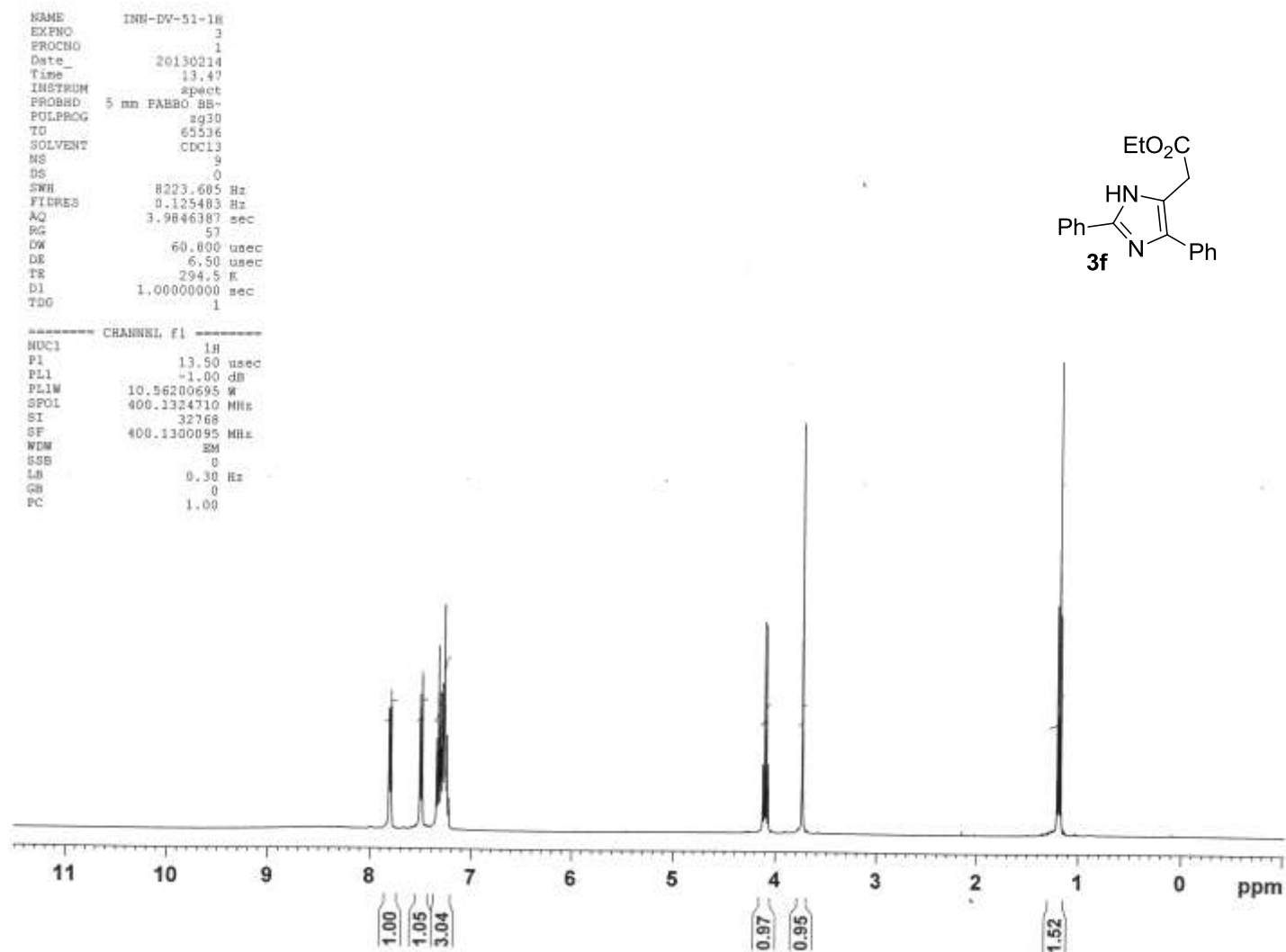


Figure S16. ^1H NMR spectrum of **3f**

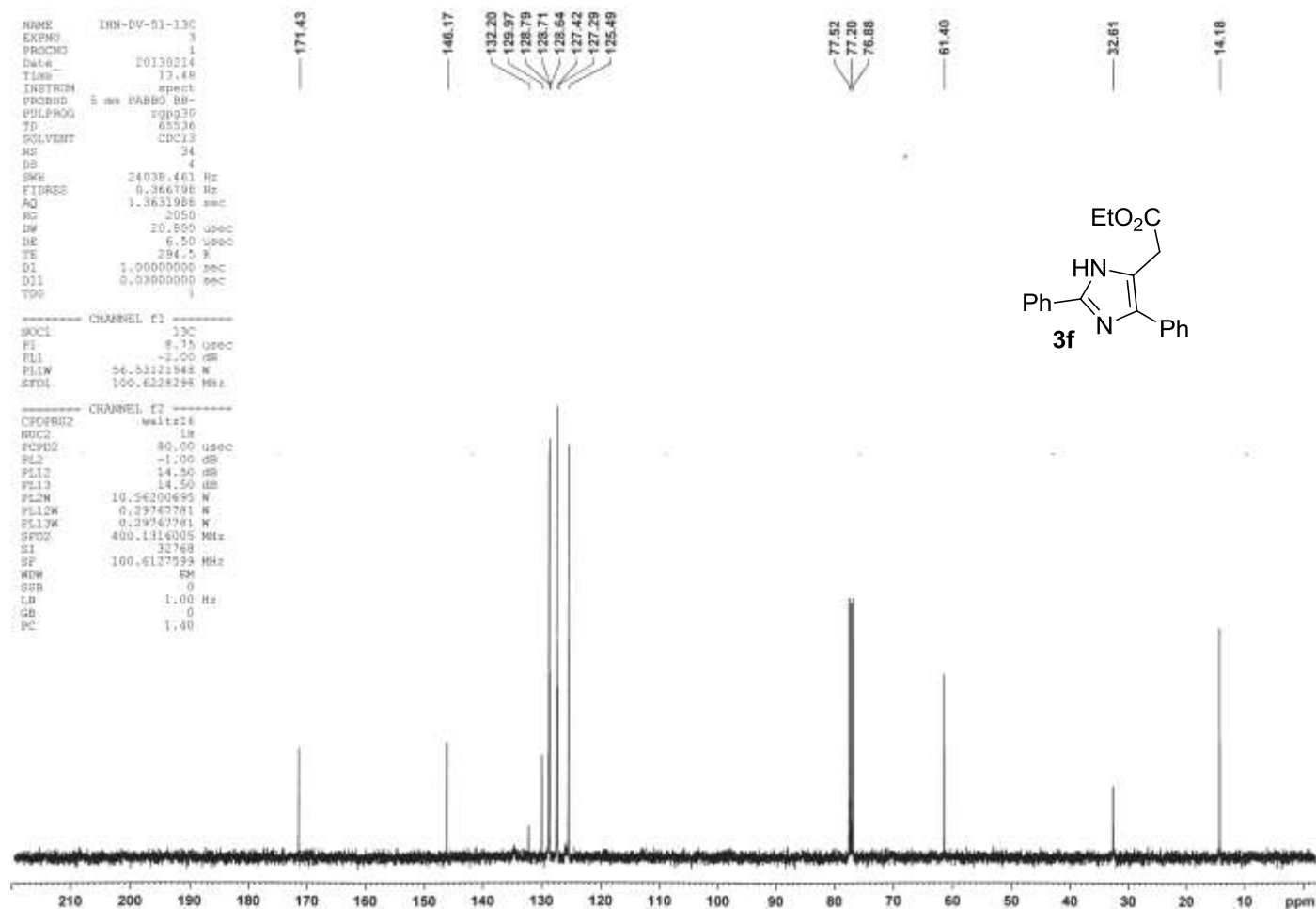


Figure S17. ¹³C NMR spectrum of **3f**

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Analysis Info

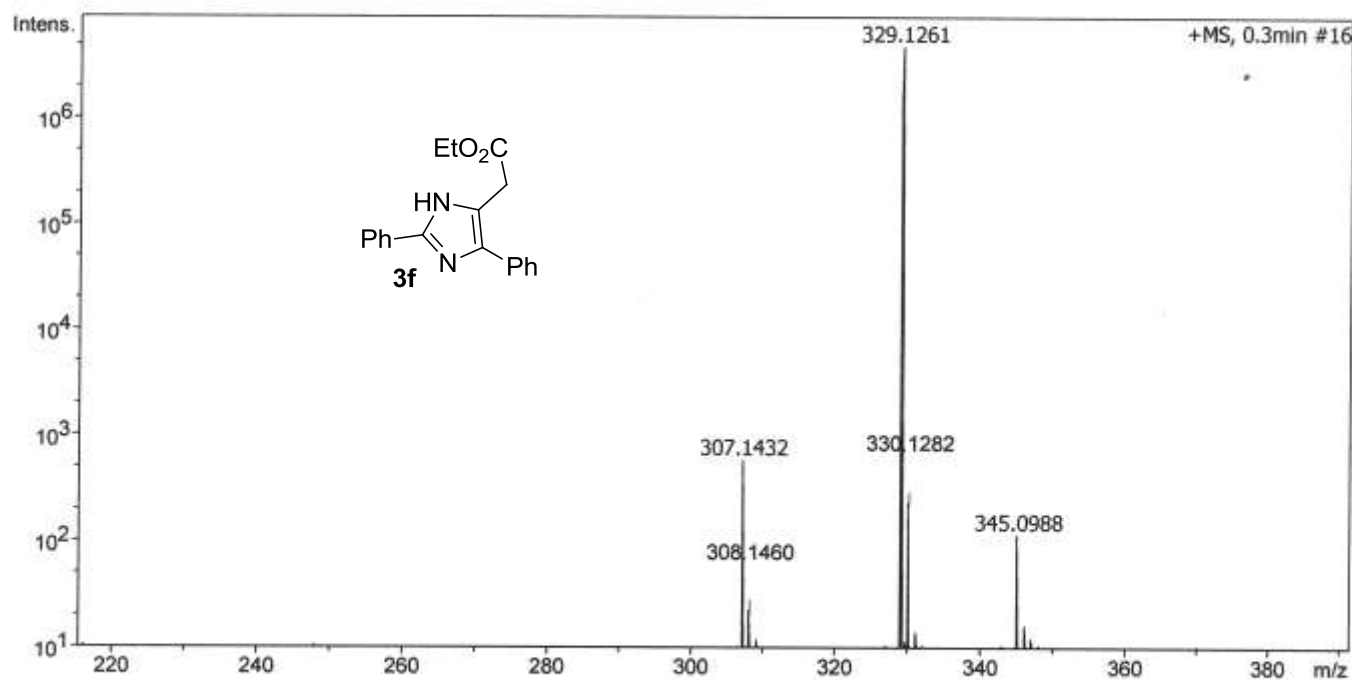
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Acquisition Date 3/6/2013 2:52:18 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
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Figure S18. HRMS spectrum of **3f**

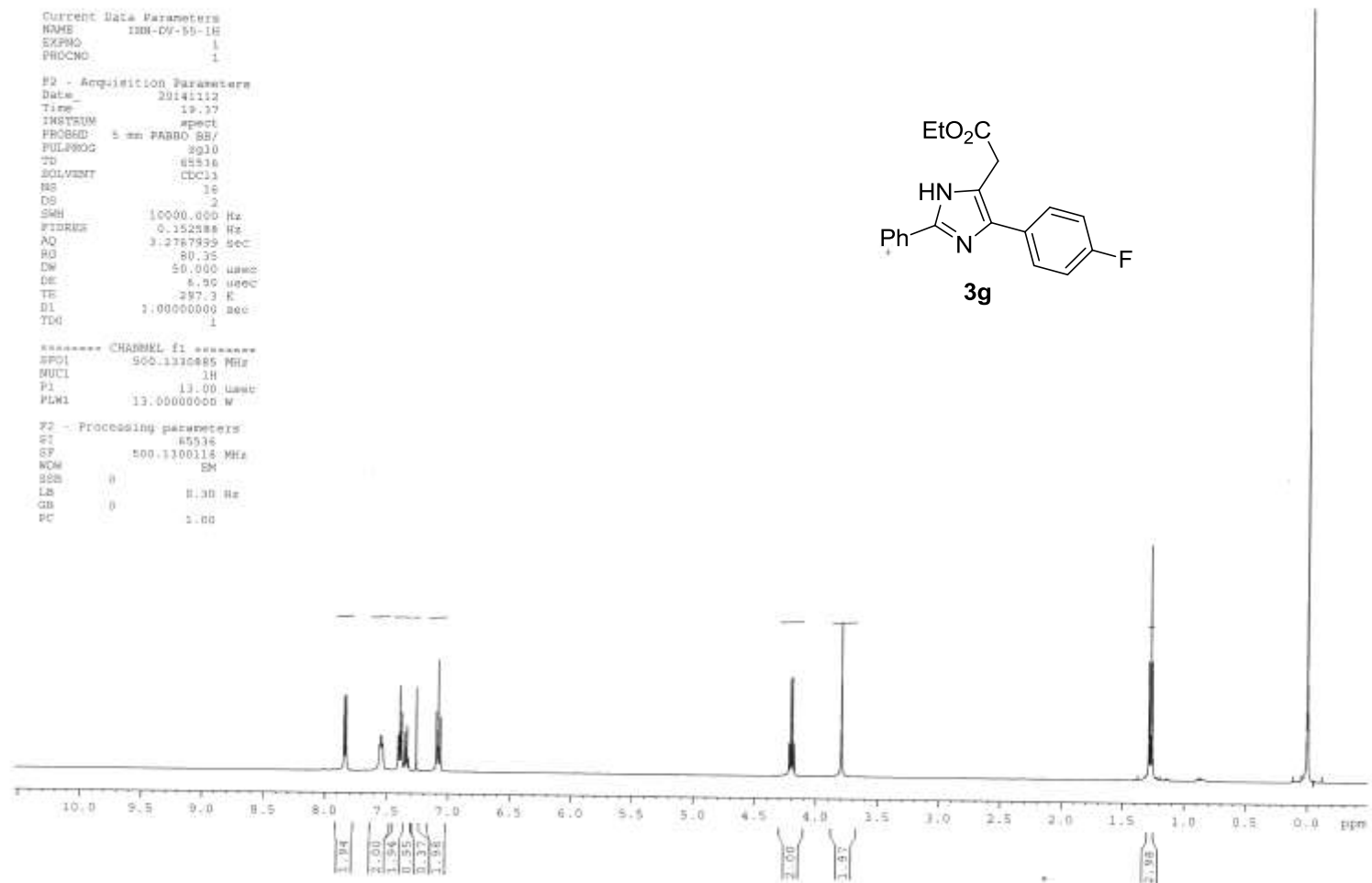


Figure S19. ^1H NMR spectrum of **3g**

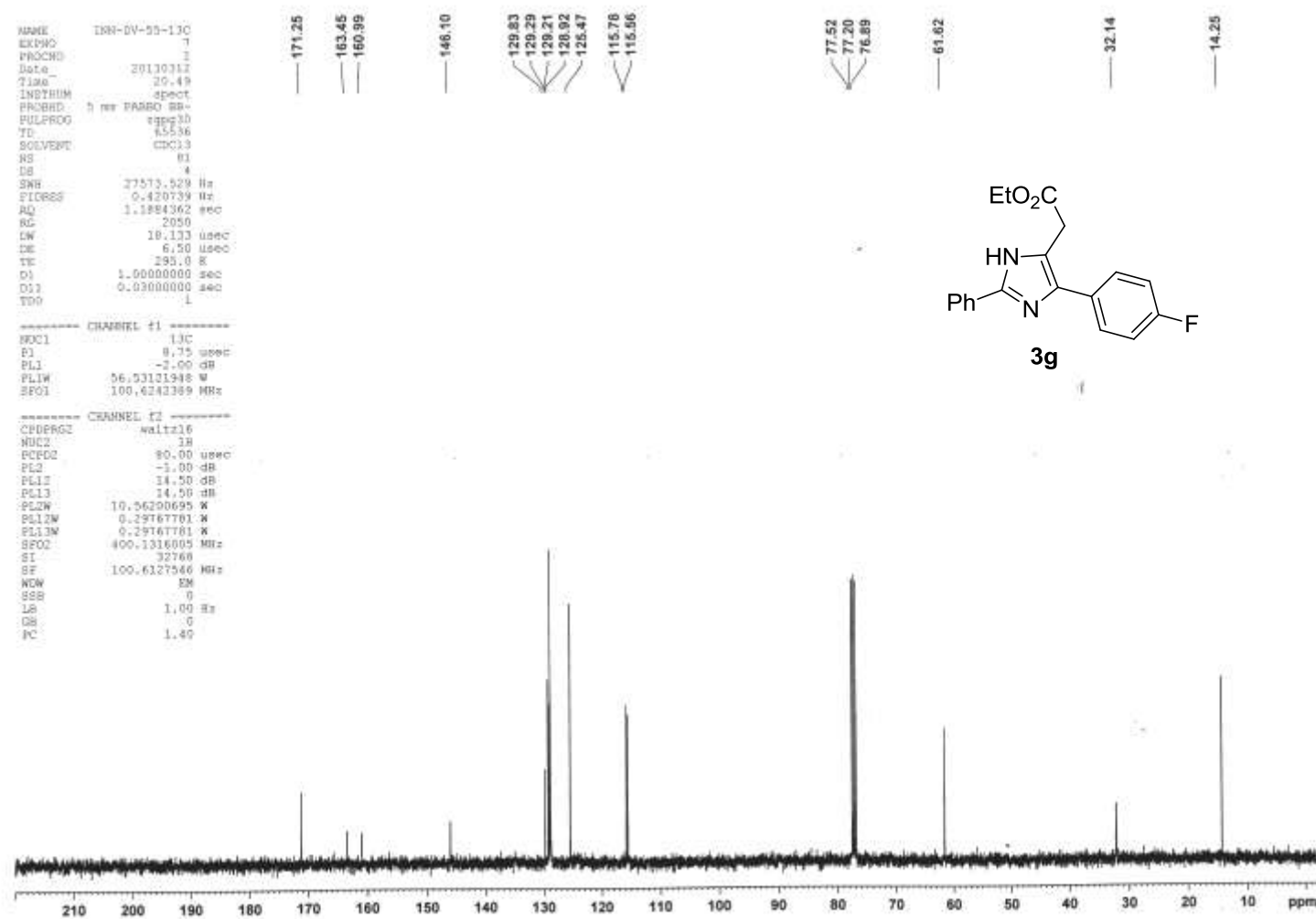


Figure S20. ¹³C NMR spectrum of **3g**

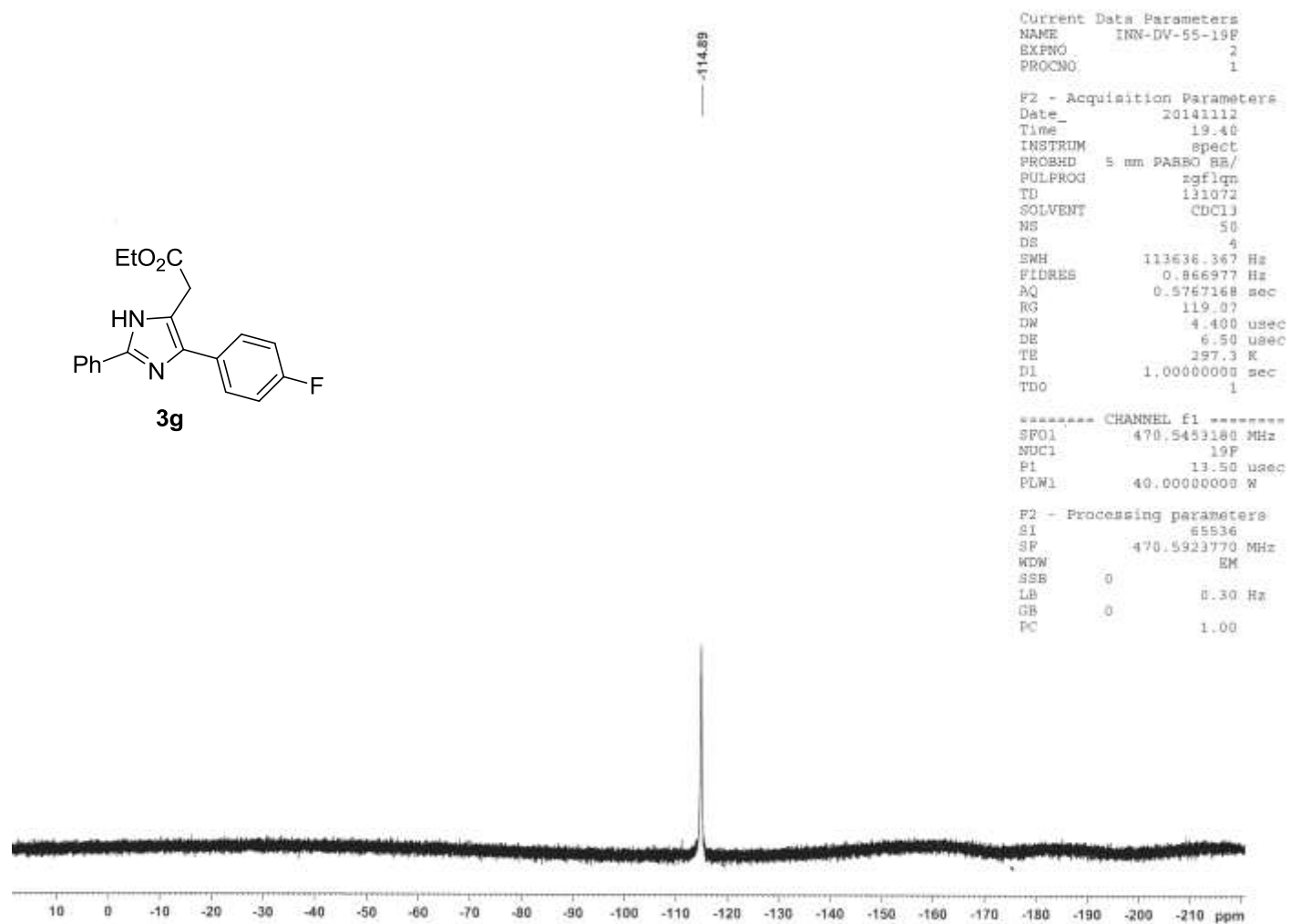


Figure S21. ^{19}F NMR spectrum of **3g**

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Analysis Info

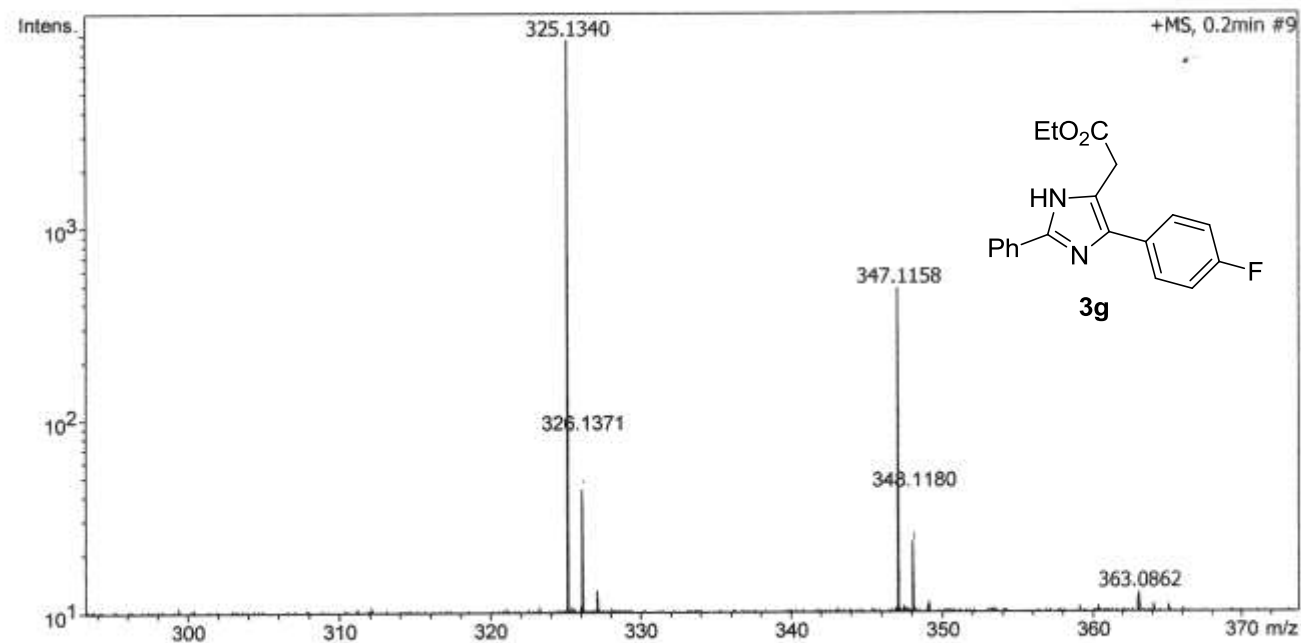
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Operator IIT-B
 Instrument maXis impact 282001.00081

Acquisition Parameter

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Scan End	1000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
325.1340	1	C19H18FN2O2	325.1347	2.0	7.8	1	100.00	11.5	even	ok

Figure S22. HRMS spectrum of **3g**

INN-TK-323-1H

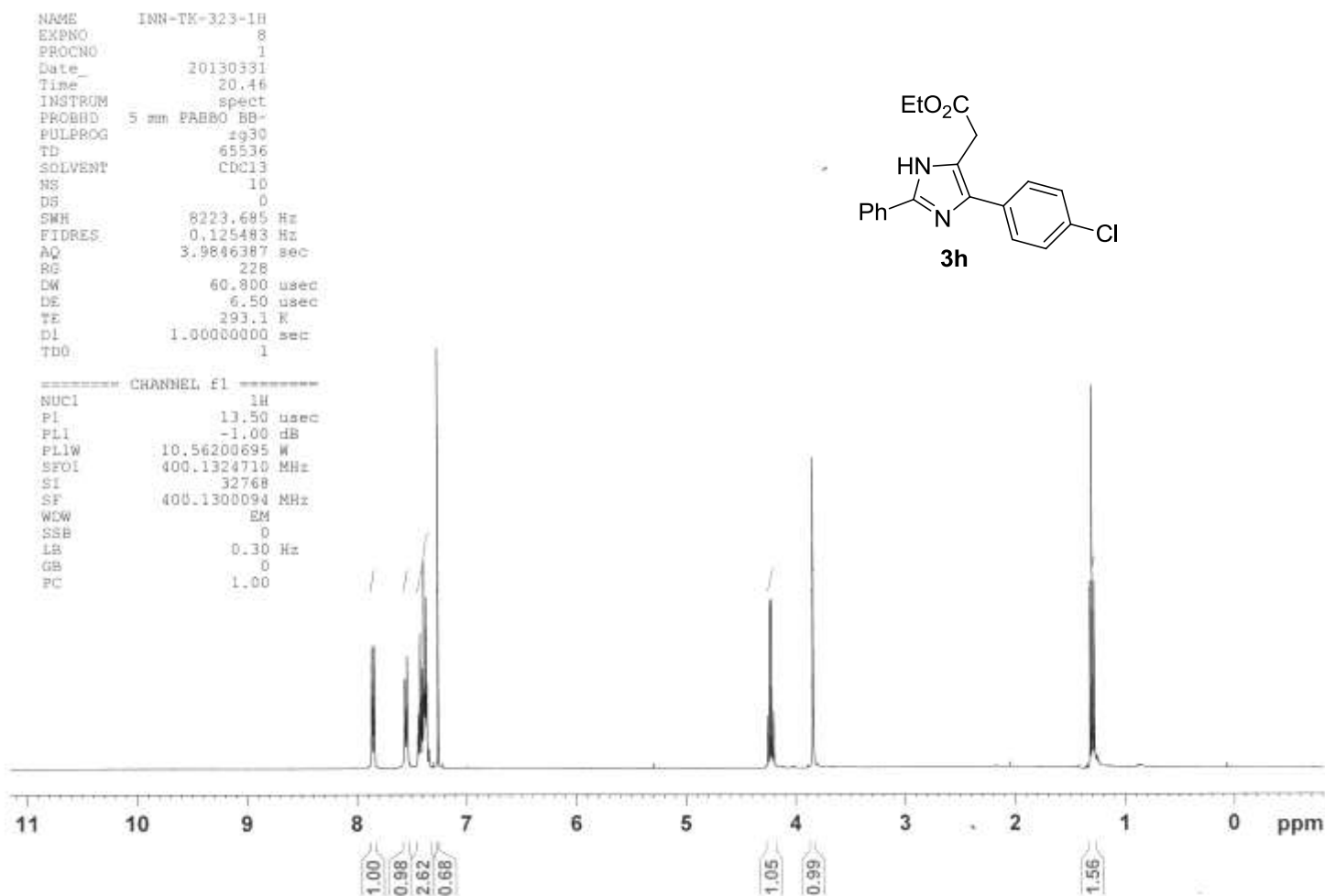


Figure S23. ^1H NMR spectrum of **3h**

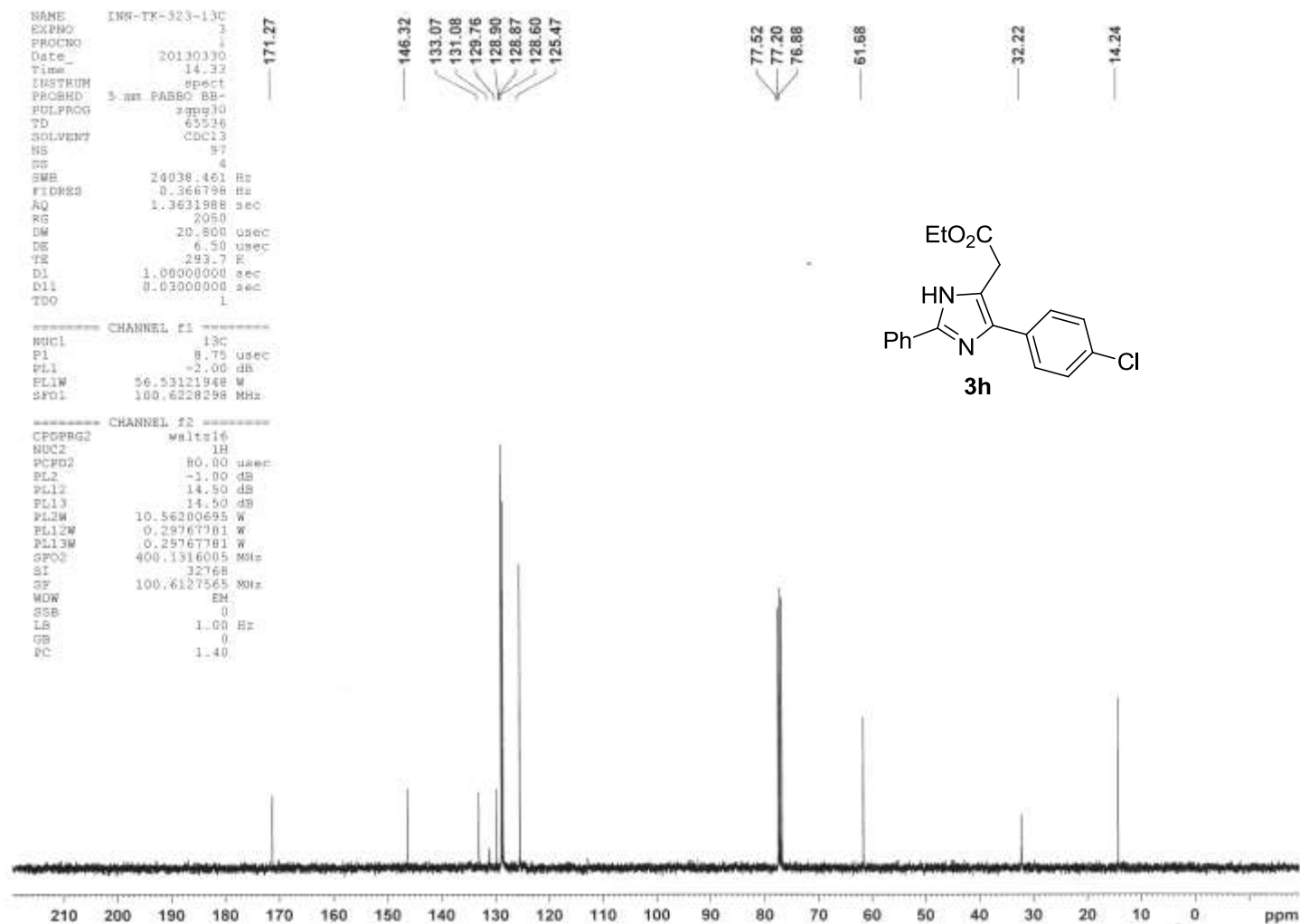


Figure S24. ^{13}C NMR spectrum of **3h**

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Analysis Info

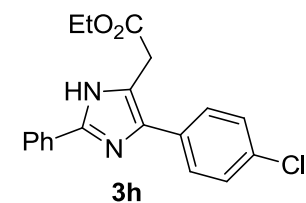
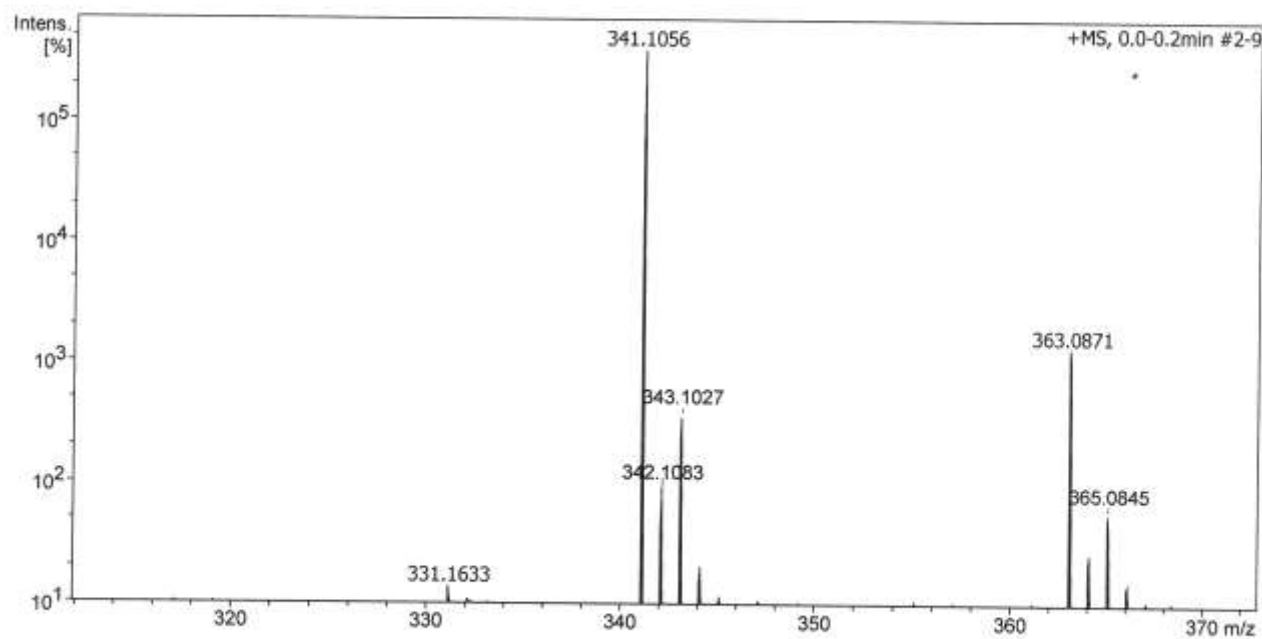
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Acquisition Date 3/26/2013 6:45:11 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

Acquisition Parameter

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Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e ⁻ Conf	N-Rule
341.1056	1	C19H18ClN2O2	341.1051	-1.3	4.9	100.00	11.5	even	ok

Figure S25. HRMS NMR spectrum of **3h**

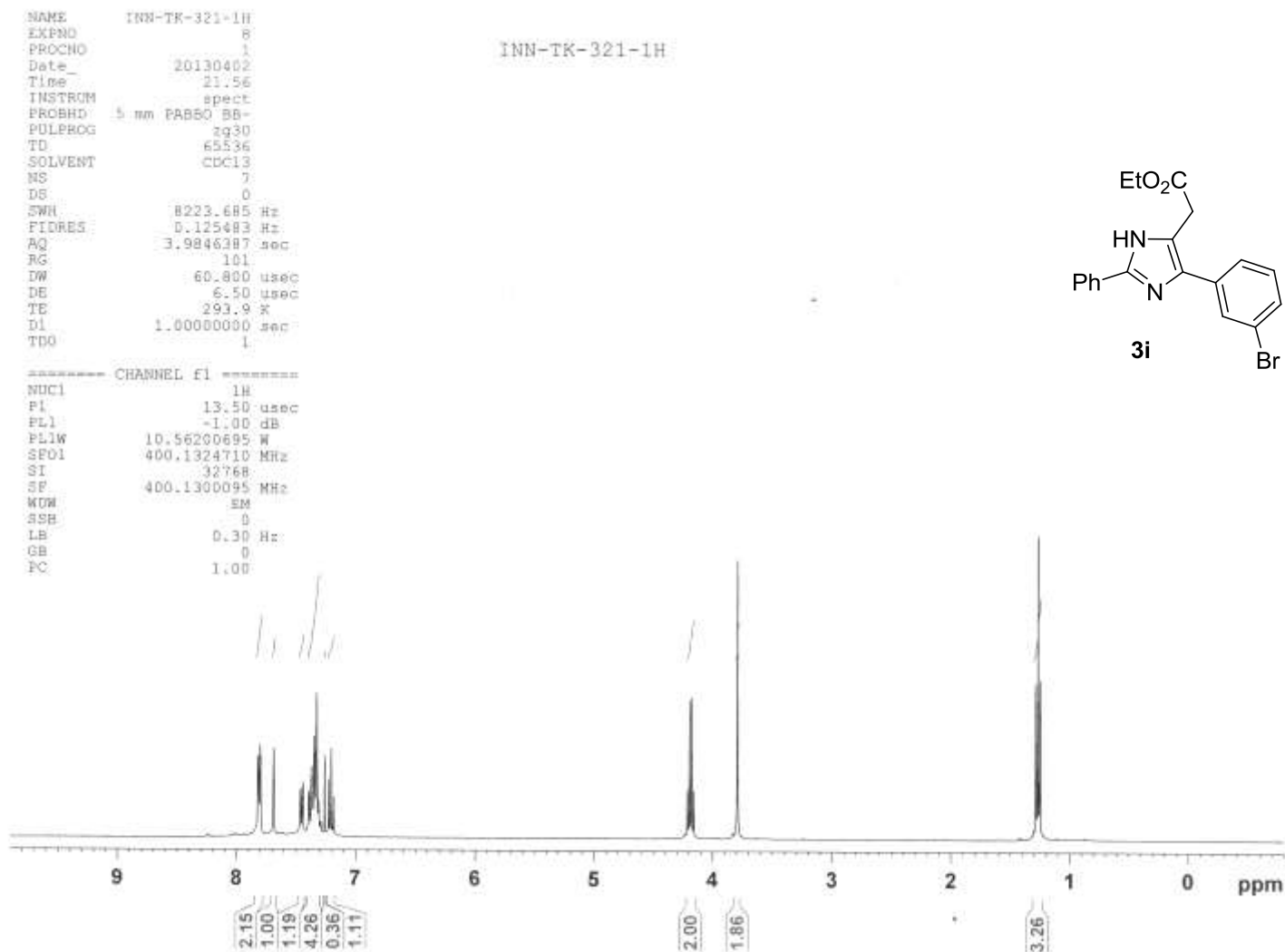


Figure S26. ^1H NMR spectrum of **3i**

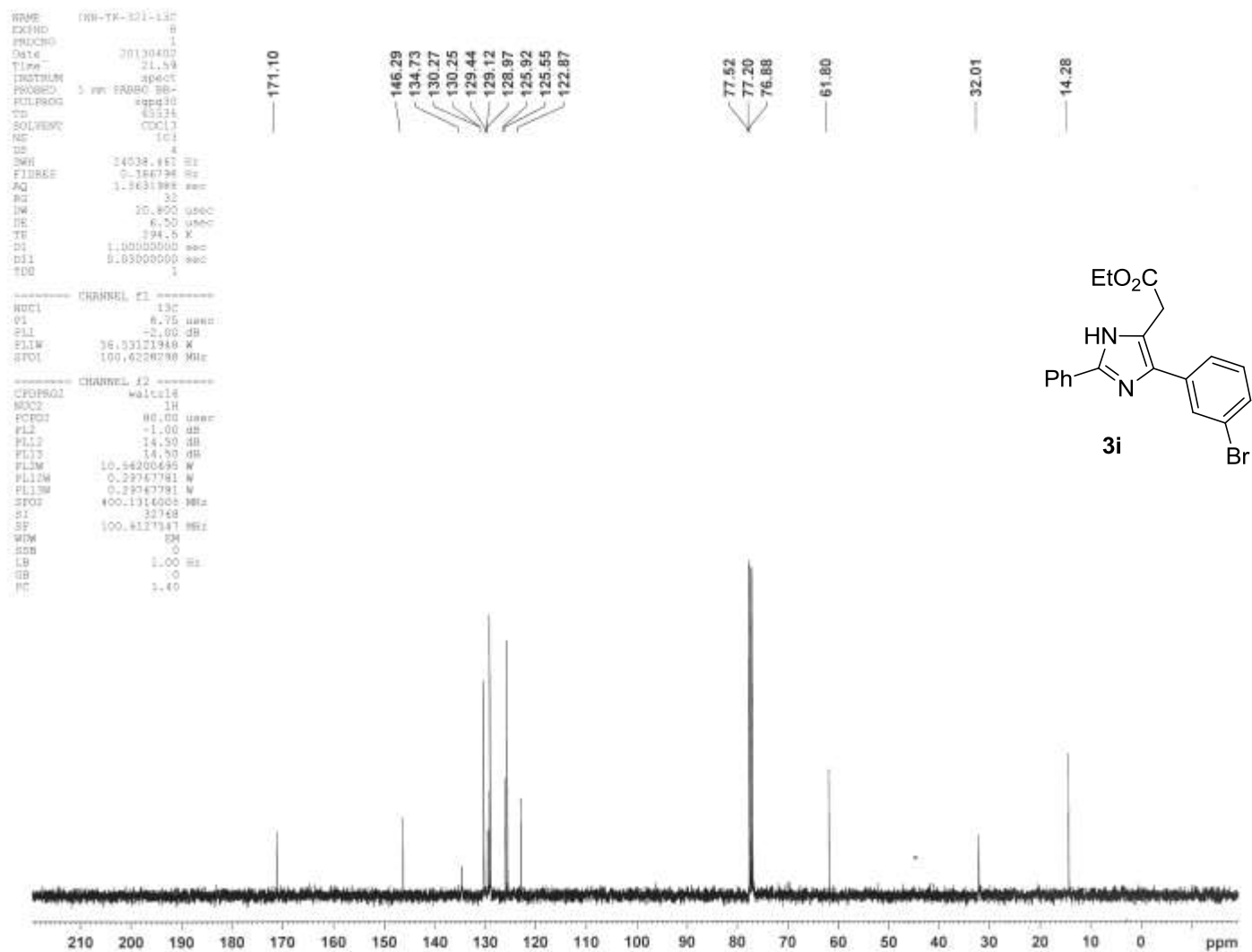


Figure S27. ¹³C NMR spectrum of **3i**

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Analysis Info

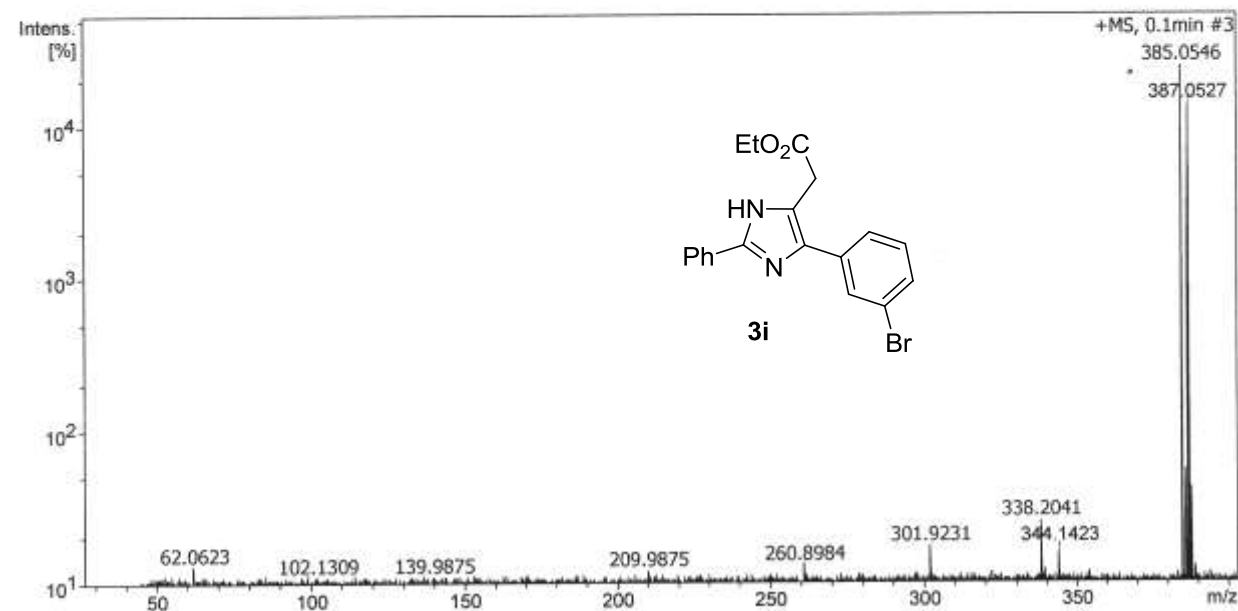
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Acquisition Date 3/15/2013 3:21:48 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

Acquisition Parameter

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Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e ⁻ Conf	N-Rule
385.0546	1	C19H18BrN2O2	385.0546	0.0	37.5	1	100.00	11.5 even	ok

Figure S28. HRMS spectrum of **3i**

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PROCNO    1
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TD        65536
SOLVENT   CDCl3
NS         7
DS         0
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         32
DW         60.800 usec
DE         6.50 usec
TE         295.6 K
D1         1.00000000 sec
TDO        1

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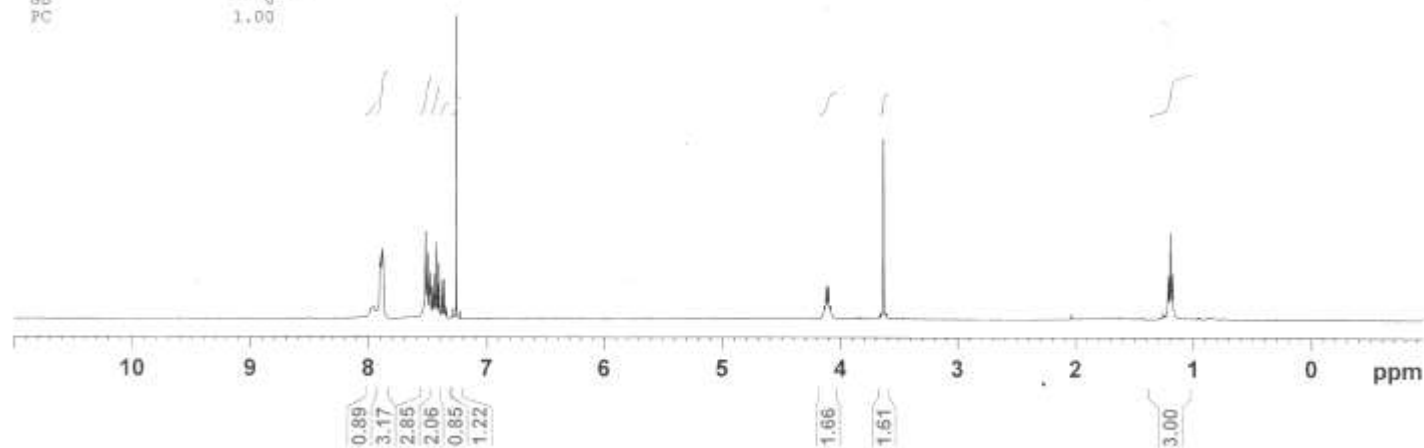
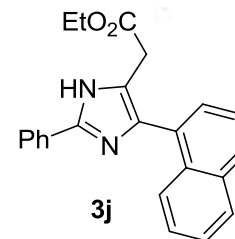


Figure S29. ^1H NMR spectrum of **3j**

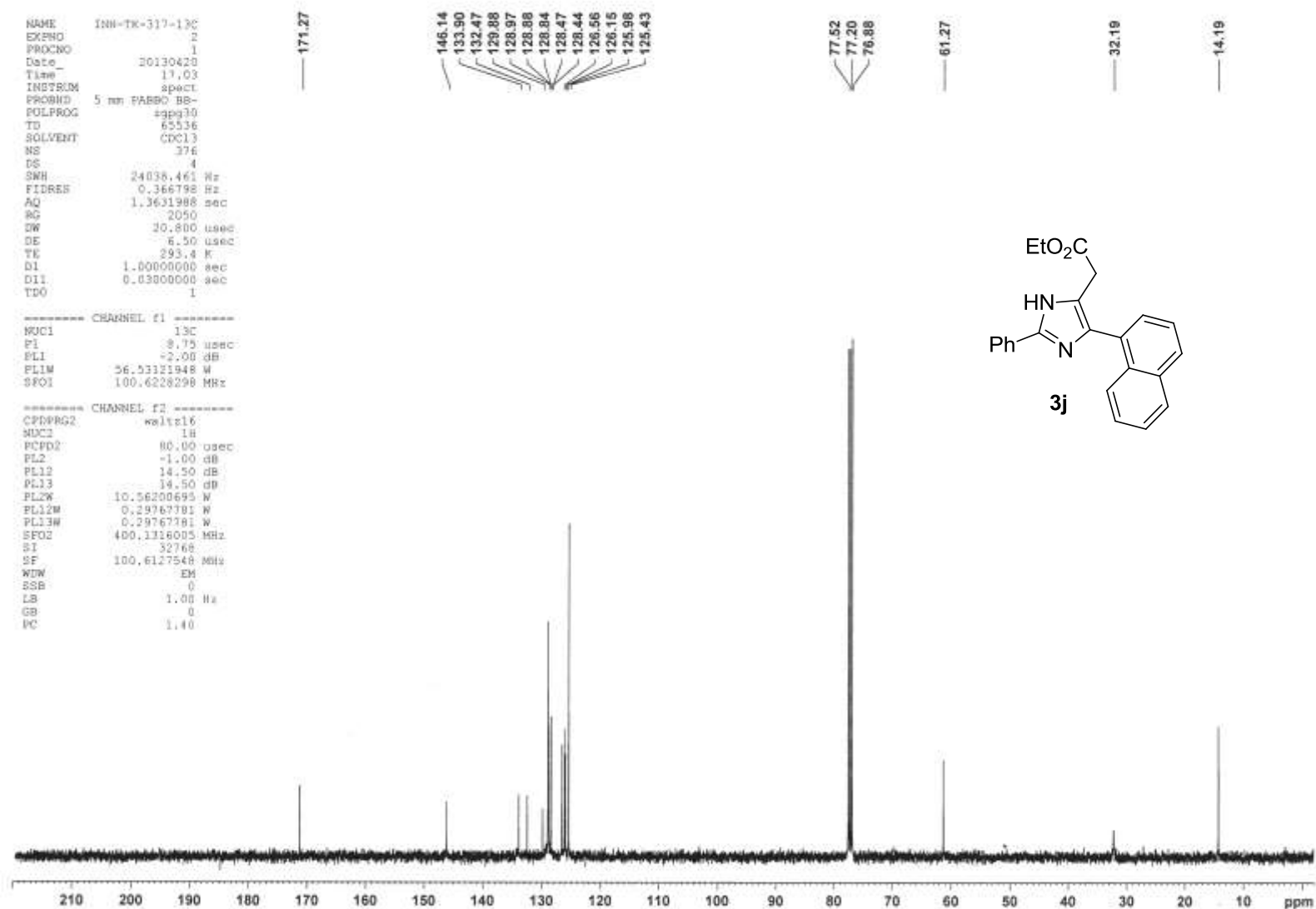


Figure S30. ¹³C NMR spectrum of **3j**

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Analysis Info

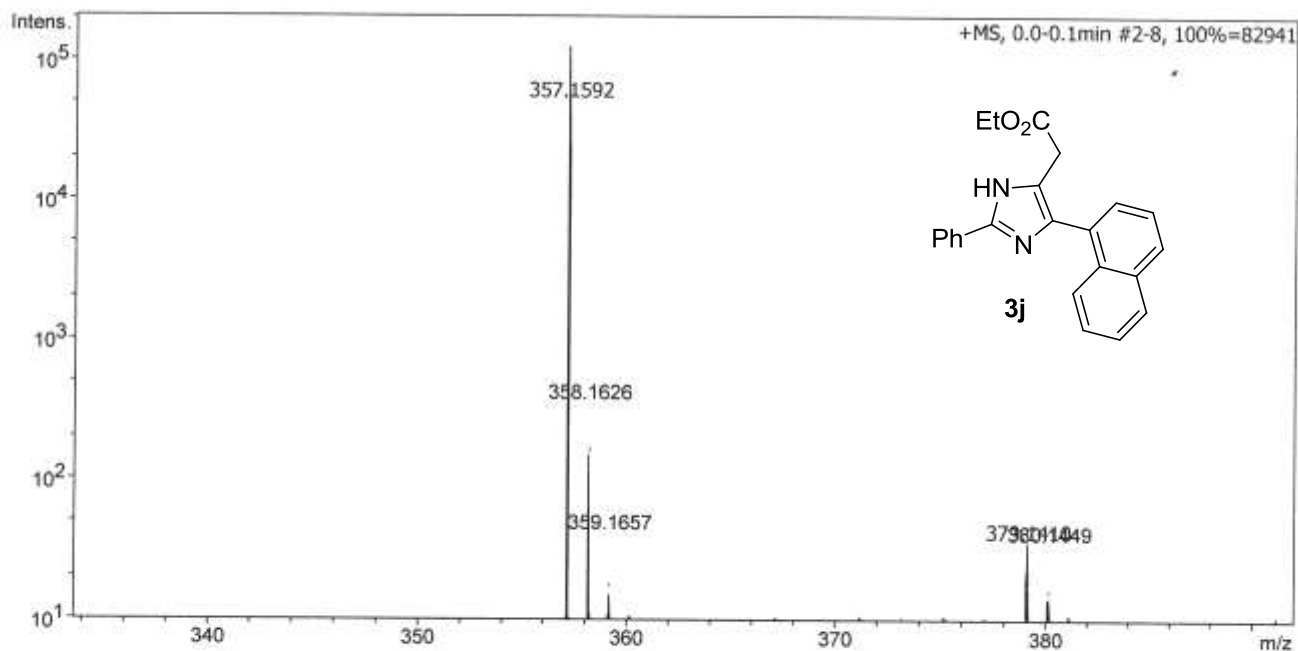
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Operator IIT-B
 Instrument maXis impact 282001.00081

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Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
357.1592	1	C23H21N2O2	357.1598	-1.5	29.2	1	100.00	14.5	even	ok

Figure S31. HRMS spectrum of **3j**

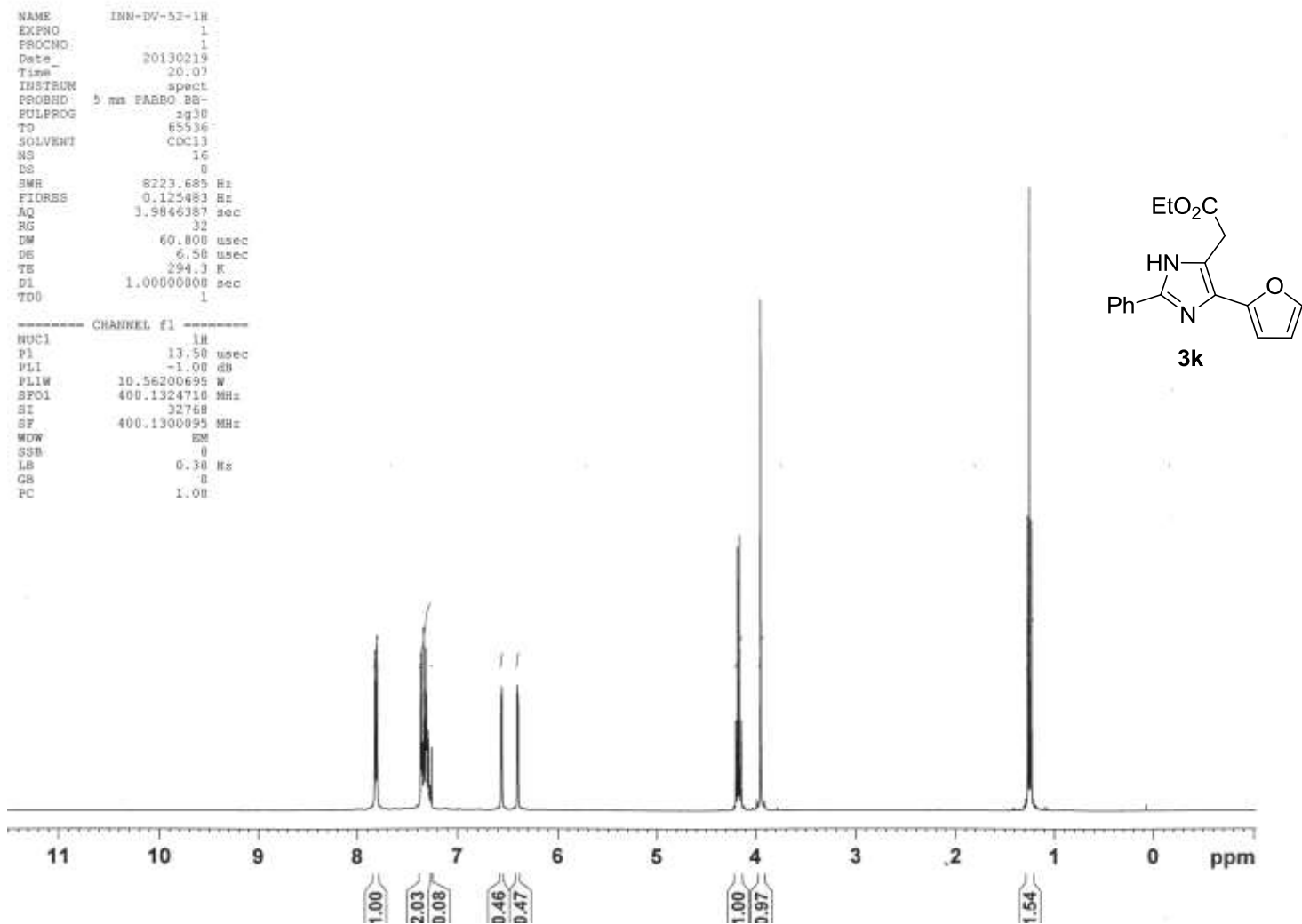


Figure S32. ¹H NMR spectrum of **3k**

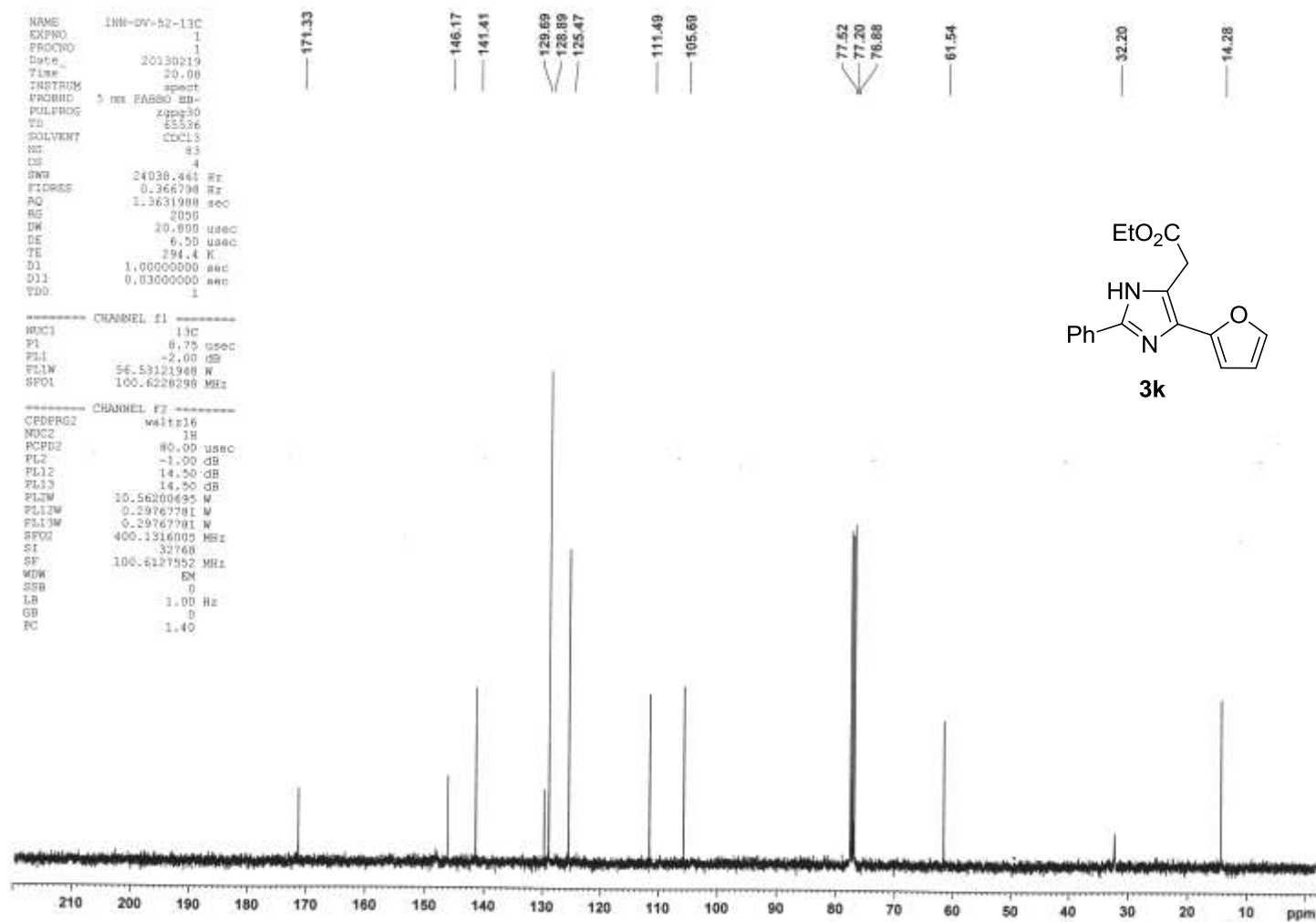


Figure S33. ¹³C NMR spectrum of **3k**

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Analysis Info

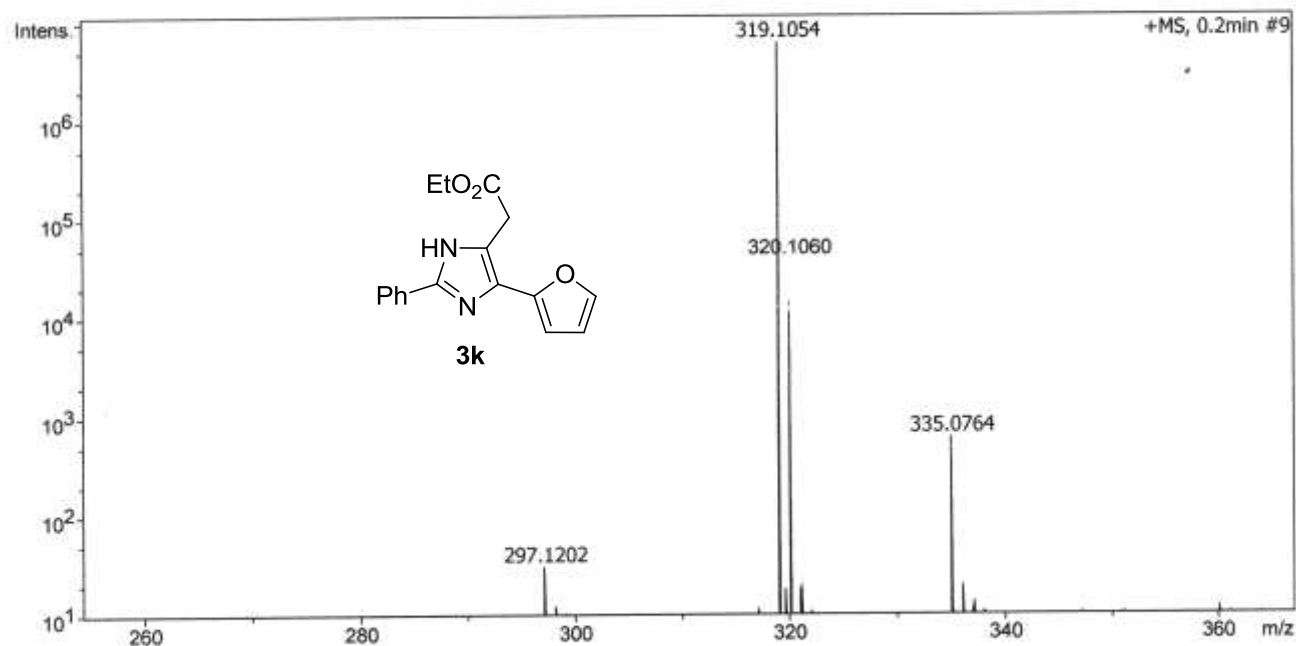
Analysis Name D:\Data\MAR-13\INN-DV-52.d
 Method Tune_pos_Standard_NAI-1000.m
 Sample Name INN-DV-52
 Comment C17H16N2O3

Acquisition Date 3/6/2013 3:08:08 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.1 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
319.1054	1	C17H16N2NaO3	319.1053	-0.2	195.2	1	100.00	10.5	even	ok

Figure S34. HRMS spectrum of **3k**

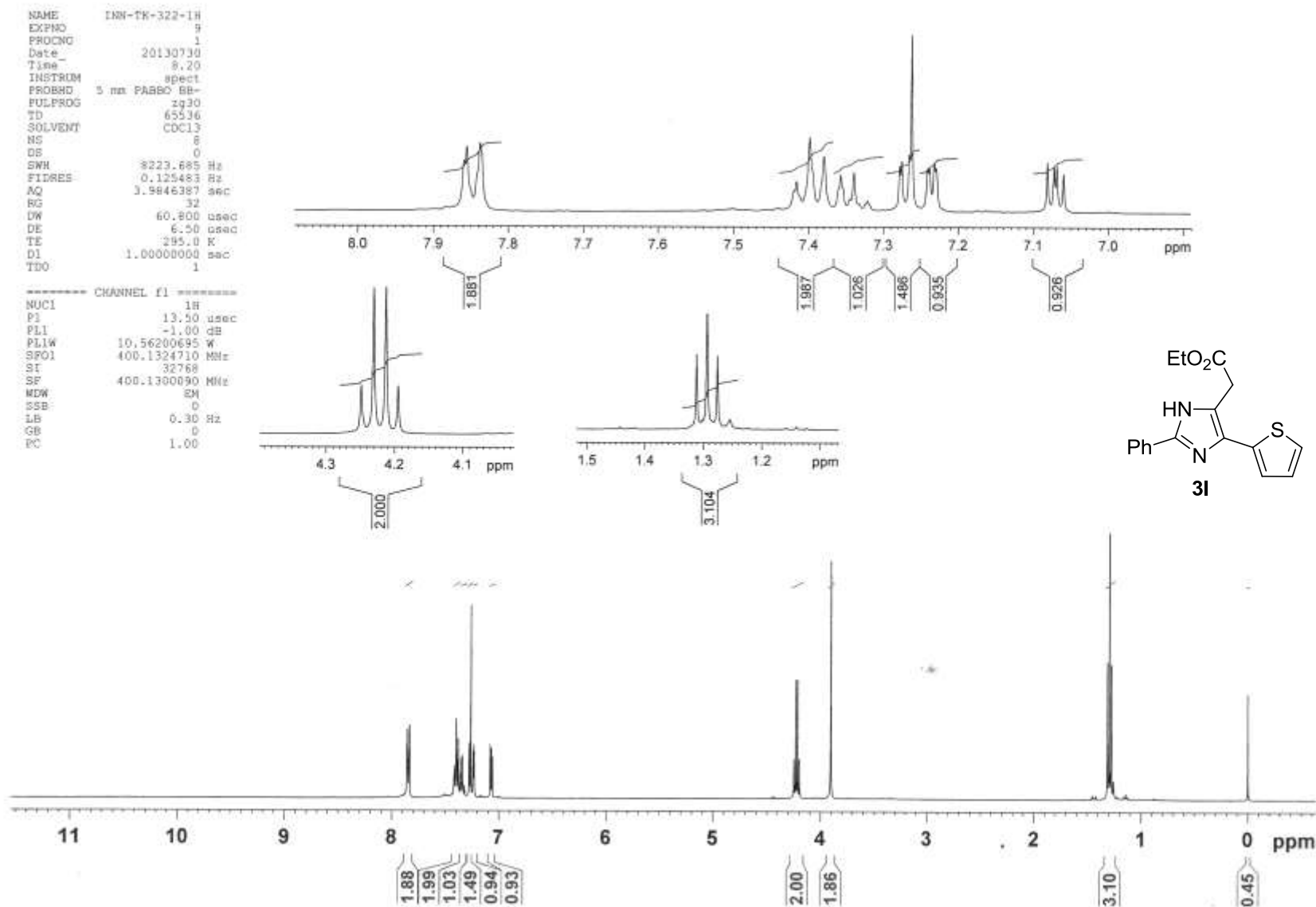


Figure S35. ^1H NMR spectrum of **3I**

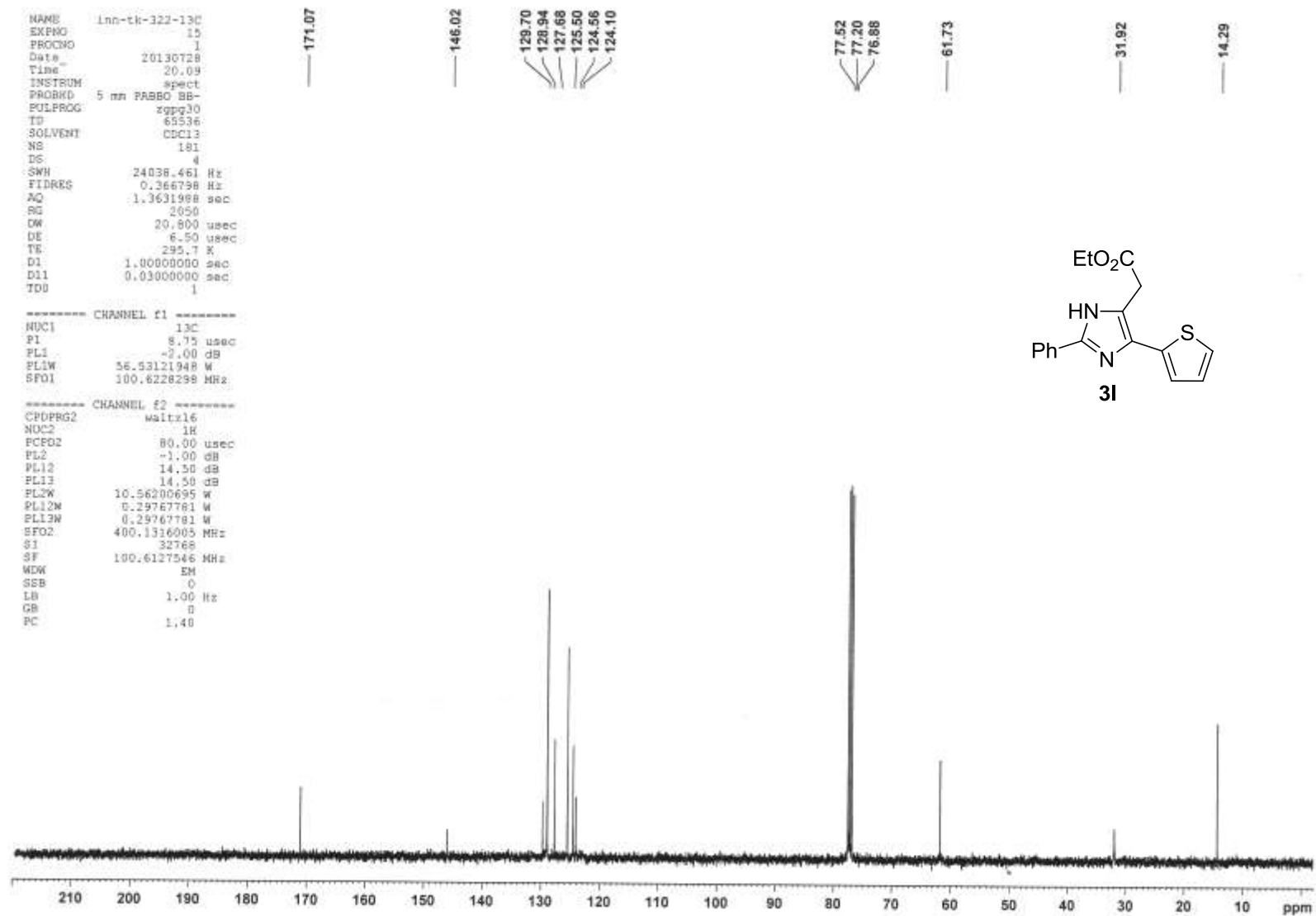


Figure S36. ¹³C NMR spectrum of **3l**

Indian Institute of Technology (B)

Analysis Info

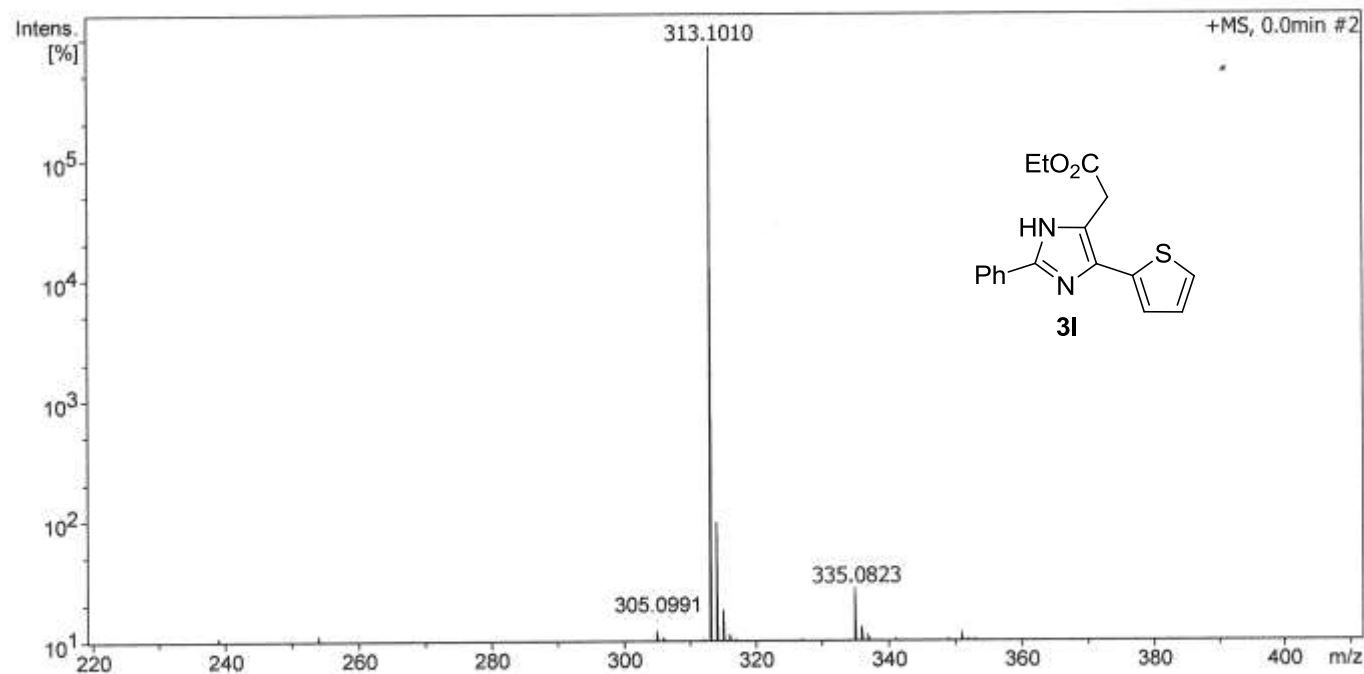
Analysis Name D:\Data\MAR-13\INN-TK-322.d
 Method Tune_pos_Standard_NAI-500.m
 Sample Name INN-TK-322
 Comment C17H16N2O2S

Acquisition Date 3/26/2013 6:52:30 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.1 Bar
Focus	Active	Set Capillary	3200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e ⁻ Conf	N-Rule
313.1010	1	C17H17N2O2S	313.1005	-1.5	7.6	1	100.00	10.5	even ok

Figure S37. HRMS spectrum of **3I**

```

NAME      inn-tk-328-1a
EXPNO     1
PROCNO    1
Date_     20130827
Time      13.33
INSTRUM   spect
PROBHD    5 mm SEI 1H/D-
PULPROG   zg30
TD        49340
SOLVENT   CDCl3
NS        8
DS        0
SMH       8223.685 Hz
FIDRES    0.166674 Hz
AQ        2.9999220 sec
RG        71.8
DM        60.800 usec
DE        6.50 usec
TE        293.2 K
D1        1.00000000 sec
TDO       1

```

```

===== CHANNEL f1 =====
NUC1      1H
P1        6.75 usec
PL1       -3.00 dB
PL1W      16.73965454 W
SF01      400.1324710 MHz
SI        32768
SF        400.1300124 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00

```

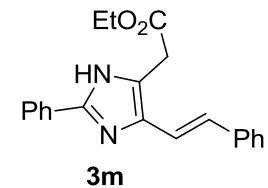
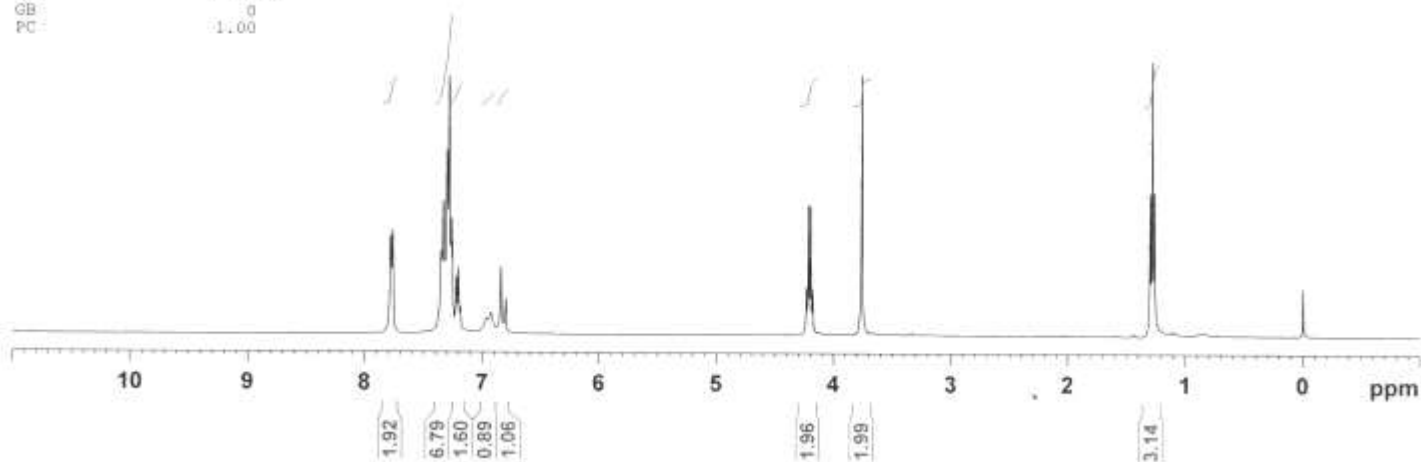


Figure S38. ¹H NMR spectrum of **3m**

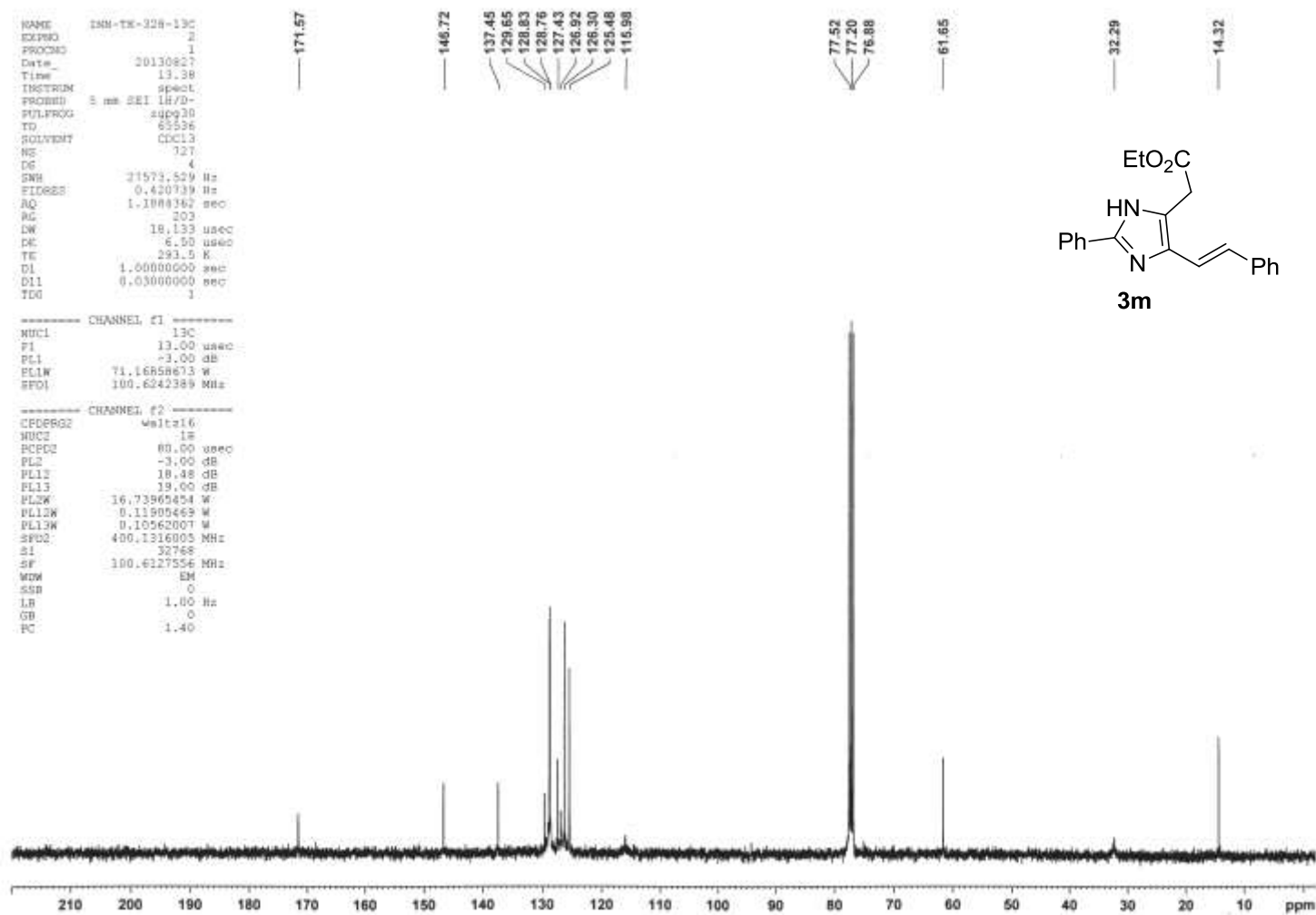


Figure S39. ¹³C NMR spectrum of **3m**

Indian Institute of Technology (B)

Analysis Info

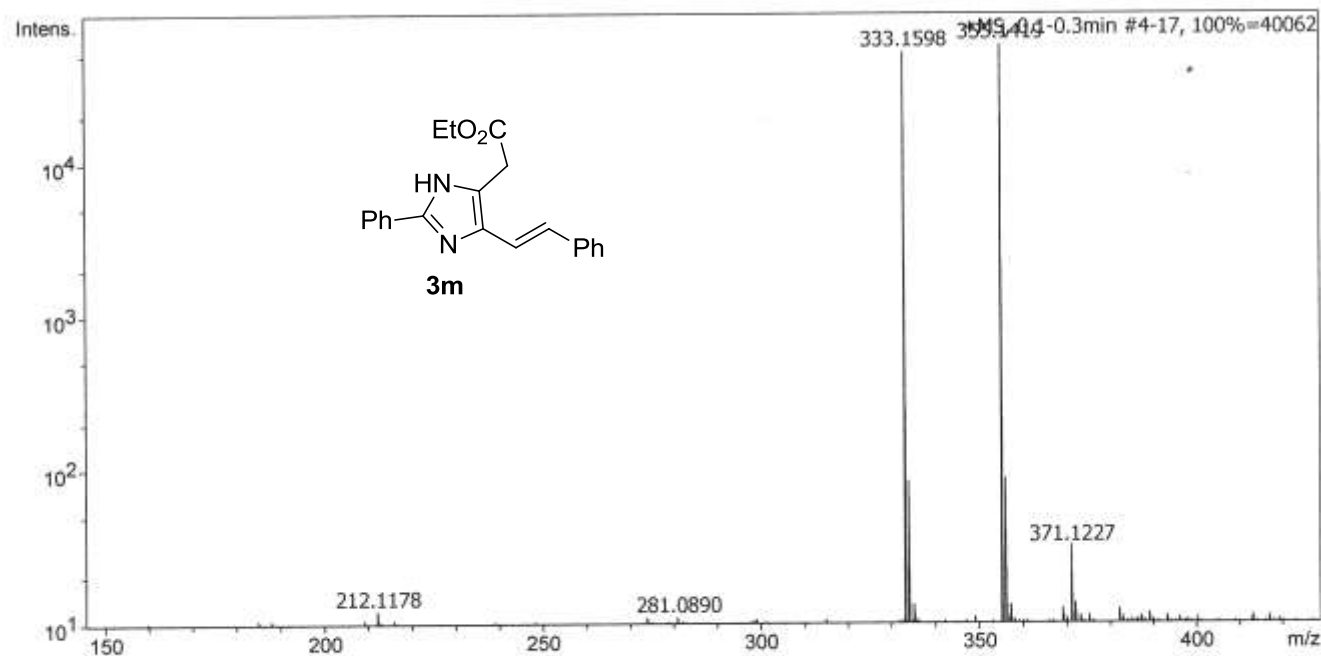
Analysis Name D:\Data\JUN-13\INN-TK-328.d
 Method Tune_pos_Standard_NAI-500.m
 Sample Name INN-TK-328
 Comment C21H20N2O2

Acquisition Date 6/10/2013 10:13:06 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.1 Bar
Focus	Active	Set Capillary	3200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
333.1598	1	C21H21N2O2	333.1598	0.2	6.6	1	100.00	12.5	even	ok

Figure S40. HRMS spectrum of **3m**

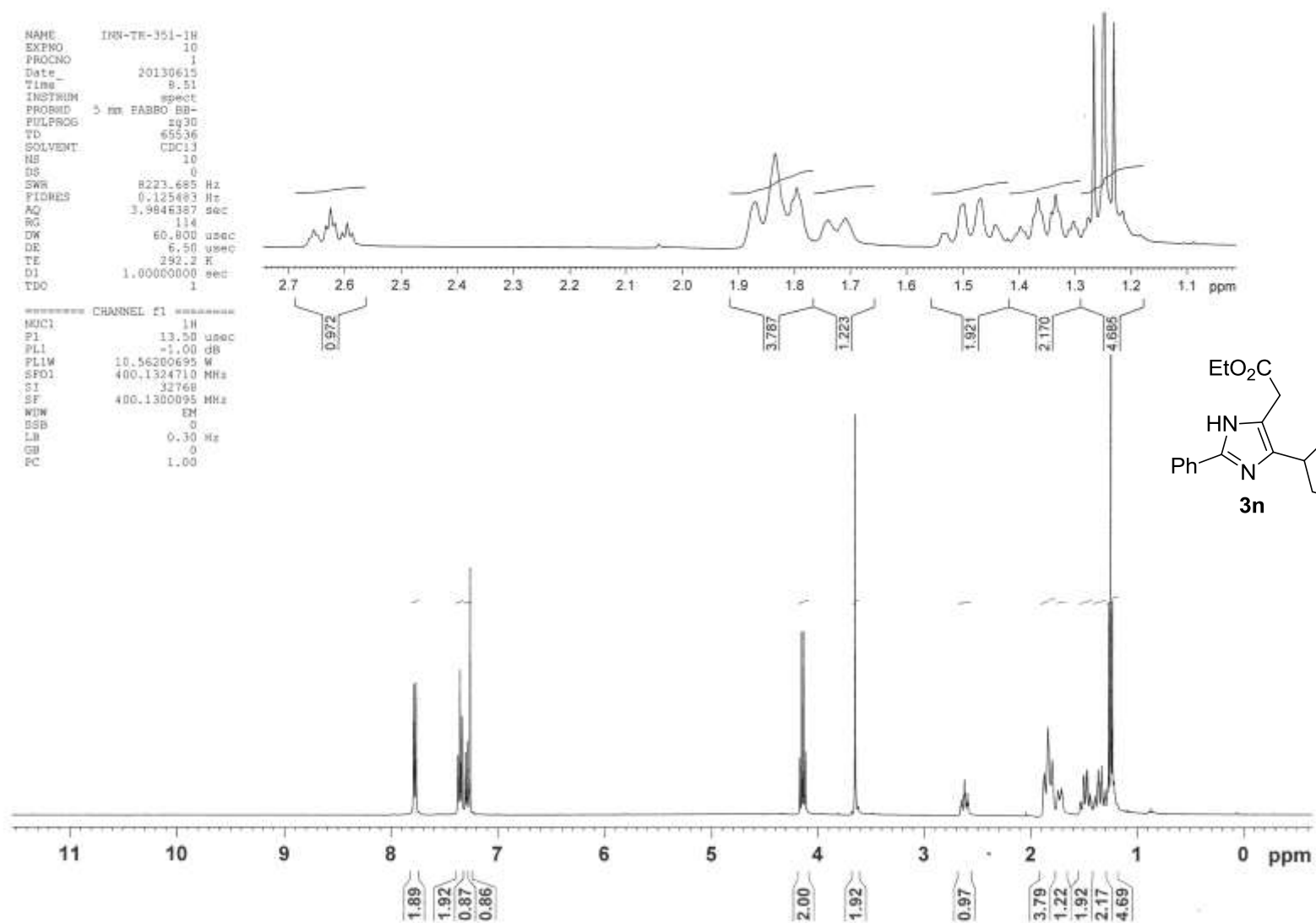


Figure S41. ^1H NMR spectrum of **3n**

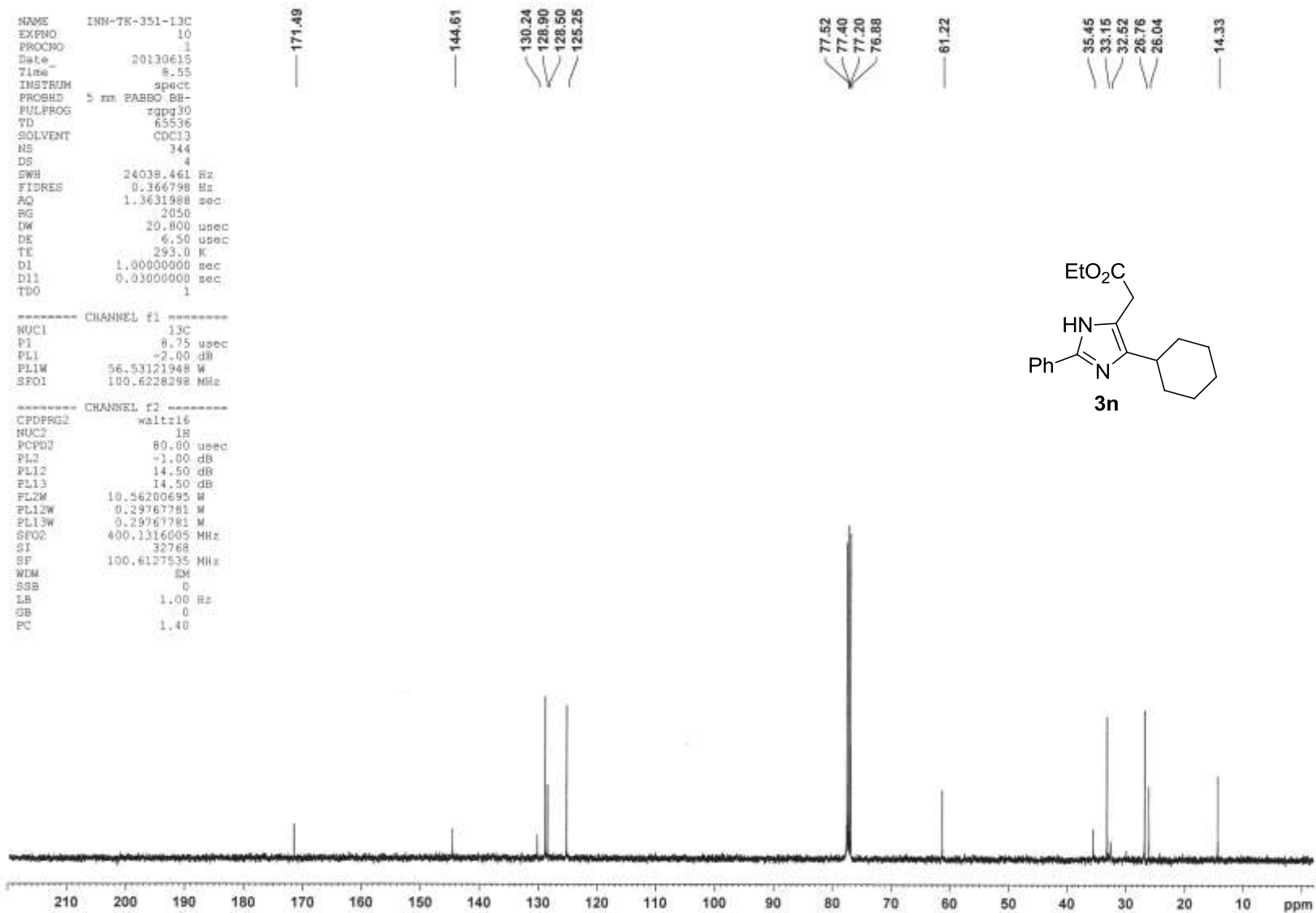


Figure S42. ¹³C NMR spectrum of **3n**

Indian Institute of Technology (B)

Analysis Info

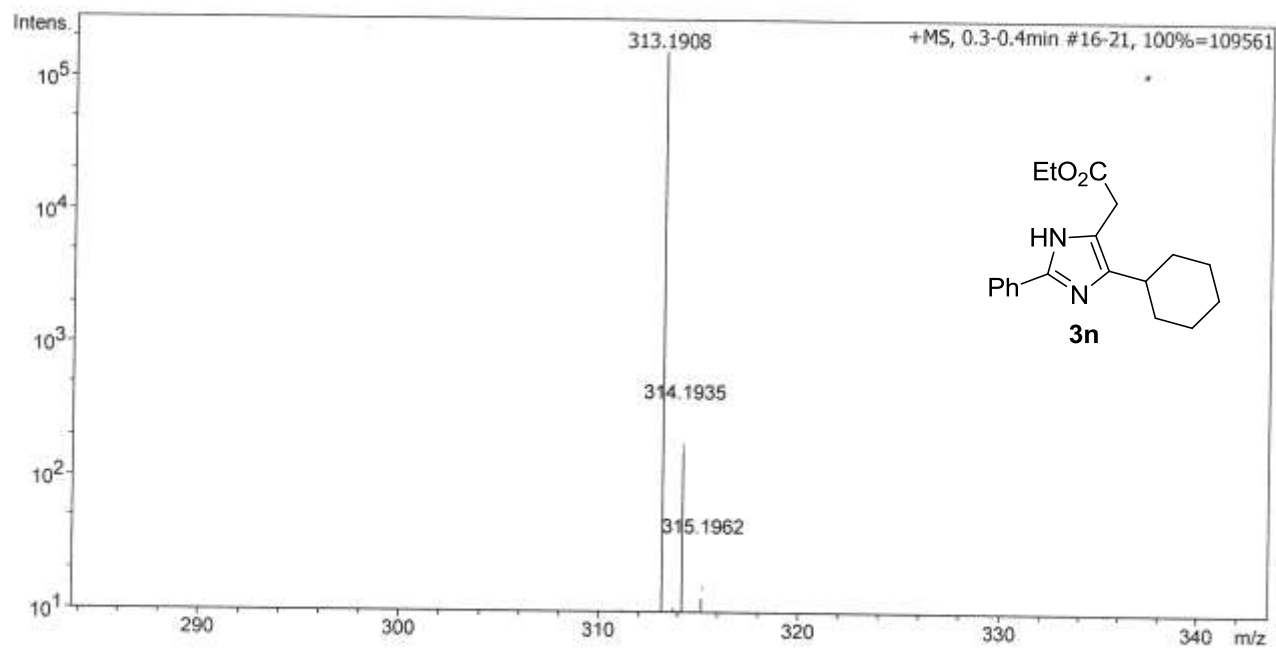
Analysis Name D:\Data\JUN-13\INN-TK-351.d
 Method Tune_pos_Standard_NAI-1000.m
 Sample Name INN-TK-351
 Comment C19H24N2O2

Acquisition Date 6/27/2013 8:53:35 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.1 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
313.1908	1	C19H25N2O2	313.1911	0.8	40.0	1	100.00	8.5	even	ok

Figure S43. HRMS spectrum of **3n**

NAME INN-TK-343-1H
 EXPNO 6
 PROCNO 1
 Date_ 20130406
 Time_ 21.46
 INSTRUM spect
 PROBHD 5 mm F4BBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 9
 DS 0
 SWH 8221.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 32
 DW 60.800 usec
 DE 6.50 usec
 TE 295.5 K
 D1 1.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 13.50 usec
 PL1 -1.00 dB
 PL1W 10.56200695 W
 SFO1 400.1324710 MHz
 SI 32768
 SF 400.1300096 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

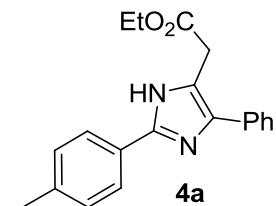
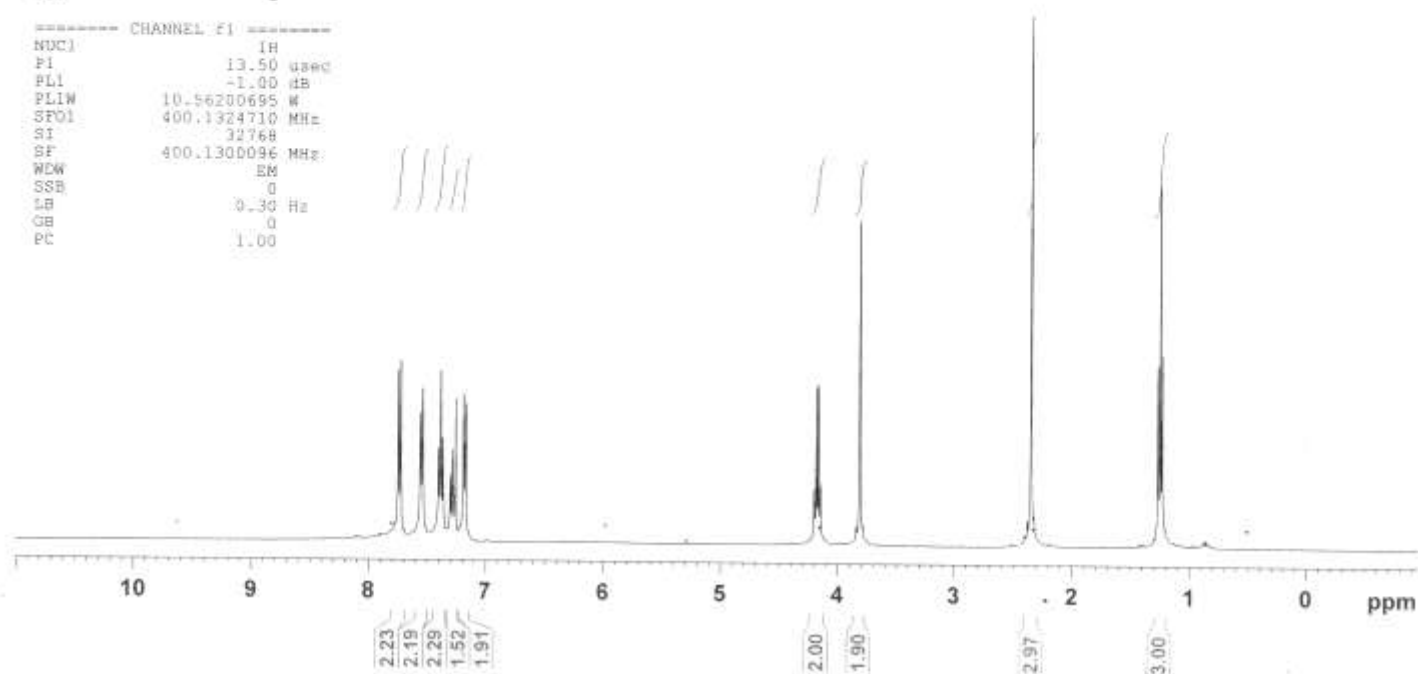


Figure S44. ¹H NMR spectrum of **4a**

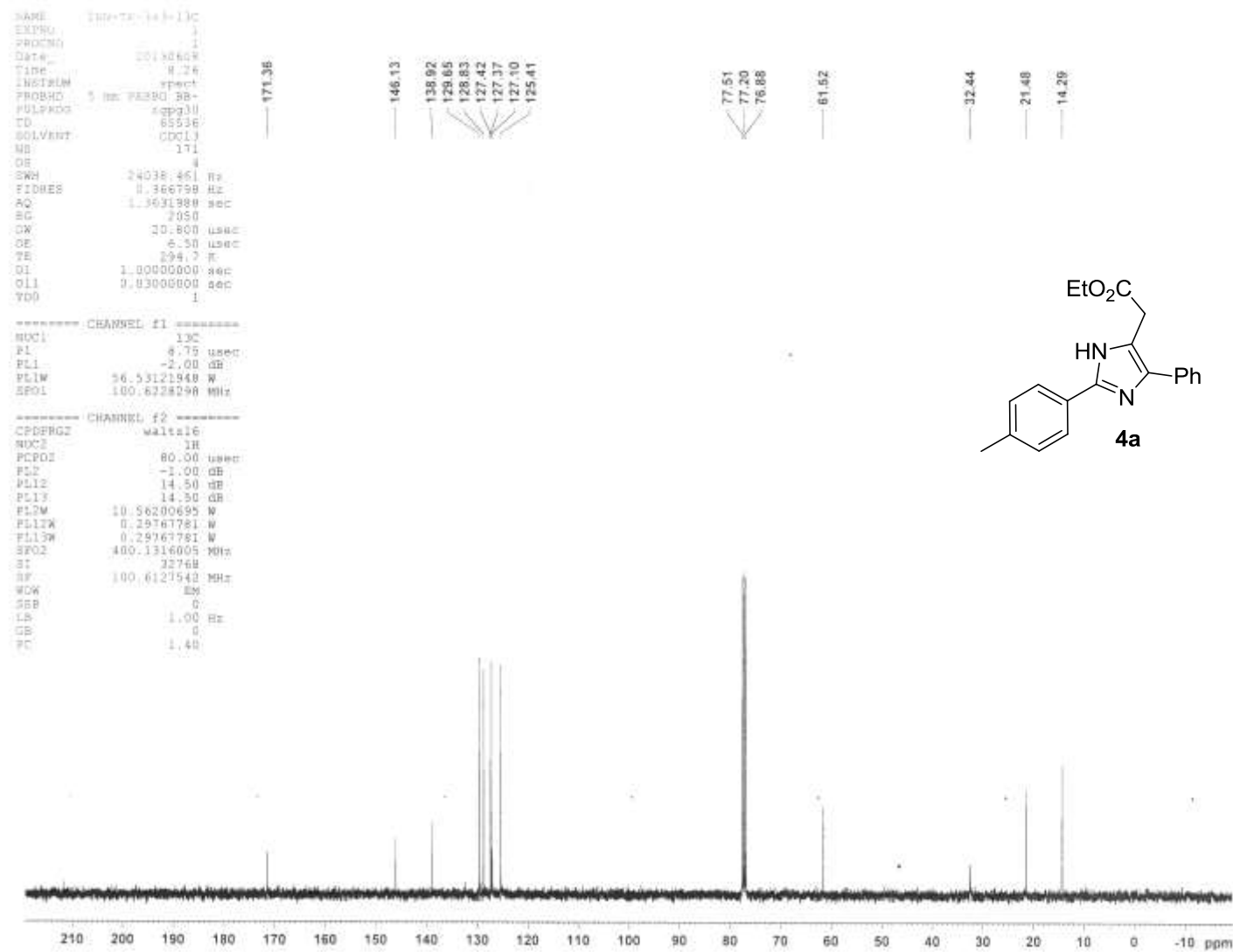


Figure S45. ¹³C NMR spectrum of **4a**

Indian Institute of Technology (B)

Analysis Info

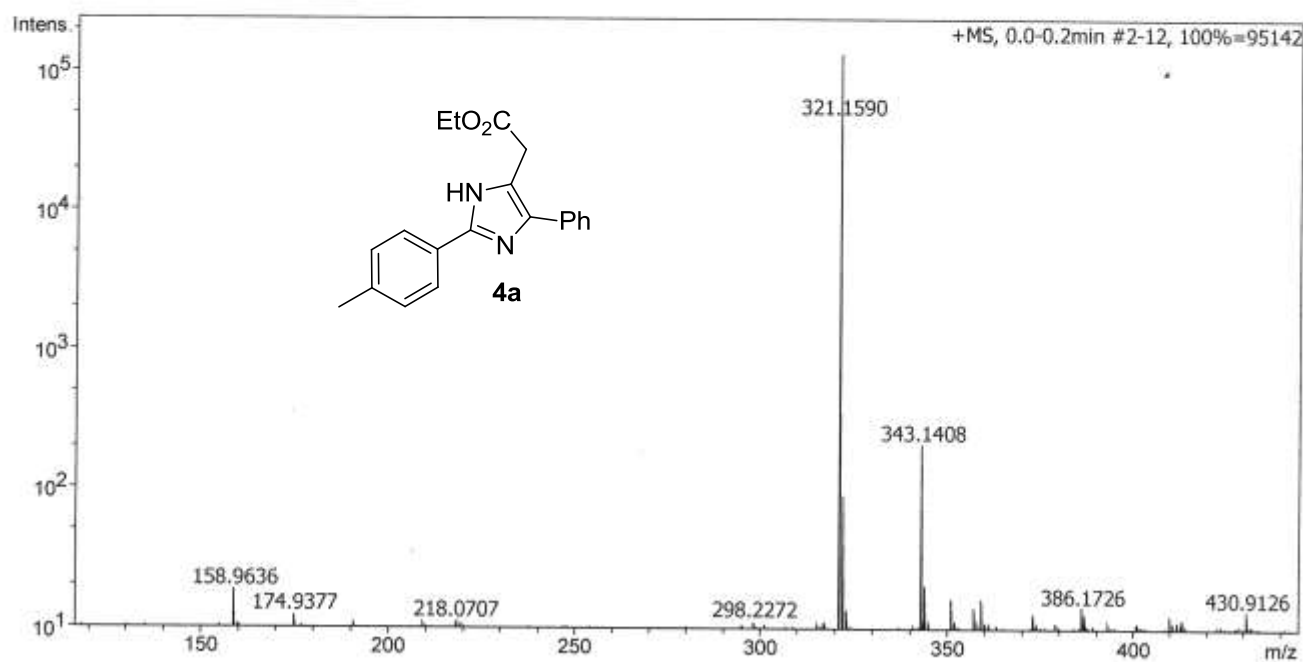
Analysis Name D:\Data\JUN-13\INN-TK-343.d
 Method Tune_pos_Standard_NAI-500.m
 Sample Name INN-TK-343
 Comment C20H20N2O2

Acquisition Date 6/10/2013 9:31:45 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.1 Bar
Focus	Active	Set Capillary	3200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
321.1590	1	C20H21N2O2	321.1598	-2.4	18.7	1	100.00	11.5	even	ok

Figure S46. HRMS spectrum of **4a**

NAME INN-TK-346-1H
 EXPNO 7
 PROCNO 1
 Date_ 20130606
 Time 21.51
 INSTRUM spect
 PROBHD 5 mm PASBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 18
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 32
 DW 60.800 usec
 DE 6.50 usec
 TE 295.5 K
 D1 1.00000000 sec
 TDO 1

INN-TK-346-1H

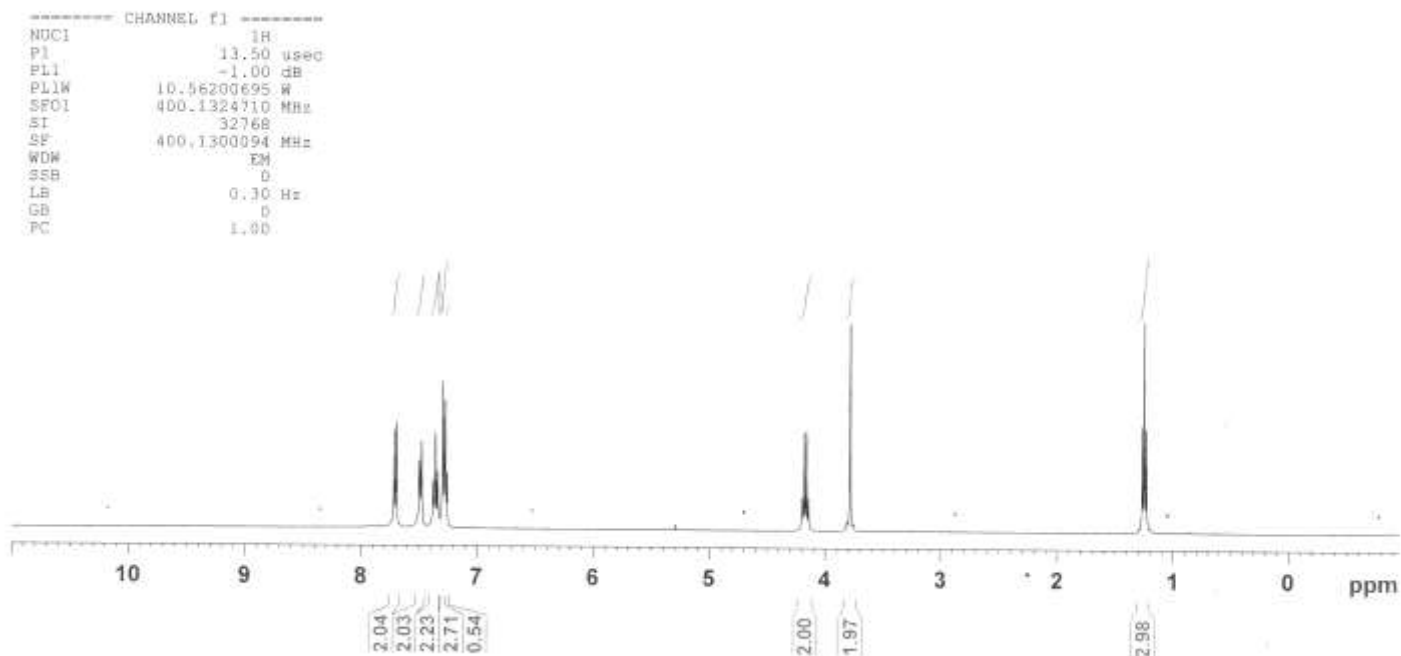
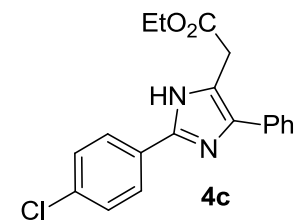


Figure S47. ^1H NMR spectrum of **4c**

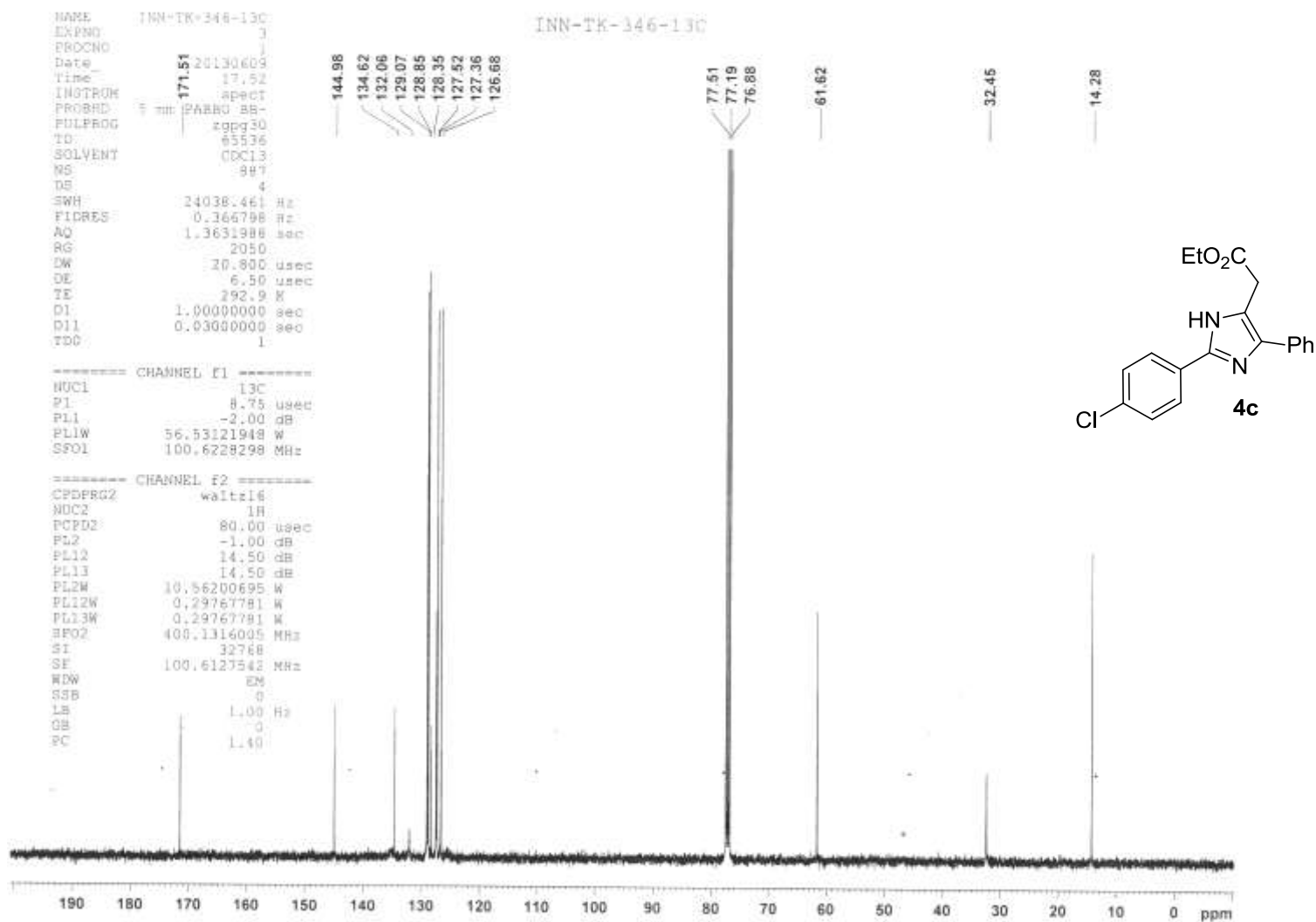


Figure S48. ^{13}C NMR spectrum of **4c**

Indian Institute of Technology (B)

Analysis Info

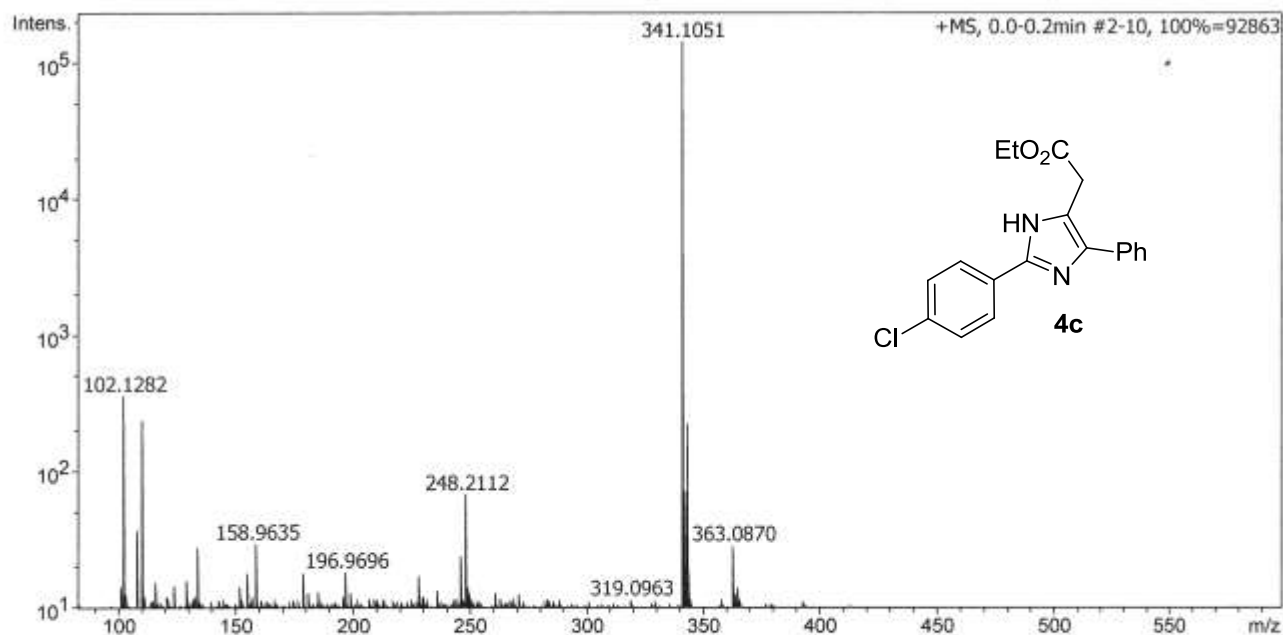
Analysis Name D:\Data\JUN-13\INN-TK-346.d
 Method Tune_pos_Standard_NAI-1000.m
 Sample Name INN-TK-346
 Comment C19H17ClN2O2

Acquisition Date 6/10/2013 5:43:10 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.1 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
341.1051	1	C19H18ClN2O2	341.1051	0.0	10.0	1	100.00	11.5	even	ok

Figure S49. HRMS spectrum of **4c**

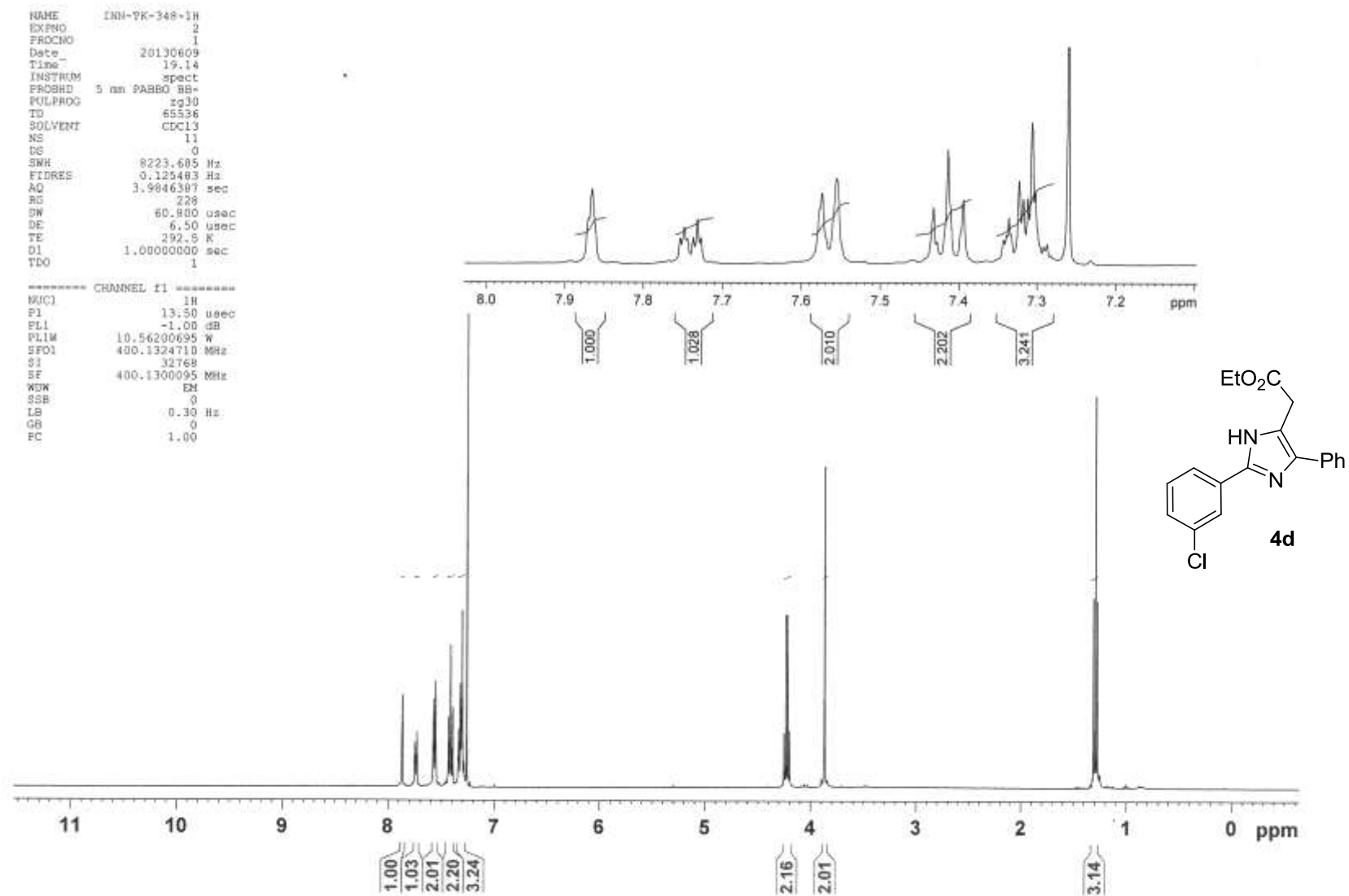


Figure S50. ^1H NMR spectrum of **4d**

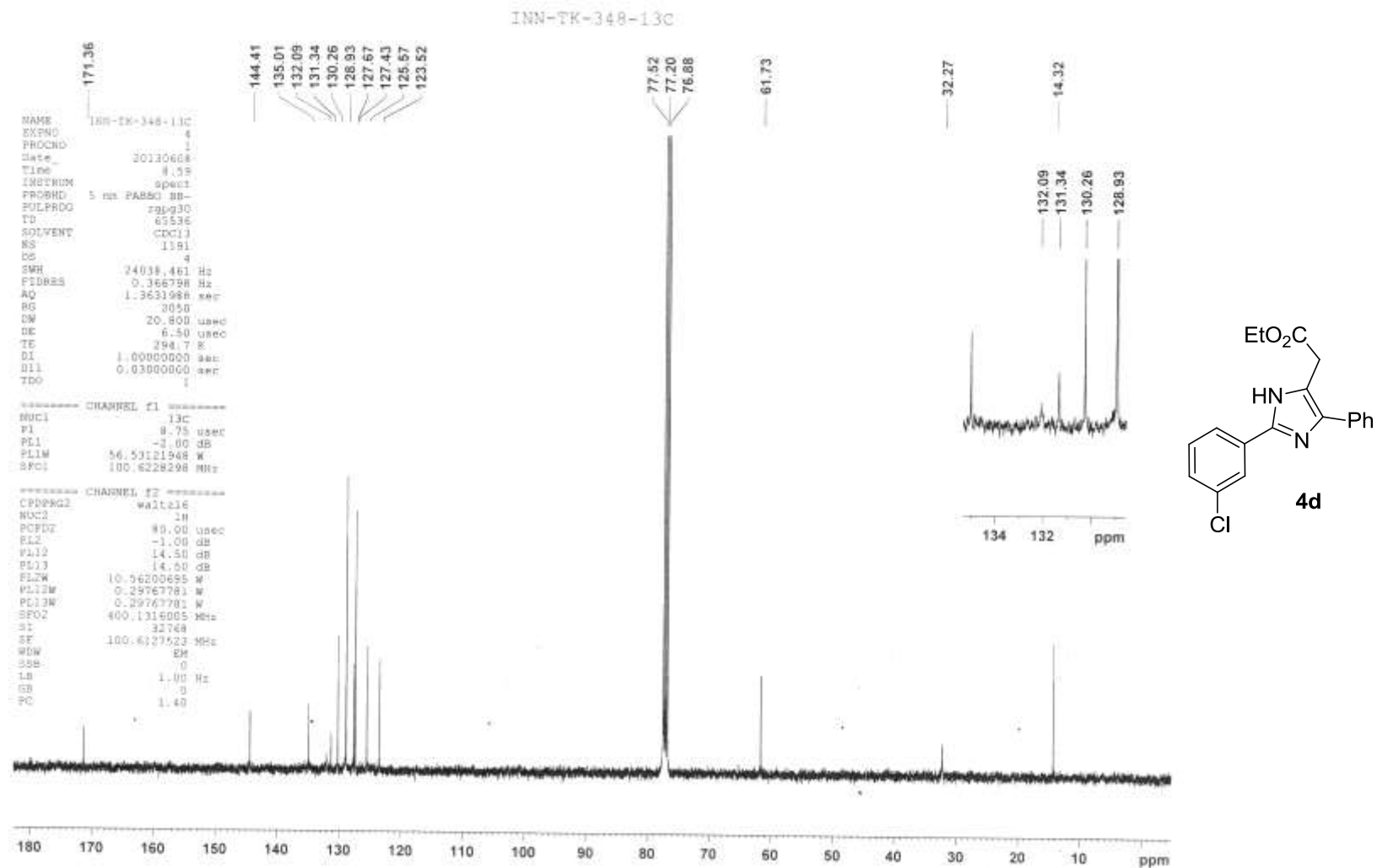


Figure S51. ¹³C NMR spectrum of **4d**

Indian Institute of Technology (B)

Analysis Info

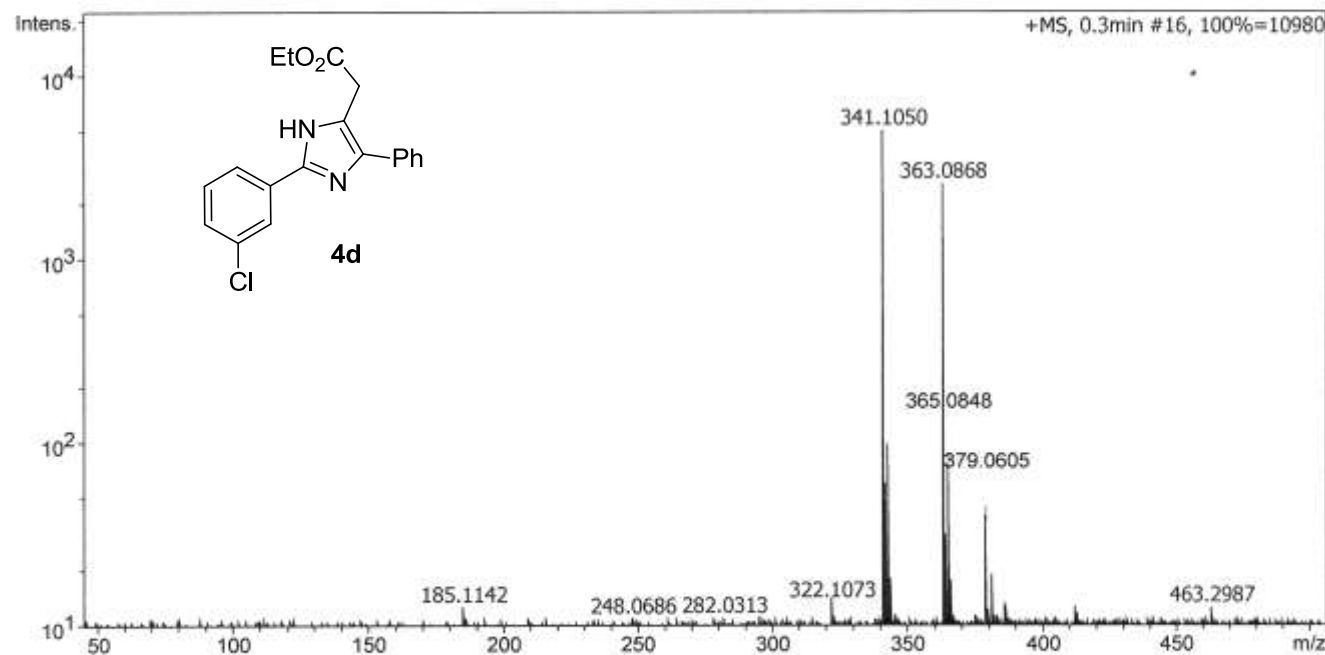
Analysis Name D:\Data\JUN-13\INN-TK-348.d
 Method Tune_pos_Standard_NAI-500.m
 Sample Name INN-TK-348
 Comment C19H17CIN2O2

Acquisition Date 6/10/2013 9:13:54 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

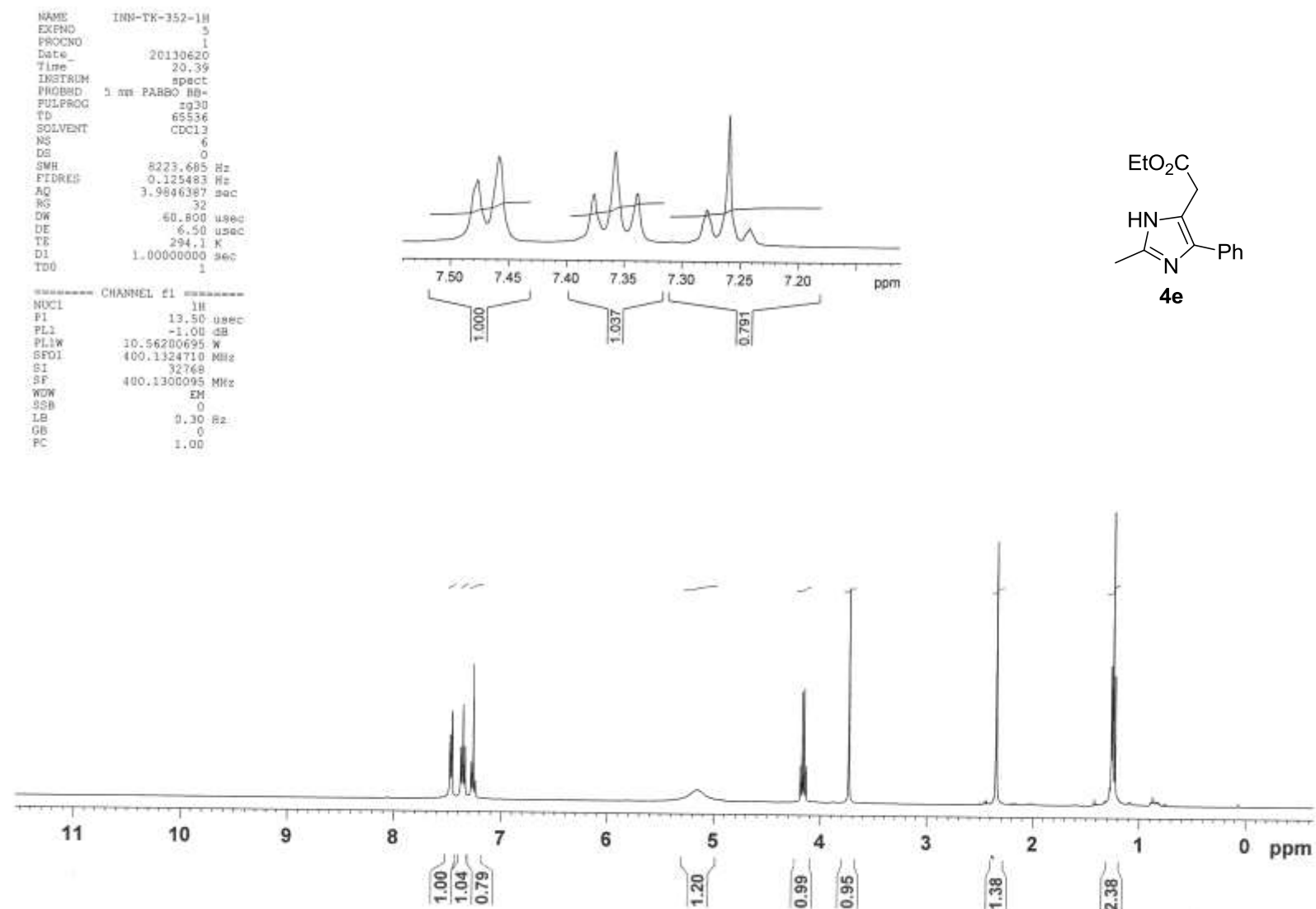
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.1 Bar
Focus	Active	Set Capillary	3200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
341.1050	1	C19H18CIN2O2	341.1051	-0.5	36.1	1	100.00	11.5	even	ok

Figure S52. HRMS spectrum of **4d**



S53. ^1H NMR spectrum of **4e**

Figure

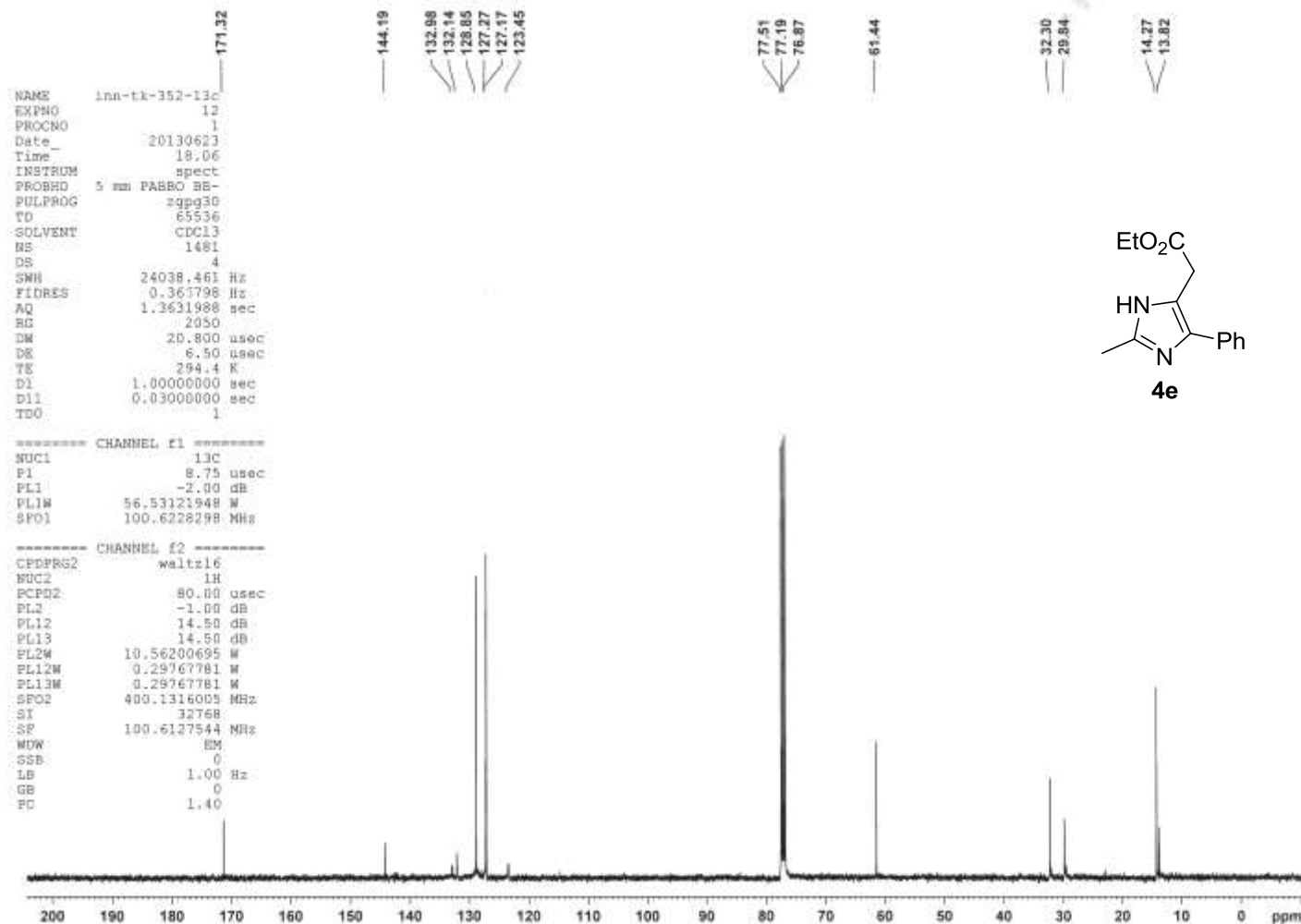


Figure S54. ¹³C NMR spectrum of **4e**

Indian Institute of Technology (B)

Analysis Info

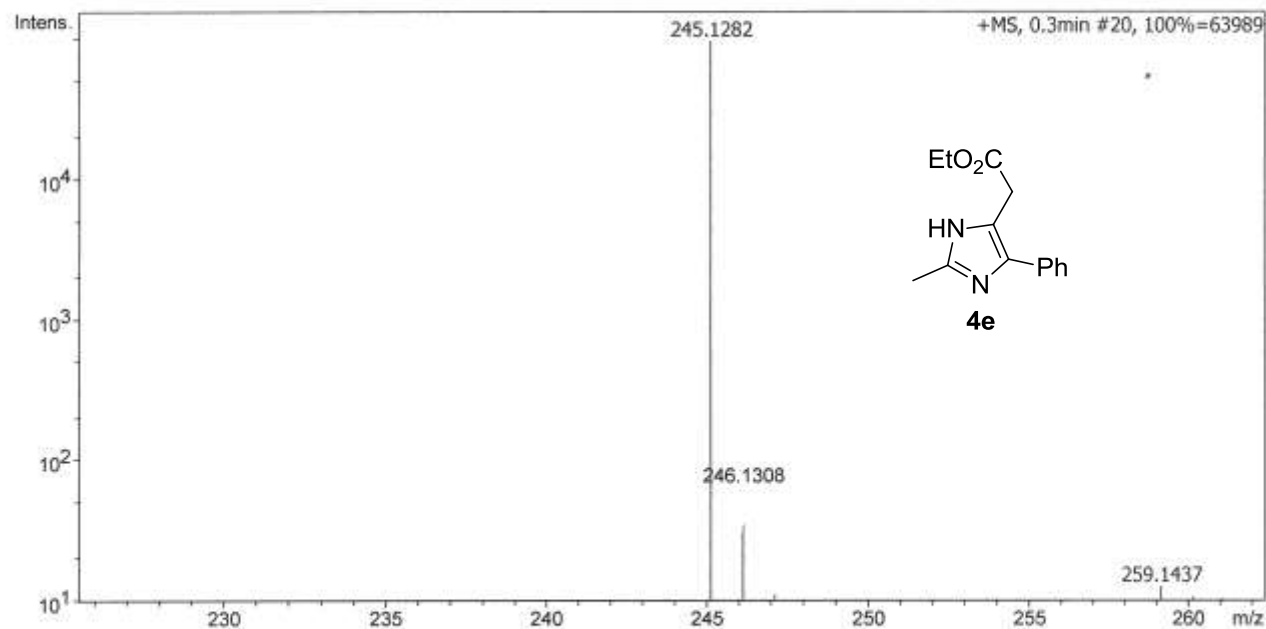
Analysis Name D:\Data\JUN-13\INN-TK-352.d
 Method Tune_pos_Standard_NAI-1000.m
 Sample Name INN-TK-352
 Comment C14H16N2O2

Acquisition Date 6/27/2013 9:01:05 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.1 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
245.1282	1	C14H17N2O2	245.1285	0.9	23.8	1	100.00	7.5	even	ok

Figure S55. HRMS spectrum of **4e**

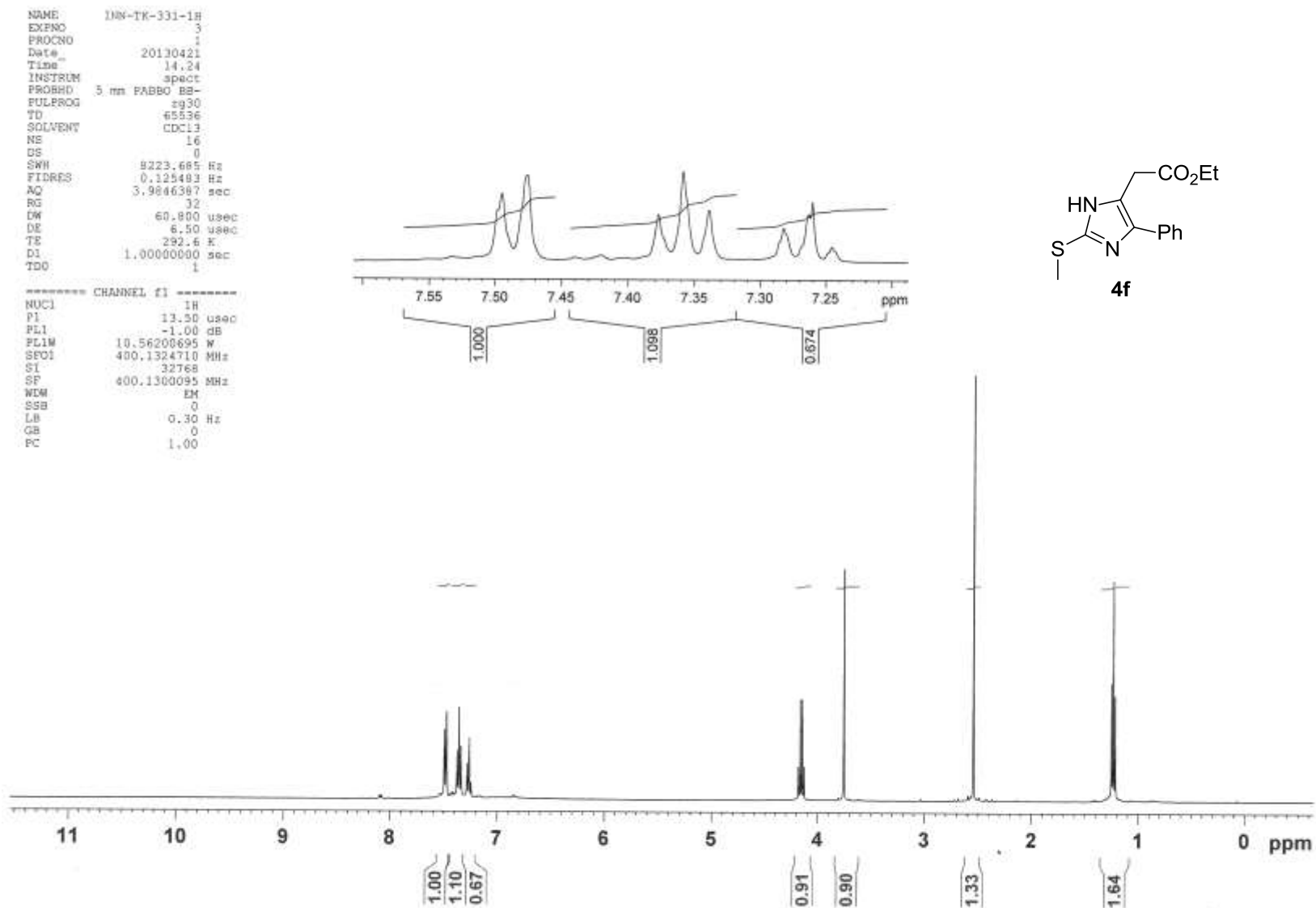


Figure S56. ^1H NMR spectrum of **4f**

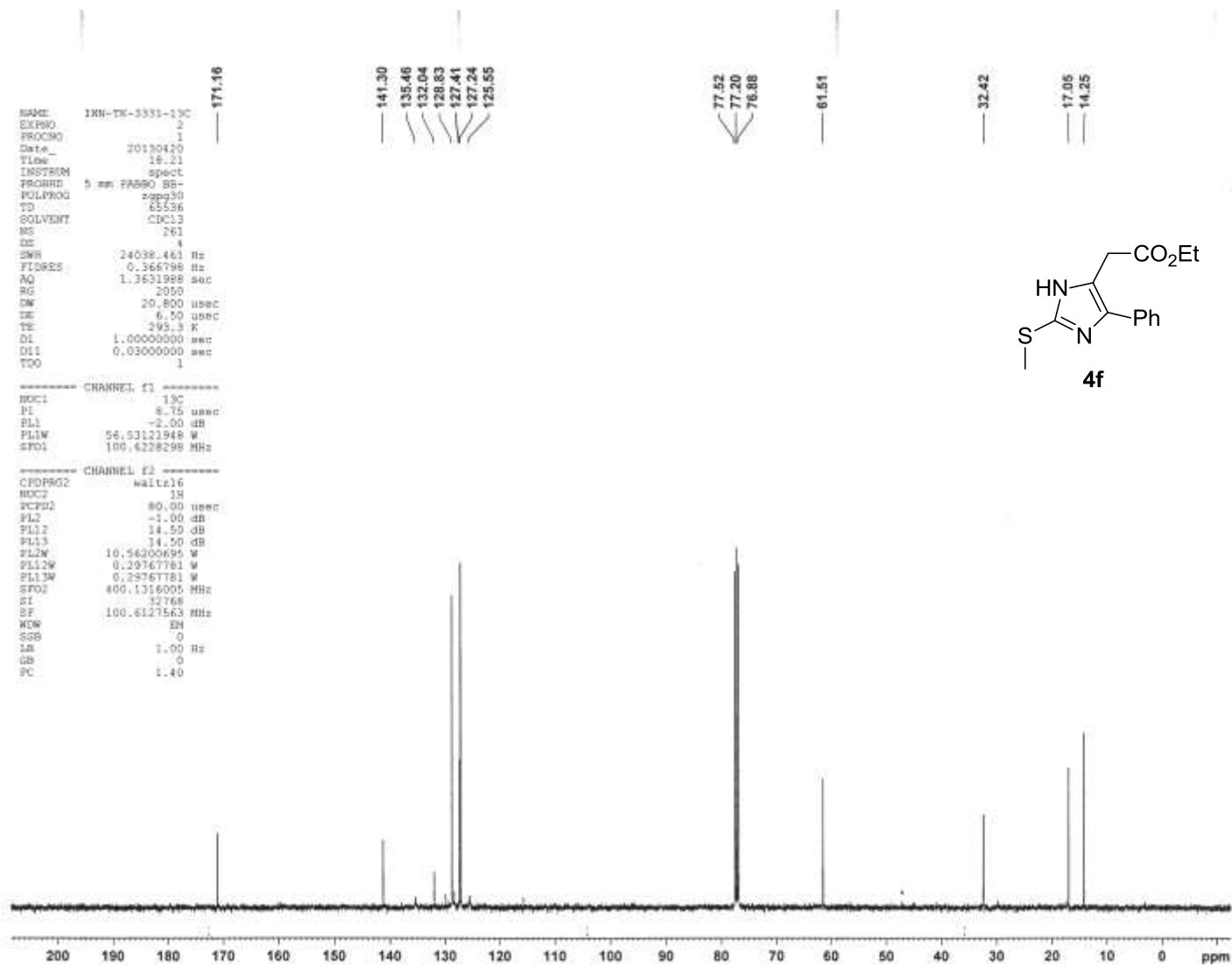


Figure S57. ¹³C NMR spectrum of **4f**

Indian Institute of Technology (B)

Analysis Info

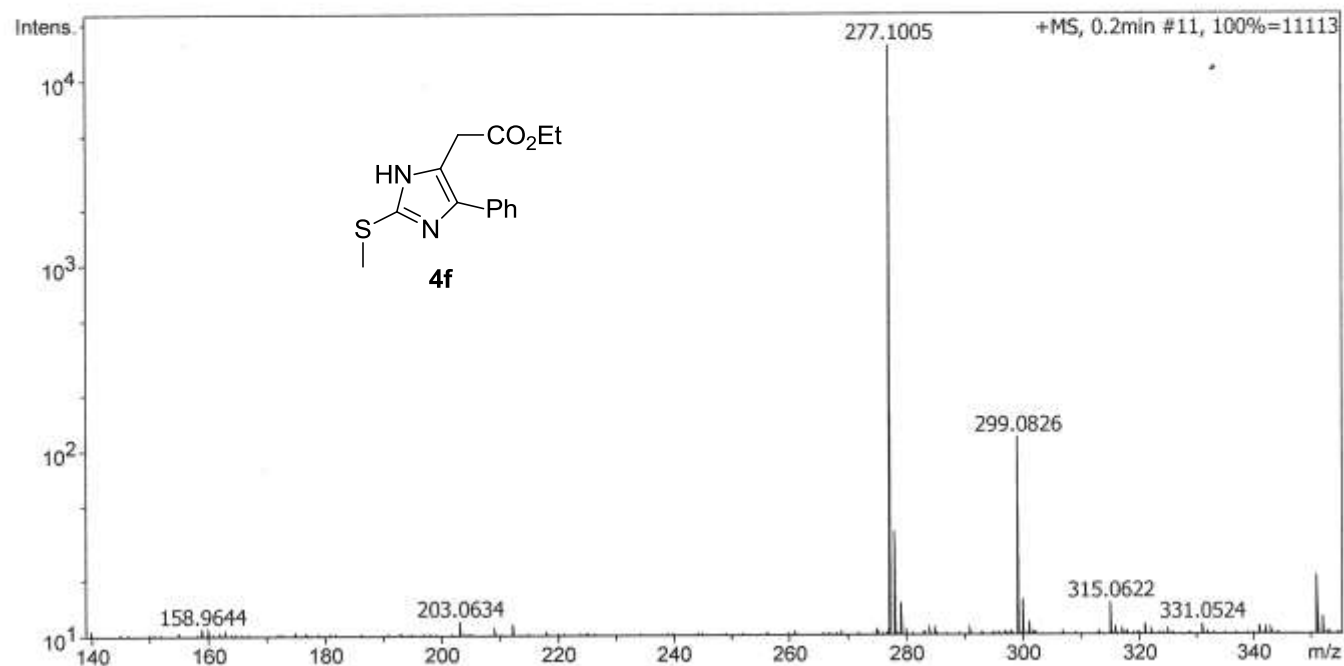
Analysis Name D:\Data\JUN-13\INN-TK-331 .d
Method Tune_pos_Standard_NAI-500.m
Sample Name INN-TK-331
Comment C14H16N2O2S

Acquisition Date 6/10/2013 9:54:24 PM

Operator IIT-B
Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.1 Bar
Focus	Active	Set Capillary	3200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
277.1005	1	C14H17N2O2S	277.1005	-0.1	7.5	1	100.00	7.5	even	ok

Figure S58. HRMS spectrum of **4f**

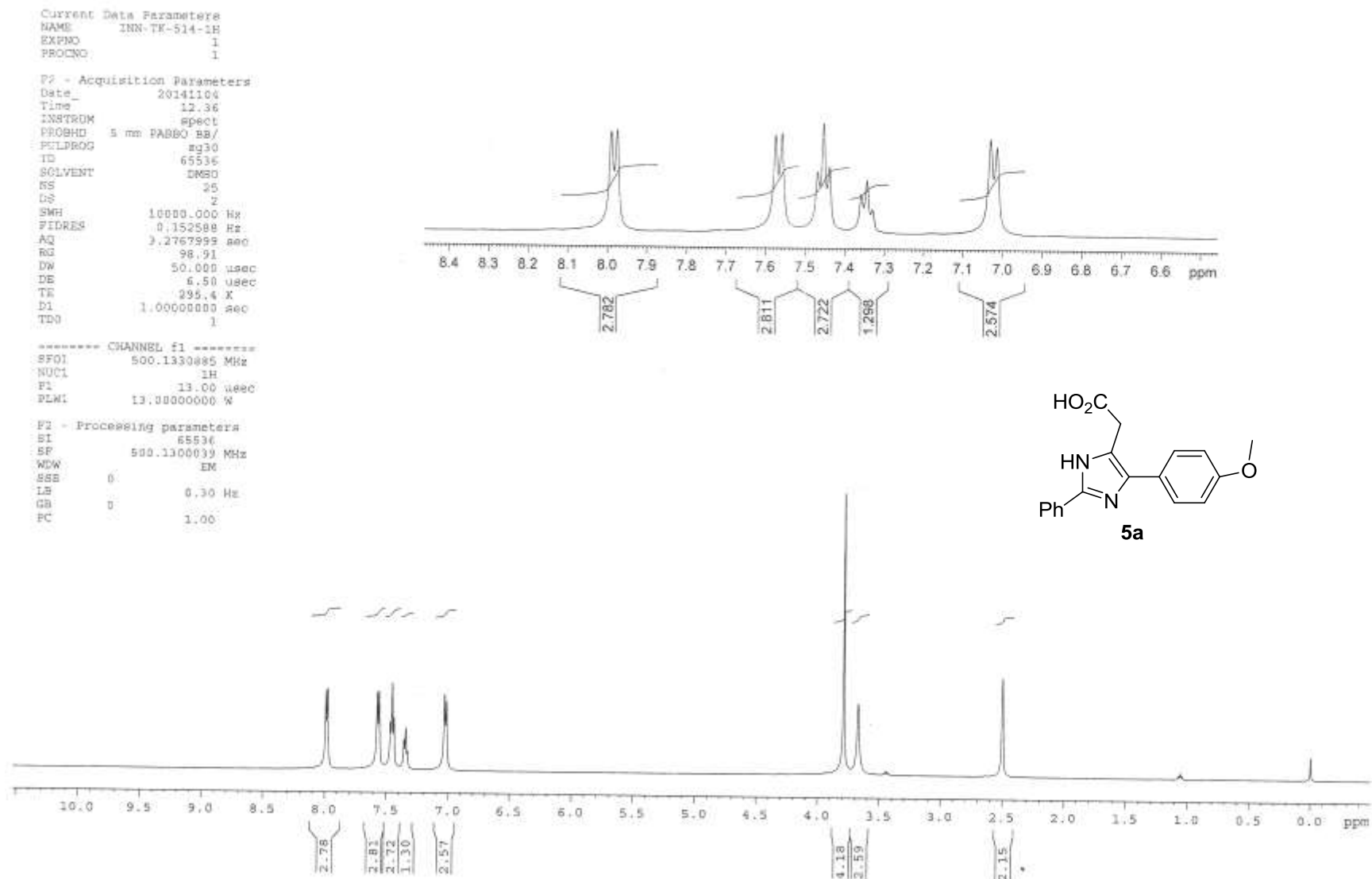


Figure S59. ^1H NMR spectrum of **5a**

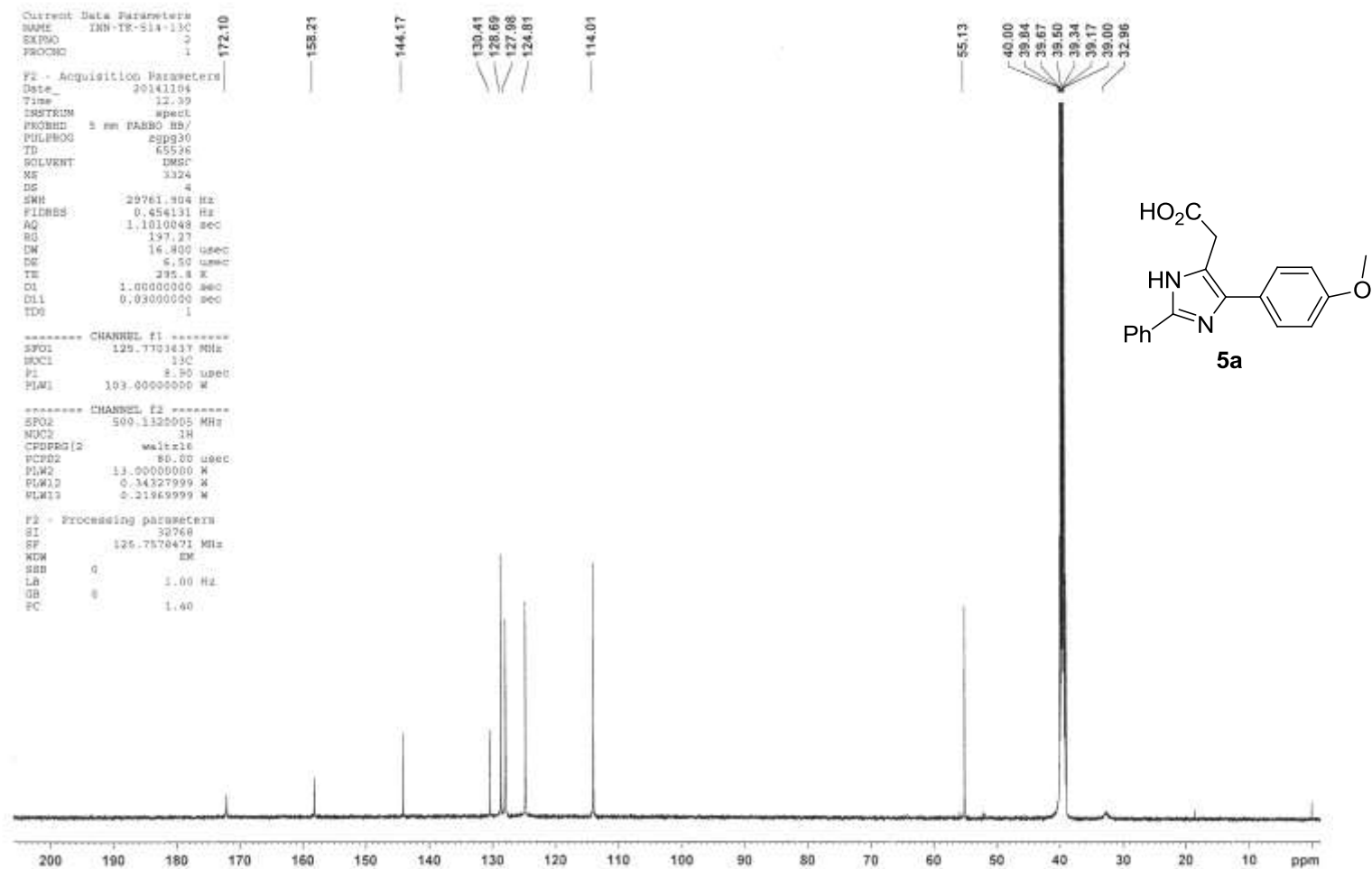


Figure S60. ¹³C NMR spectrum of **5a**

DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

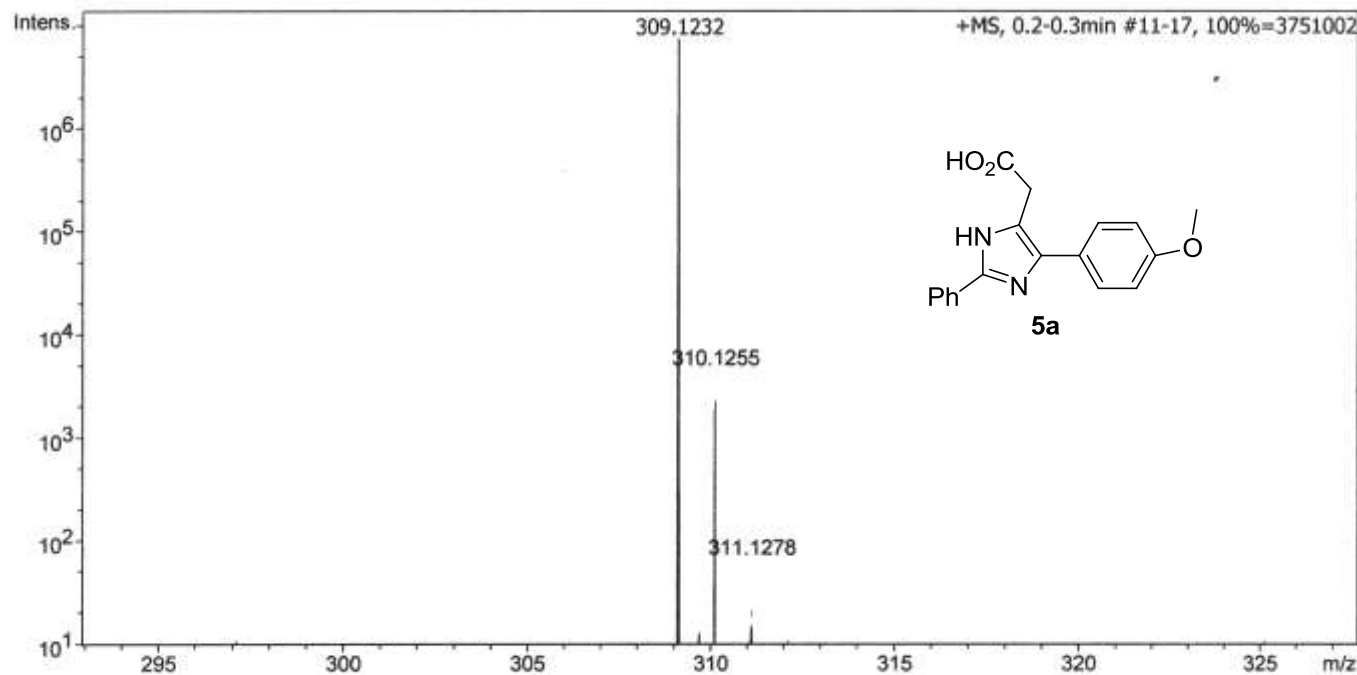
Analysis Name D:\Data\NOV-14\INN-TK-514.d
 Method Tune_pos_NAICSI-1000.m
 Sample Name INN-TK-514
 Comment C18H16N2O3

Acquisition Date 11/10/2014 7:21:10 PM

Operator CPR IN
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
309.1232	1	C18H17N2O3	309.1234	0.4	104.8	1	100.00	11.5	even	ok

Figure S61. HRMS spectrum of **5a**

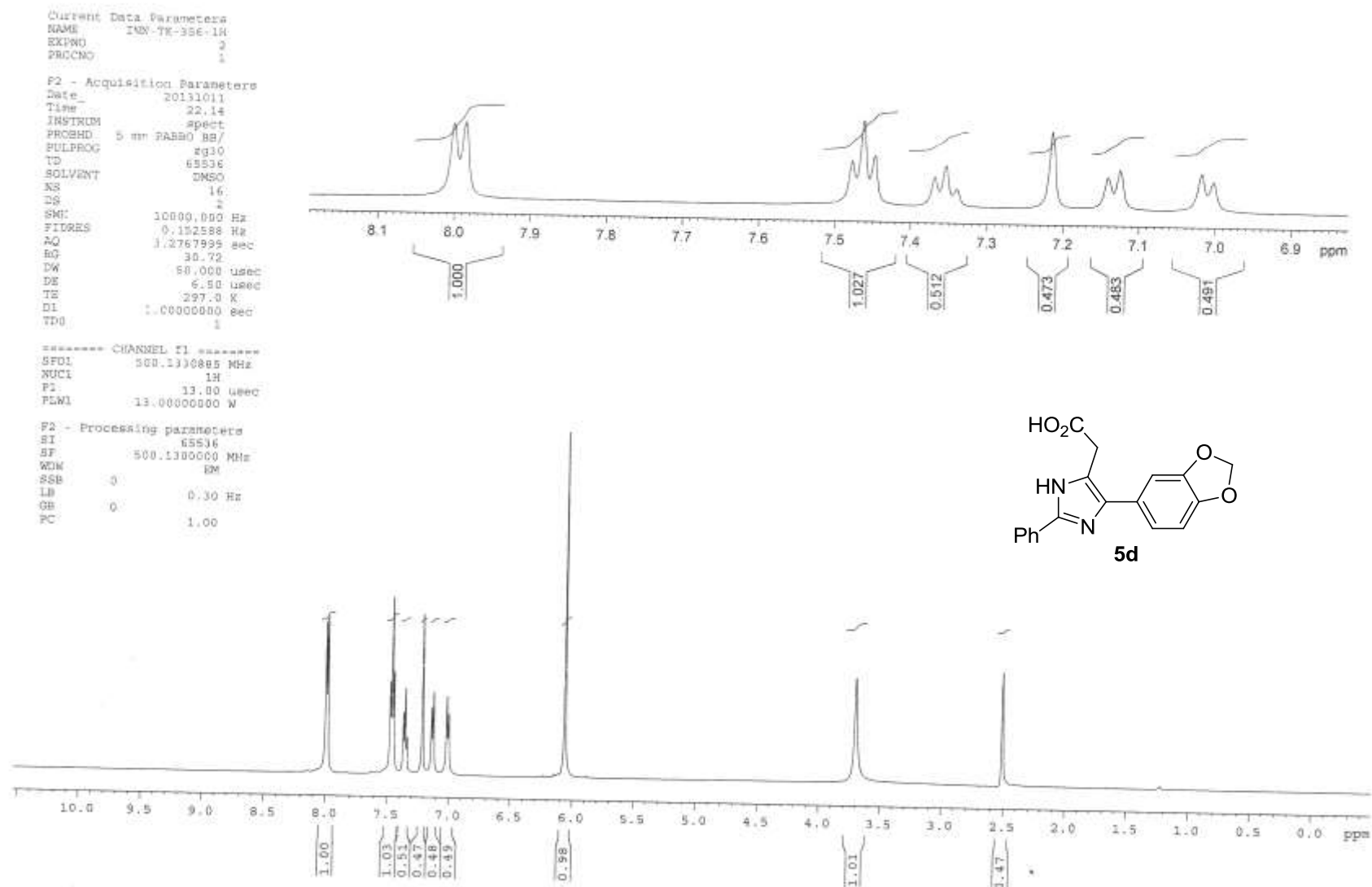


Figure S62. ^1H NMR spectrum of **5d**

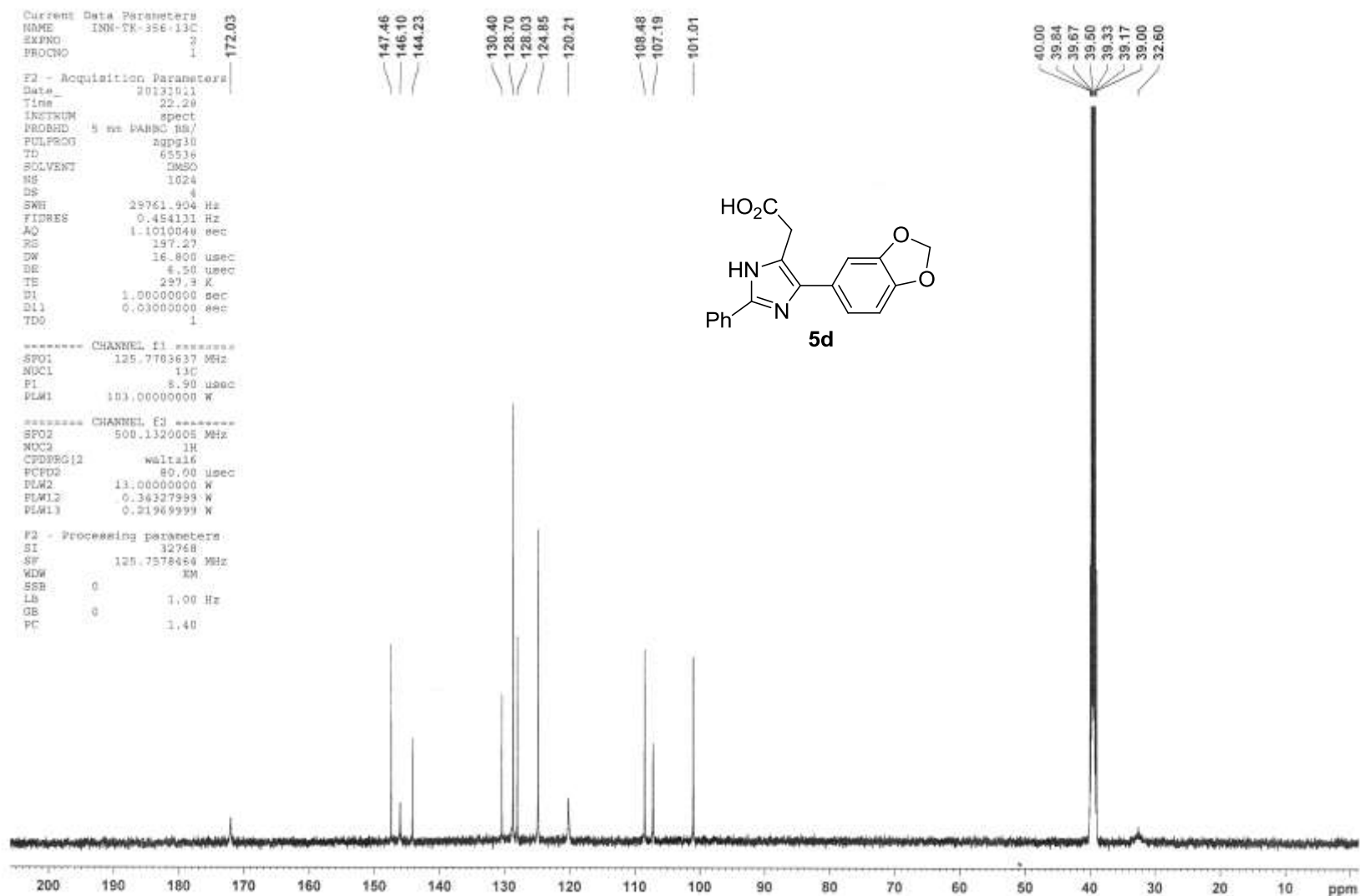


Figure S63. ^{13}C NMR spectrum of **5d**

Indian Institute of Technology (B)

Analysis Info

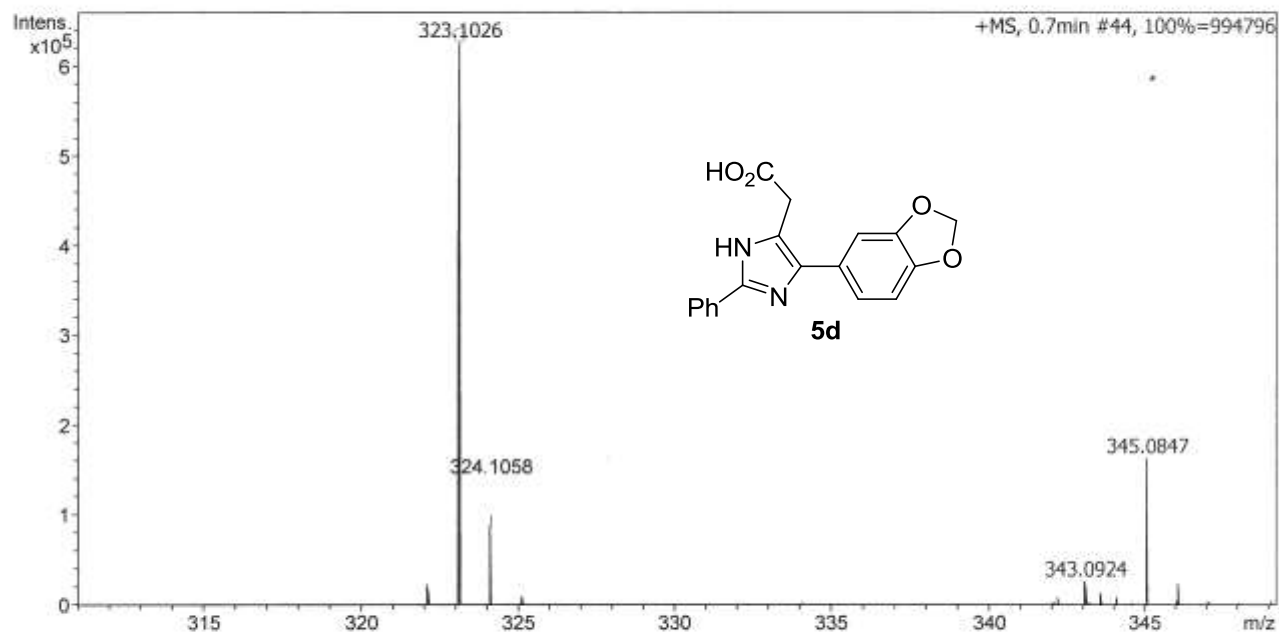
Analysis Name D:\Data\JULY_13\INN-TK-356.d
 Method Tune_pos_Standard_NAI-1500.m
 Sample Name INN-TK-356
 Comment C18H14N2O4

Acquisition Date 7/26/2013 3:28:29 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.1 Bar
Focus	Active	Set Capillary	3200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
323.1026	1	C18H15N2O4	323.1026	0.0	37.5	1	100.00	12.5	even	ok

Figure S64. HRMS spectrum of **5d**

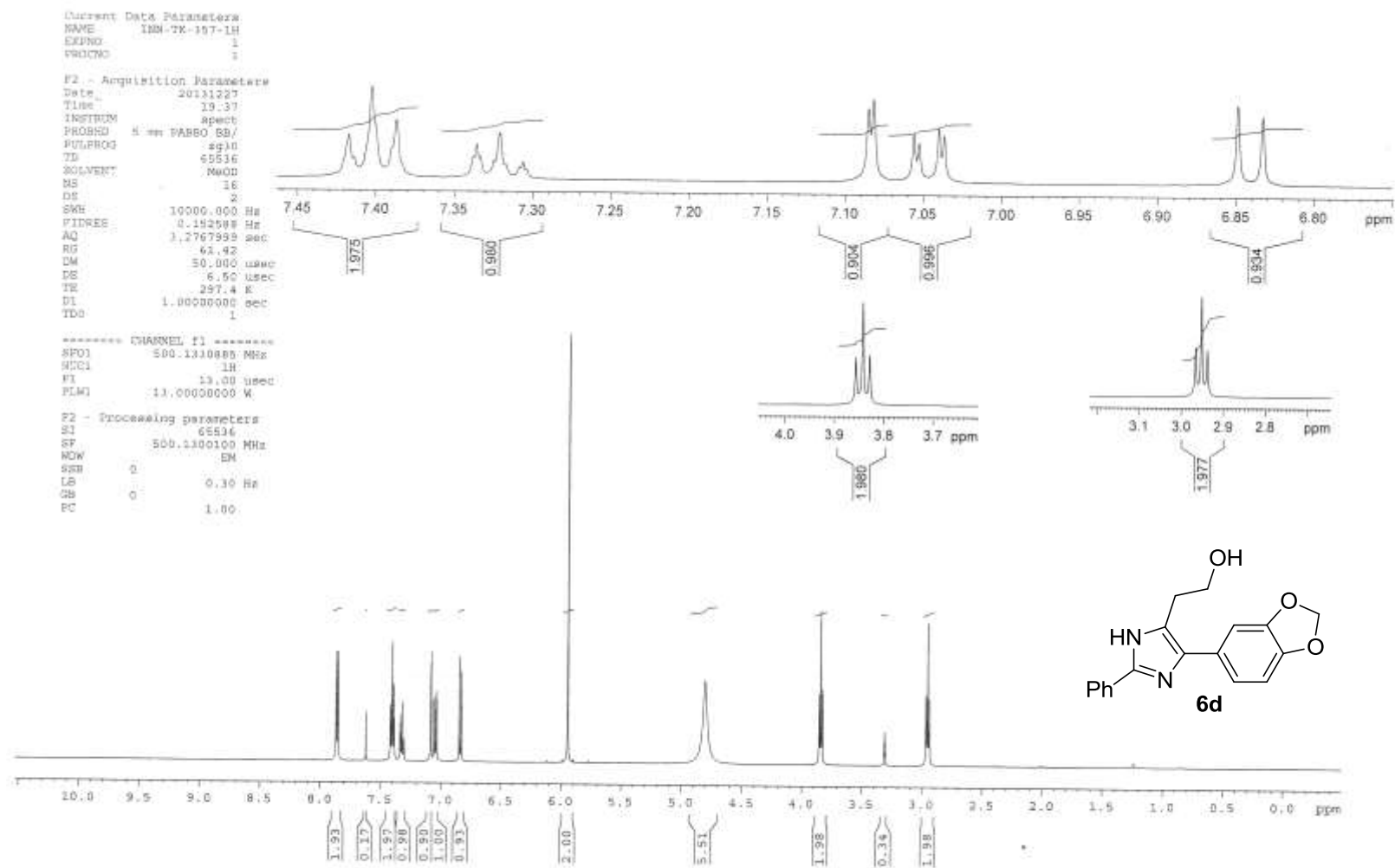


Figure S65. ^1H NMR spectrum of **6d**

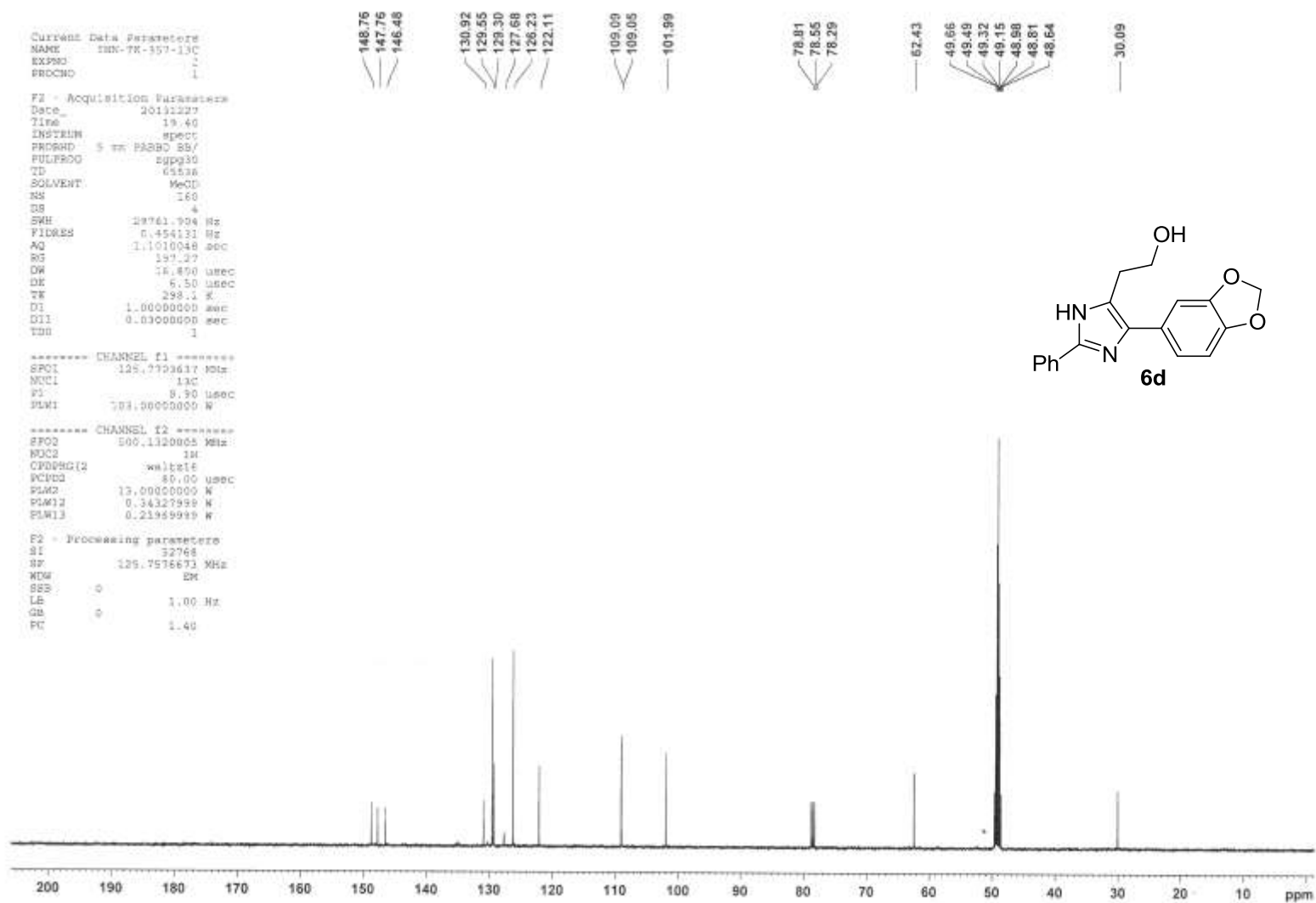


Figure S66. ^{13}C NMR spectrum of **6d**

Indian Institute of Technology (B)

Analysis Info

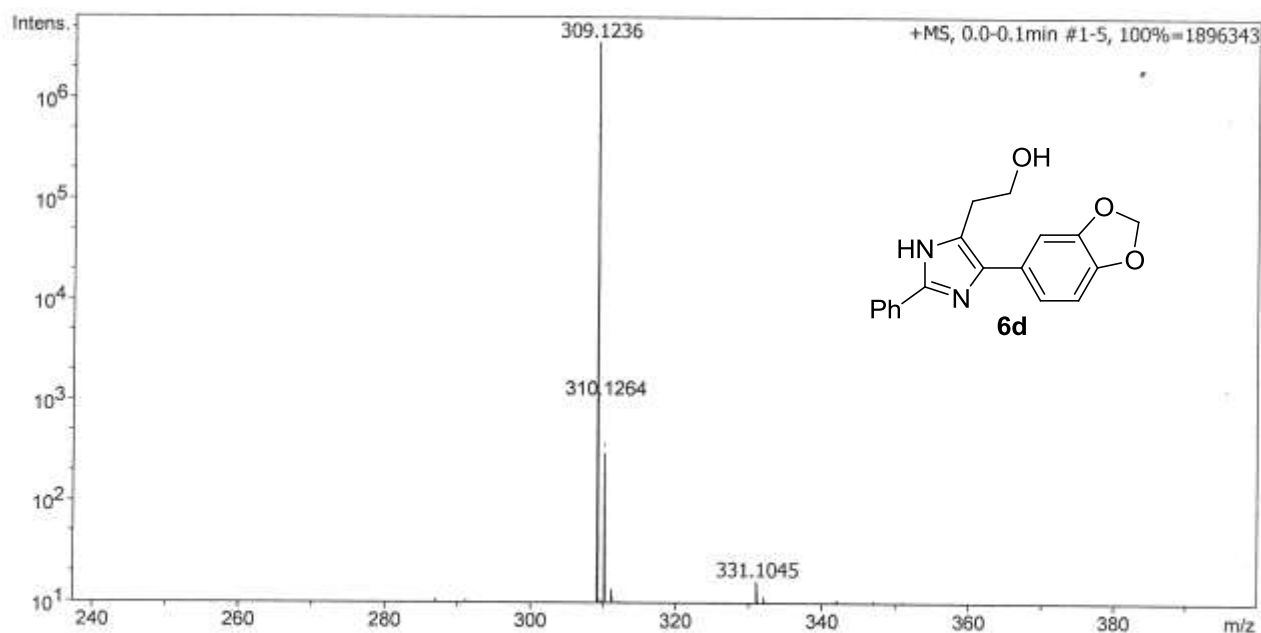
Analysis Name D:\Data\DEC-13\INN-TK-357.d
 Method Tune_pos_Standard_NAI-1000.m
 Sample Name INN-TK-357
 Comment C18HH16O3N2

Acquisition Date 12/31/2013 3:29:59 PM

Operator INN-IN
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
309.1236	1	C18H17N2O3	309.1234	0.7	36.0	1	100.00	11.5	even	ok

Figure S67. HRMS spectrum of **6d**

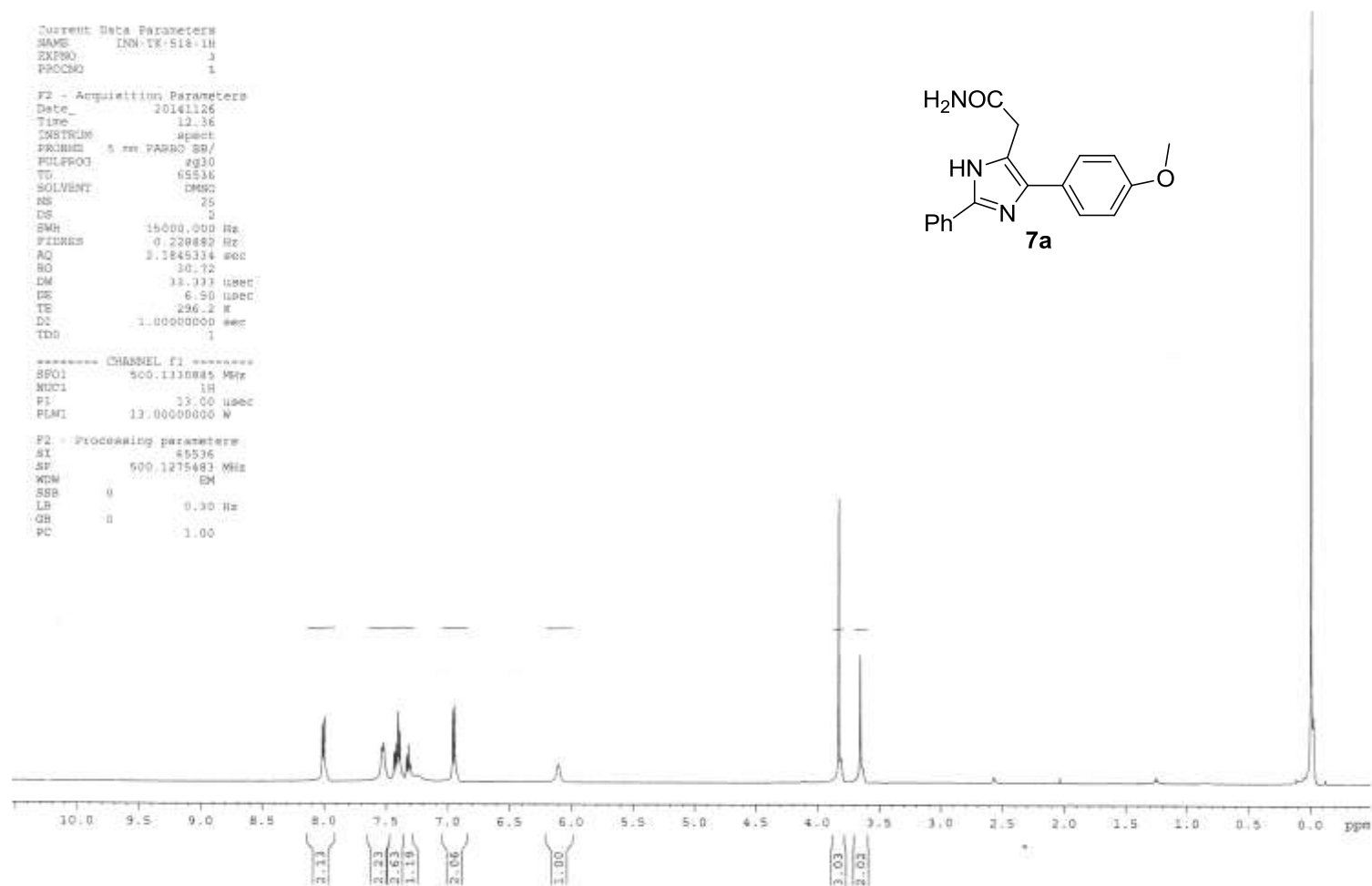


Figure S68. ^1H NMR spectrum of **7a**

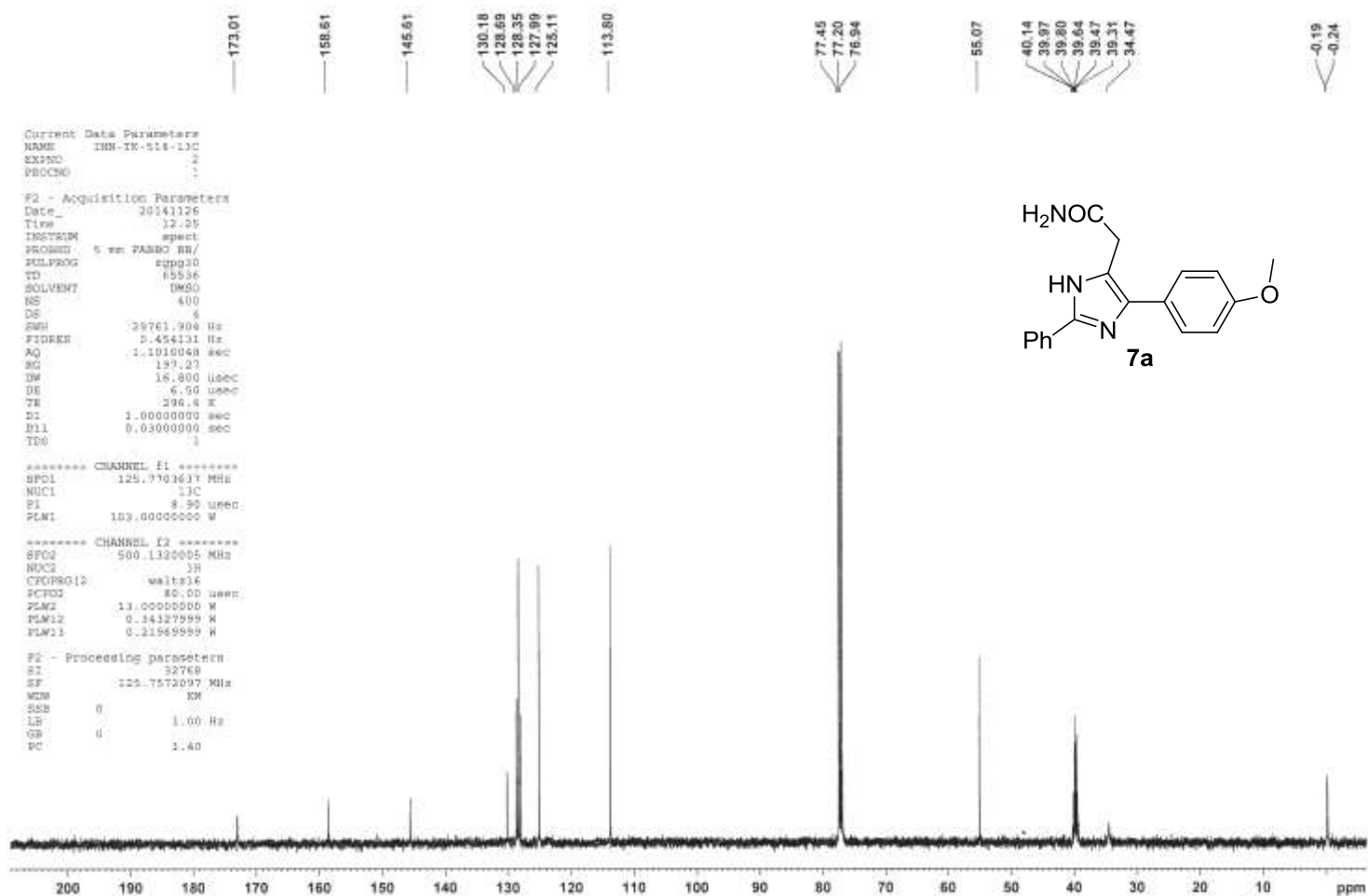


Figure S69. ^{13}C NMR spectrum of **7a**

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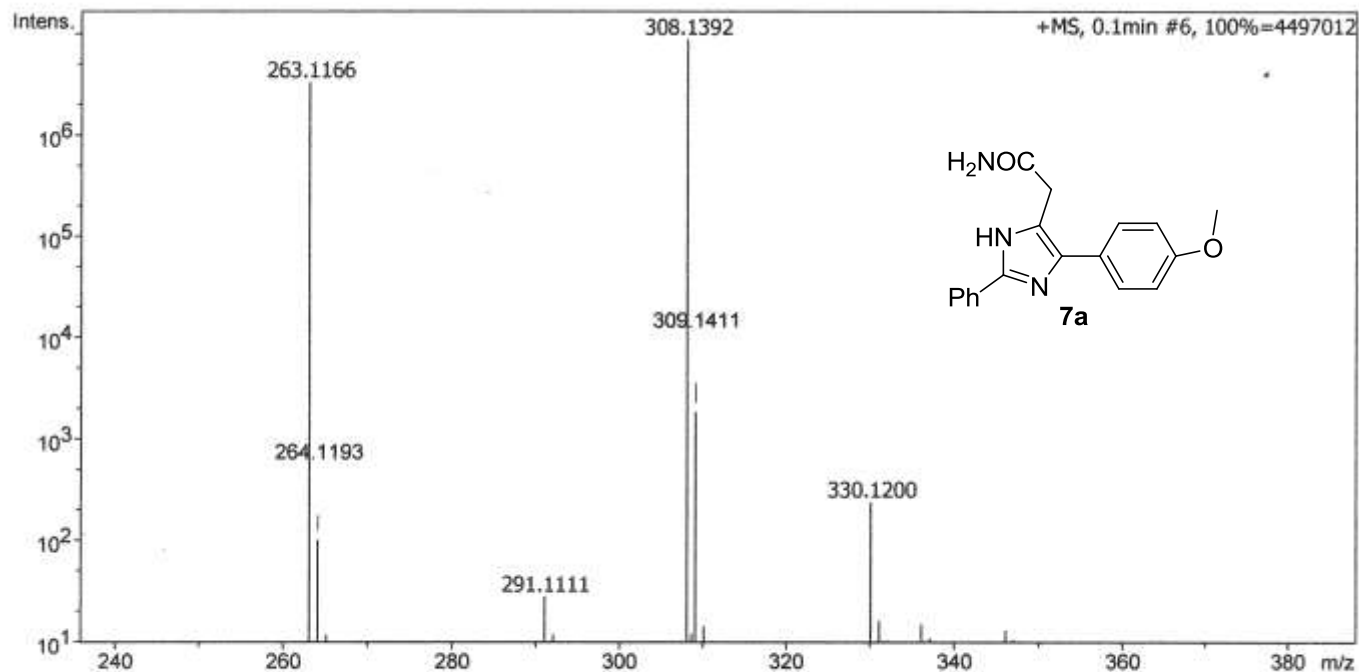
Analysis Info

Analysis Name D:\Data\NOV-14\INN-TK-518.d
 Method Tune_pos_NAICSI-500.m
 Sample Name INN-TK-518
 Comment C18H17N3O2

Acquisition Date 11/26/2014 1:26:39 PM
 Operator DM OUT
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
308.1392	1	C18H18N3O2	308.1394	-0.6	99.9	1	100.00	11.5	even	ok

Figure S70. HRMS spectrum of **7a**

```

NAME      INH-TK-359-1H-
EXPNO     7
PROCNO     1
Date_      20130813
Time       14.33
INSTRUM    spect
PROBHD     5 mm PABBO BB-
PULPROG    zg30
TD         65536
SOLVENT    MeOD
NS         8
DS         0
SWH         8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         32
DW         60.800 usec
DE         6.50 usec
TE         294.4 K
D1         1.00000000 sec
TD0        1

```

```

===== CHANNEL f1 =====
NUC1       1H
P1         13.50 usec
PL1        -1.00 dB
PL1W       10.56200695 W
SFO1       400.1324710 MHz
SI         32768
SF         400.1300095 MHz
WDW         EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00

```

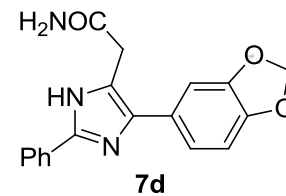
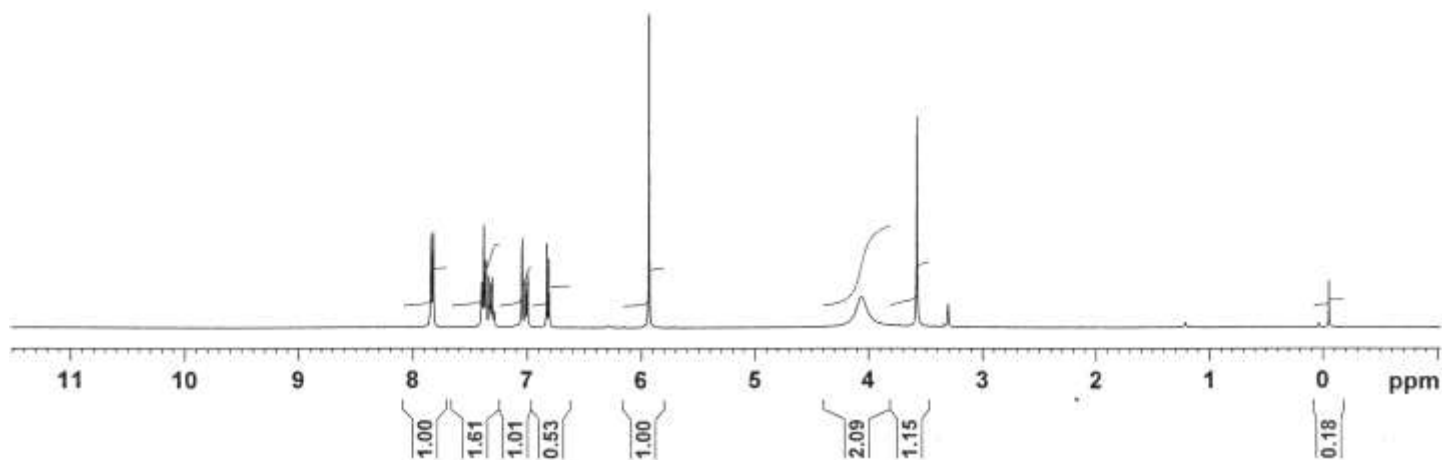


Figure S71. ¹H NMR spectrum of **7d**

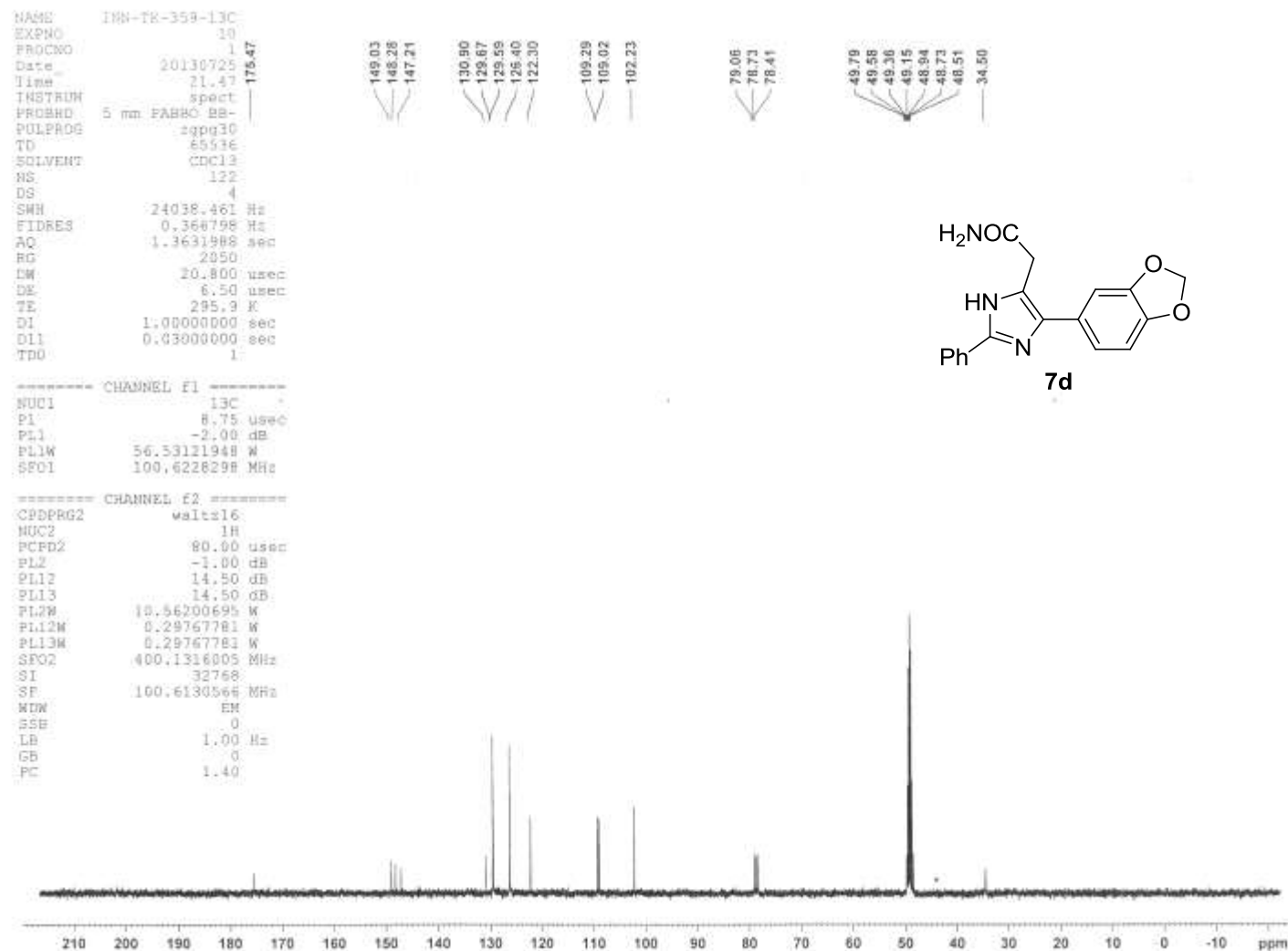


Figure S72. ^{13}C NMR spectrum of **7d**

Indian Institute of Technology (B)

Analysis Info

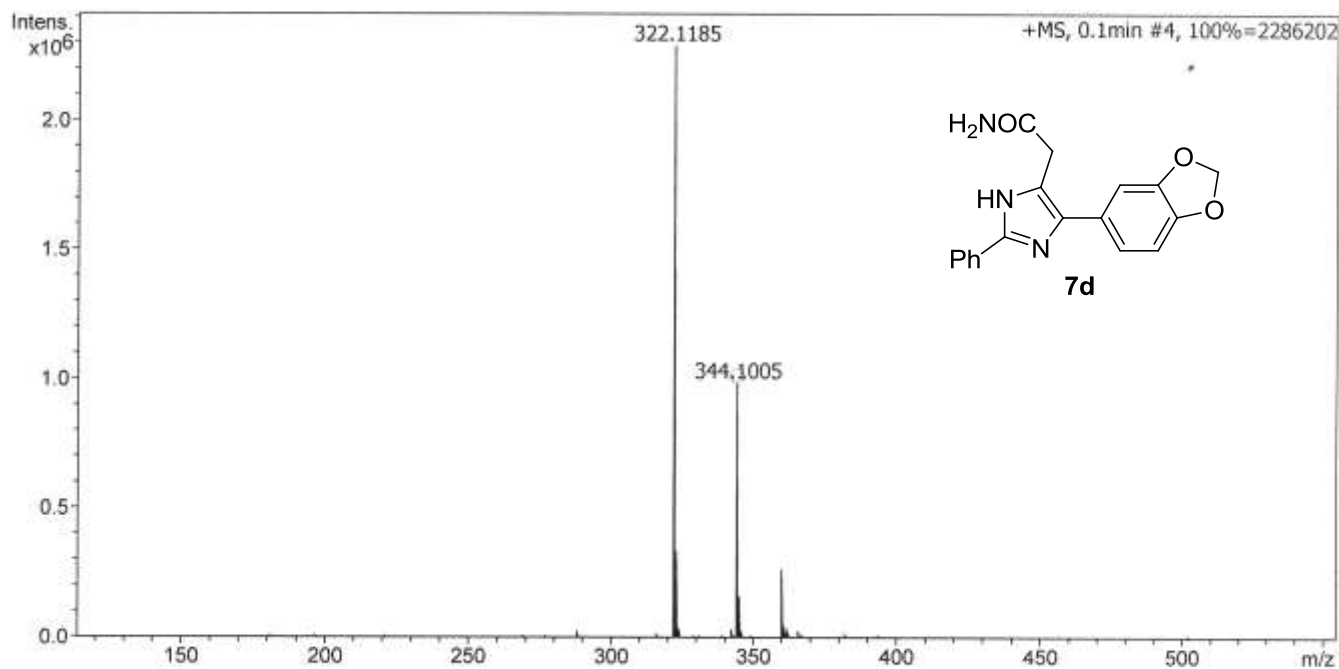
Analysis Name D:\Data\JULY_13\INN-TK-359.d
 Method Tune_pos_Standard_NAI-1500.m
 Sample Name INN-TK-359
 Comment C18H15N3O3

Acquisition Date 7/26/2013 3:02:29 PM

Operator IIT-B
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.1 Bar
Focus	Active	Set Capillary	3200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
344.1005	1	C18H15N3NaO3	344.1006	0.2	26.1	1	100.00	12.5	even	ok

Figure S73. HRMS spectrum of **7d**