Supporting information for

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

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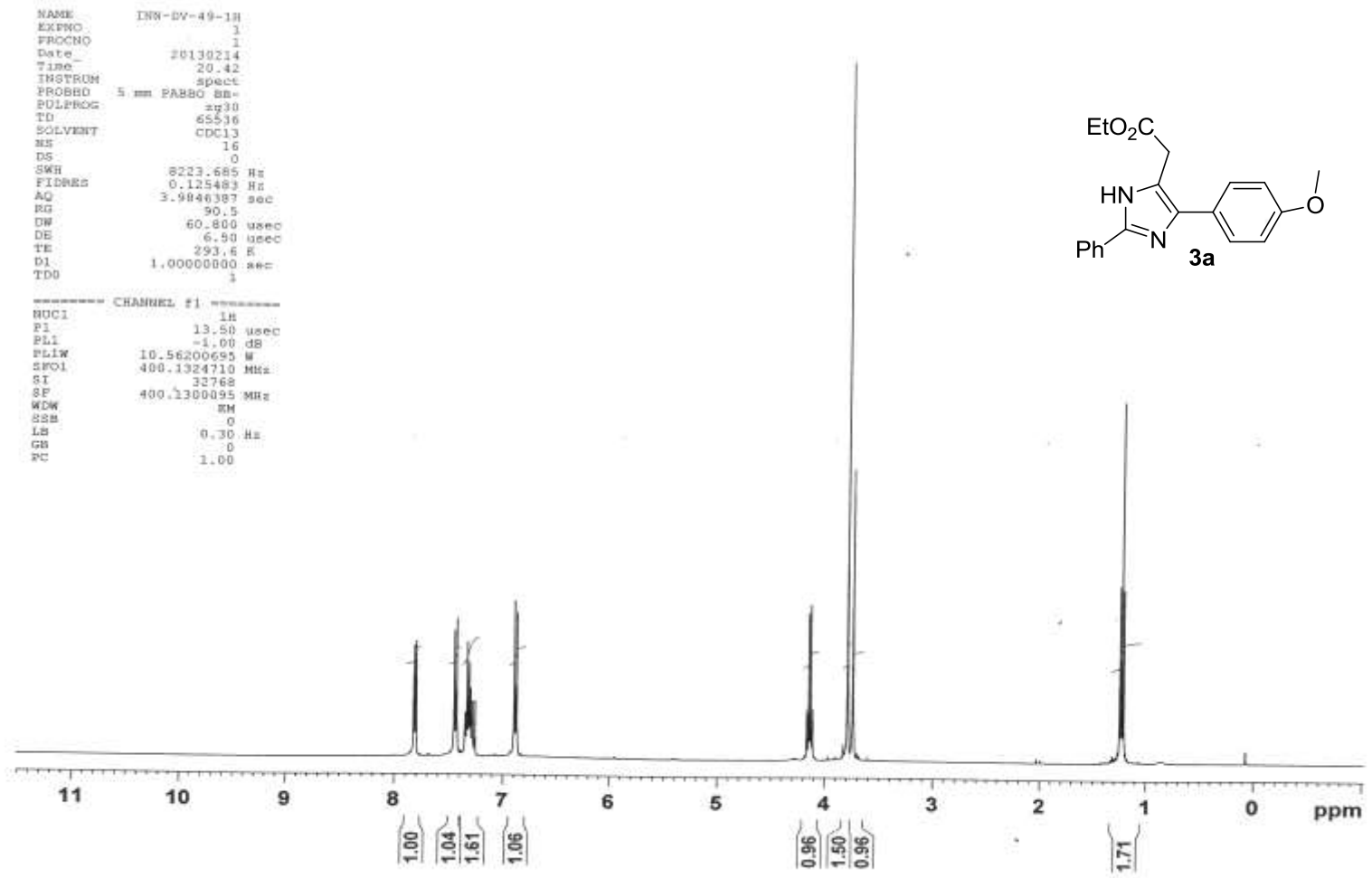

Figure S1.[1]H NMR spectrum of **3a**

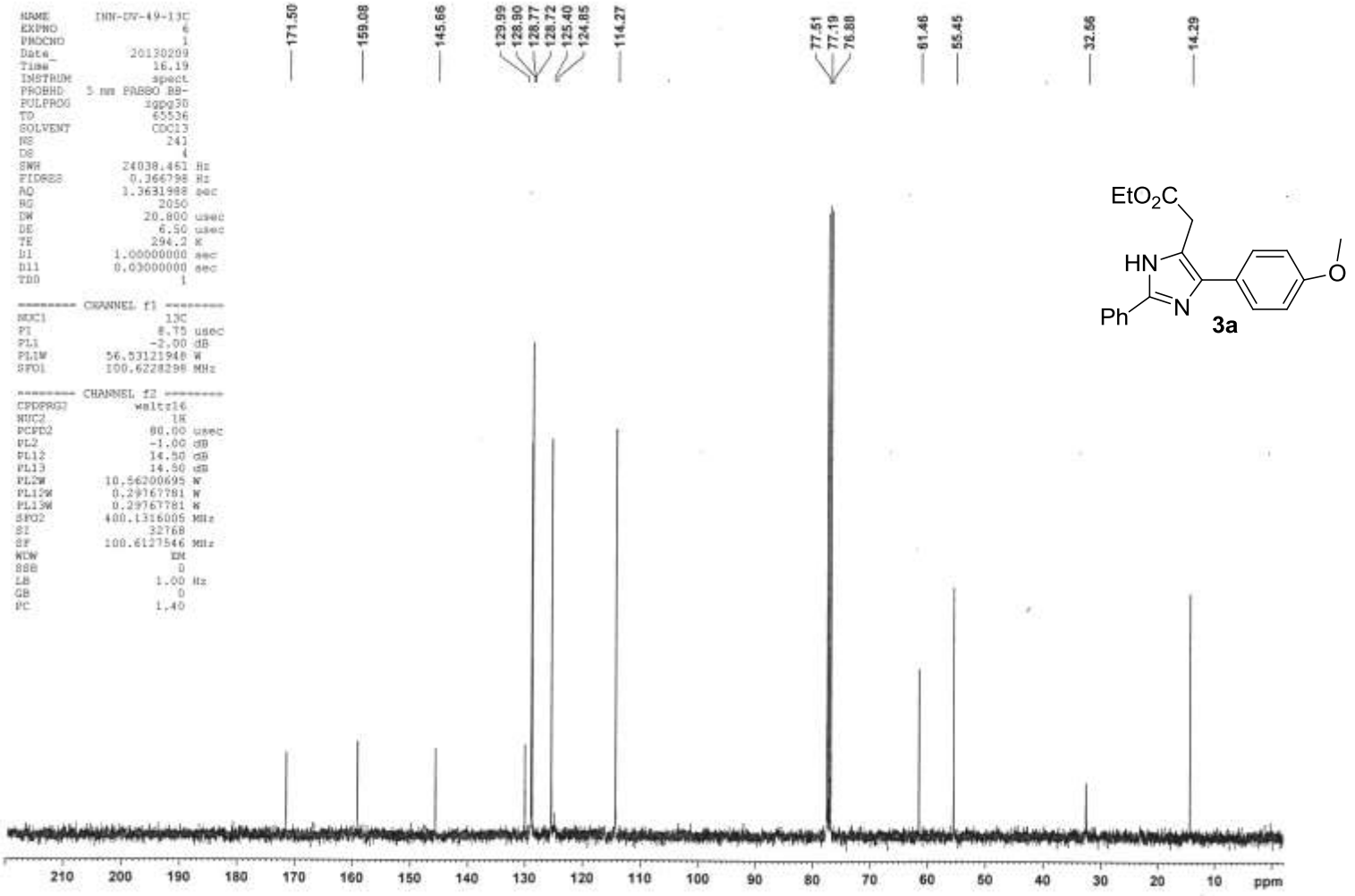

Figure S2. ^{13}C NMR spectrum of **3a**

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

Analysis Info

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Sample Name	INN-DV-49	Instrument	maXis impact 282001.00081
Comment	C20H20N2O3		

Acquisition Parameter

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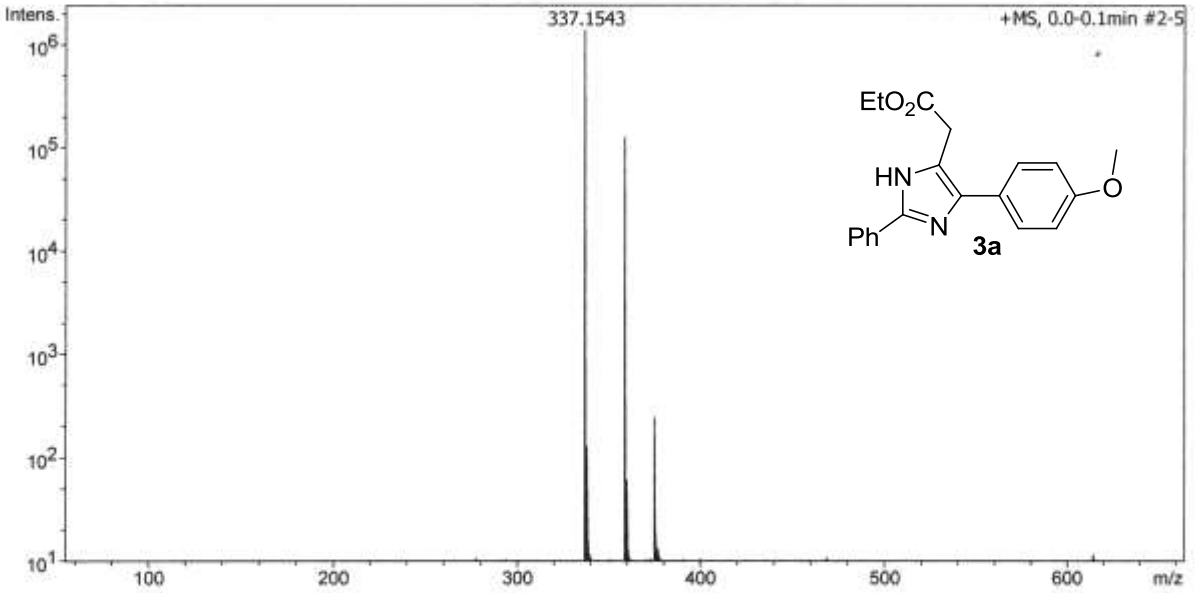

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
337.1543	1	C20H21N2O3	337.1547	1.0	9.0	1	100.00	11.5	even	ok

Figure S3. HRMS spectrum of **3a**

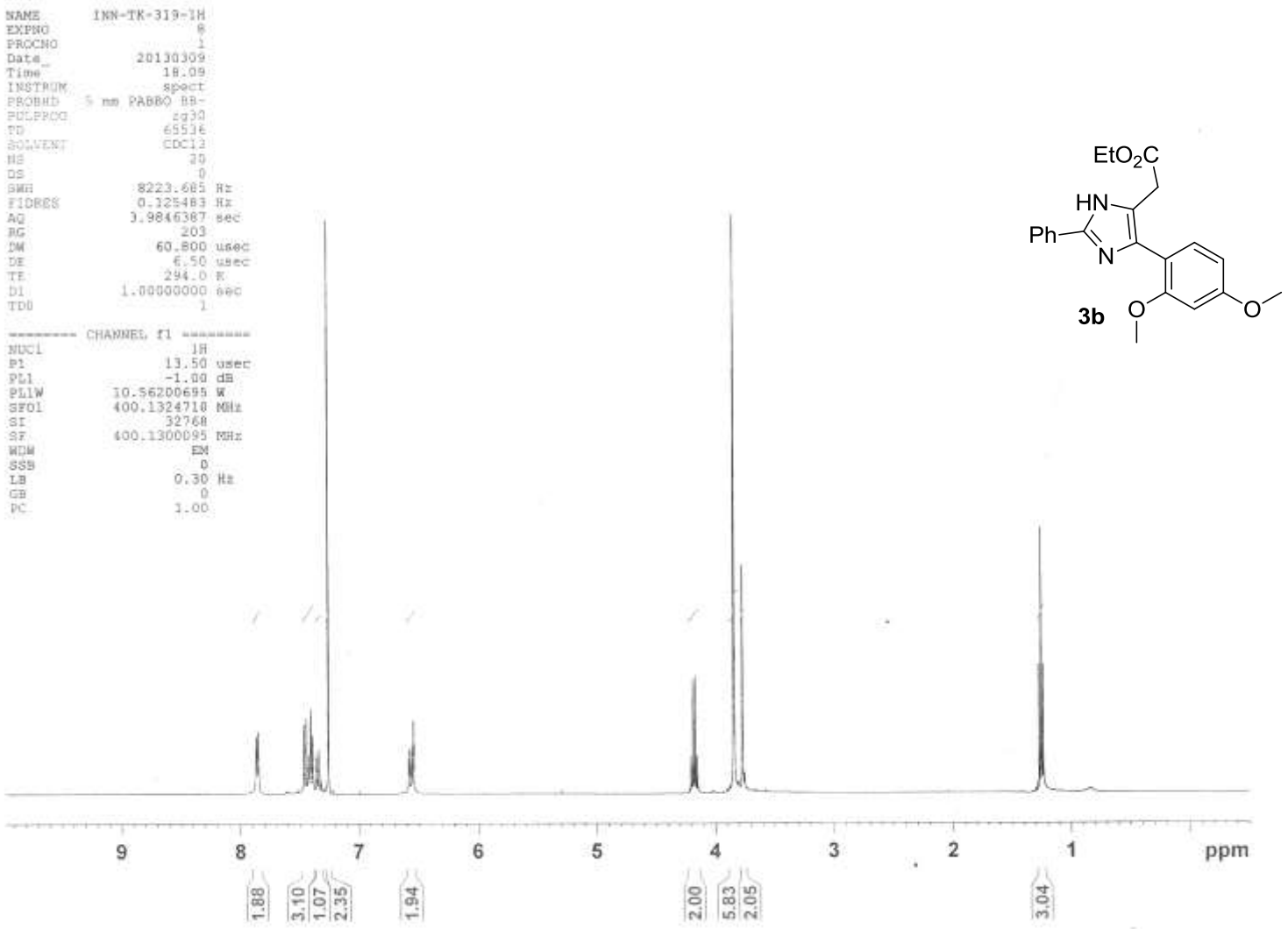

Figure S4. ^{1}H NMR spectrum of **3b**

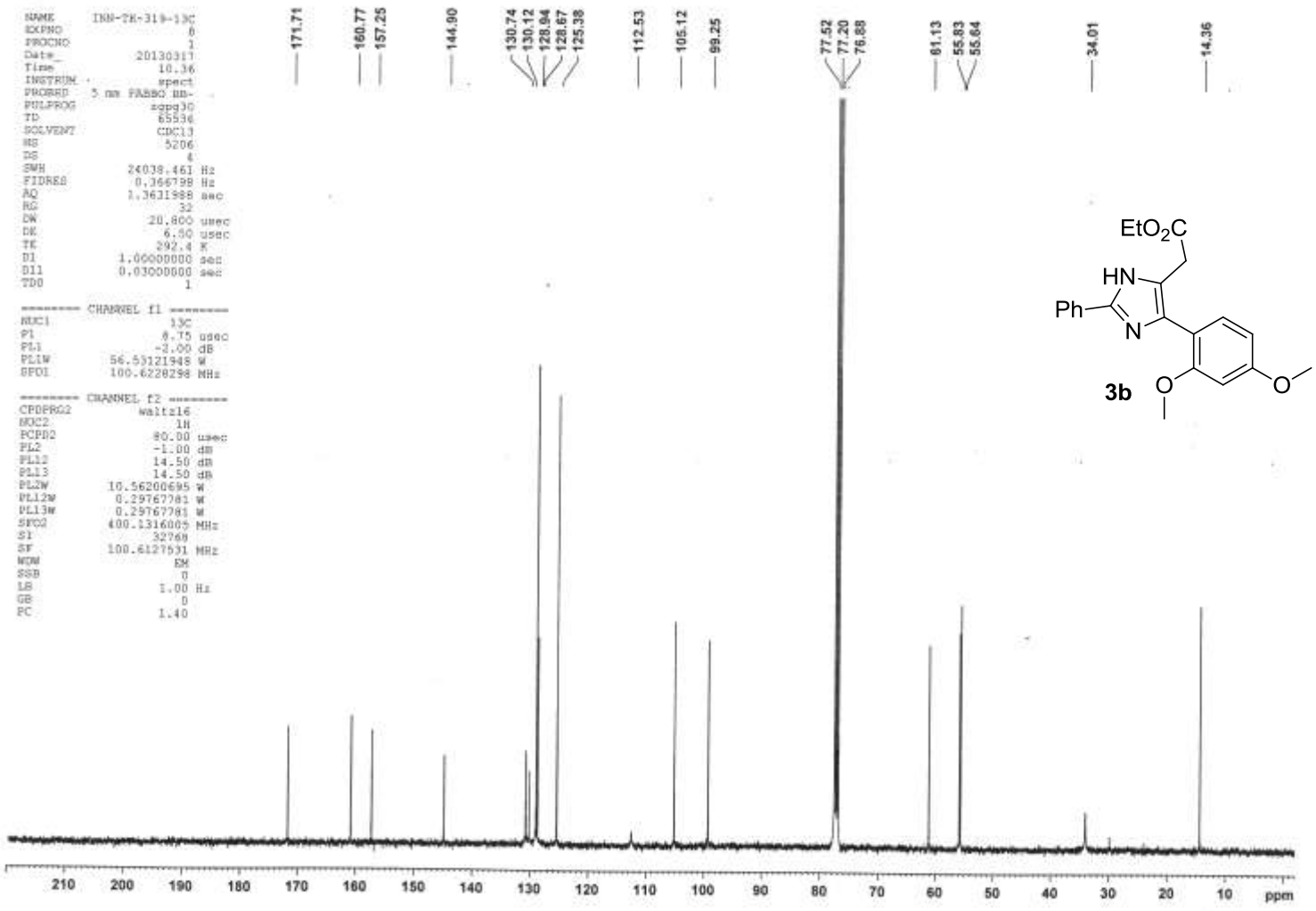

Figure S5. ^{13}C NMR spectrum of **3b**

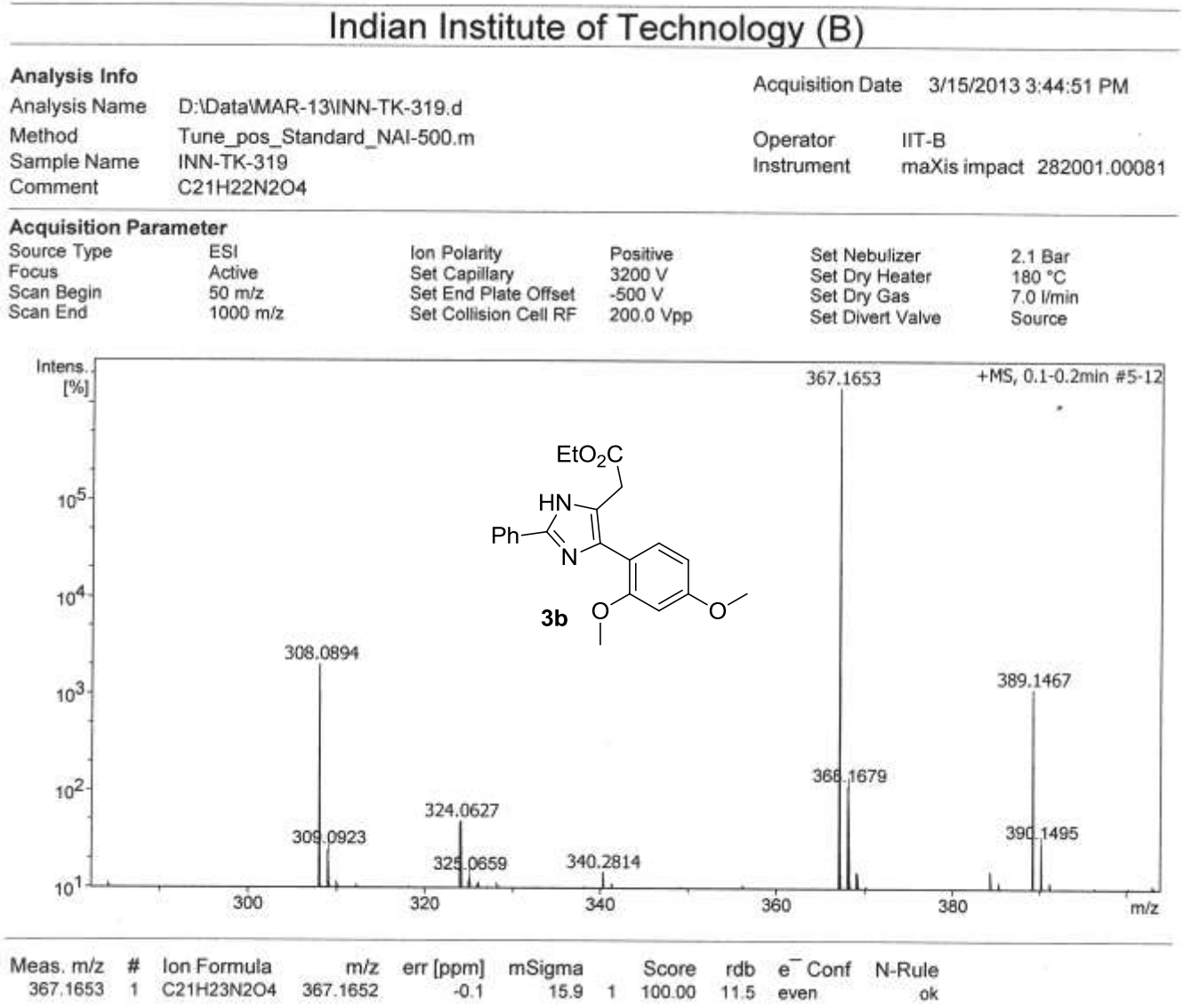

Figure S6. HRMS spectrum of **3b**

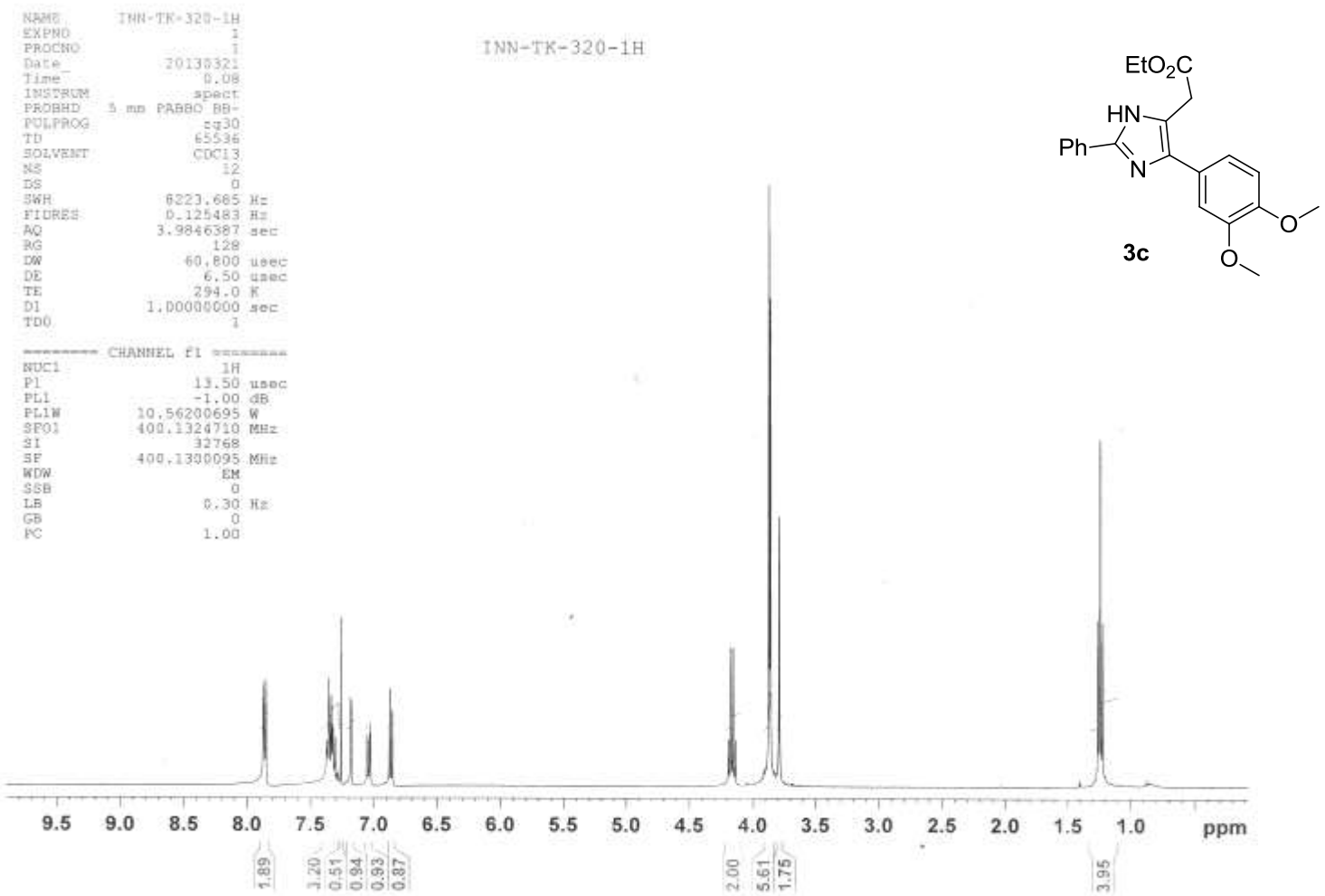

Figure S7. ^{1}H NMR spectrum of **3c**

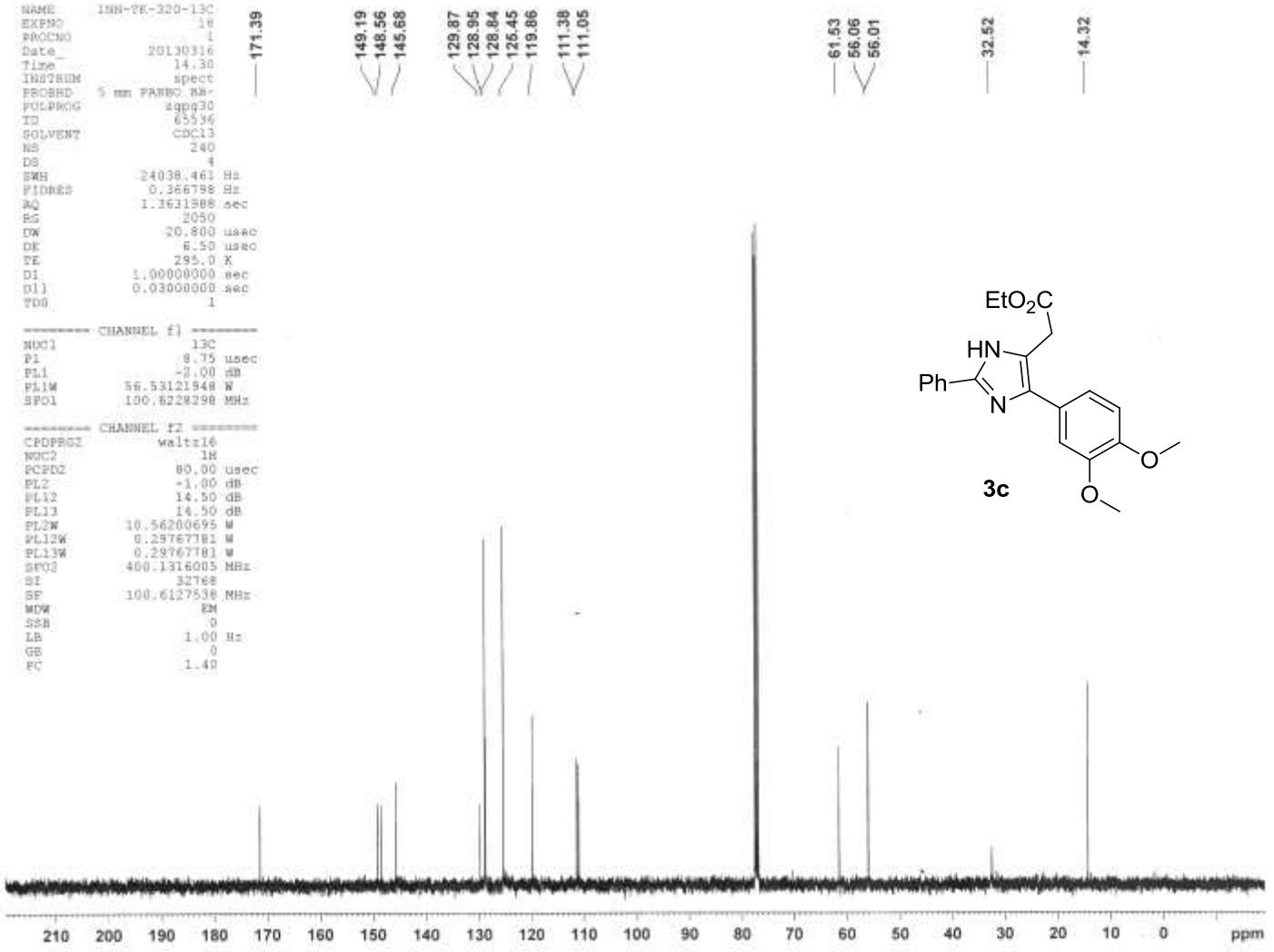

Figure S8. ^{13}C NMR spectrum of **3c**

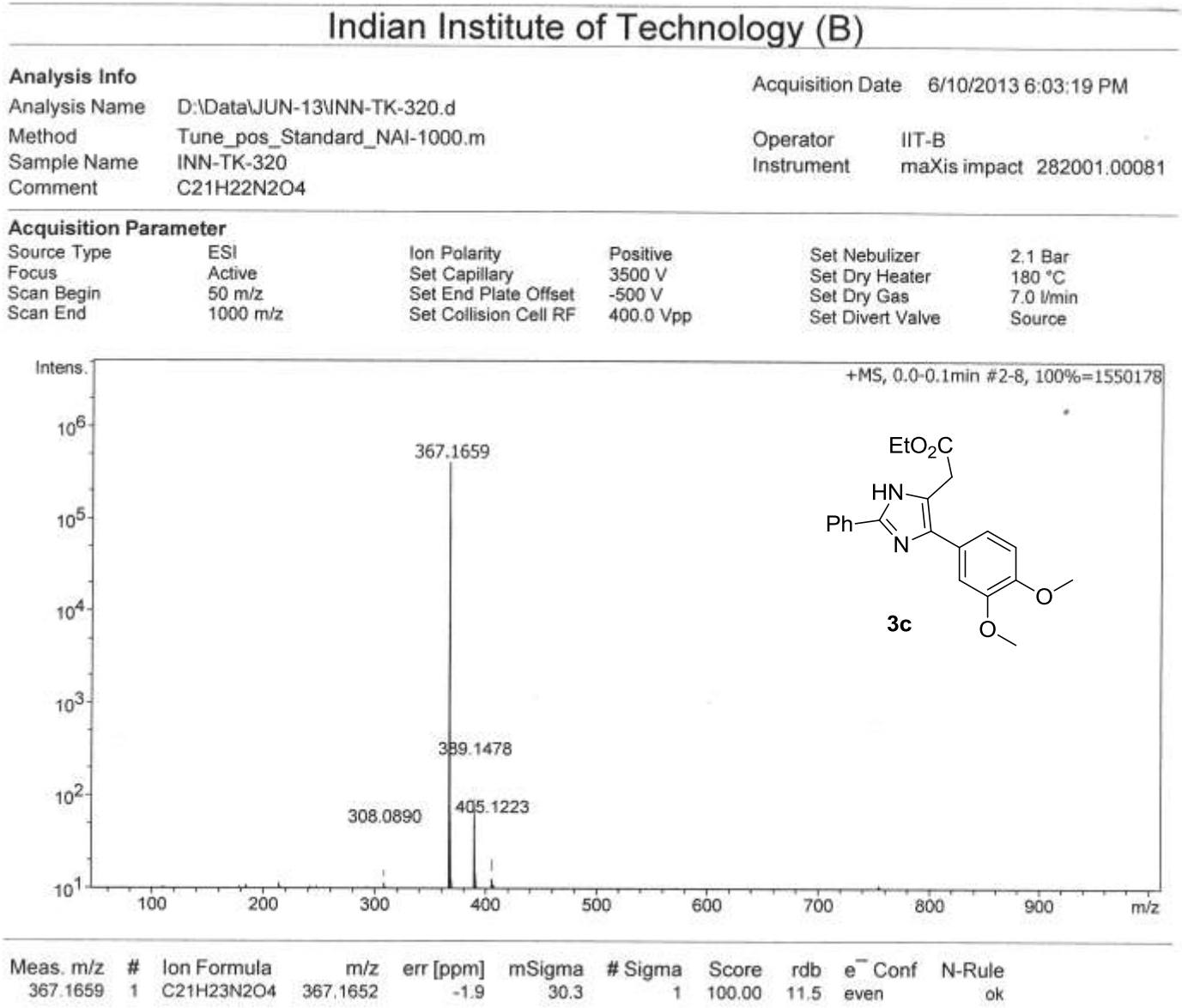

Figure S9. HRMS spectrum of **3c**

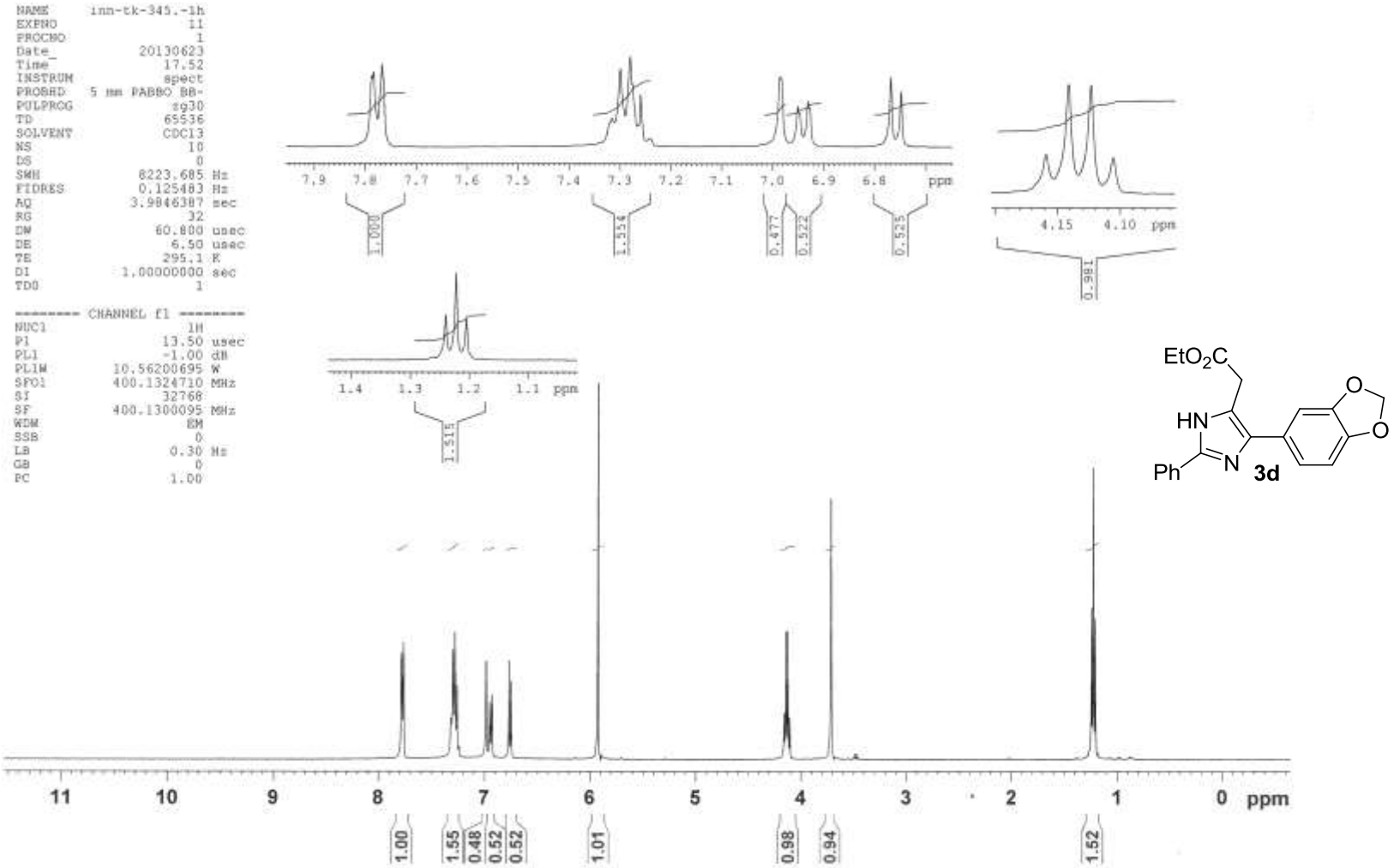

Figure S10. ^{1}H NMR spectrum of **3d**

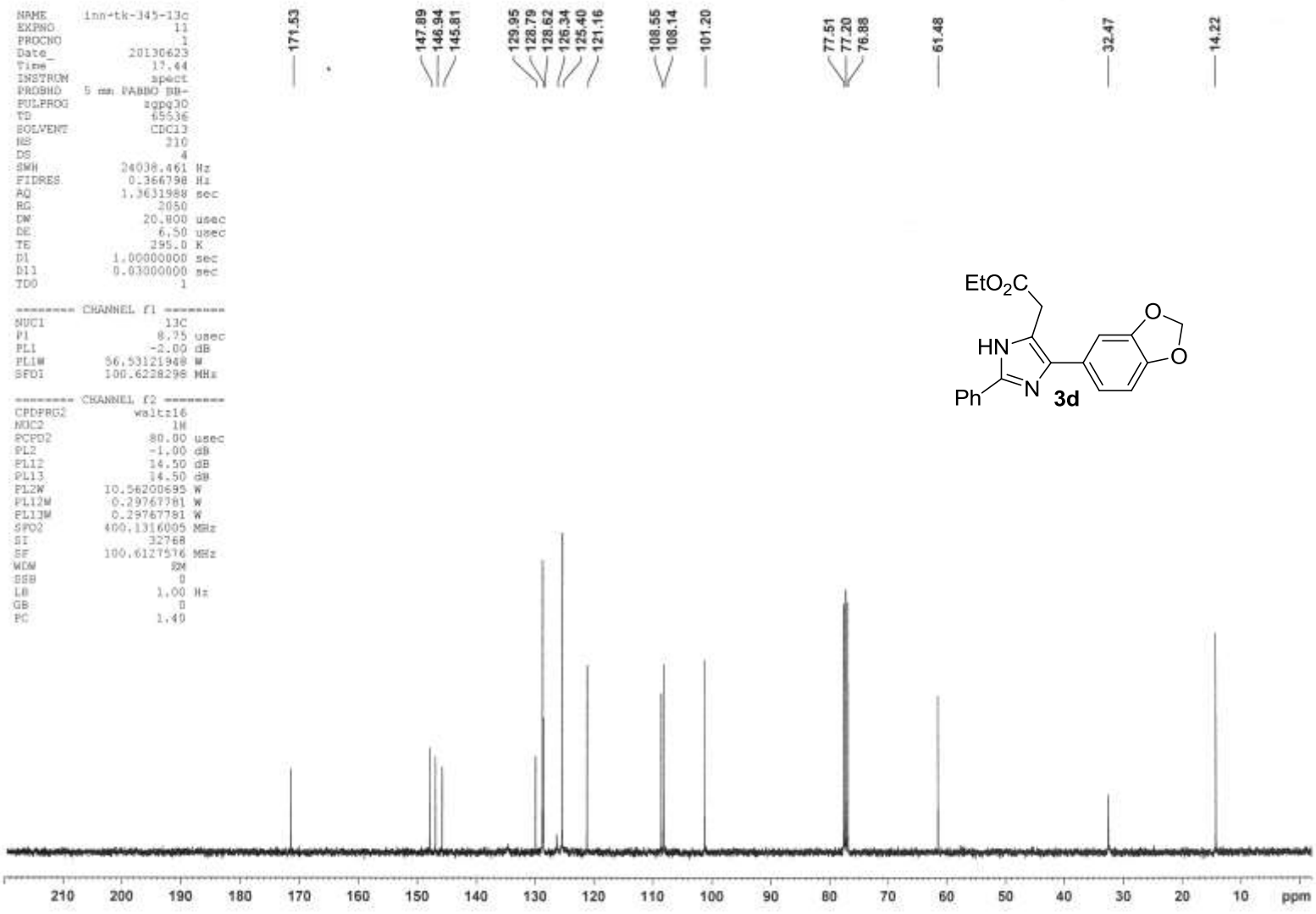

Figure S11. ^{13}C NMR spectrum of **3d**

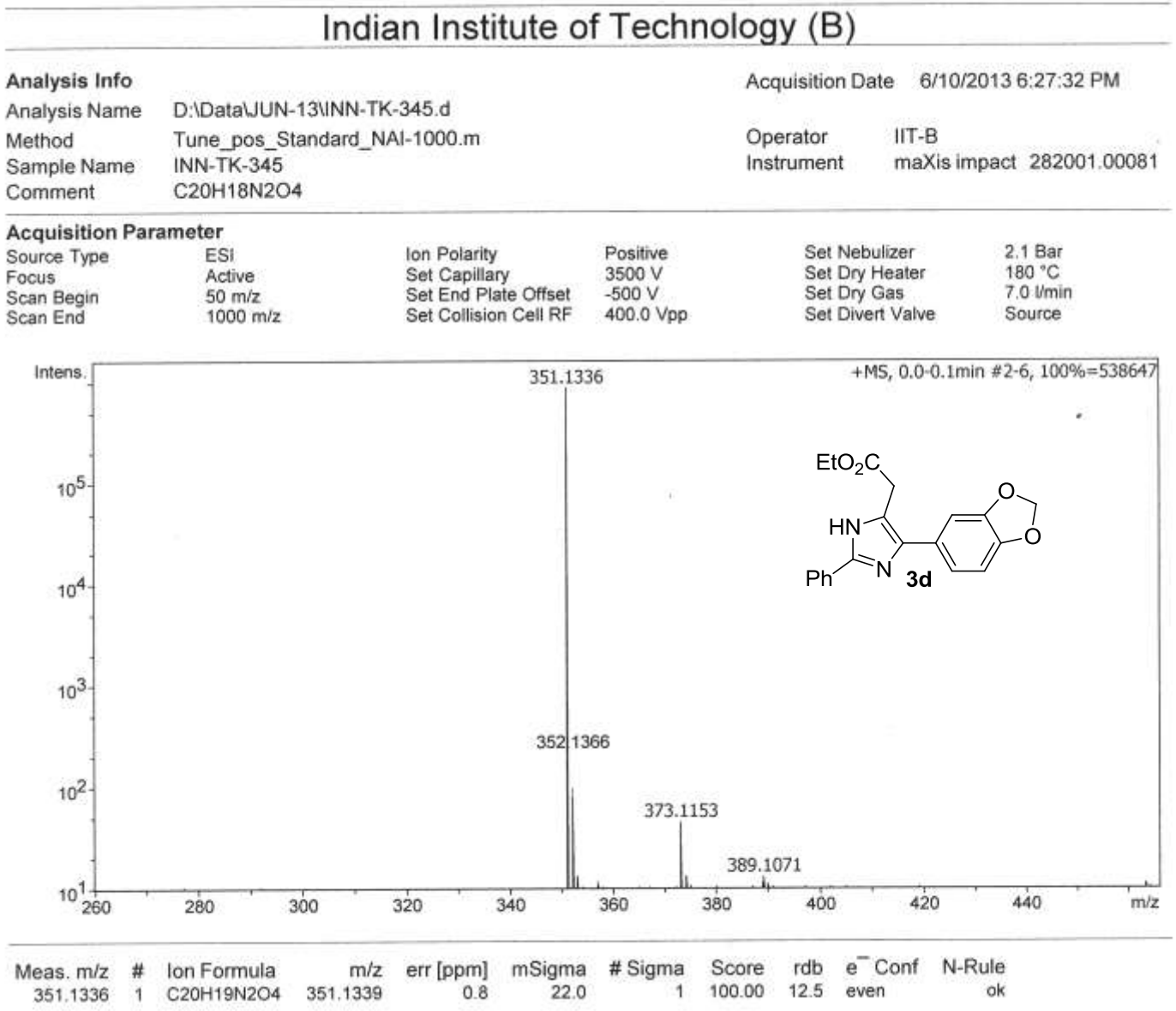

Figure S12. HRMS spectrum of **3d**

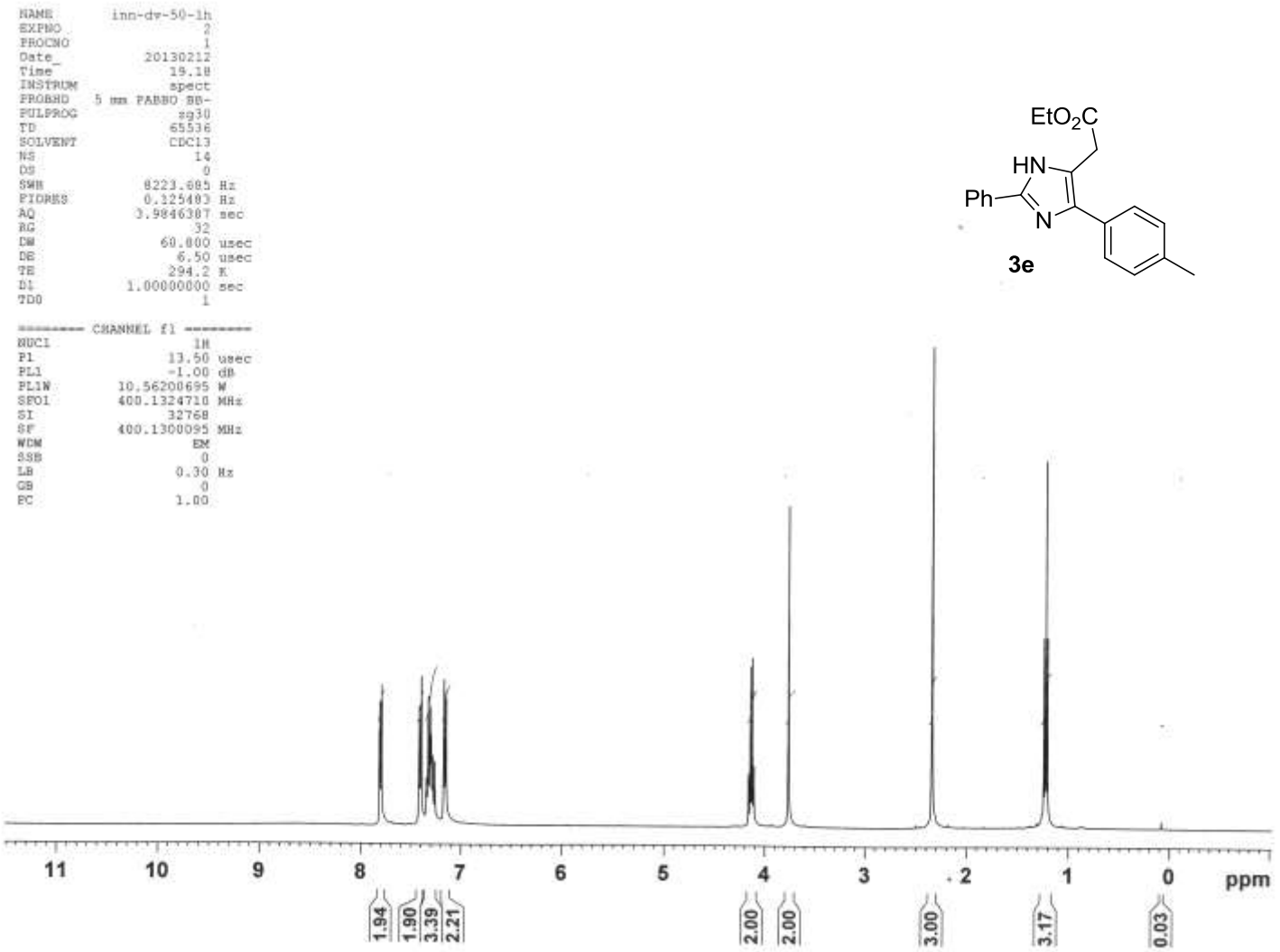

Figure S13. ^{1}H NMR spectrum of **3e**

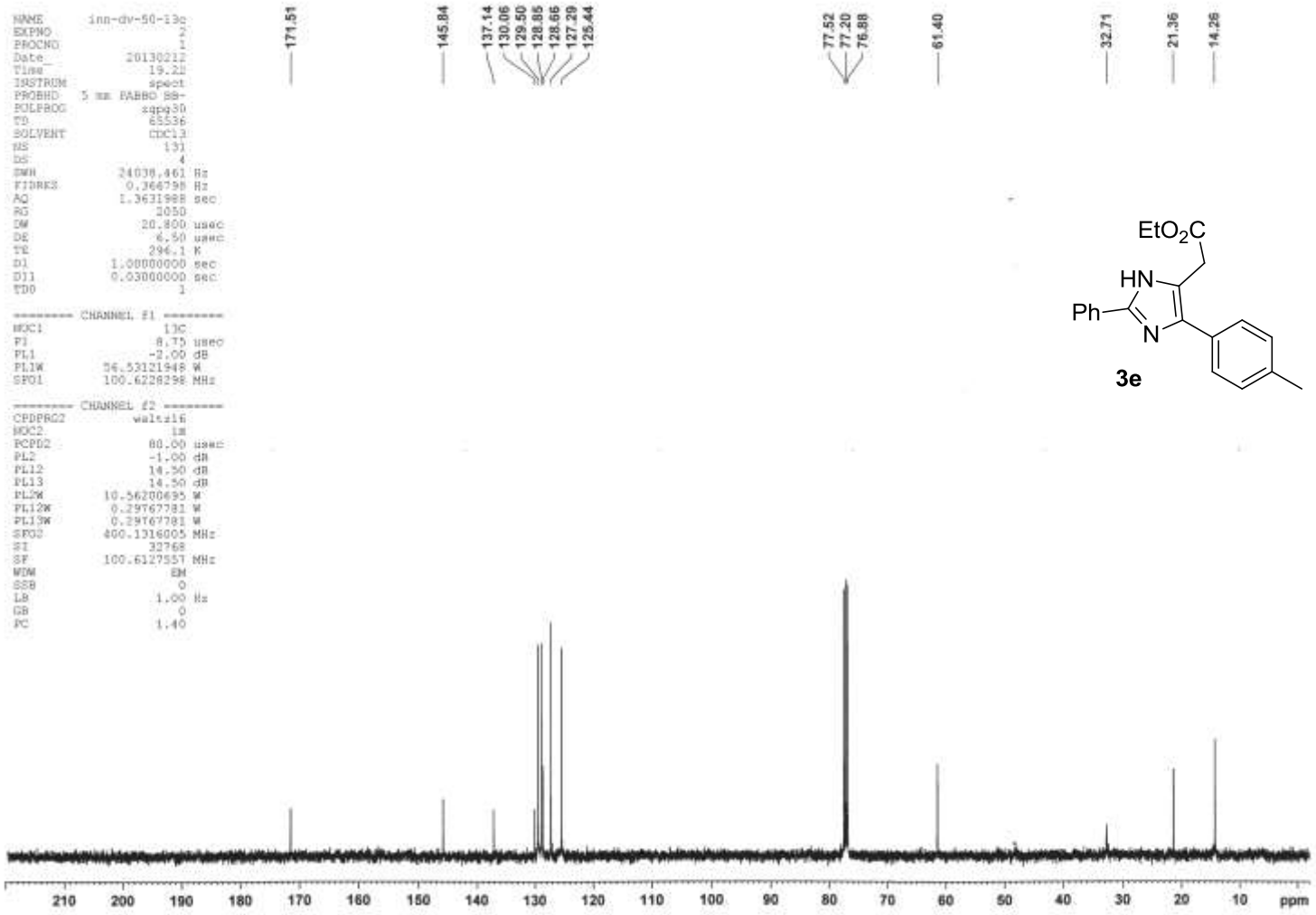

Figure S14. ^{13}C NMR spectrum of **3e**

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Analysis Info

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Sample Name	INN-DV-50	Instrument	maXis impact 282001.00081
Comment	C20H20N2O2		

Acquisition Parameter

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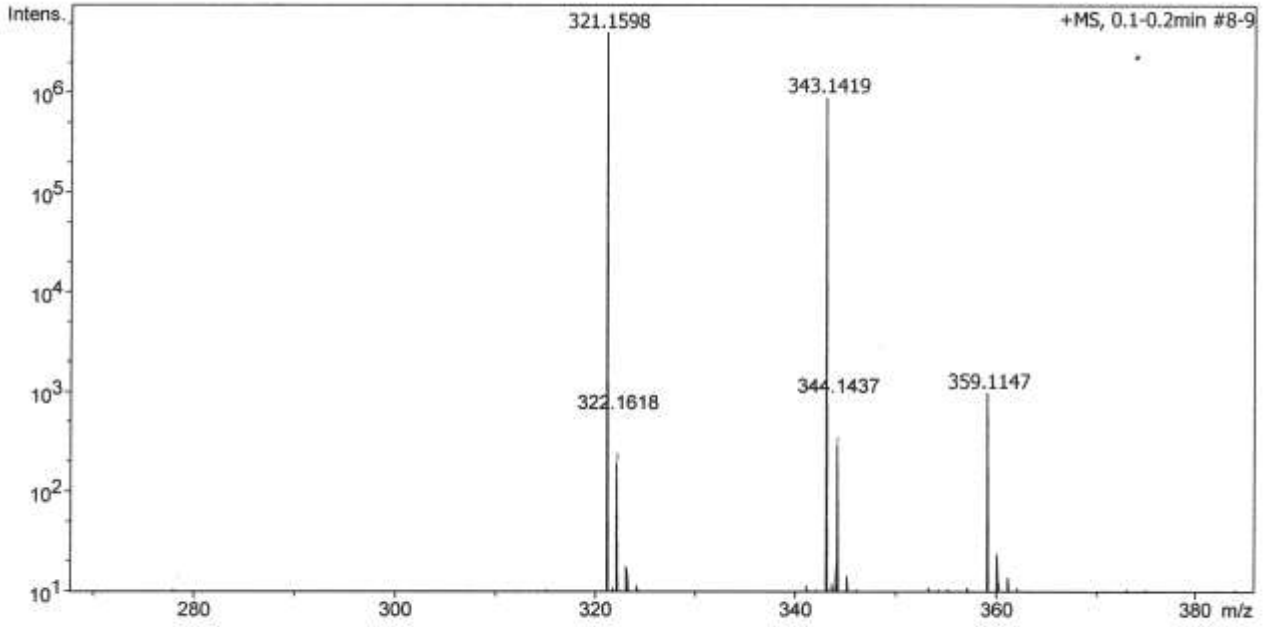
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
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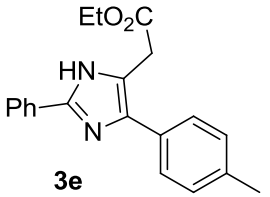

3e

Figure S15. HRMS spectrum of **3e**

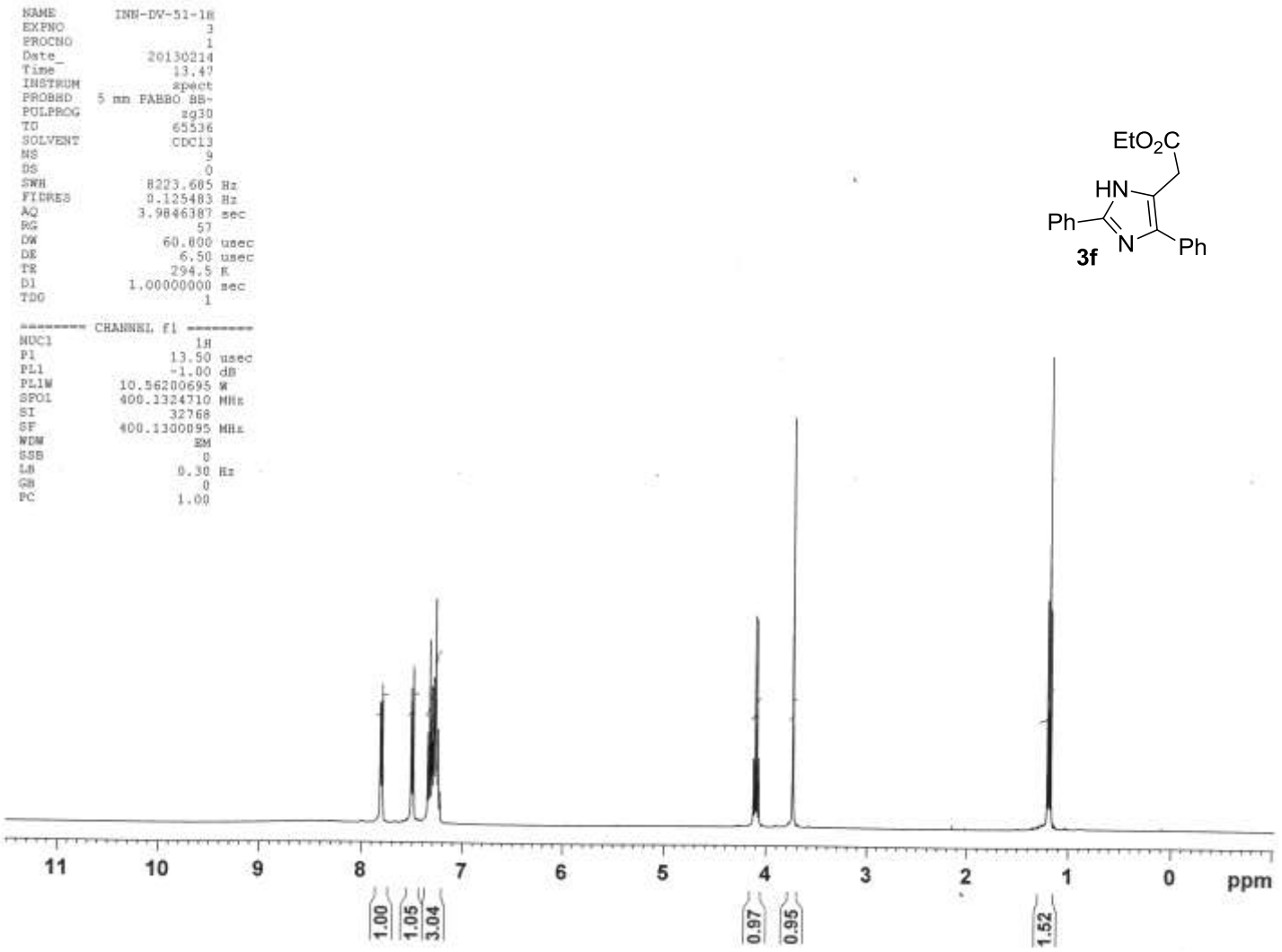

Figure S16. ^{1}H NMR spectrum of **3f**

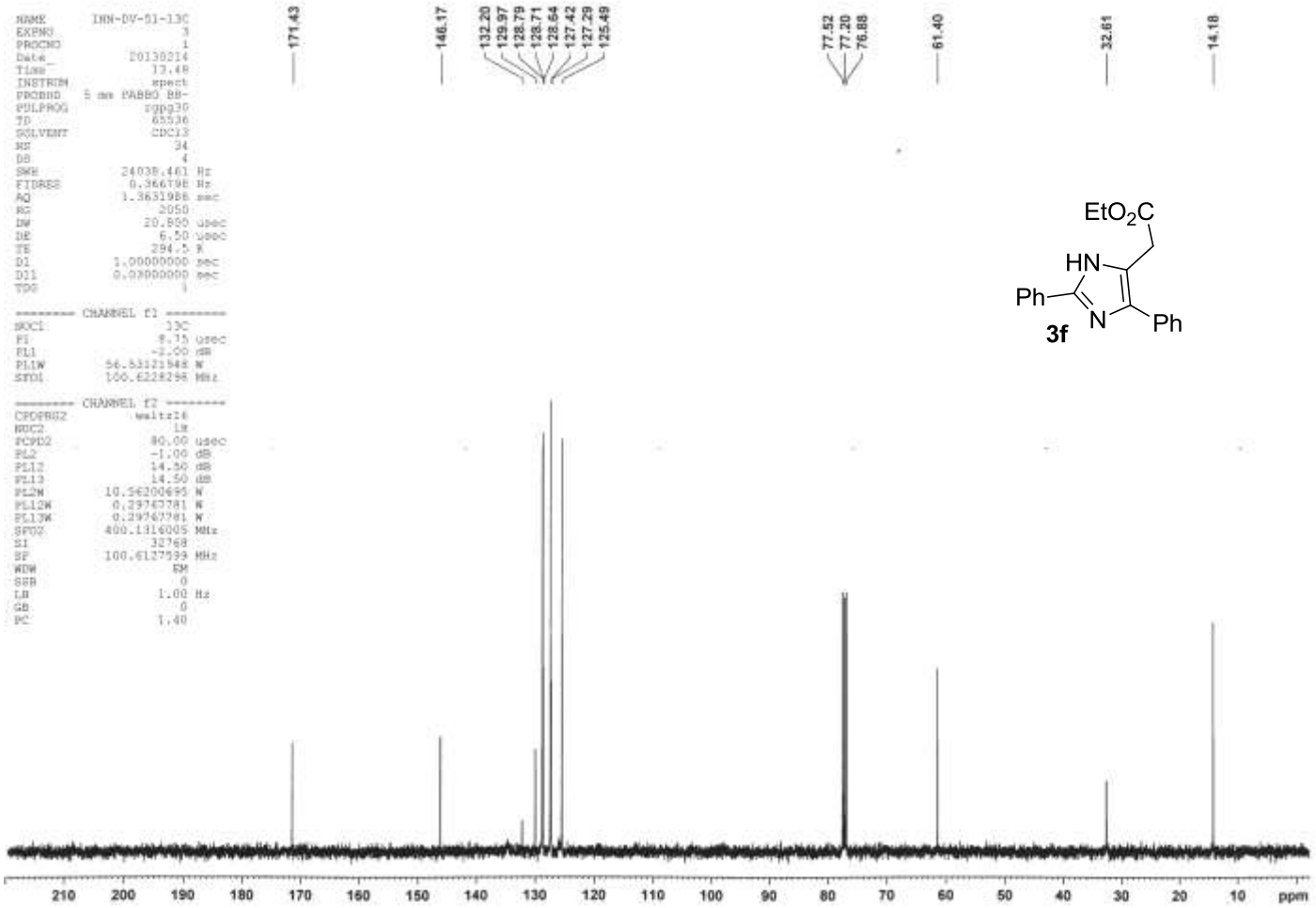

Figure S17. ^{13}C NMR spectrum of **3f**

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Analysis Info

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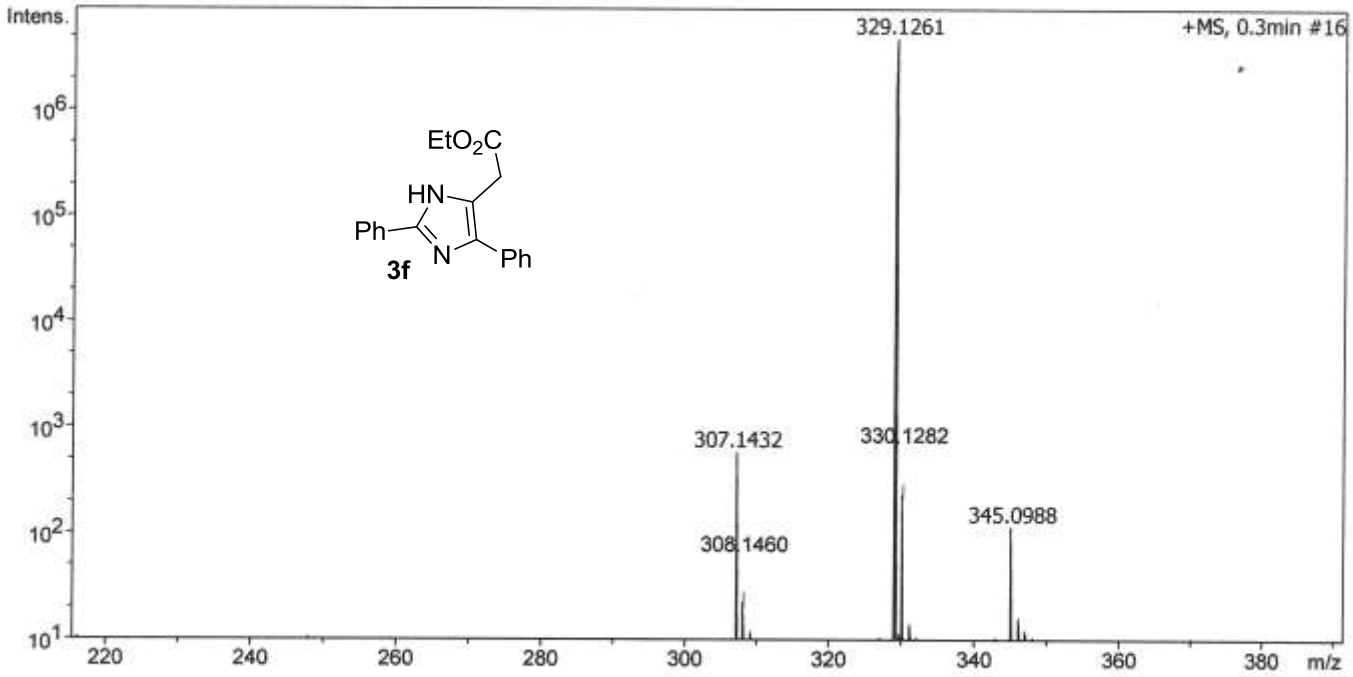
Method	Tune_pos_Standard_NAI-1000.m	Operator	IIT-B
Sample Name	INN-DV-51	Instrument	maXis impact 282001.00081
Comment	C19H18N2O2		

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
329.1261	1	C19H18N2NaO2	329.1260	-0.0	15.4	1	100.00	11.5	even	ok

Figure S18. HRMS spectrum of **3f**

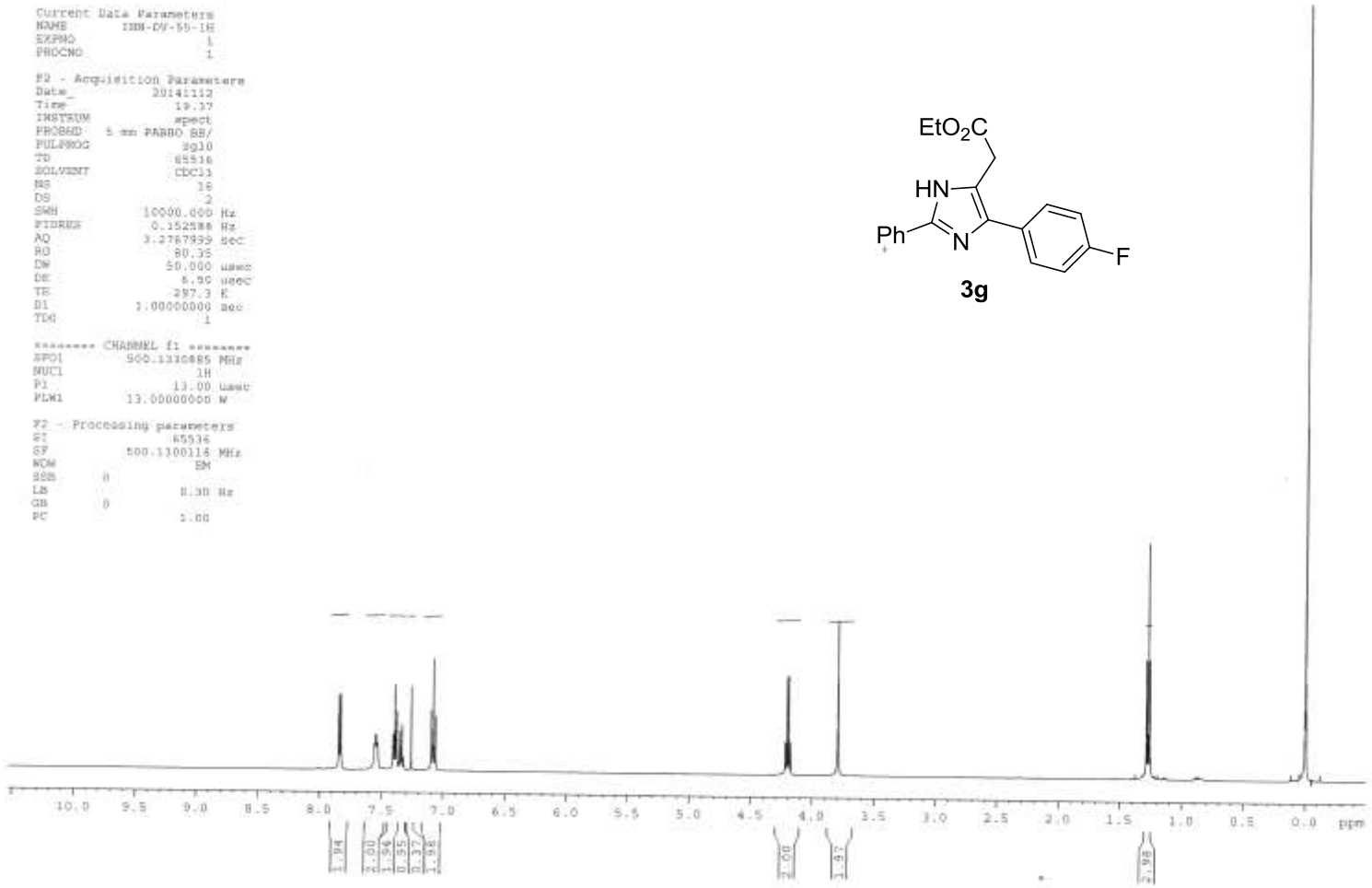


Figure S19. ^{1}H NMR spectrum of **3g**

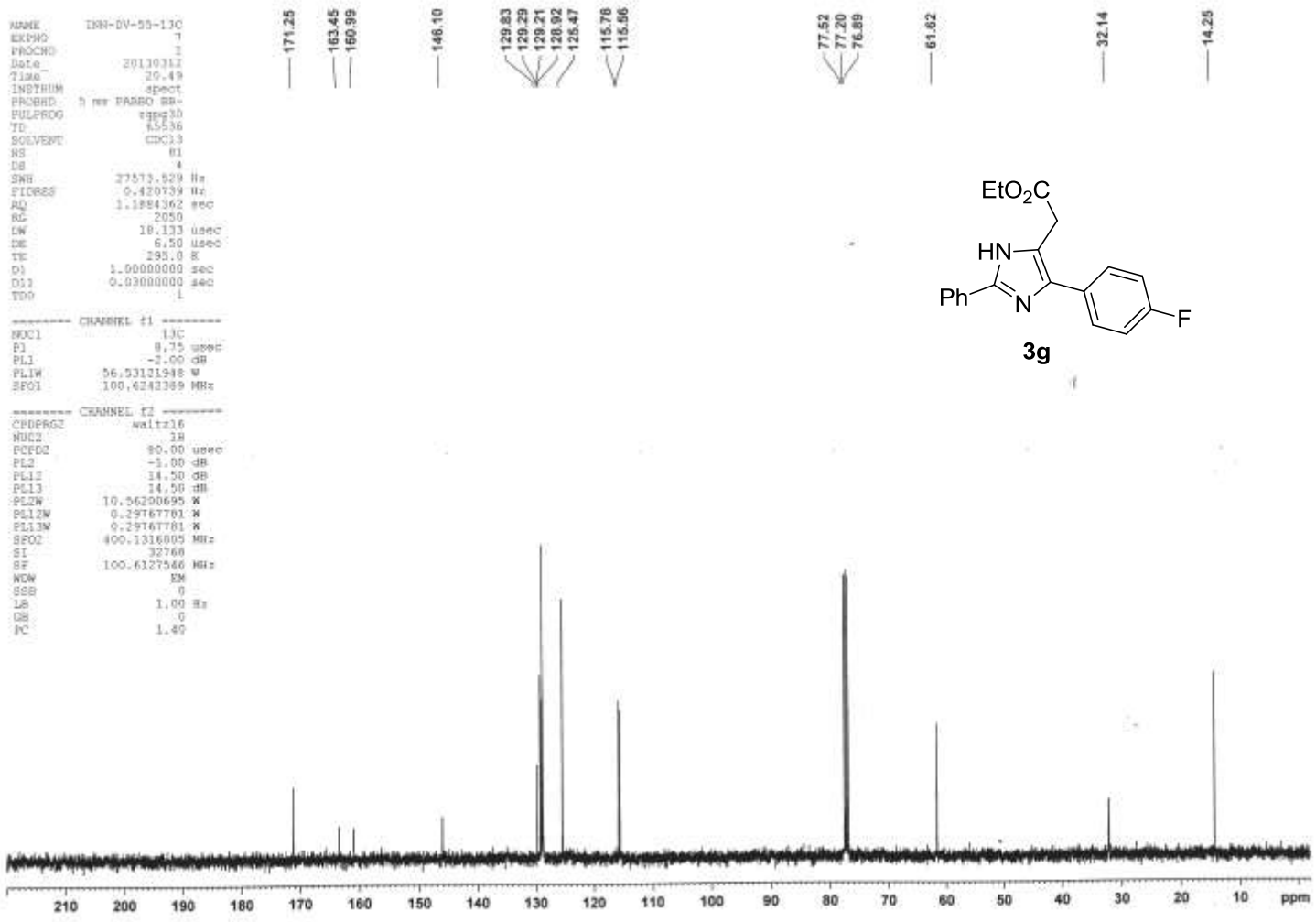


Figure S20. ^{13}C NMR spectrum of **3g**

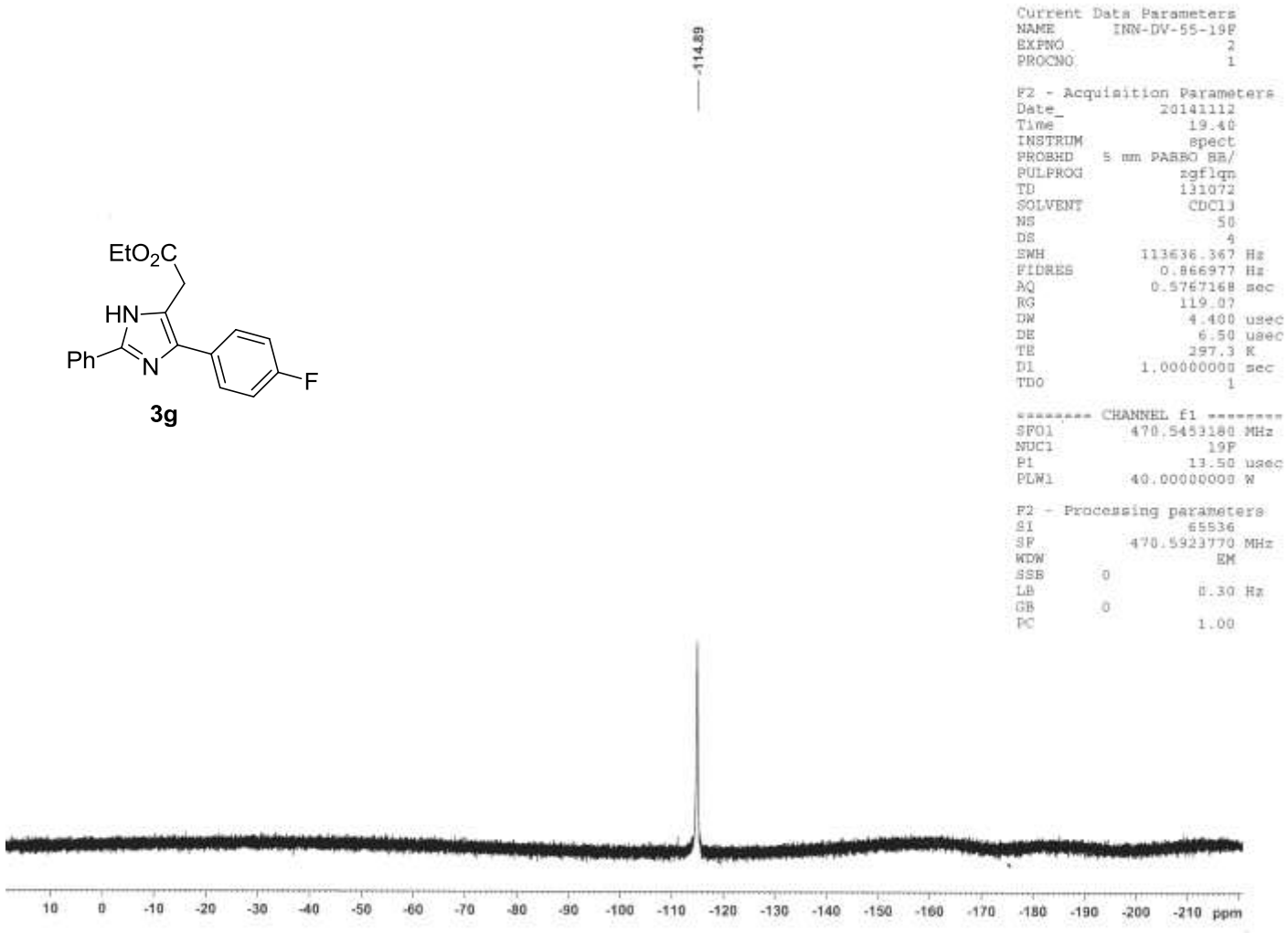


Figure S21. ^{19}F NMR spectrum of **3g**

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Analysis Info

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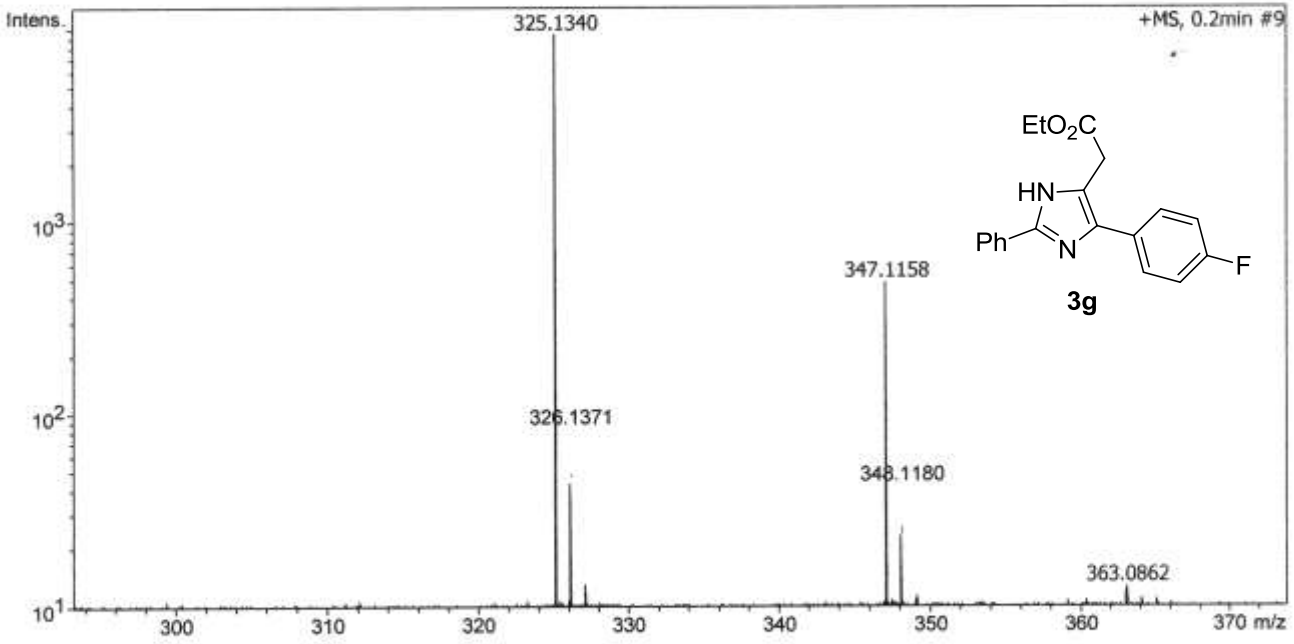
Sample Name	INN-DV-55	Instrument	maXis impact 282001.00081
Comment	C19H17FN2O2		

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
325.1340	1	C19H18FN2O2	325.1347	2.0	7.8	1	100.00	11.5	even	ok

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

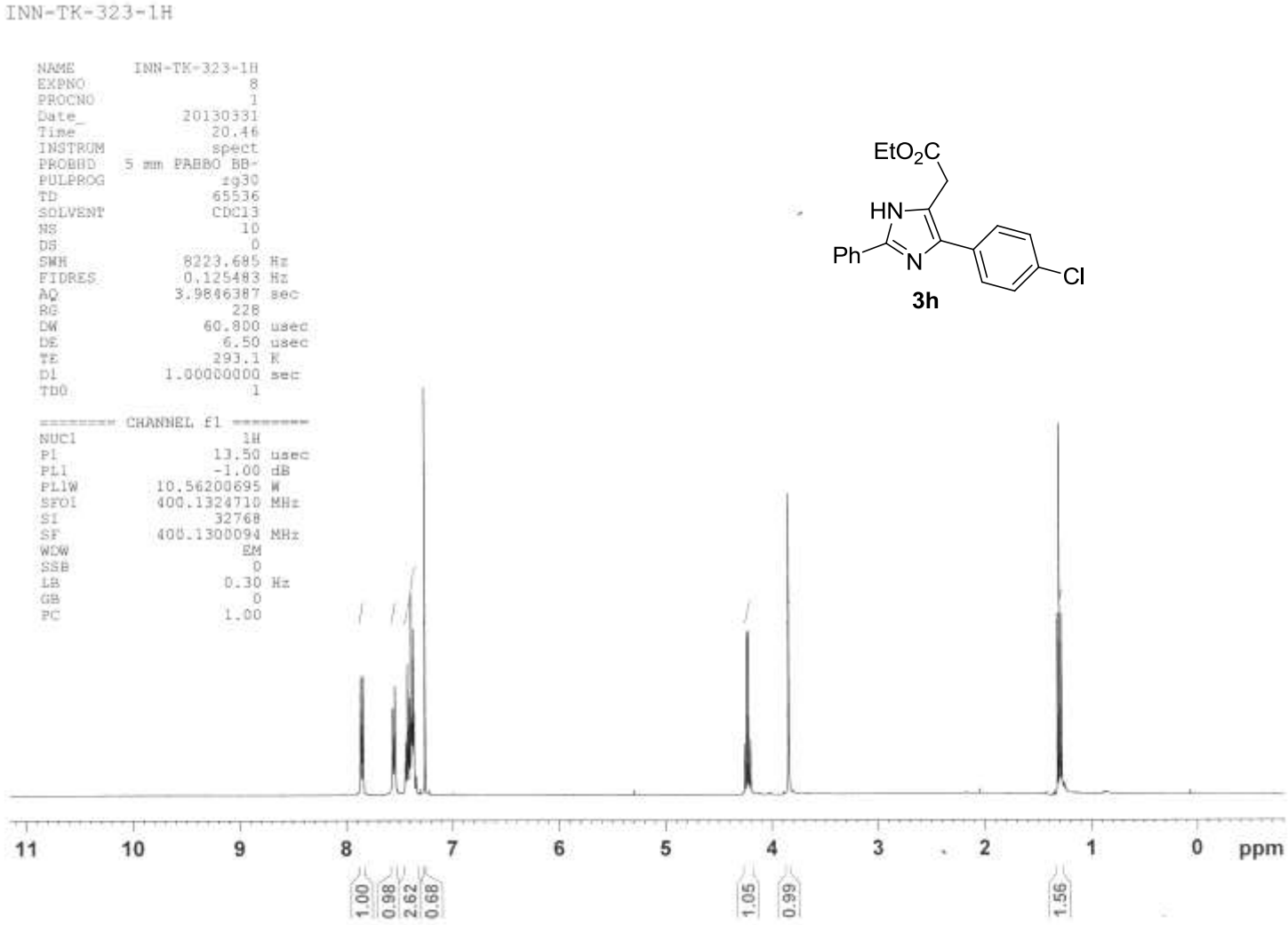


Figure S23. ^{1}H NMR spectrum of **3h**

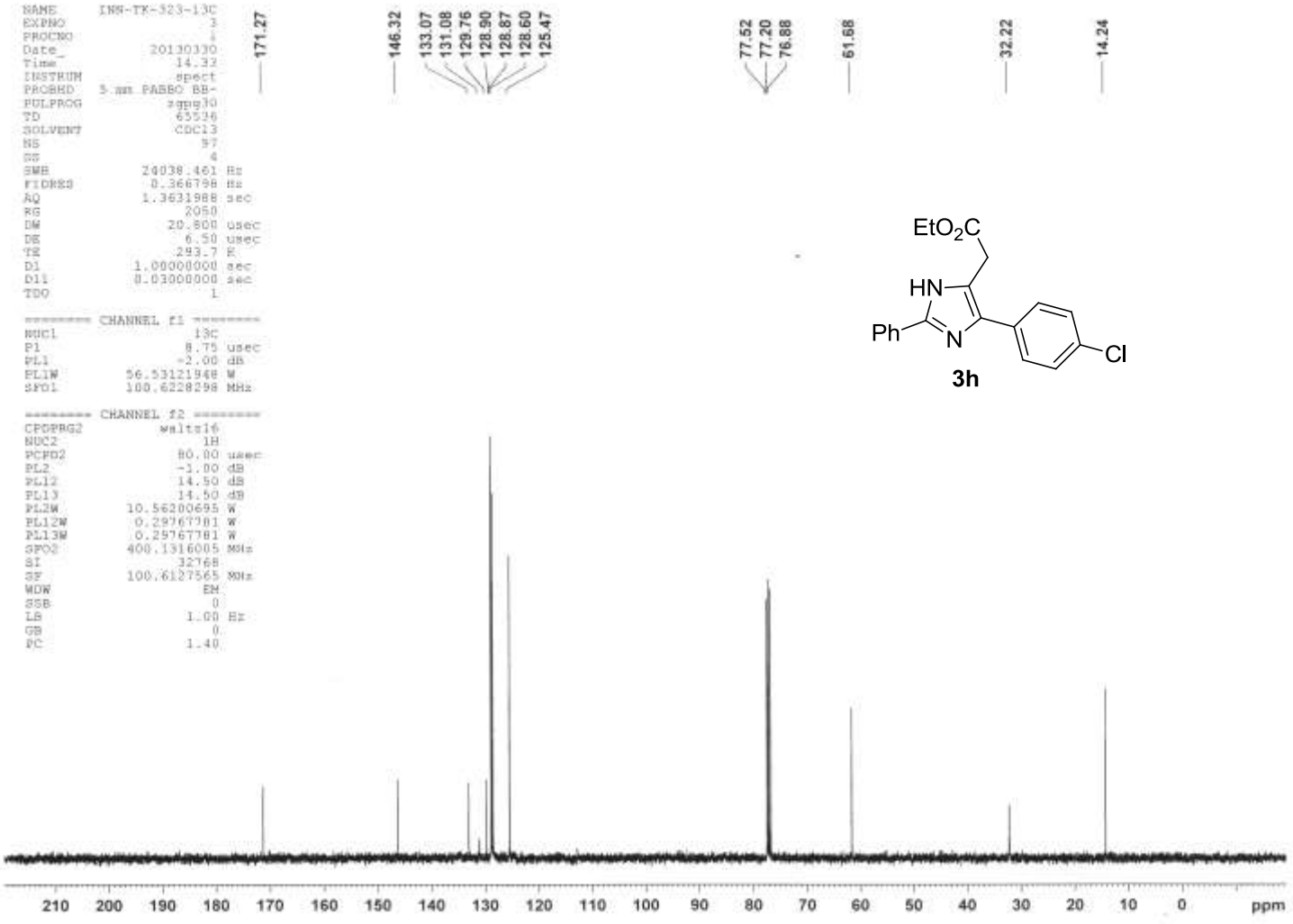
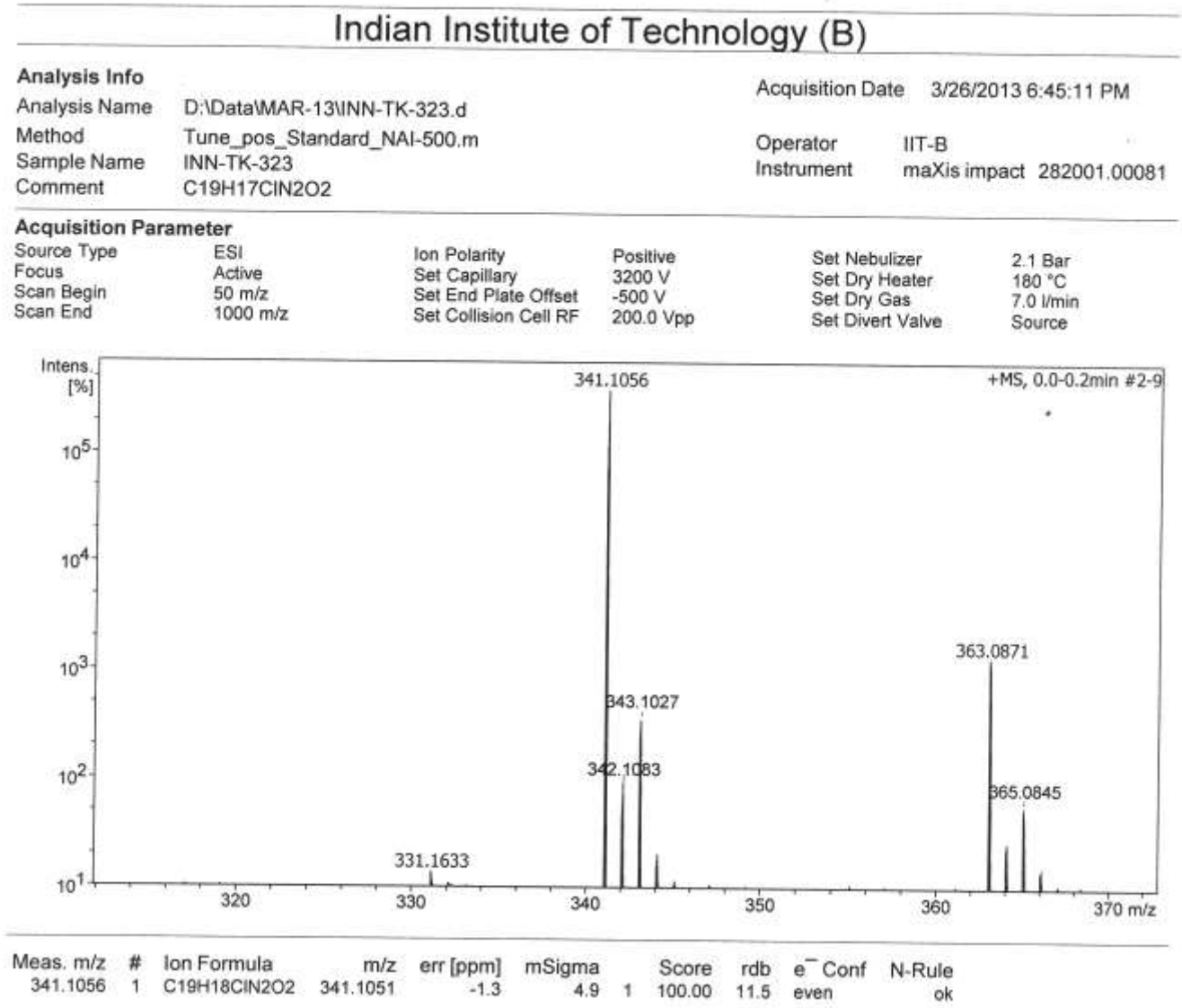
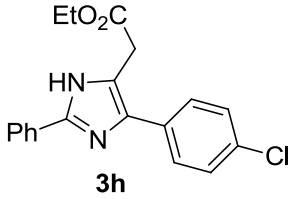


Figure S24. ^{13}C NMR spectrum of **3h**





3h

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

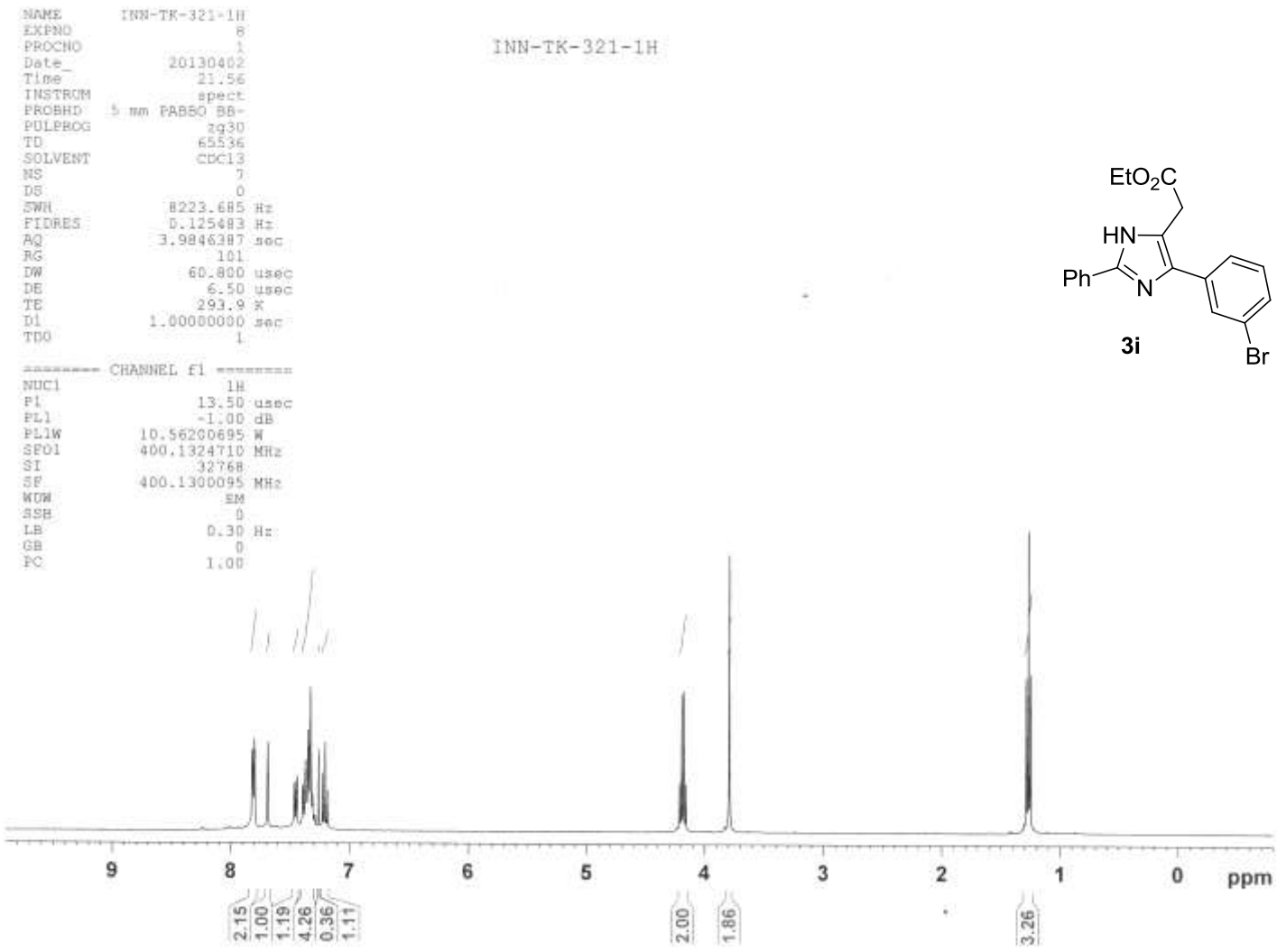


Figure S26. ^{1}H NMR spectrum of **3i**

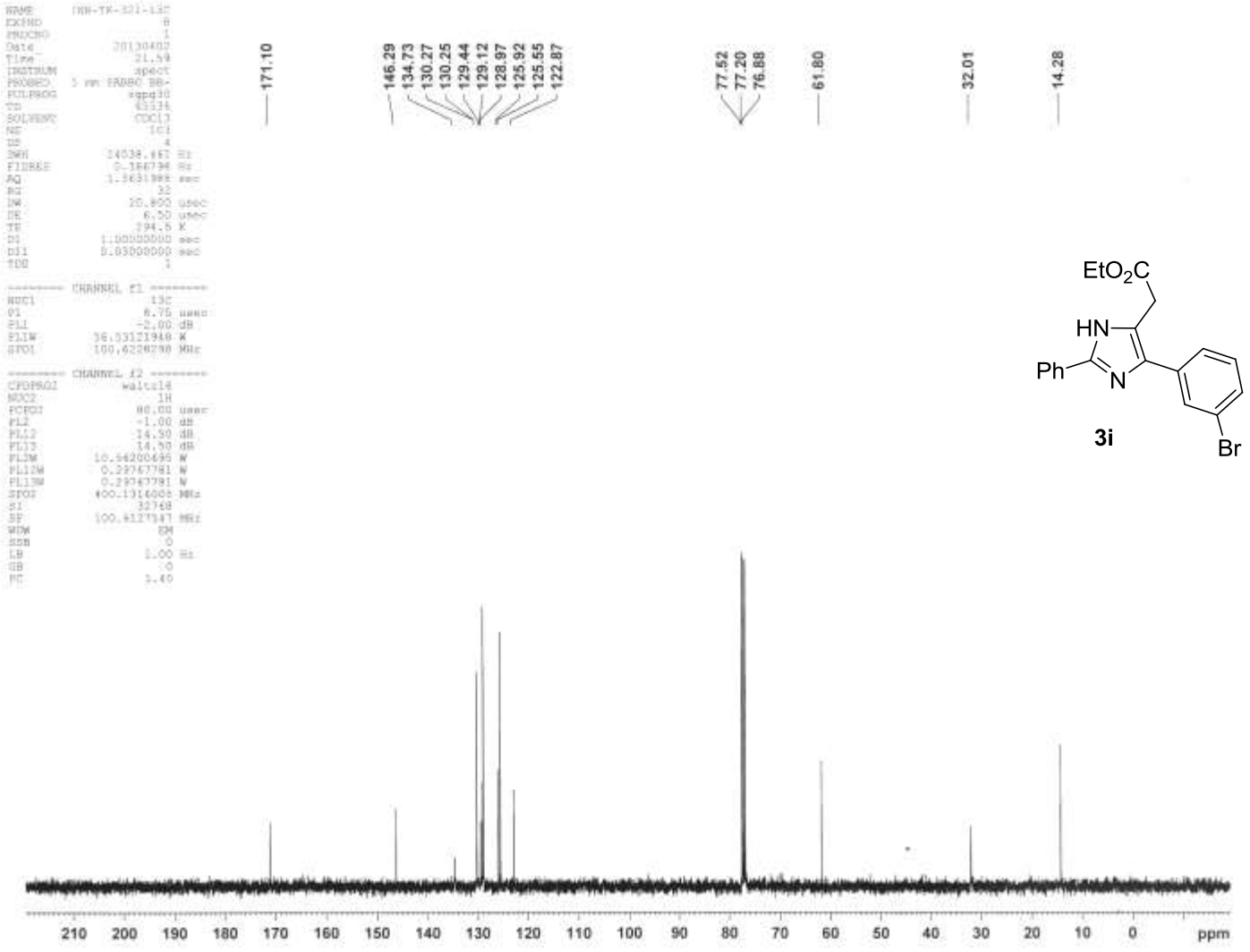


Figure S27. ^{13}C NMR spectrum of **3i**

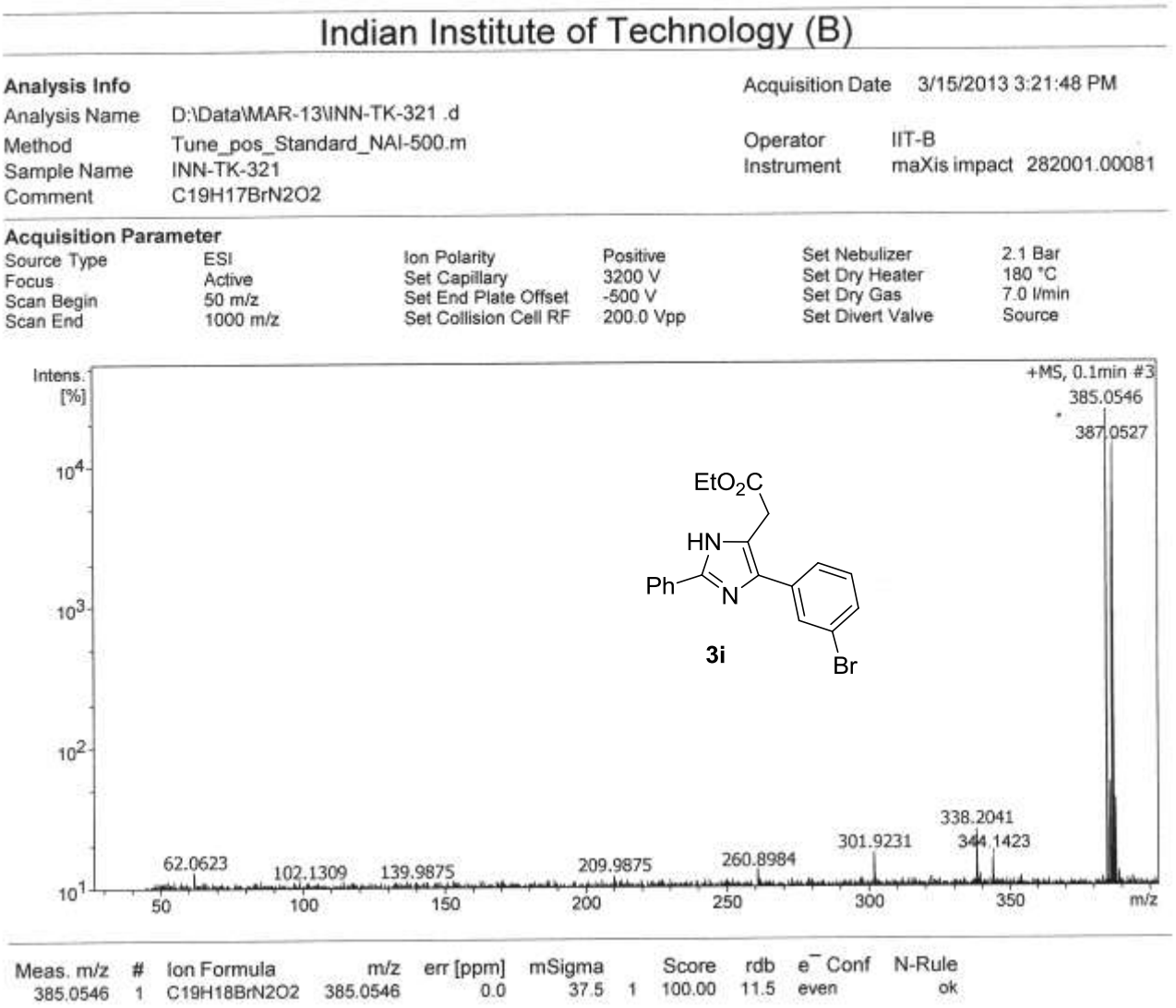


Figure S28. HRMS spectrum of **3i**

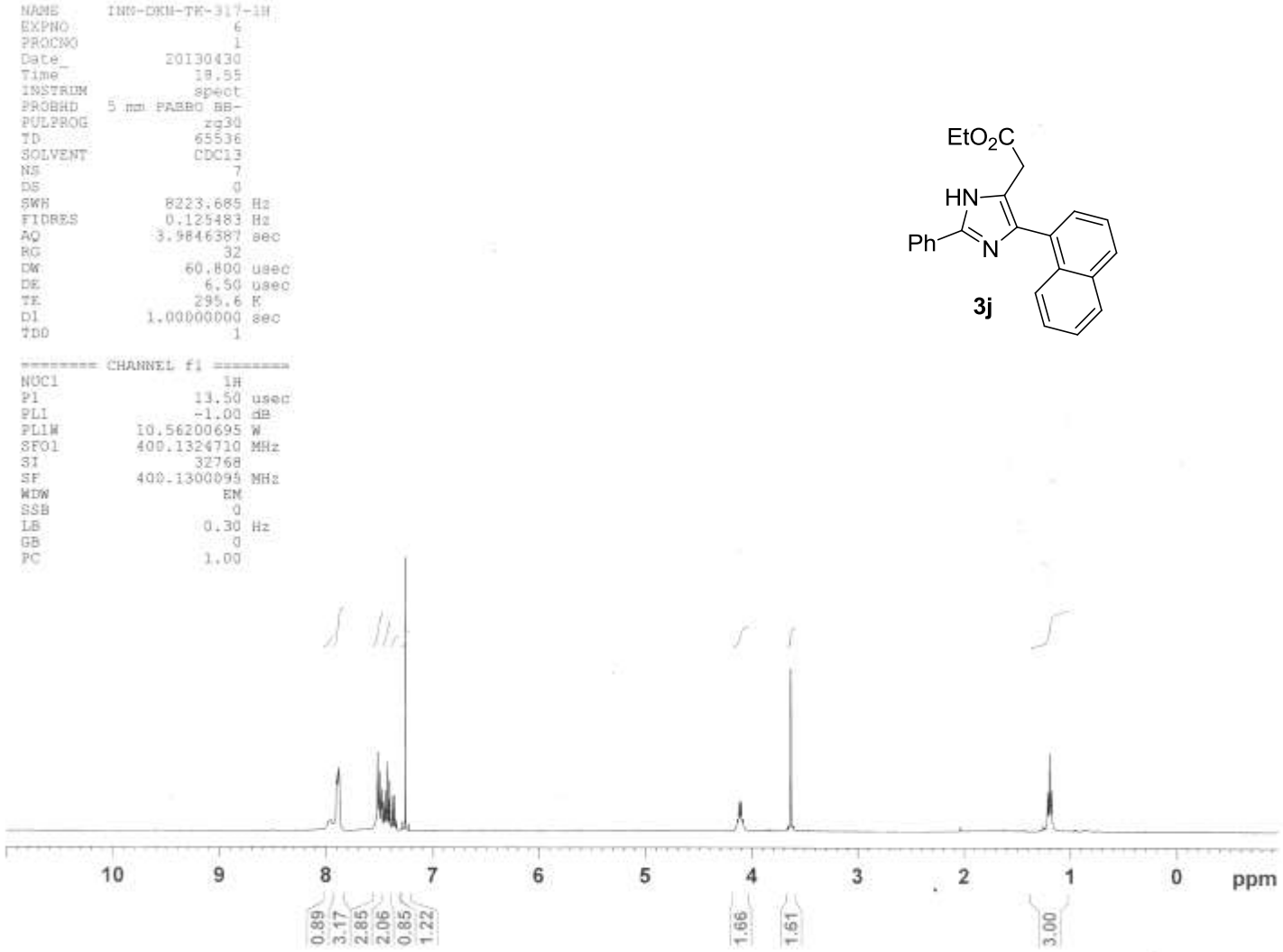


Figure S29. ^{1}H NMR spectrum of **3j**

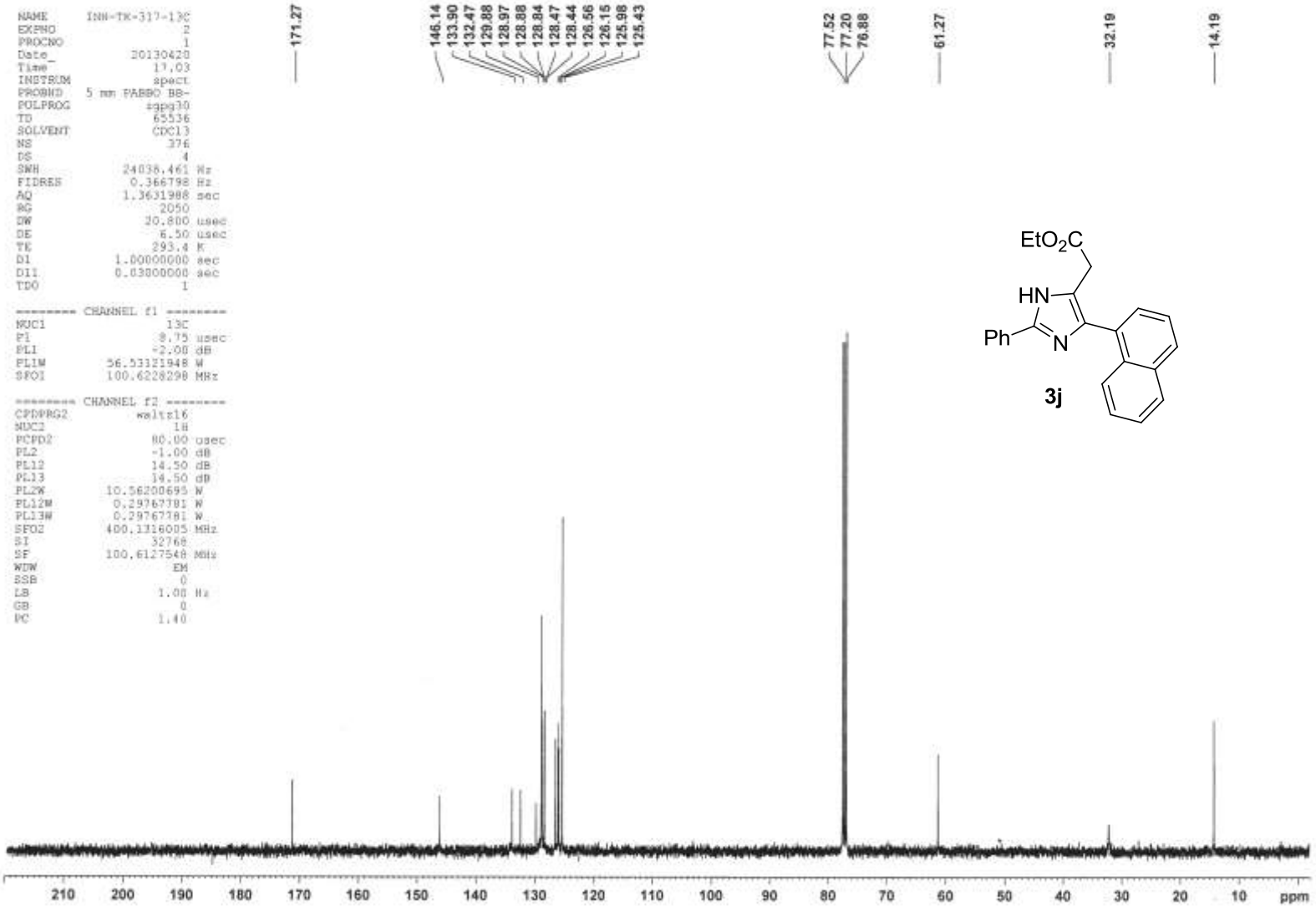


Figure S30. ^{13}C NMR spectrum of **3j**

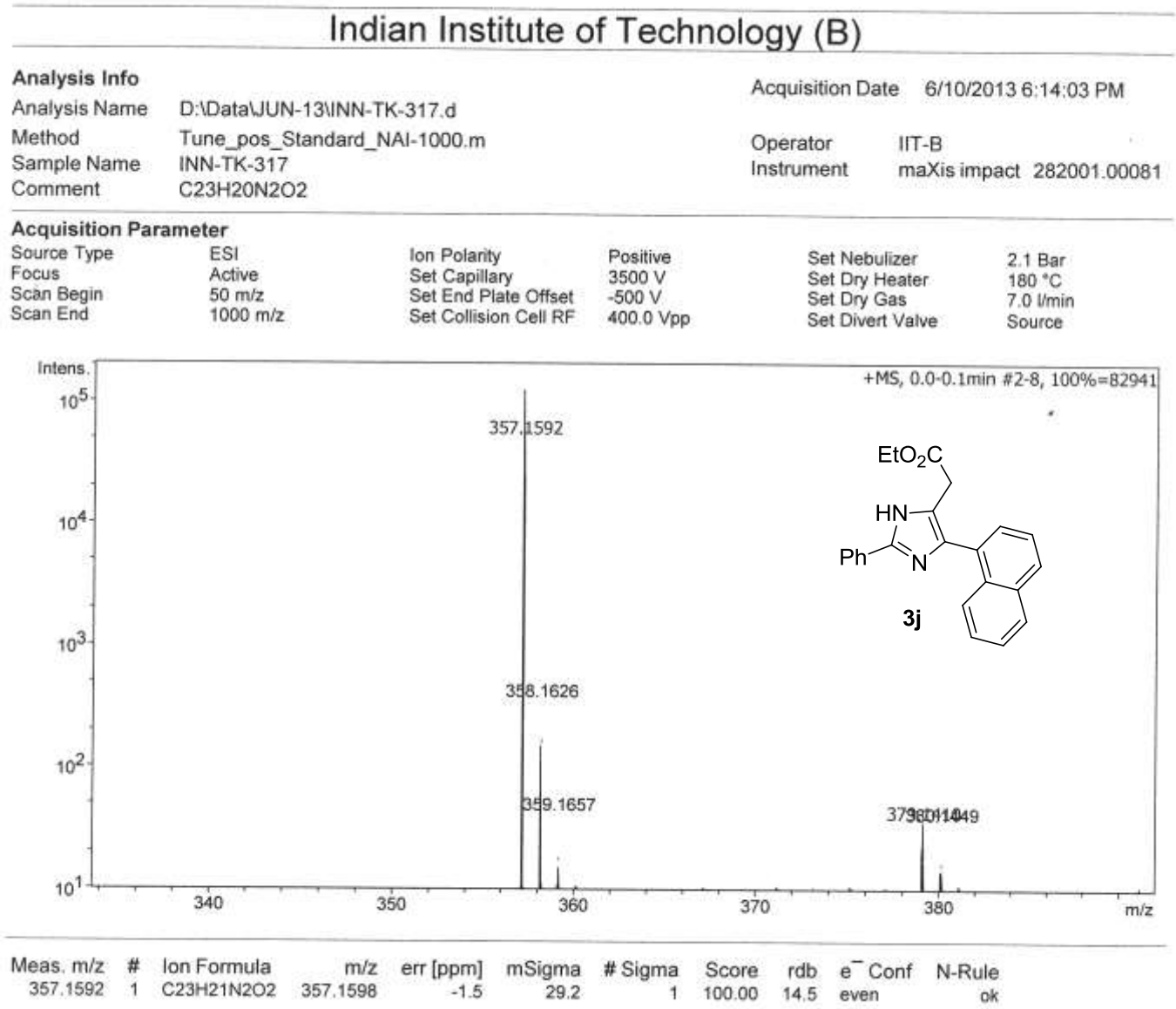


Figure S31. HRMS spectrum of **3j**

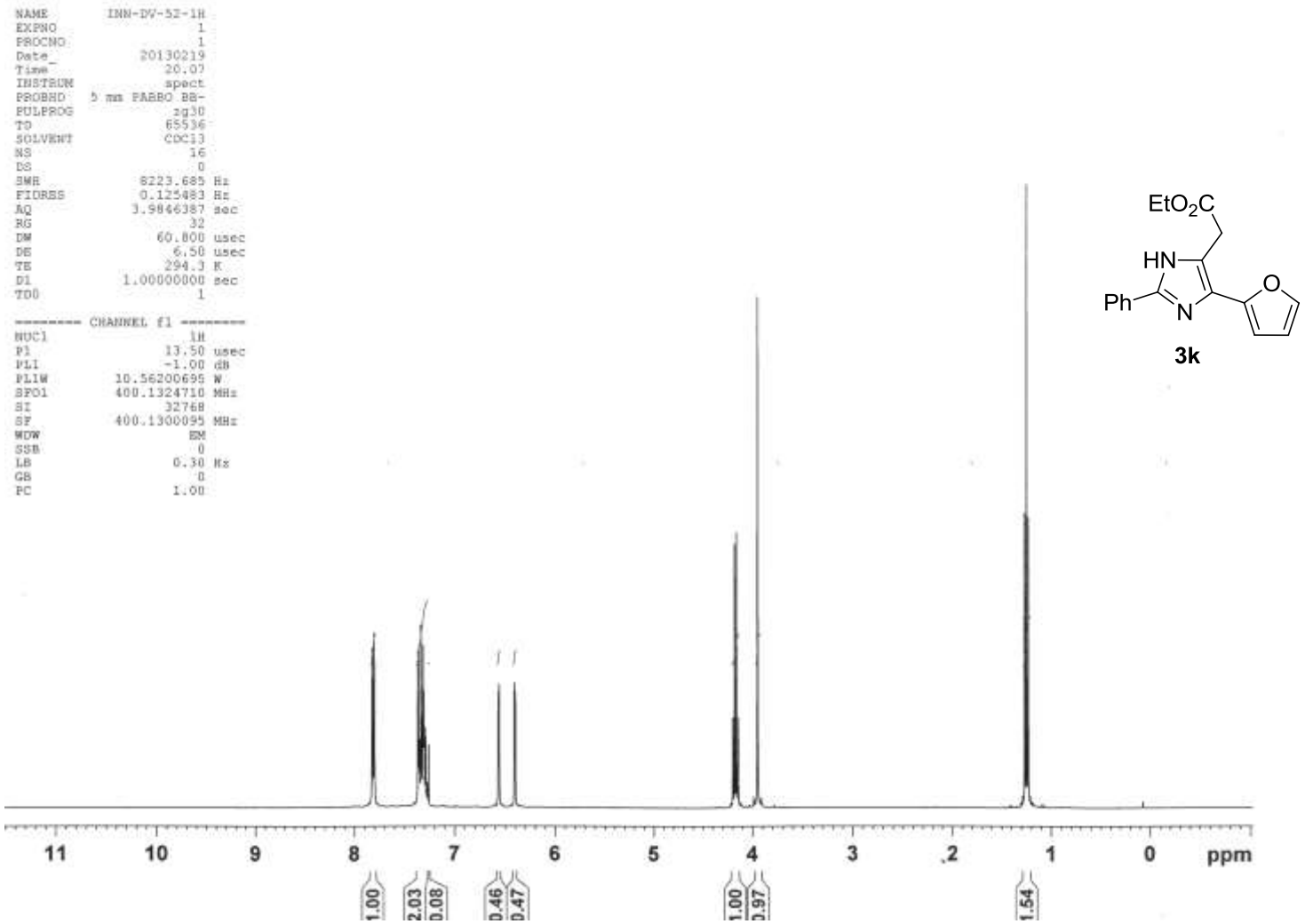


Figure S32. ^{1}H NMR spectrum of **3k**

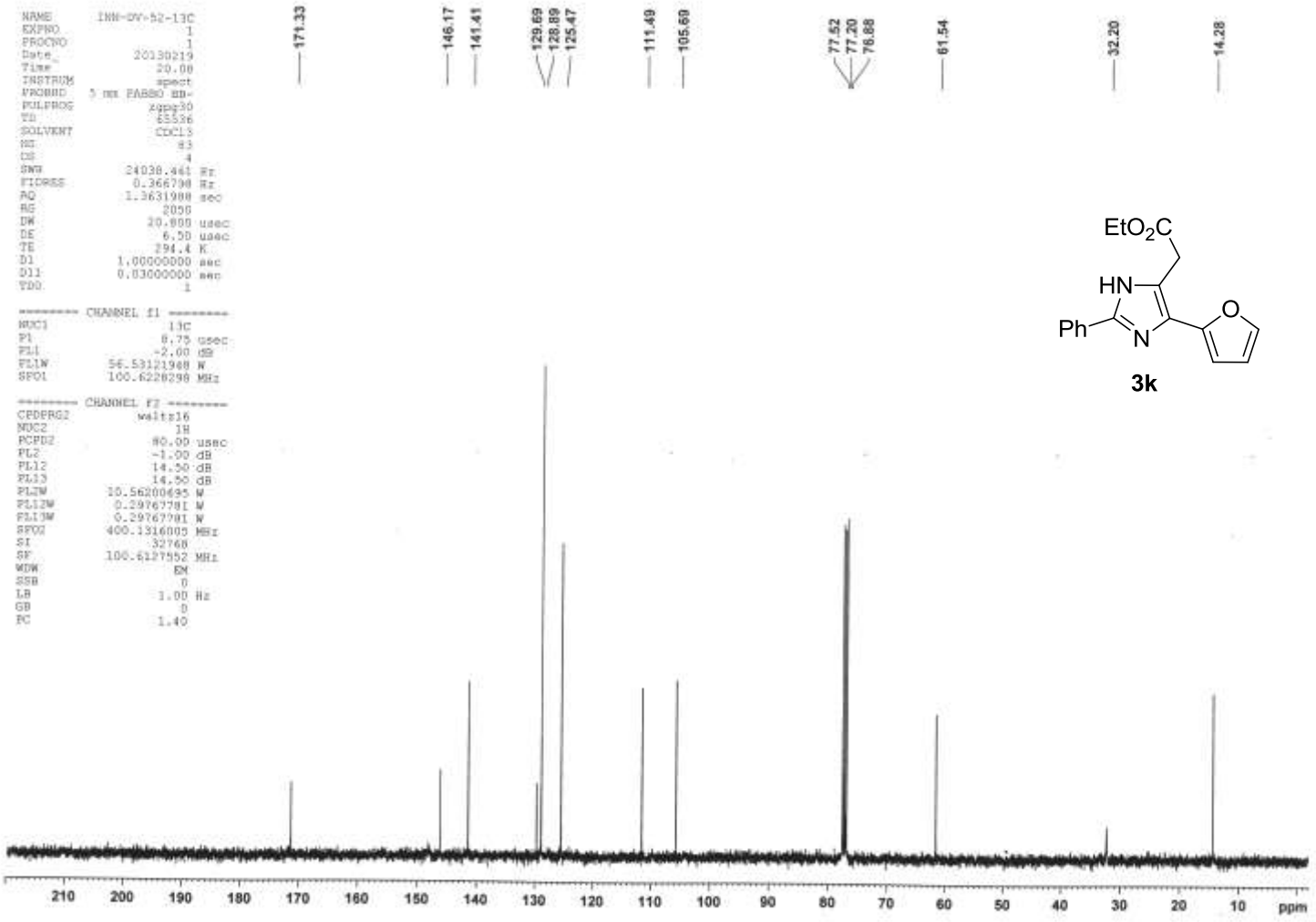


Figure S33. ^{13}C NMR spectrum of **3k**

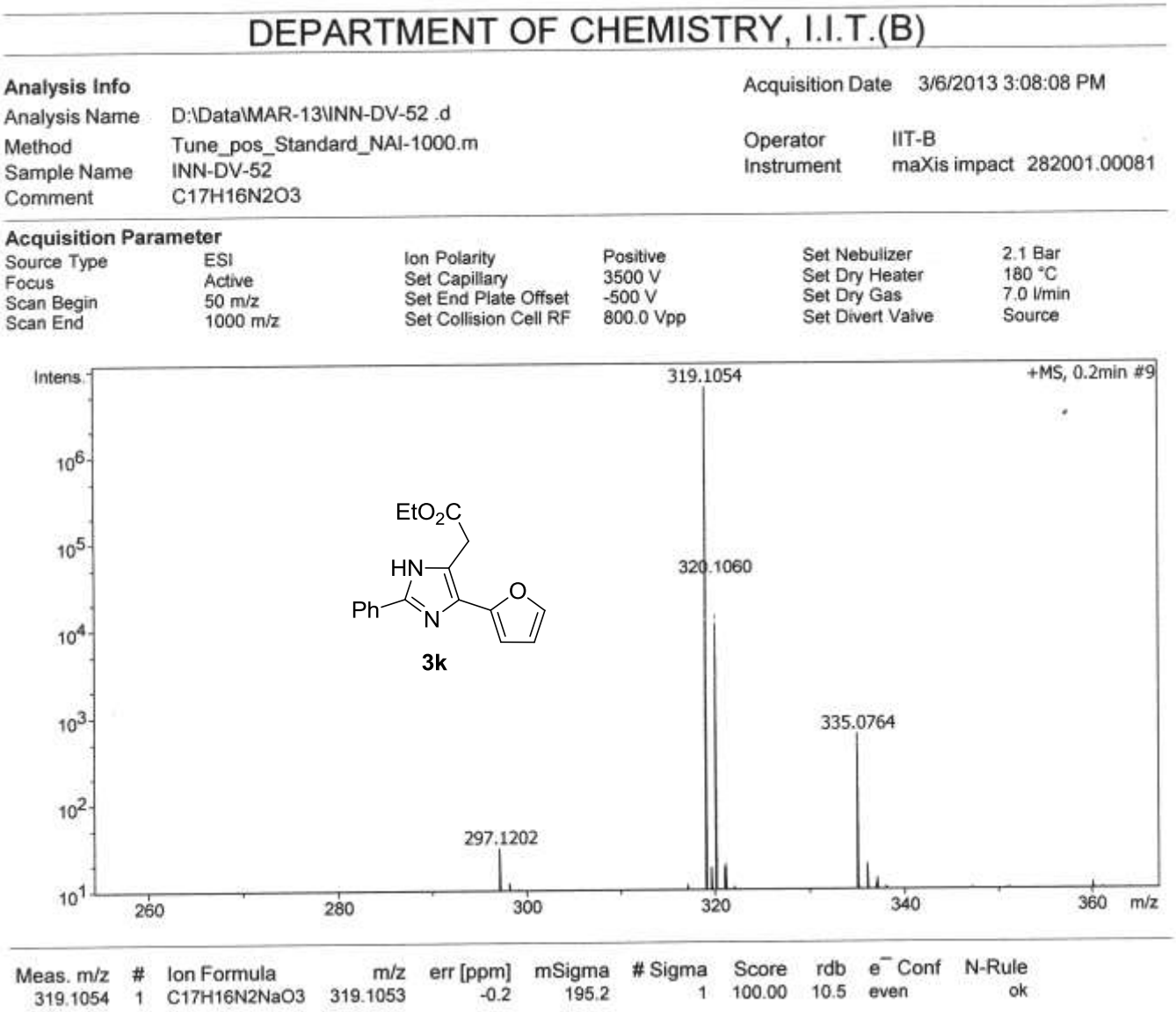


Figure S34. HRMS spectrum of **3k**

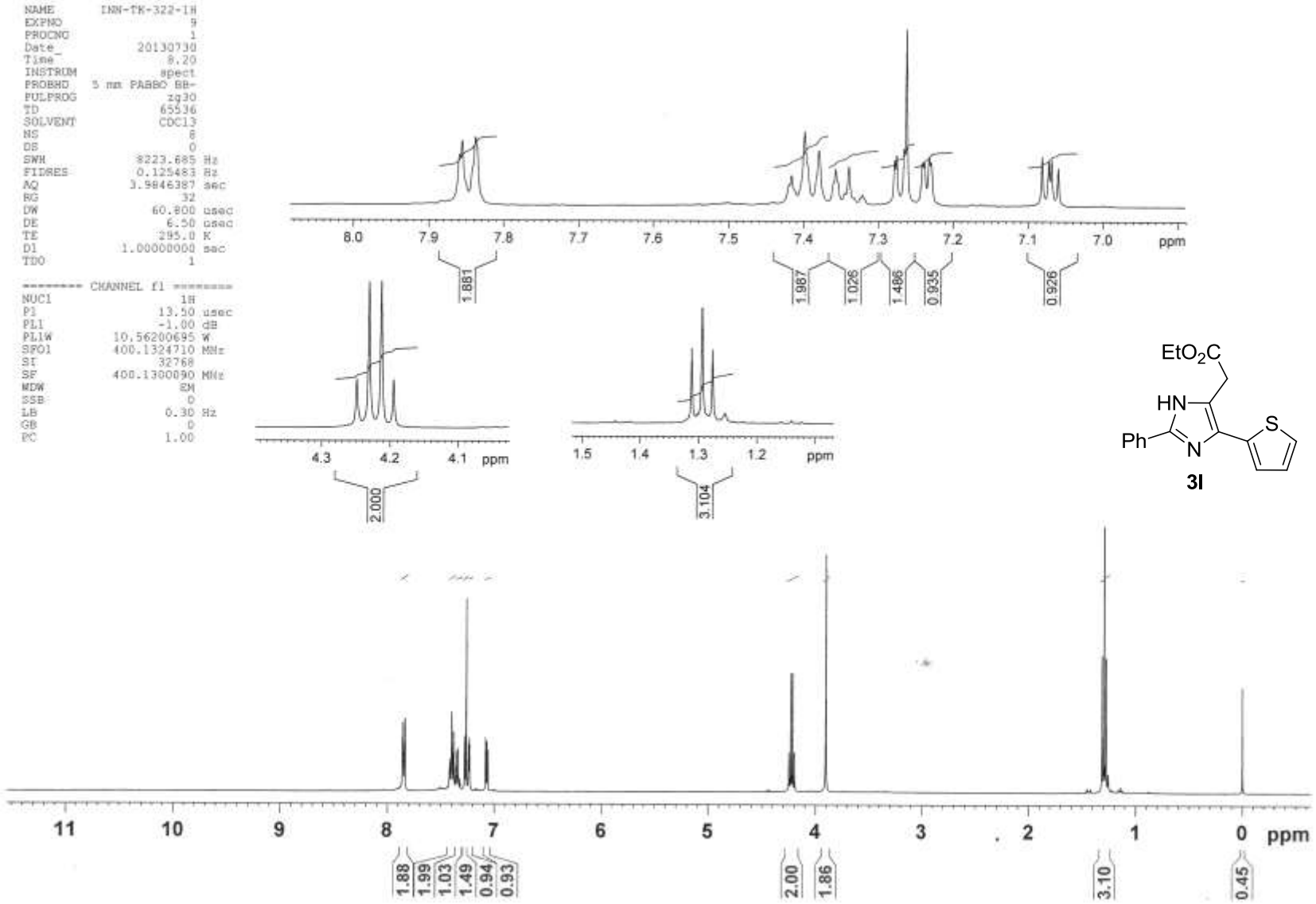


Figure S35. ^{1}H NMR spectrum of **3l**

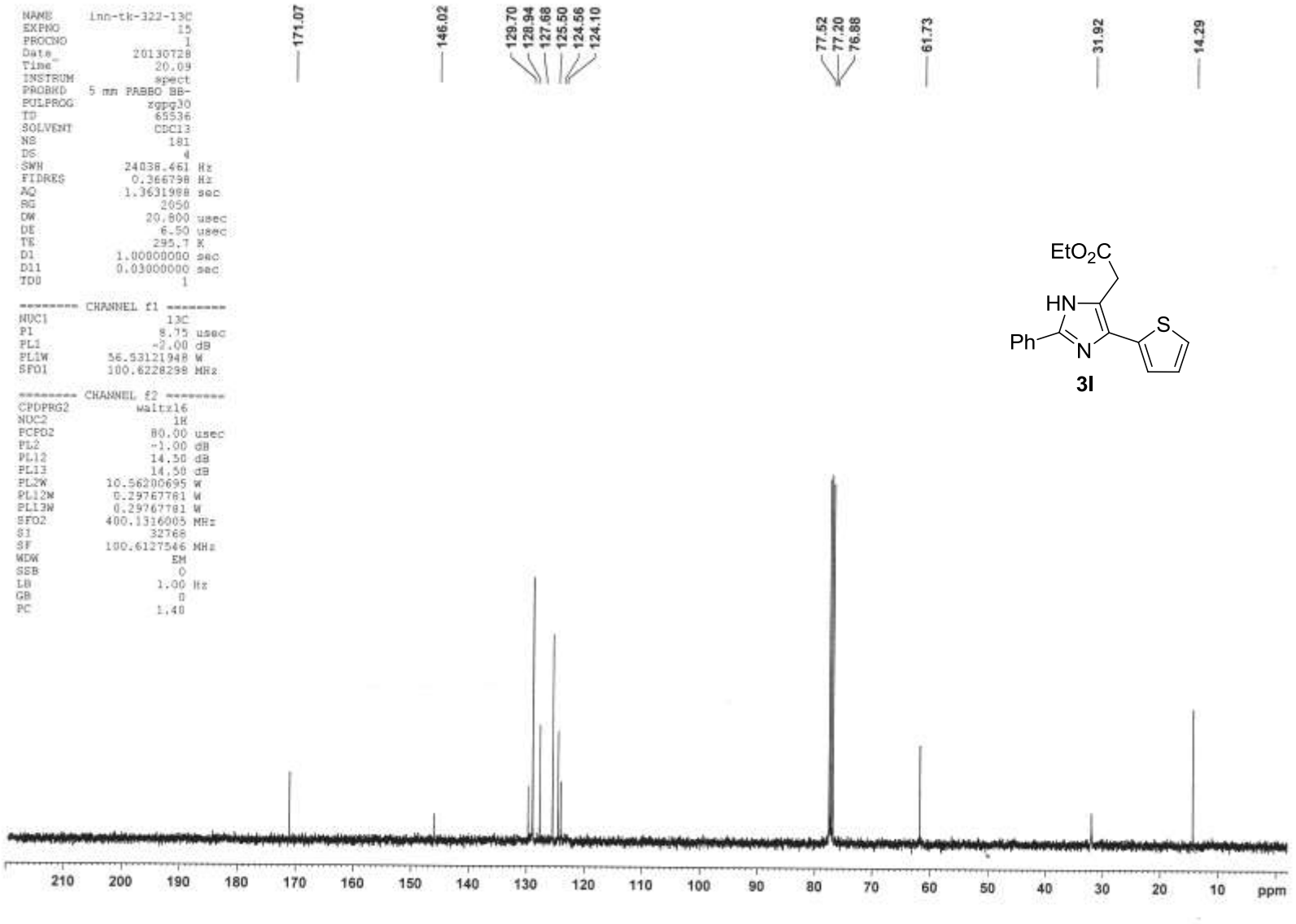


Figure S36. ^{13}C NMR spectrum of **3l**

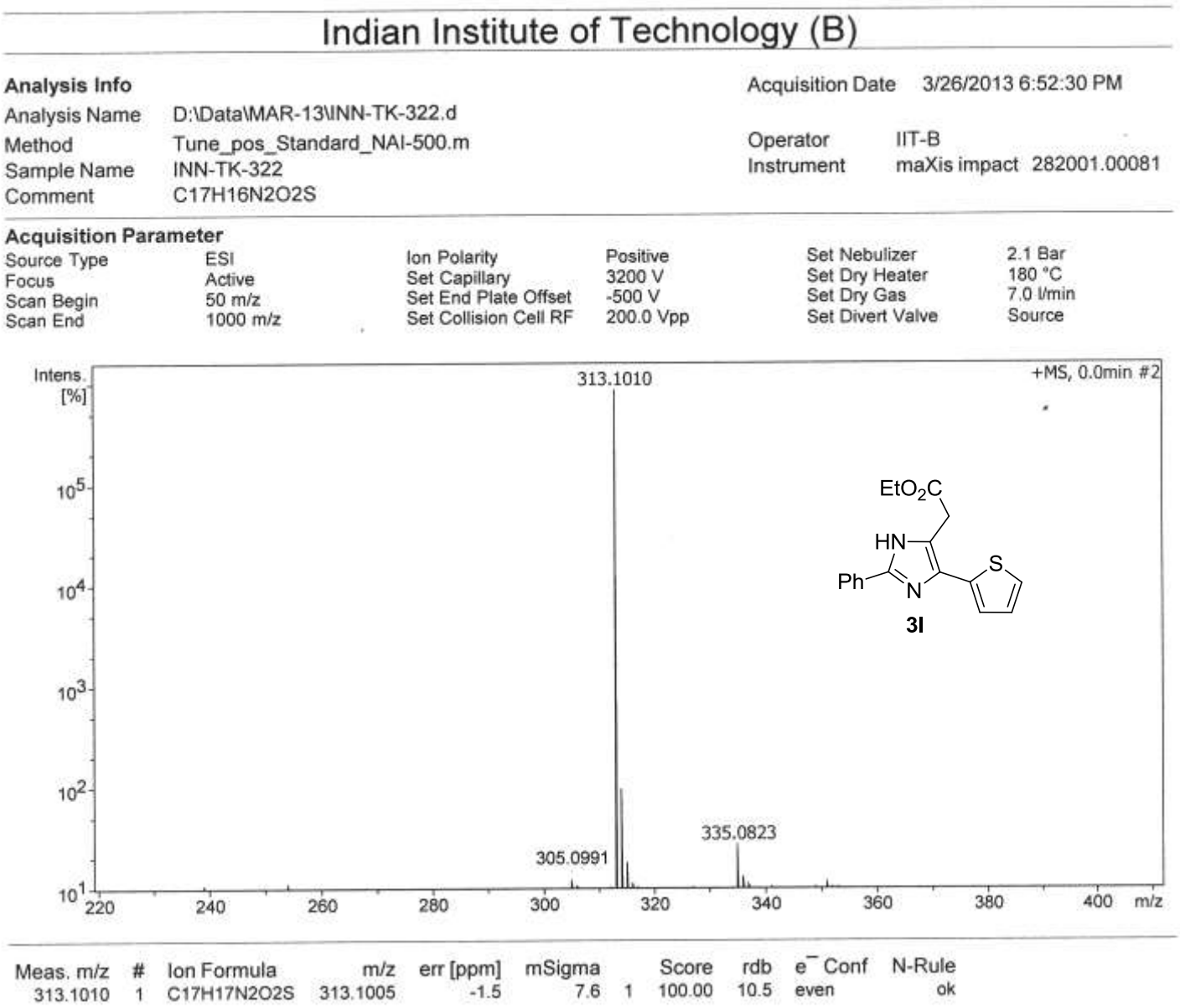


Figure S37. HRMS spectrum of **3l**

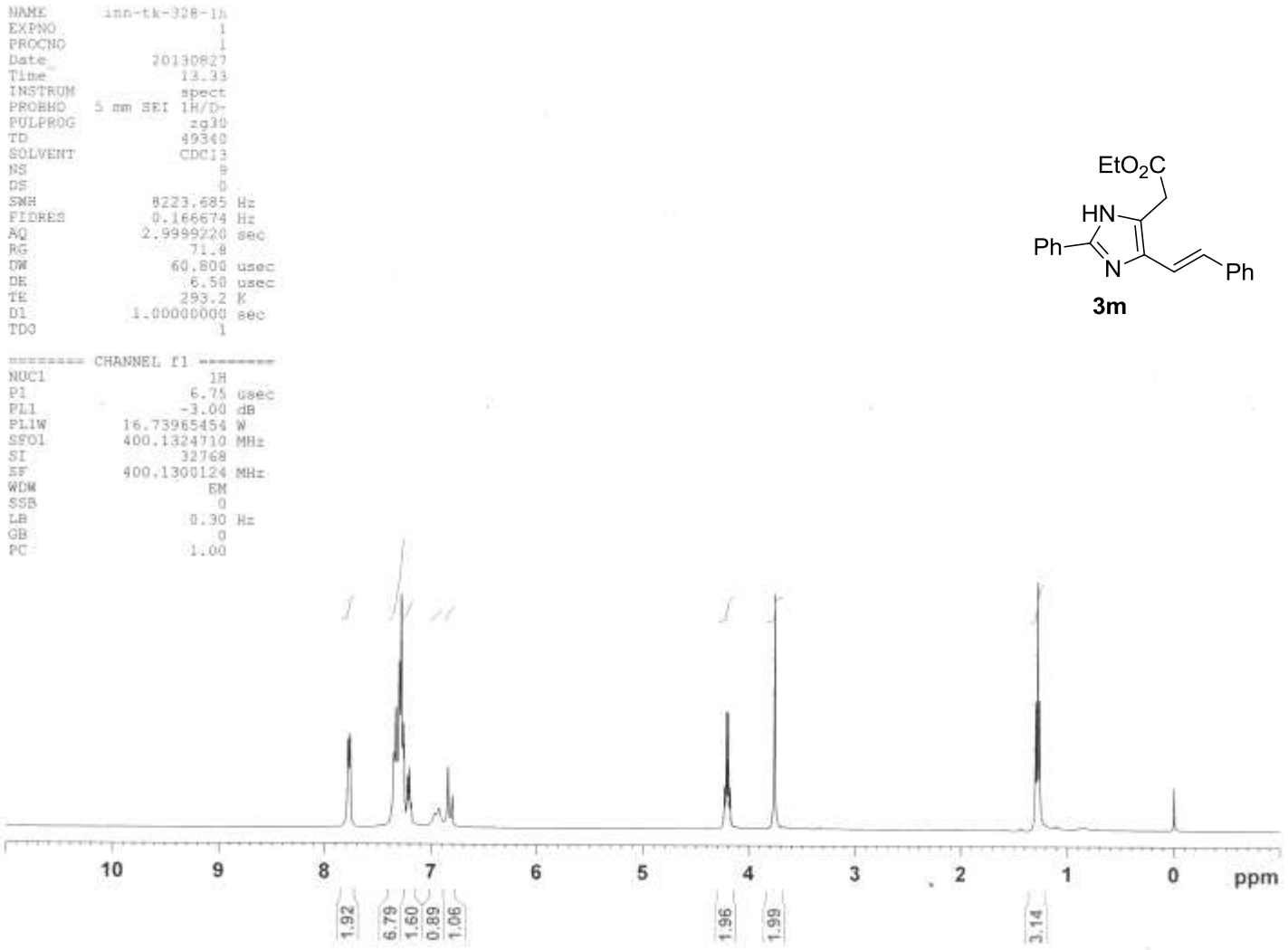


Figure S38. ^{1}H NMR spectrum of **3m**

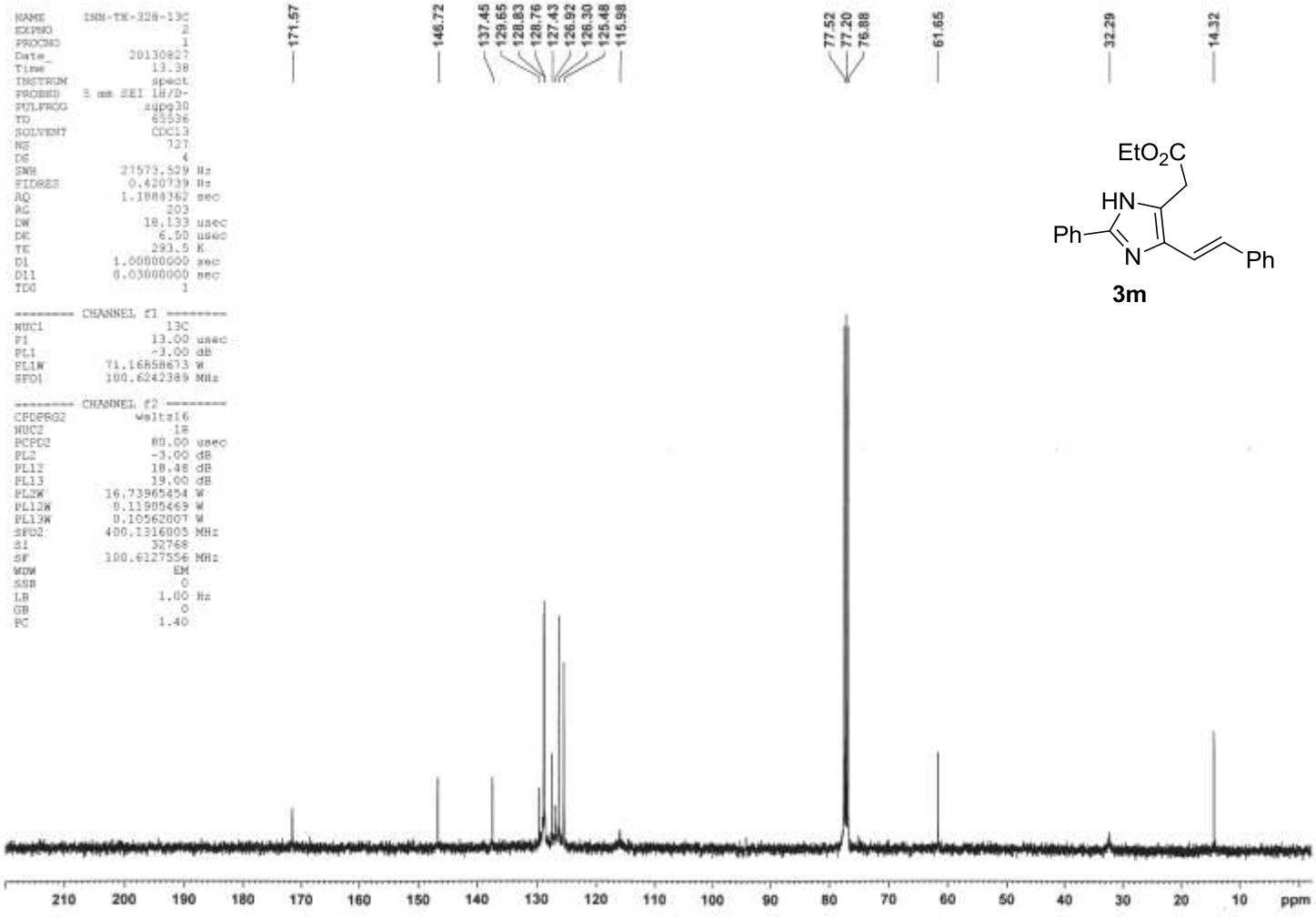


Figure S39. ^{13}C NMR spectrum of **3m**

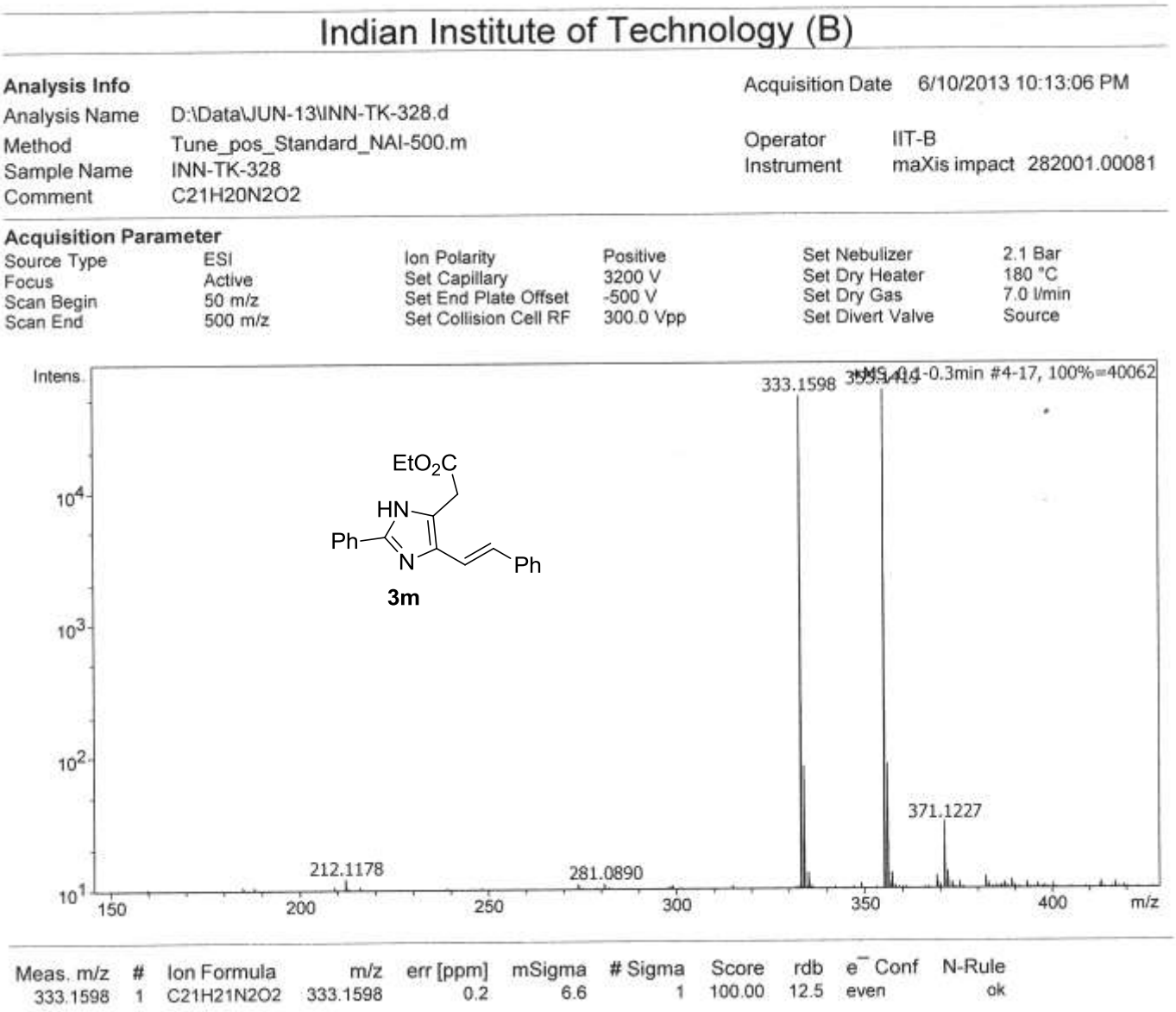


Figure S40. HRMS spectrum of **3m**

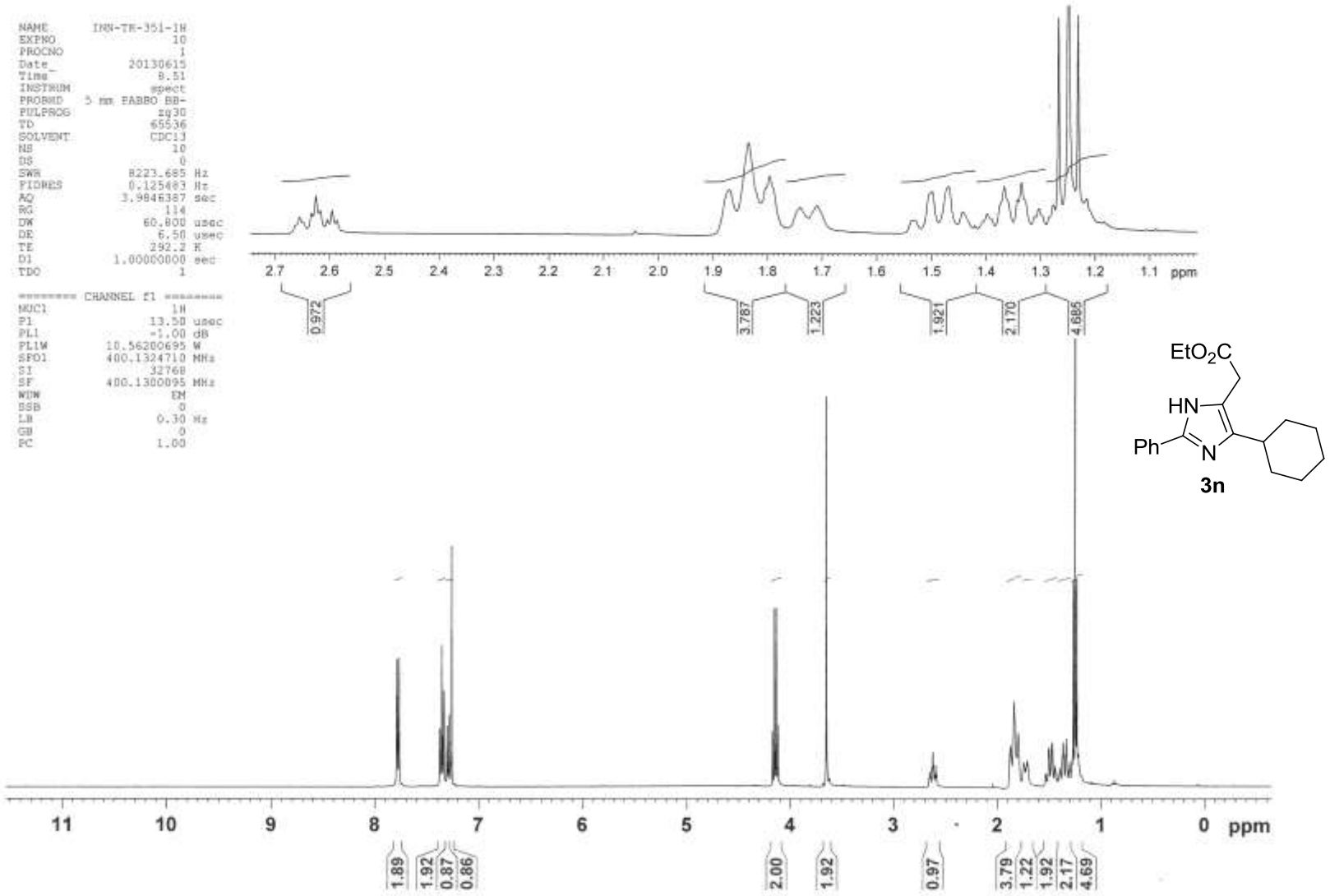


Figure S41. ^{1}H NMR spectrum of **3n**

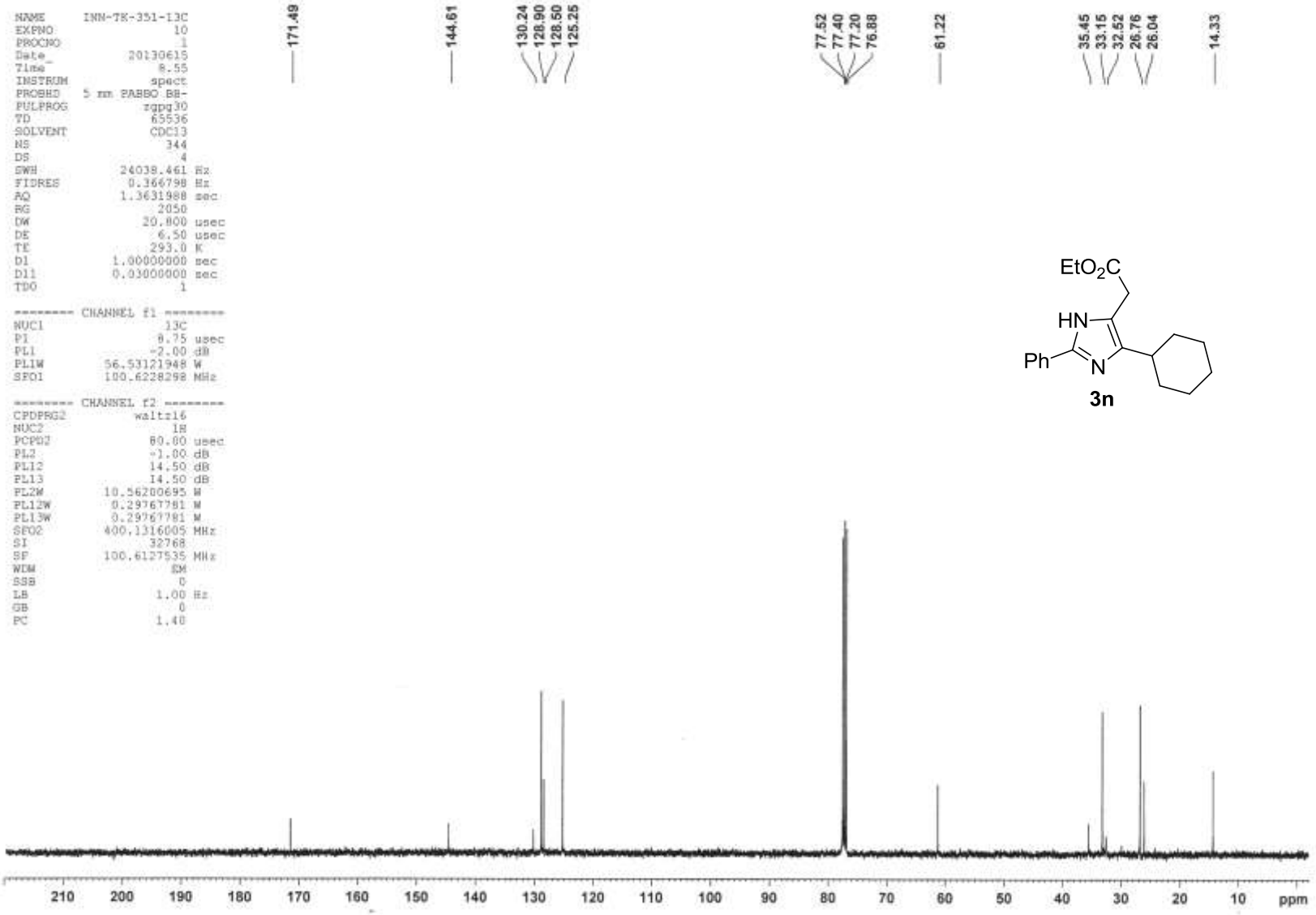


Figure S42. ^{13}C NMR spectrum of **3n**

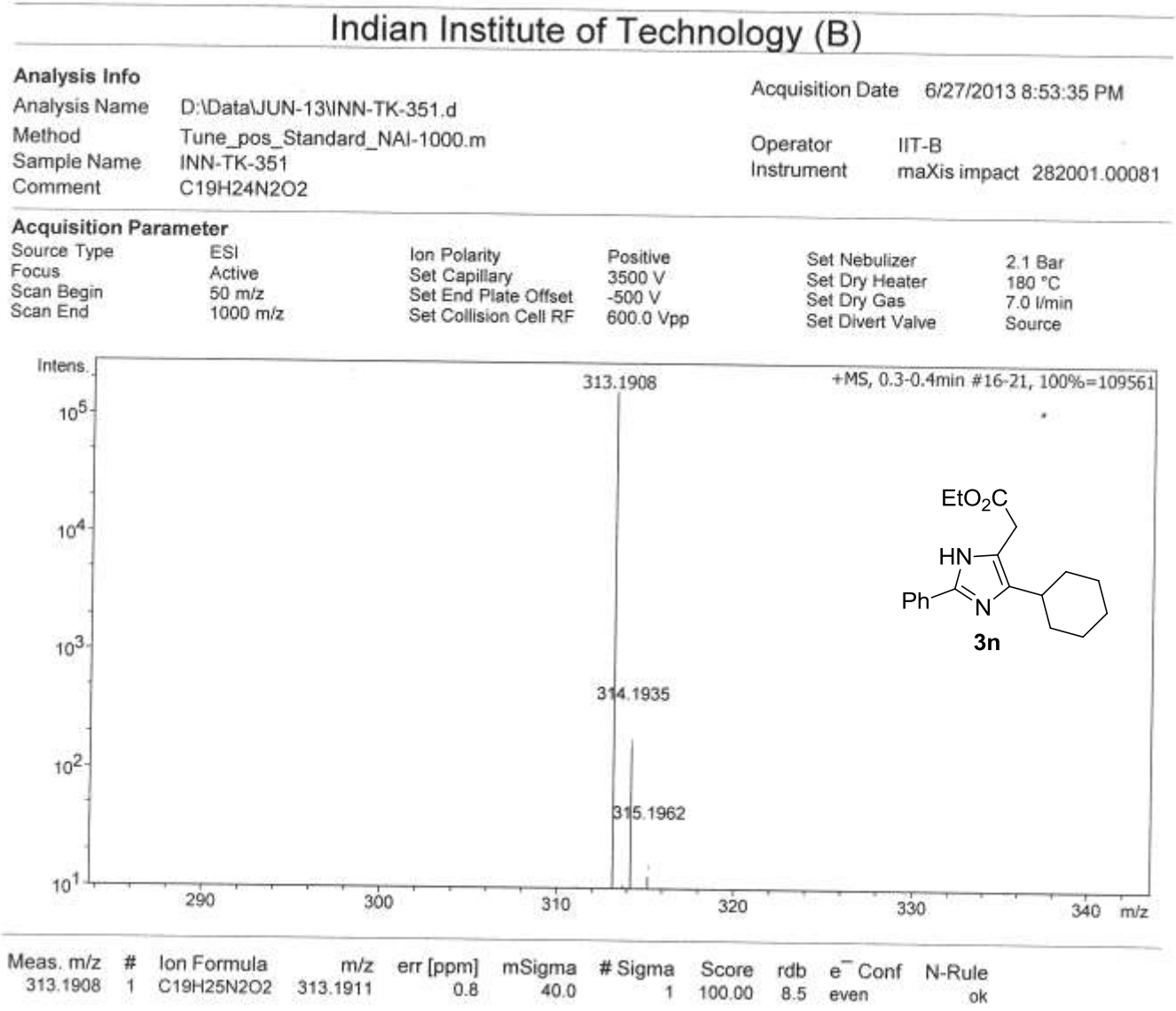


Figure S43. HRMS spectrum of **3n**

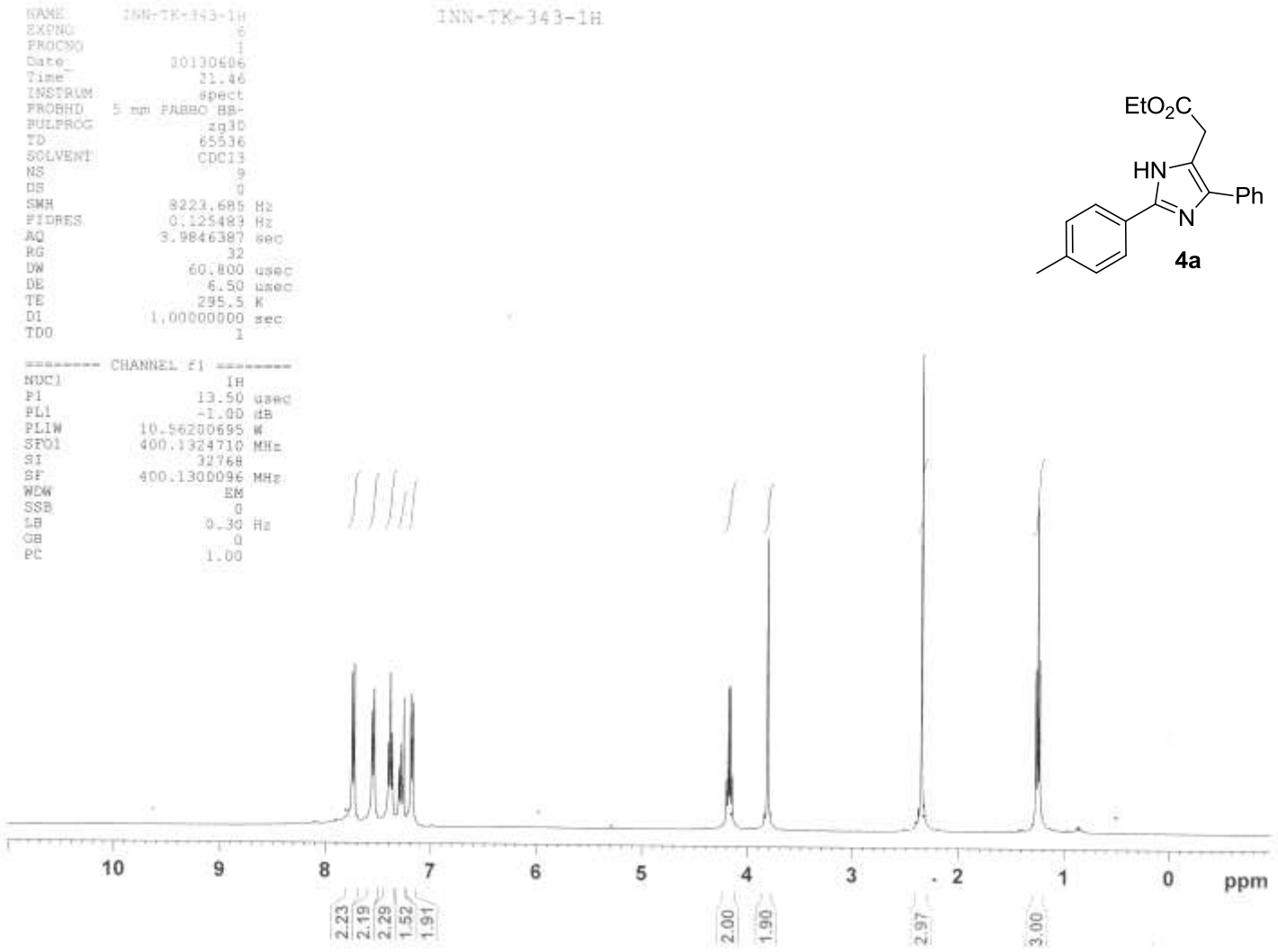


Figure S44. ^{1}H NMR spectrum of **4a**

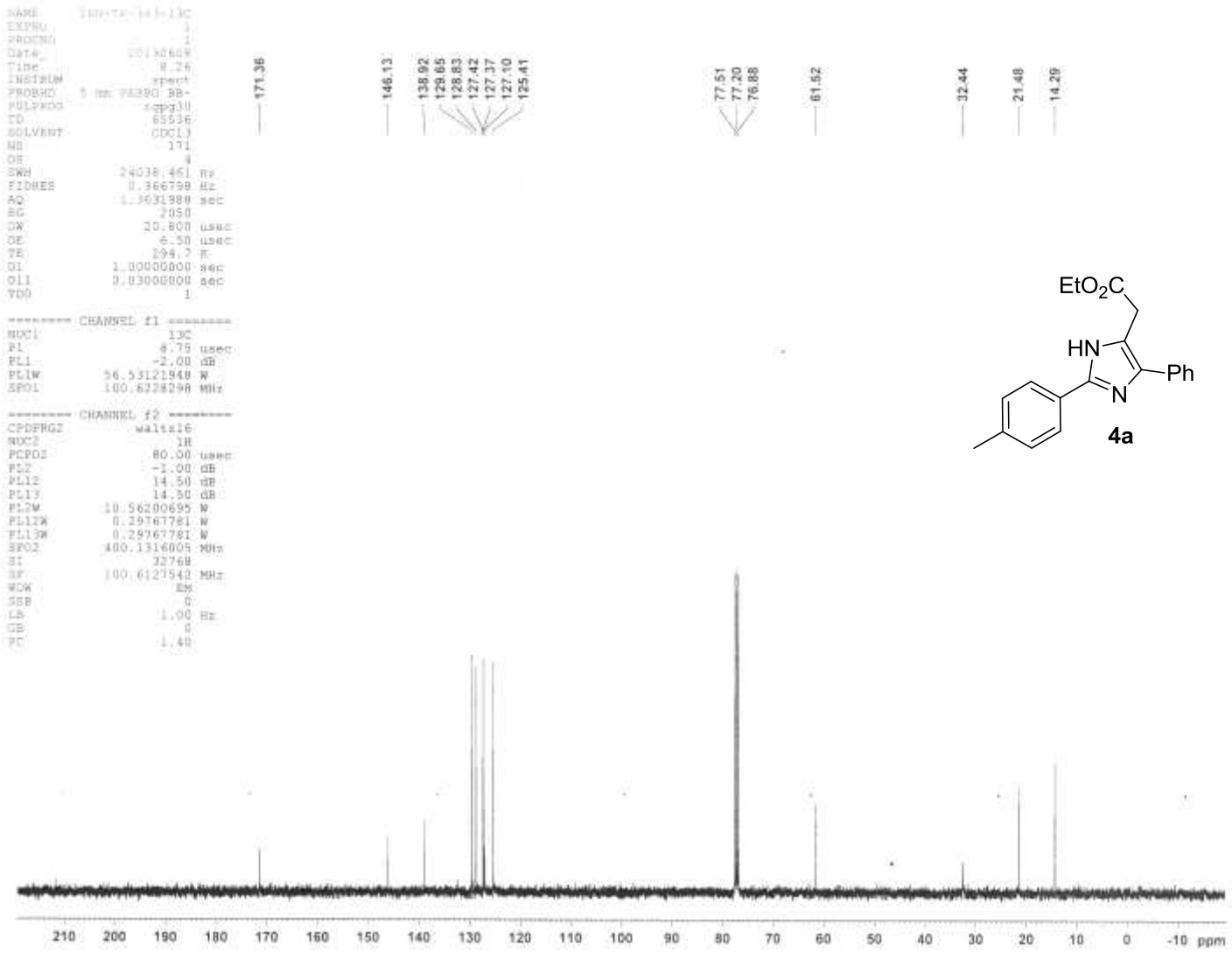


Figure S45. ^{13}C NMR spectrum of **4a**

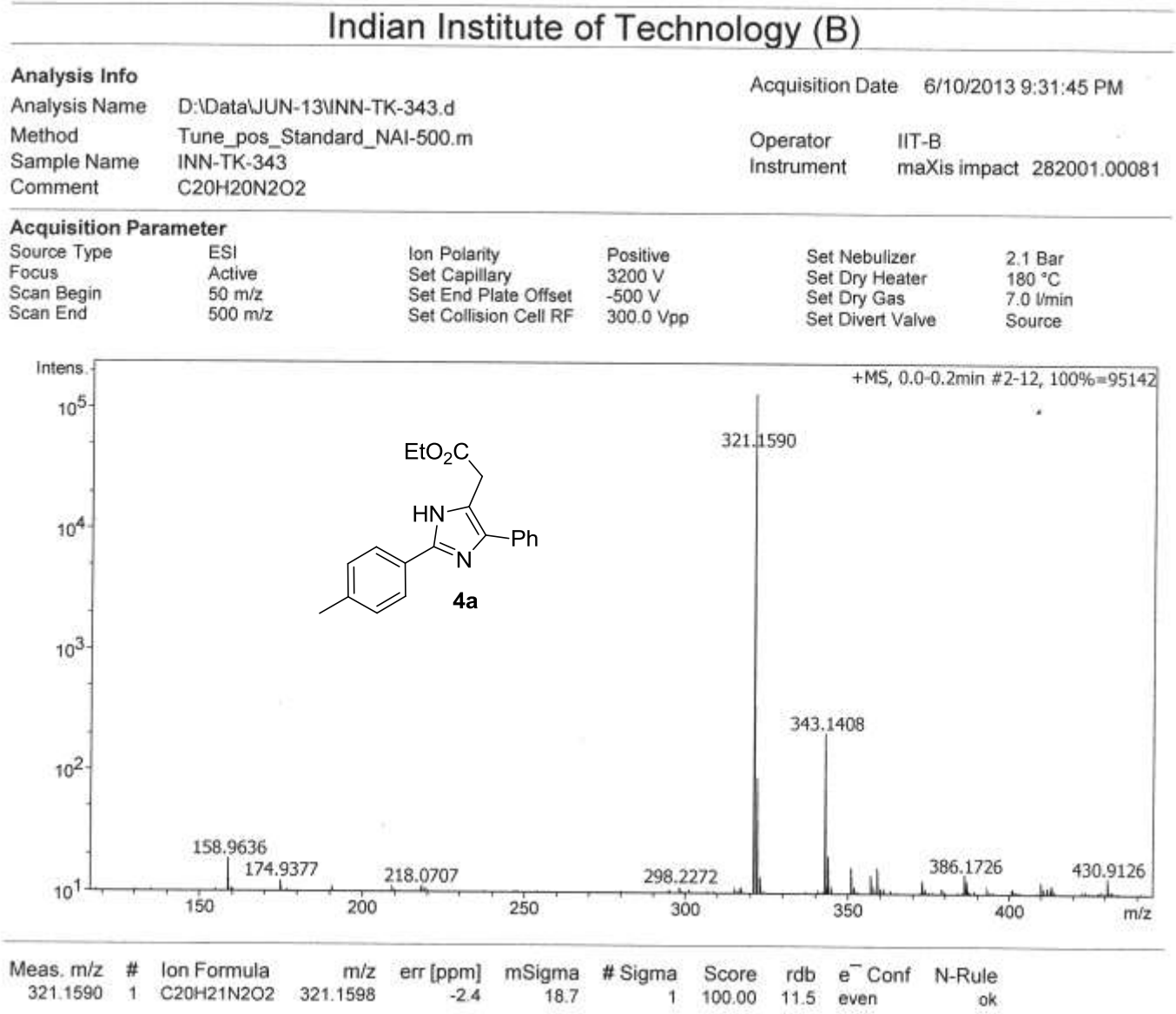


Figure S46. HRMS spectrum of **4a**

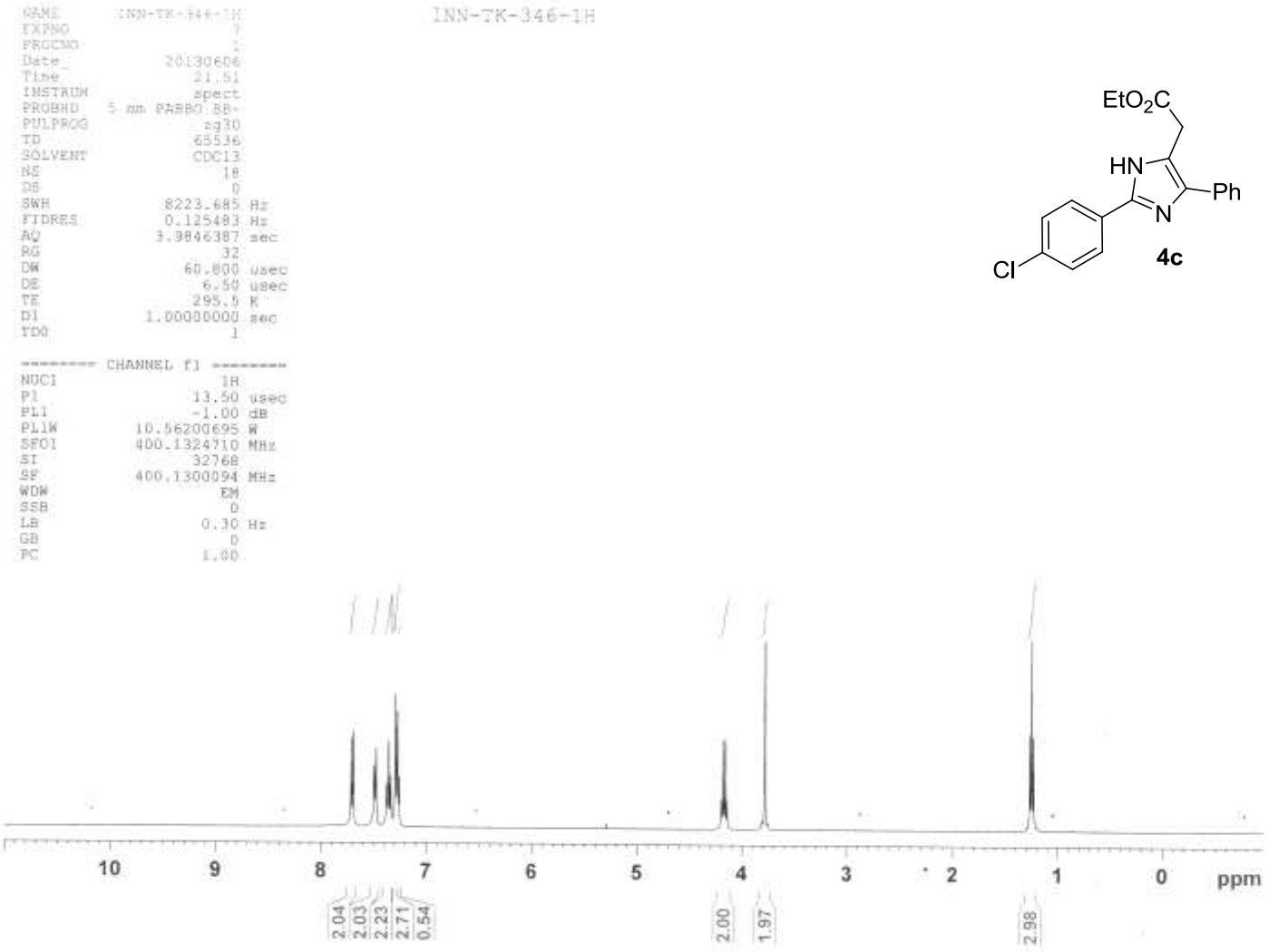


Figure S47. ^{1}H NMR spectrum of **4c**

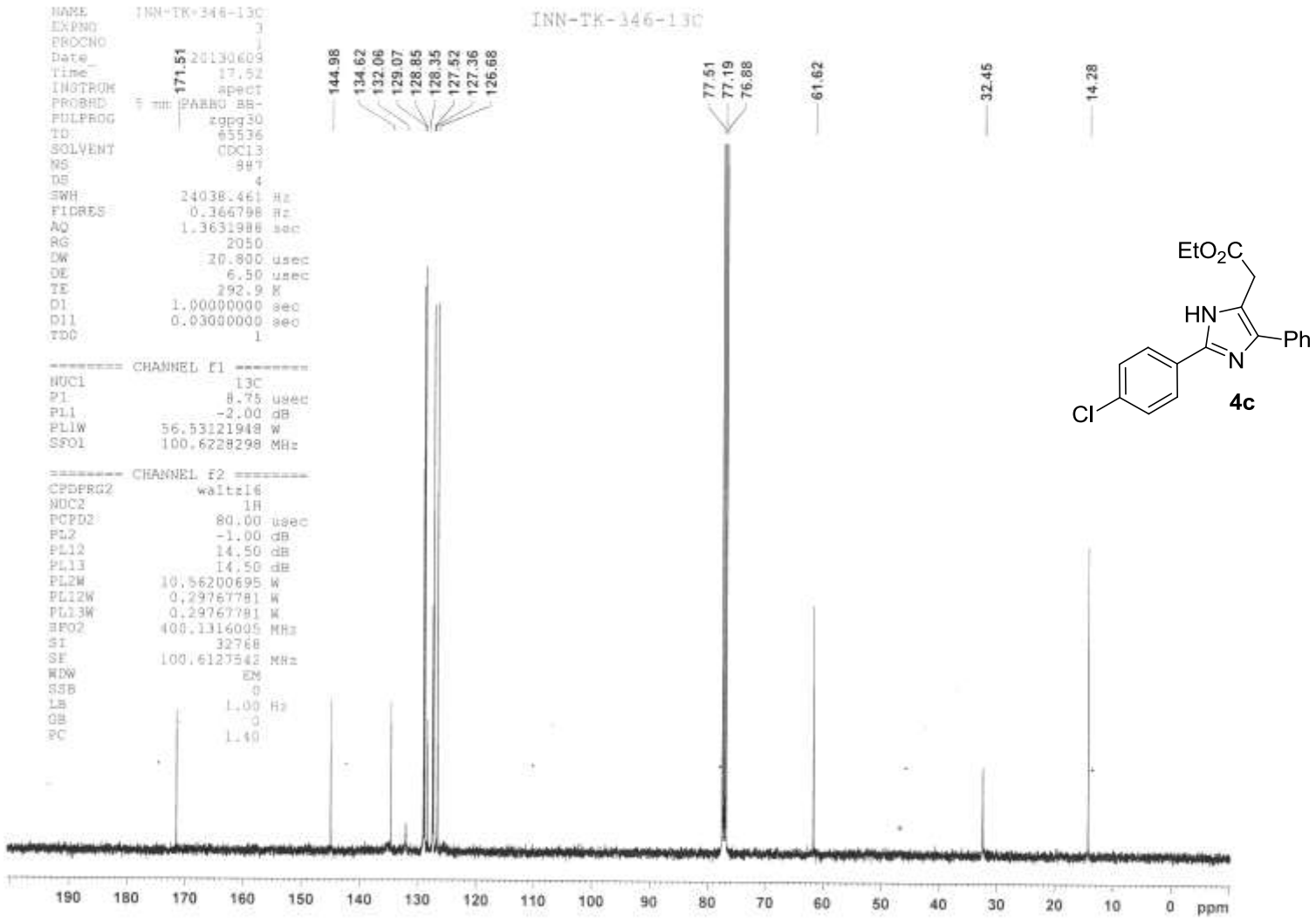


Figure S48. ^{13}C NMR spectrum of **4c**

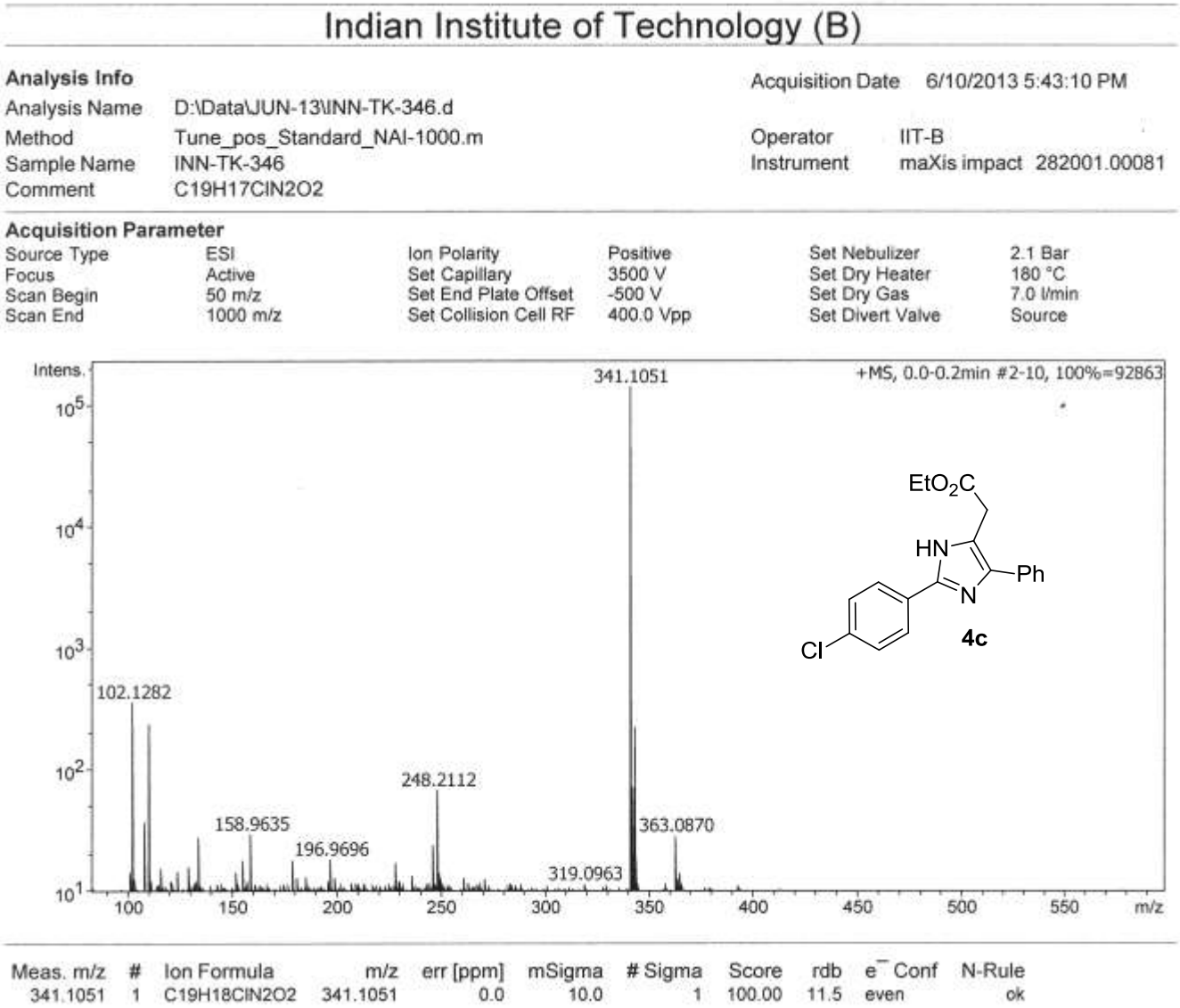


Figure S49. HRMS spectrum of **4c**

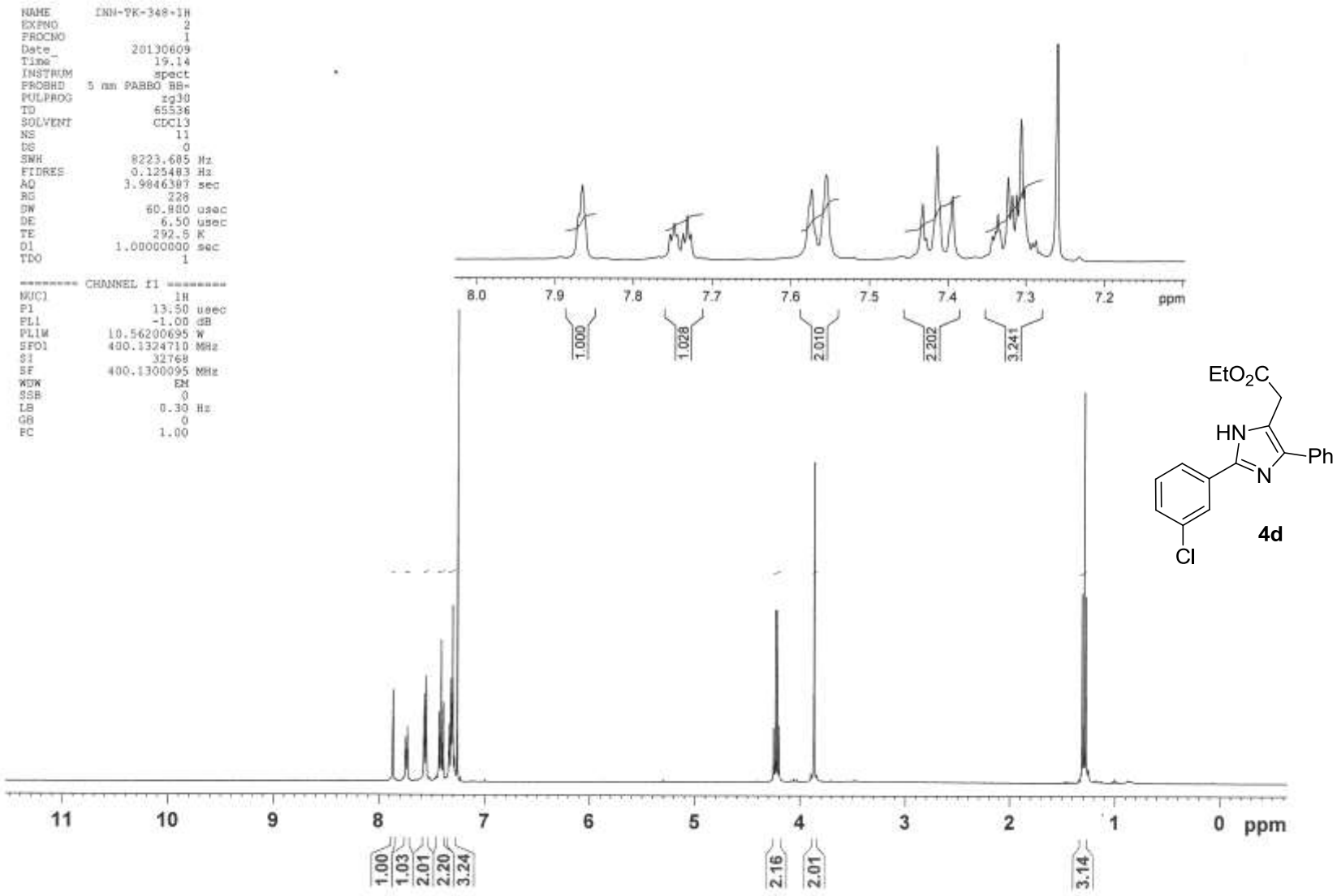


Figure S50. ^{1}H NMR spectrum of **4d**

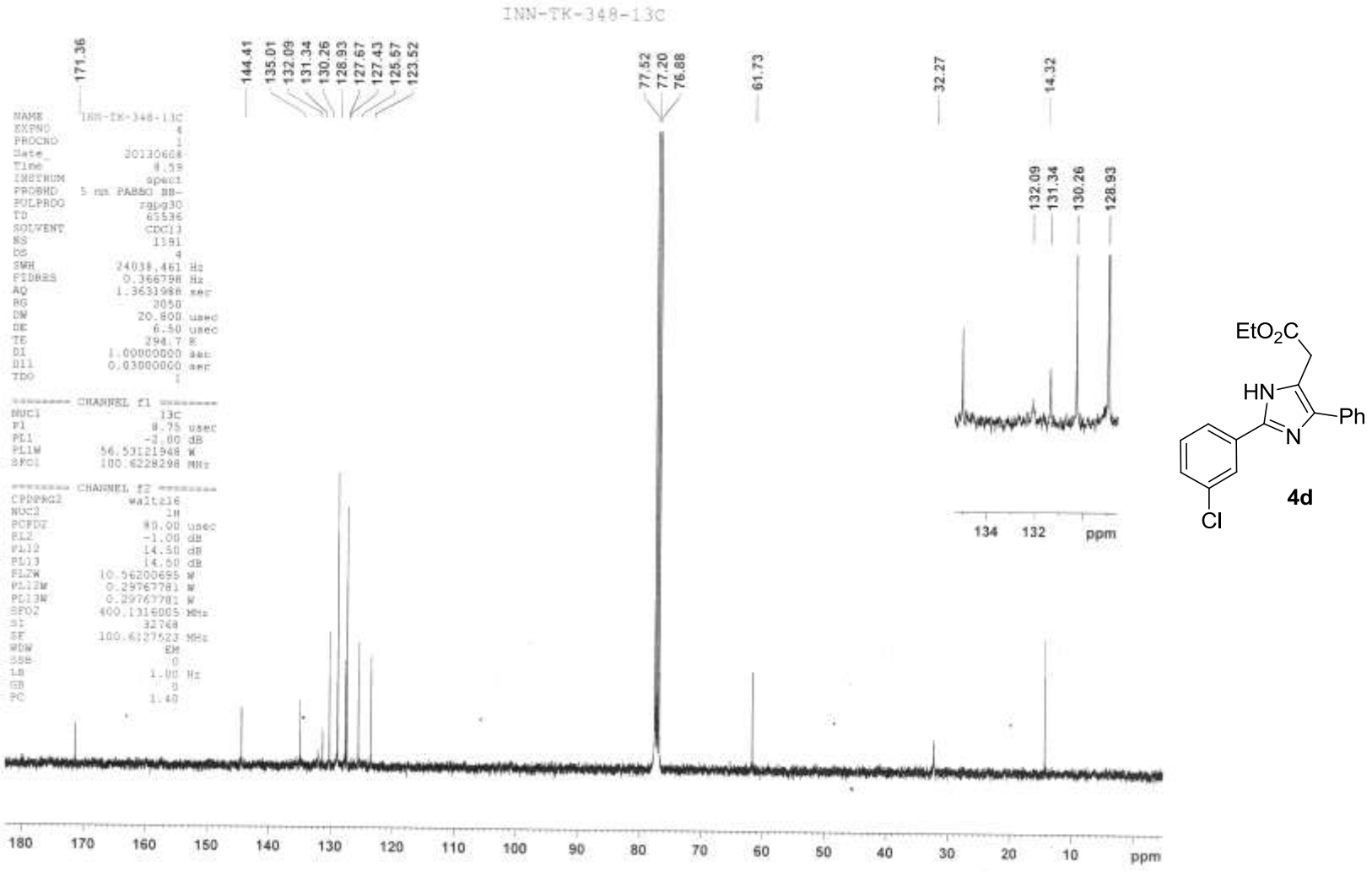


Figure S51. ^{13}C NMR spectrum of **4d**

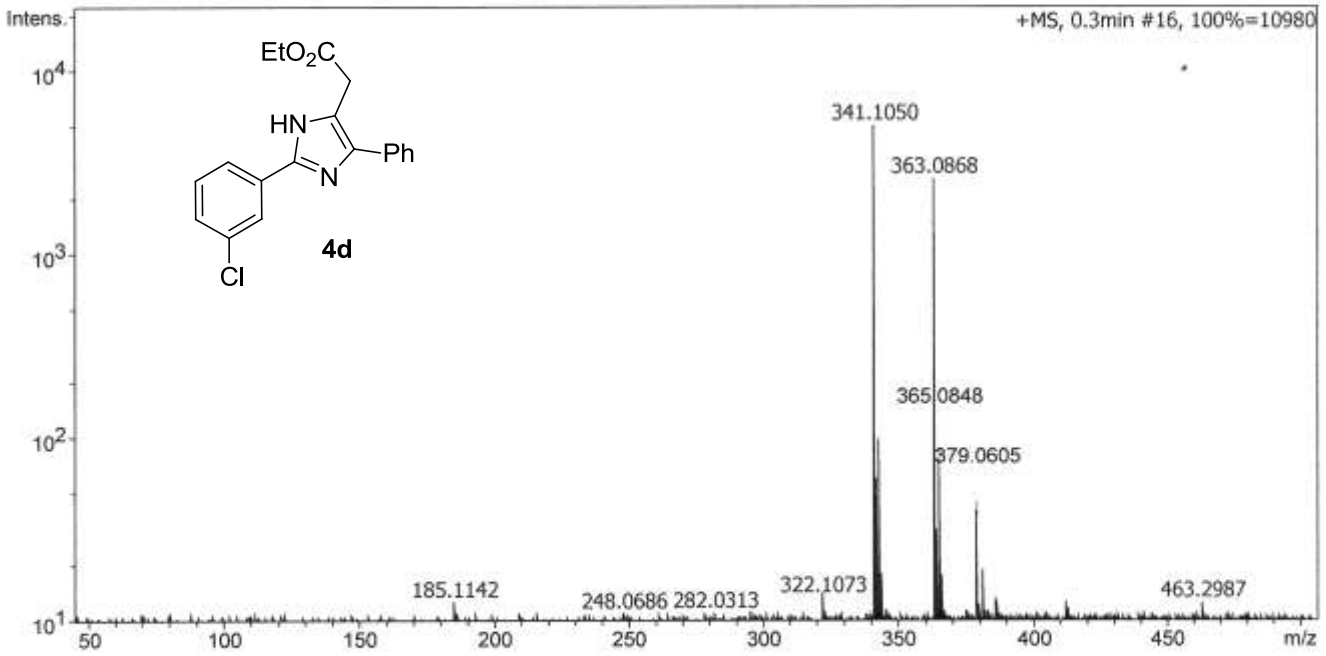
Indian Institute of Technology (B)

Analysis Info

Analysis Name	D:\Data\JUN-13\INN-TK-348.d	Acquisition Date	6/10/2013 9:13:54 PM
Method	Tune_pos_Standard_NAI-500.m	Operator	IIT-B
Sample Name	INN-TK-348	Instrument	maXis impact 282001.00081
Comment	C19H17ClN2O2		

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	C19H18ClN2O2	341.1051	-0.5	36.1	1	100.00	11.5	even	ok

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

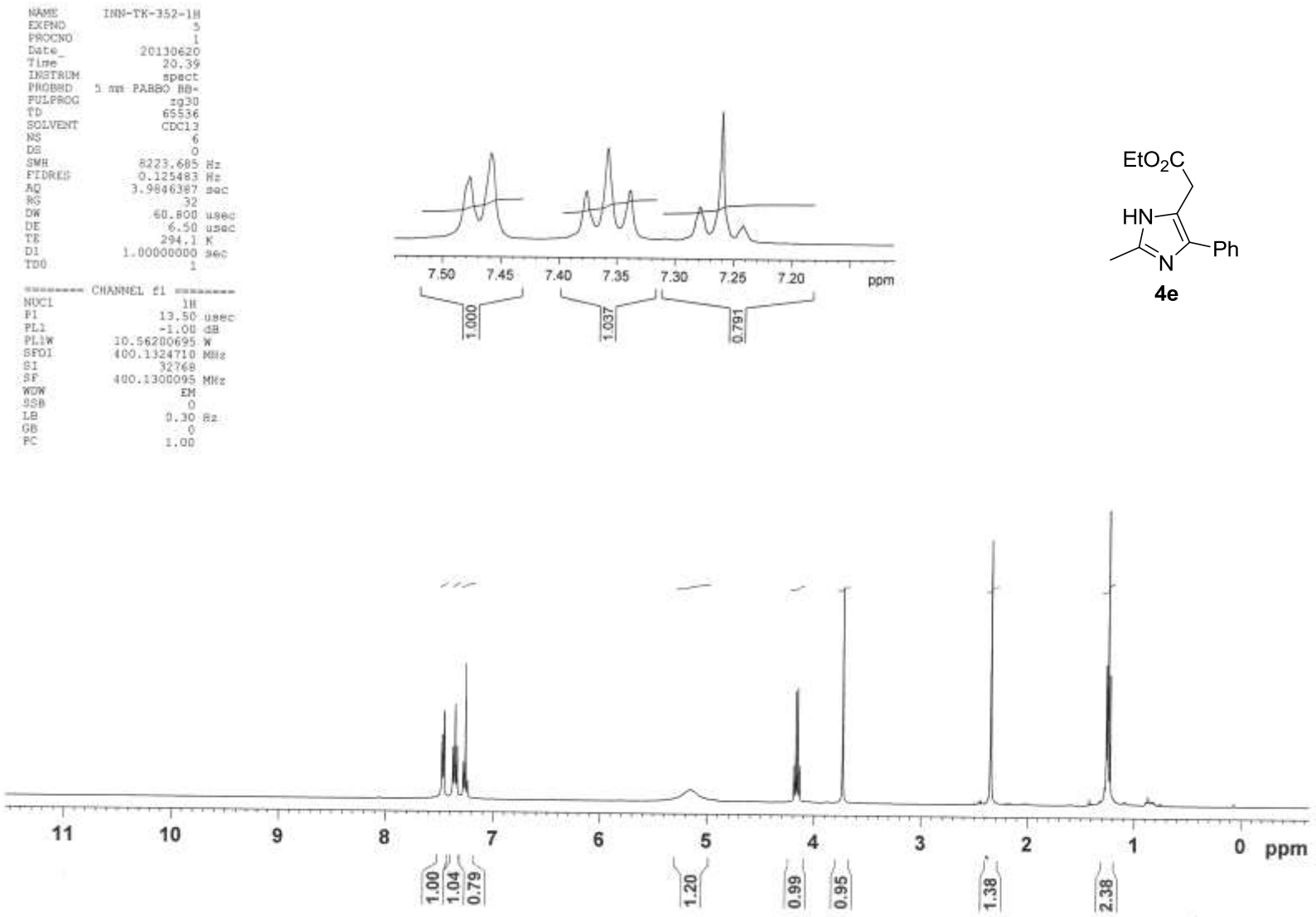


Figure S53. ^{1}H NMR spectrum of **4e**

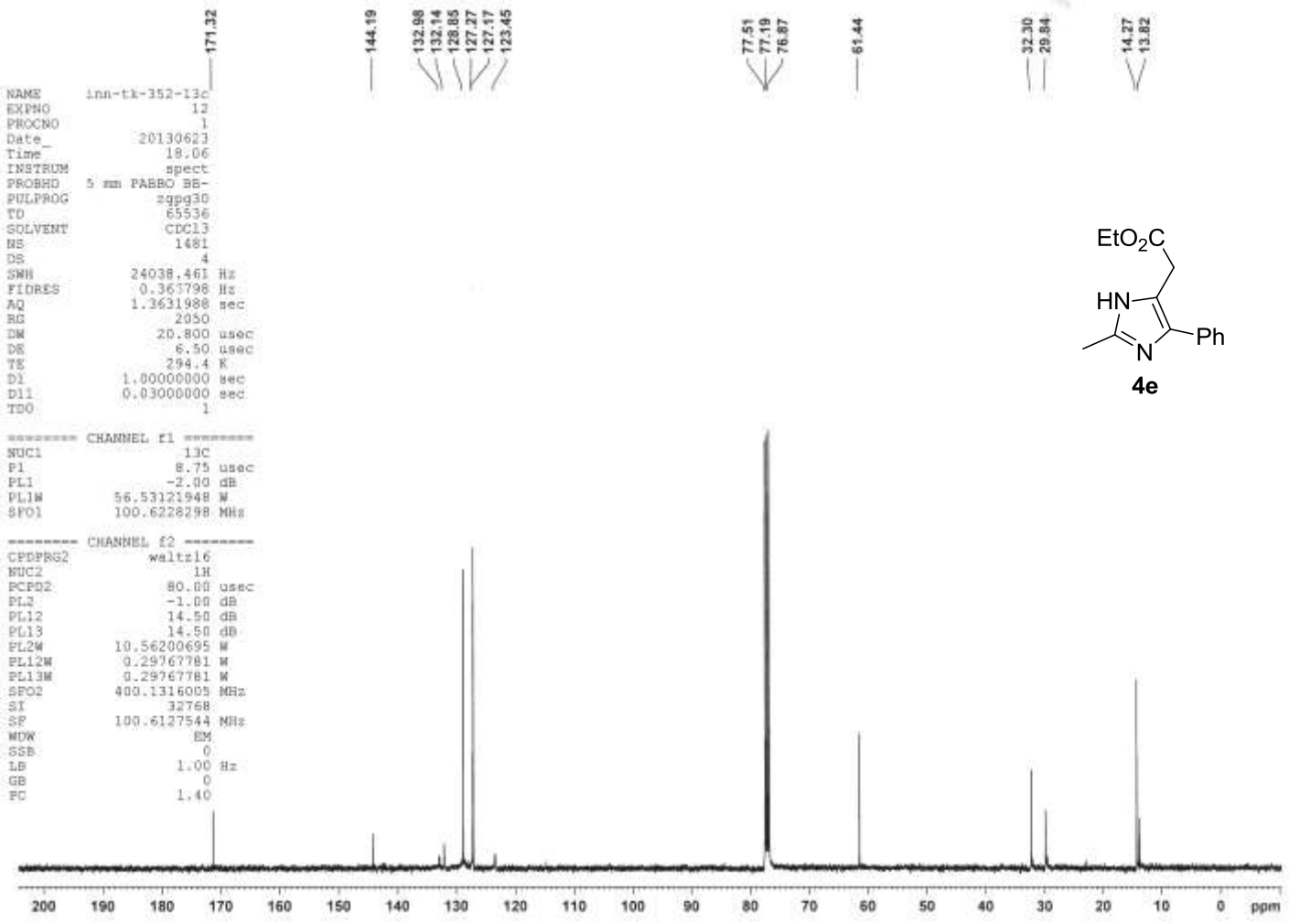


Figure S54. ^{13}C NMR spectrum of **4e**

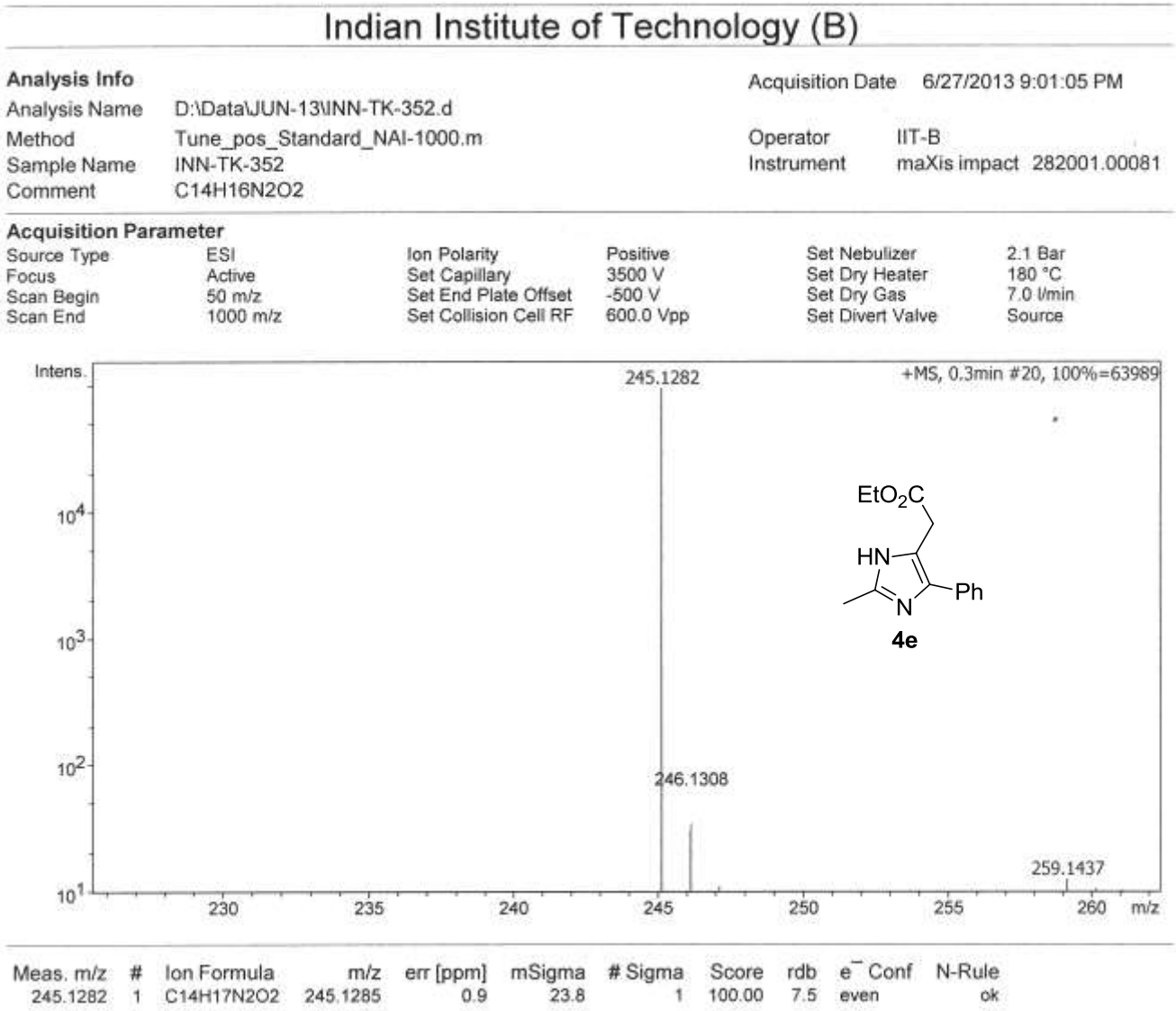


Figure S55. HRMS spectrum of **4e**

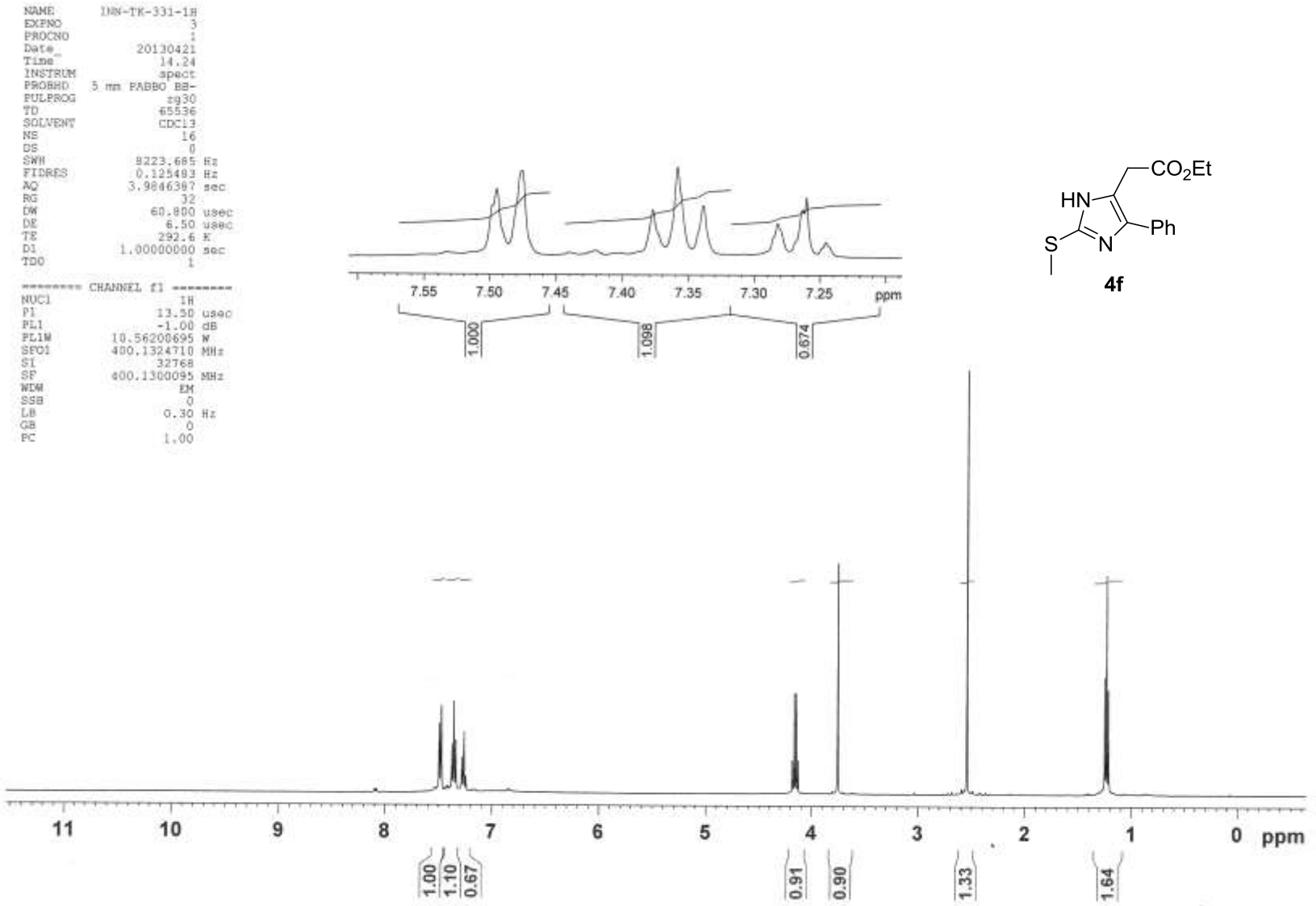


Figure S56. ^{1}H NMR spectrum of **4f**

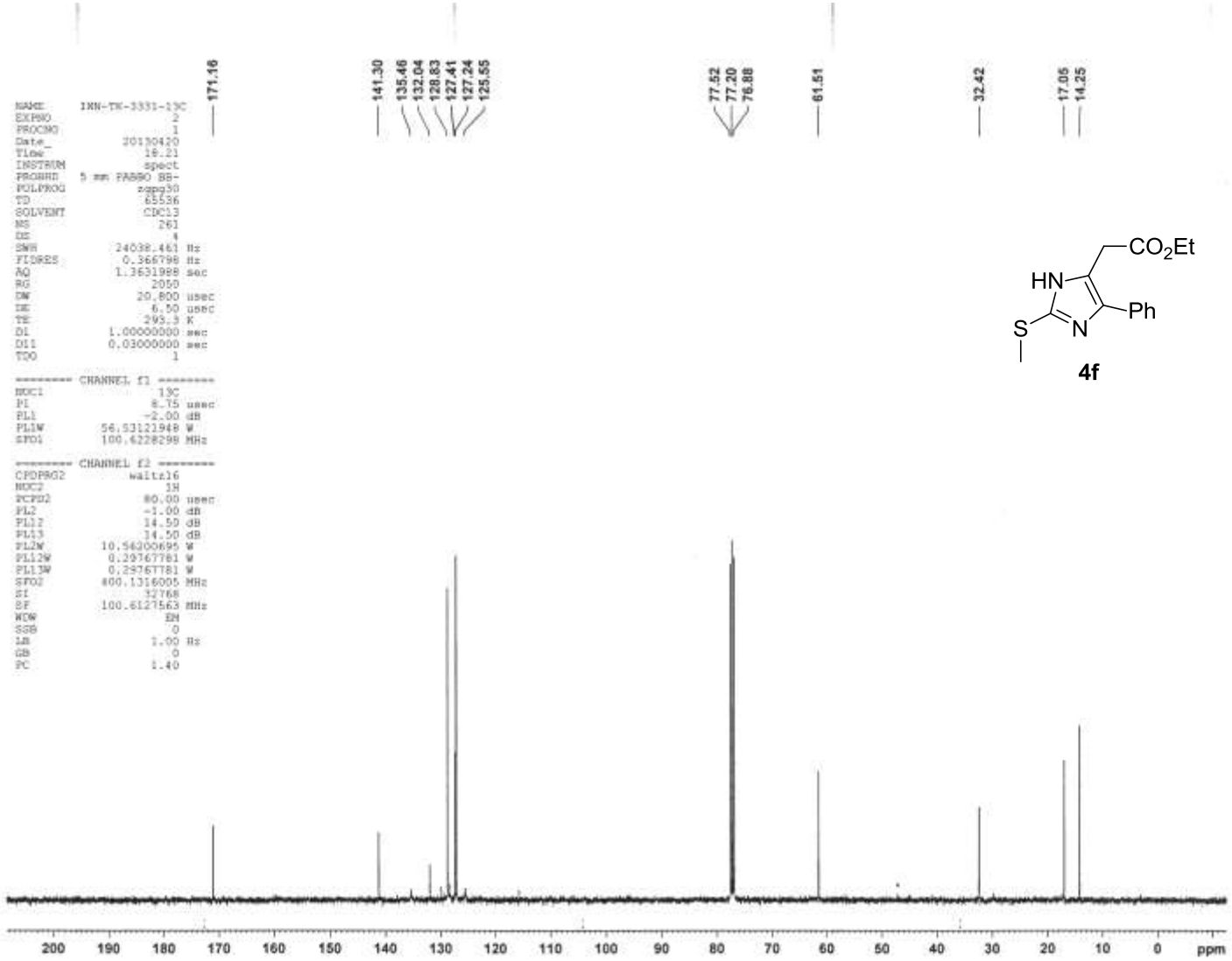


Figure S57. ^{13}C NMR spectrum of **4f**

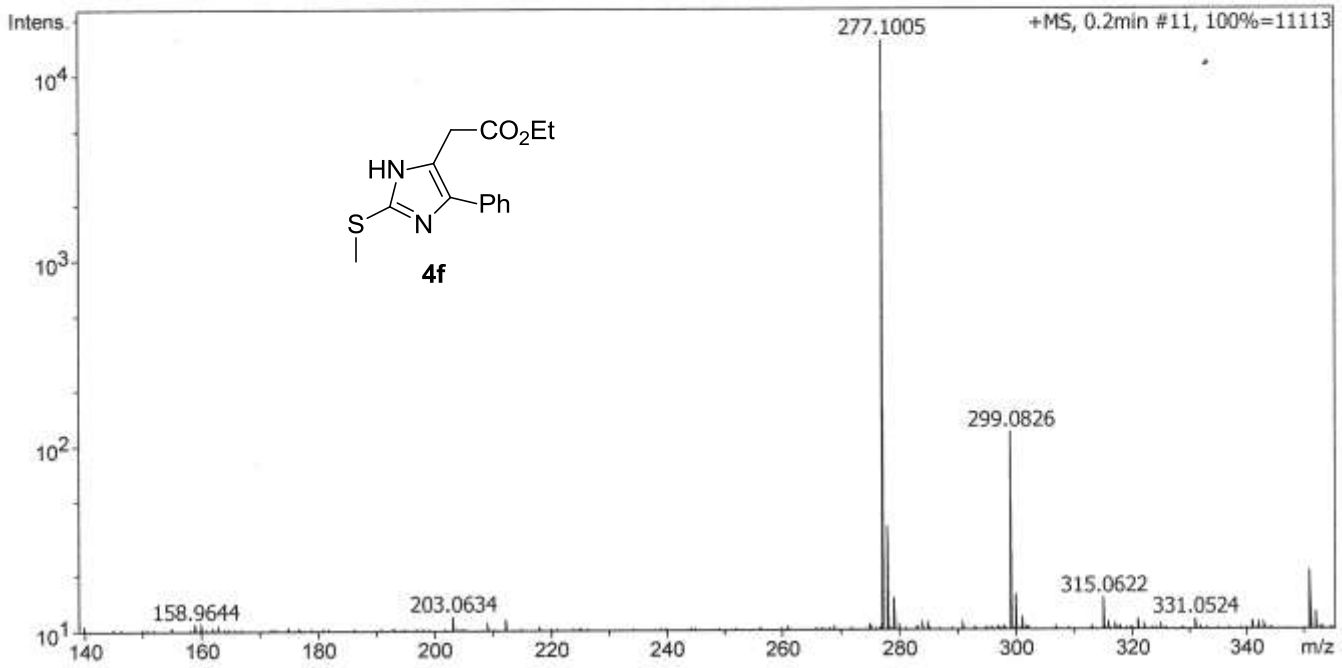
Indian Institute of Technology (B)

Analysis Info

Analysis Name	D:\Data\JUN-13\INN-TK-331 .d	Acquisition Date	6/10/2013 9:54:24 PM
Method	Tune_pos_Standard_NAI-500.m	Operator	IIT-B
Sample Name	INN-TK-331	Instrument	maXis impact 282001.00081
Comment	C14H16N2O2S		

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**

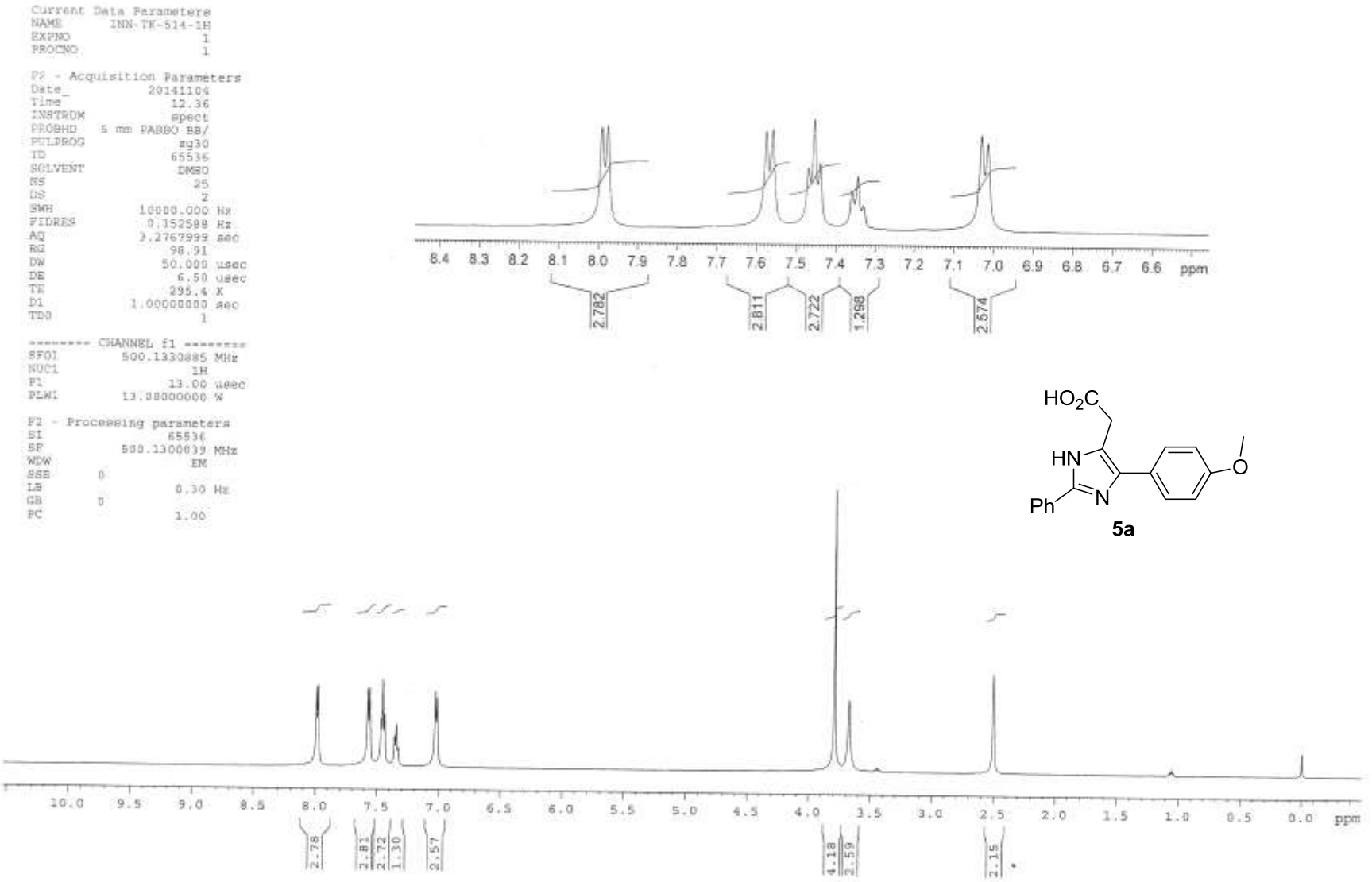


Figure S59. ^{1}H NMR spectrum of **5a**

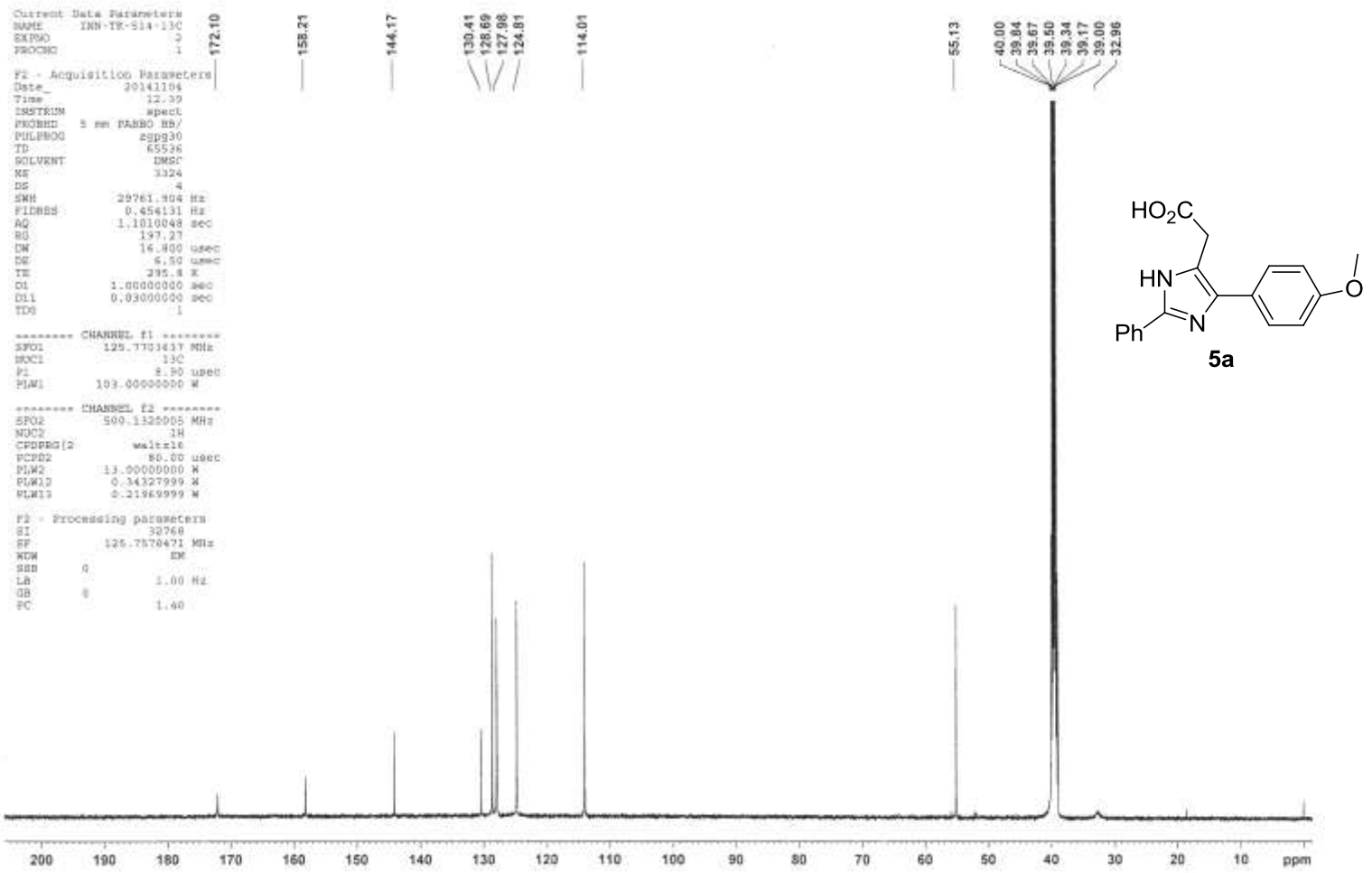


Figure S60. ^{13}C NMR spectrum of **5a**

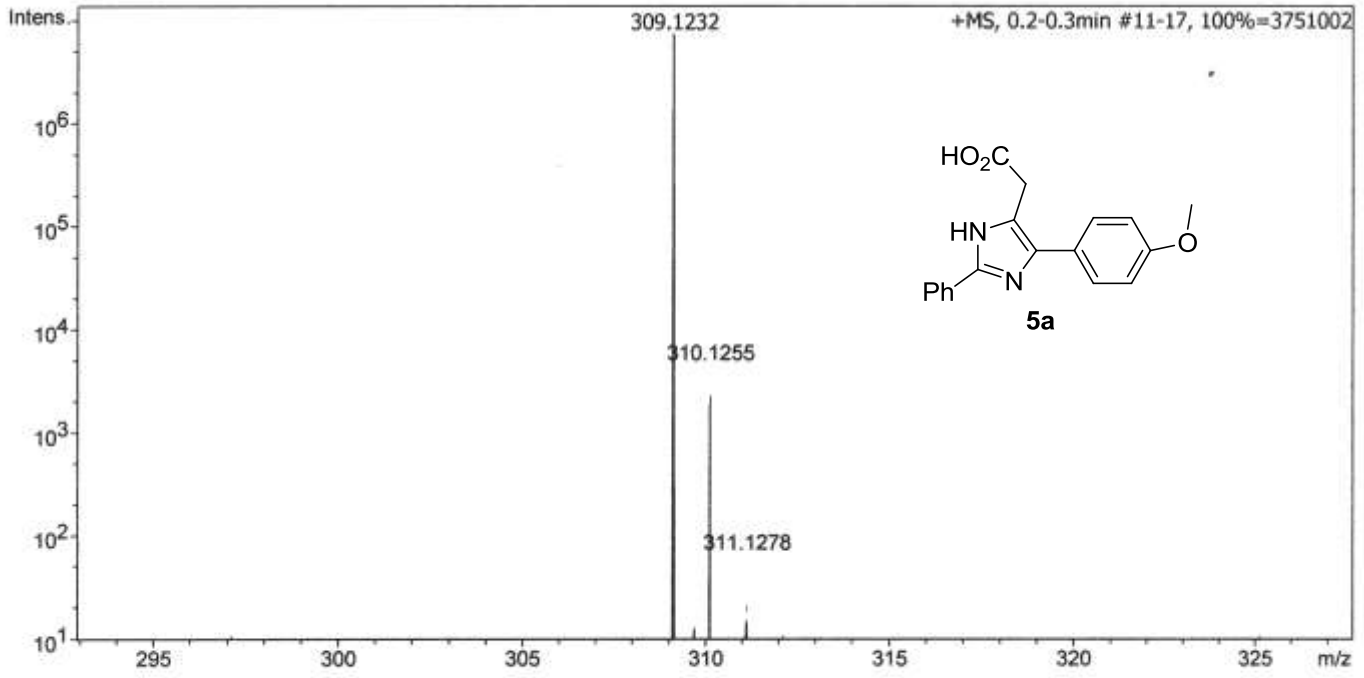
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\NOV-14\INN-TK-514.d	Acquisition Date	11/10/2014 7:21:10 PM
Method	Tune_pos_NAICSI-1000.m	Operator	CPR IN
Sample Name	INN-TK-514	Instrument	maXis impact 282001.00081
Comment	C18H16N2O3		

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**

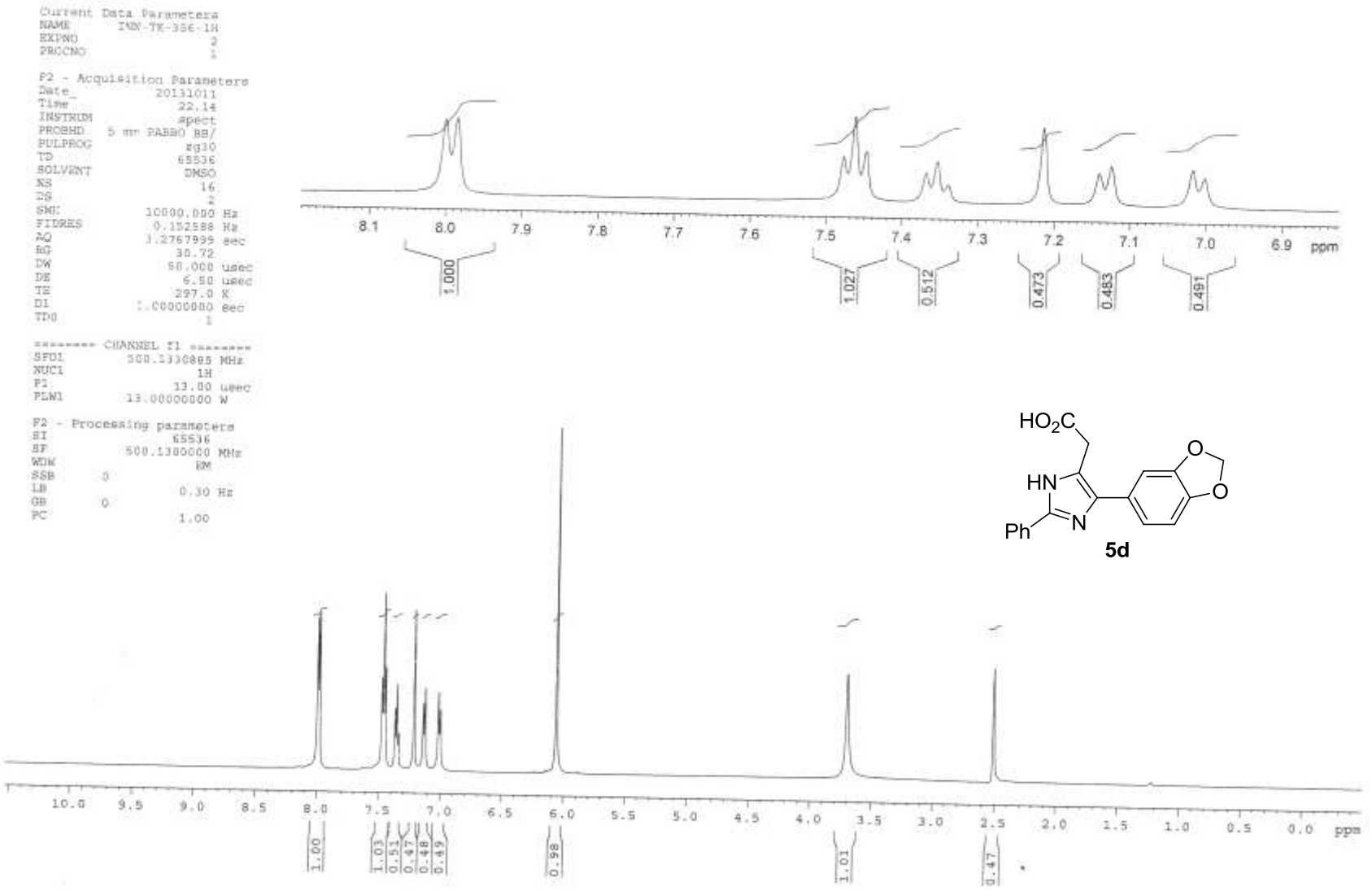


Figure S62. ^{1}H NMR spectrum of **5d**

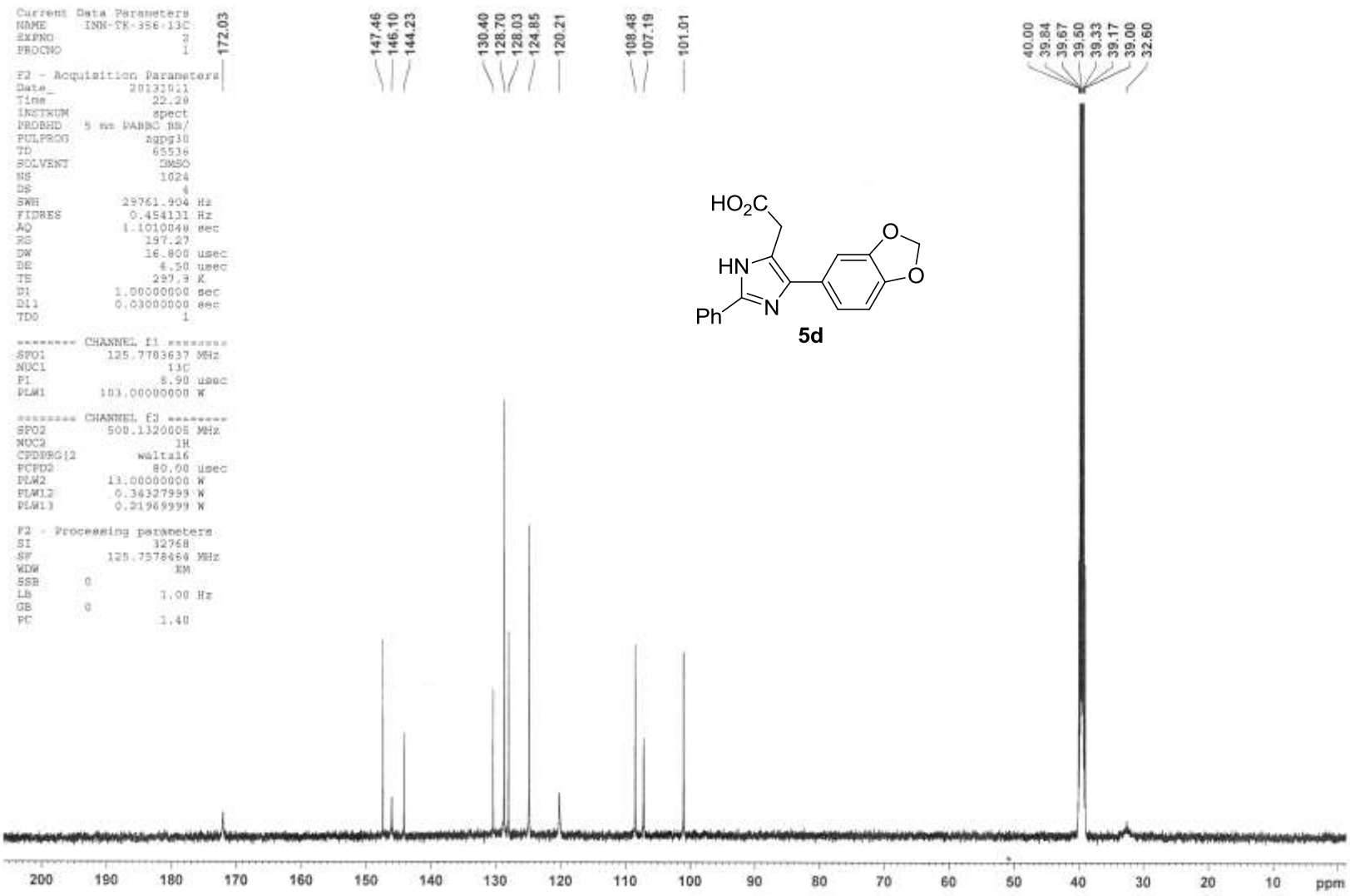


Figure S63. ^{13}C NMR spectrum of **5d**

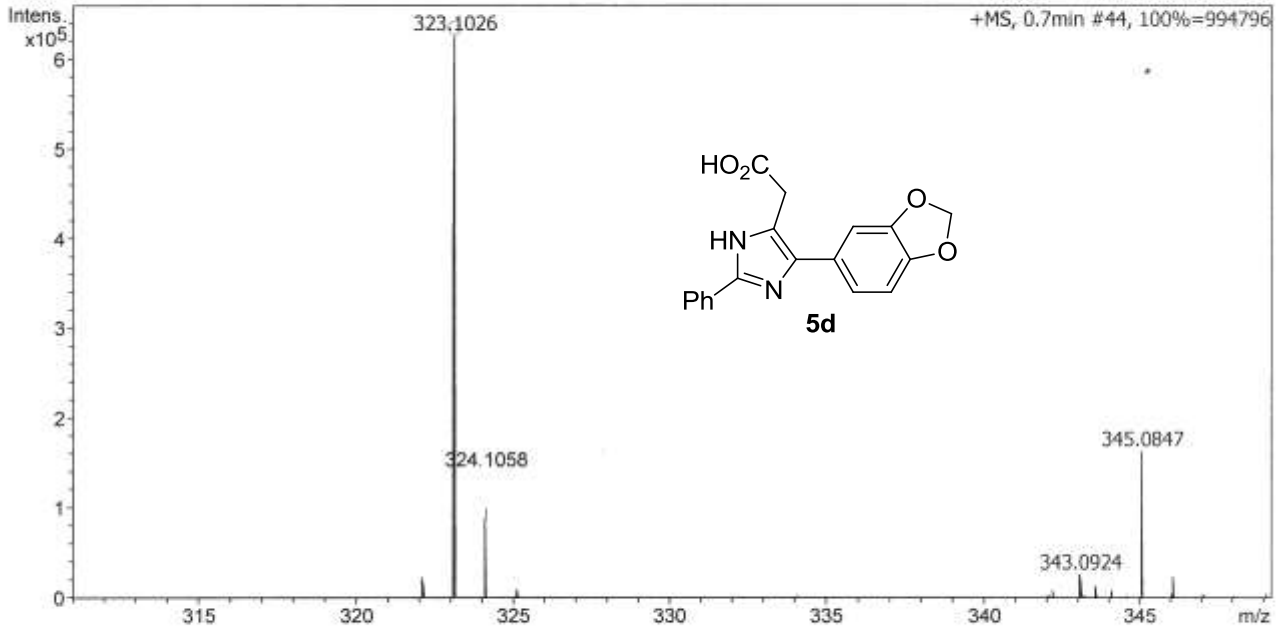
Indian Institute of Technology (B)

Analysis Info

Analysis Name	D:\Data\JULY_13\INN-TK-356.d	Acquisition Date	7/26/2013 3:28:29 PM
Method	Tune_pos_Standard_NAI-1500.m	Operator	IIT-B
Sample Name	INN-TK-356	Instrument	maXis impact 282001.00081
Comment	C18H14N2O4		

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**

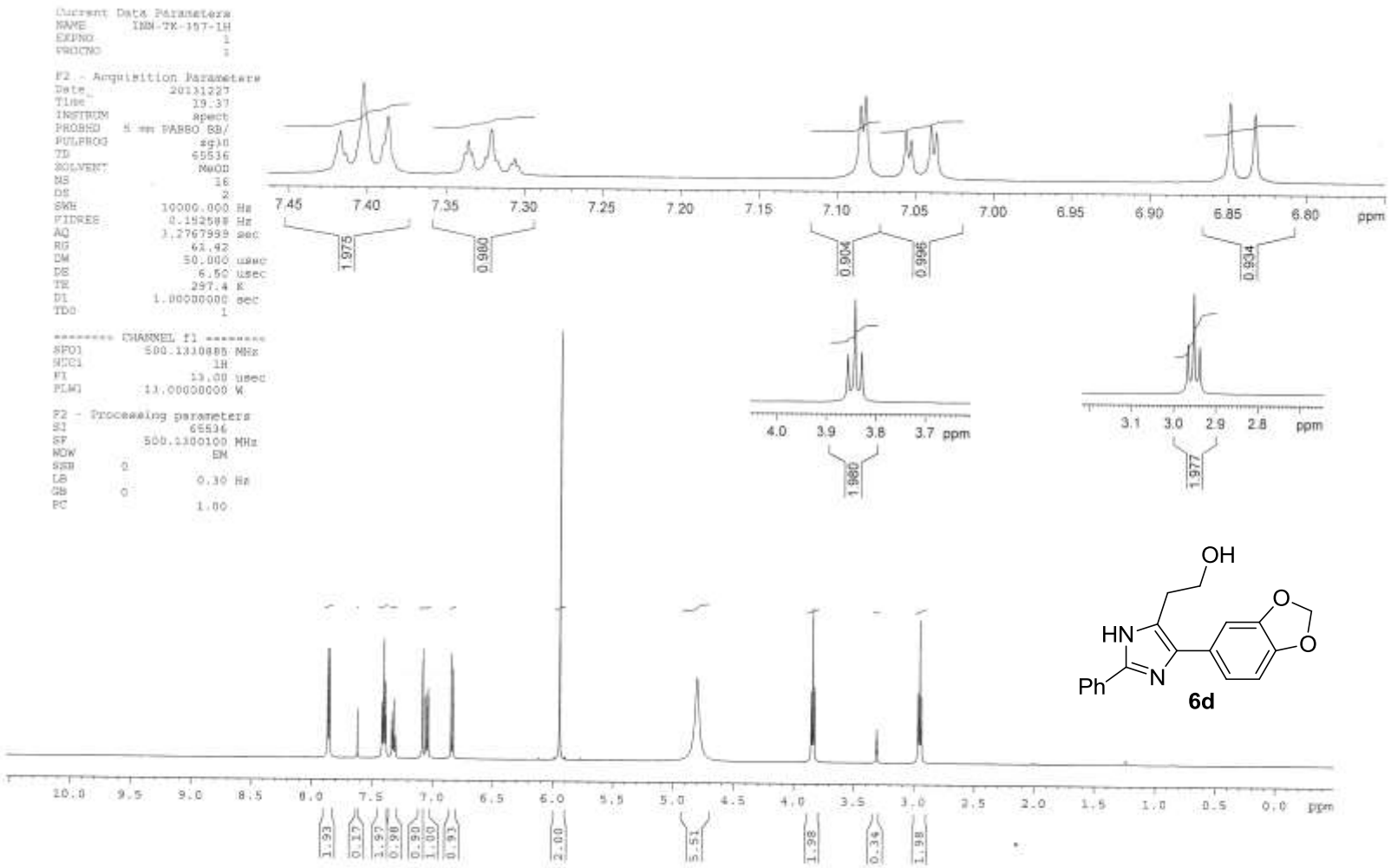


Figure S65. ^{1}H NMR spectrum of **6d**

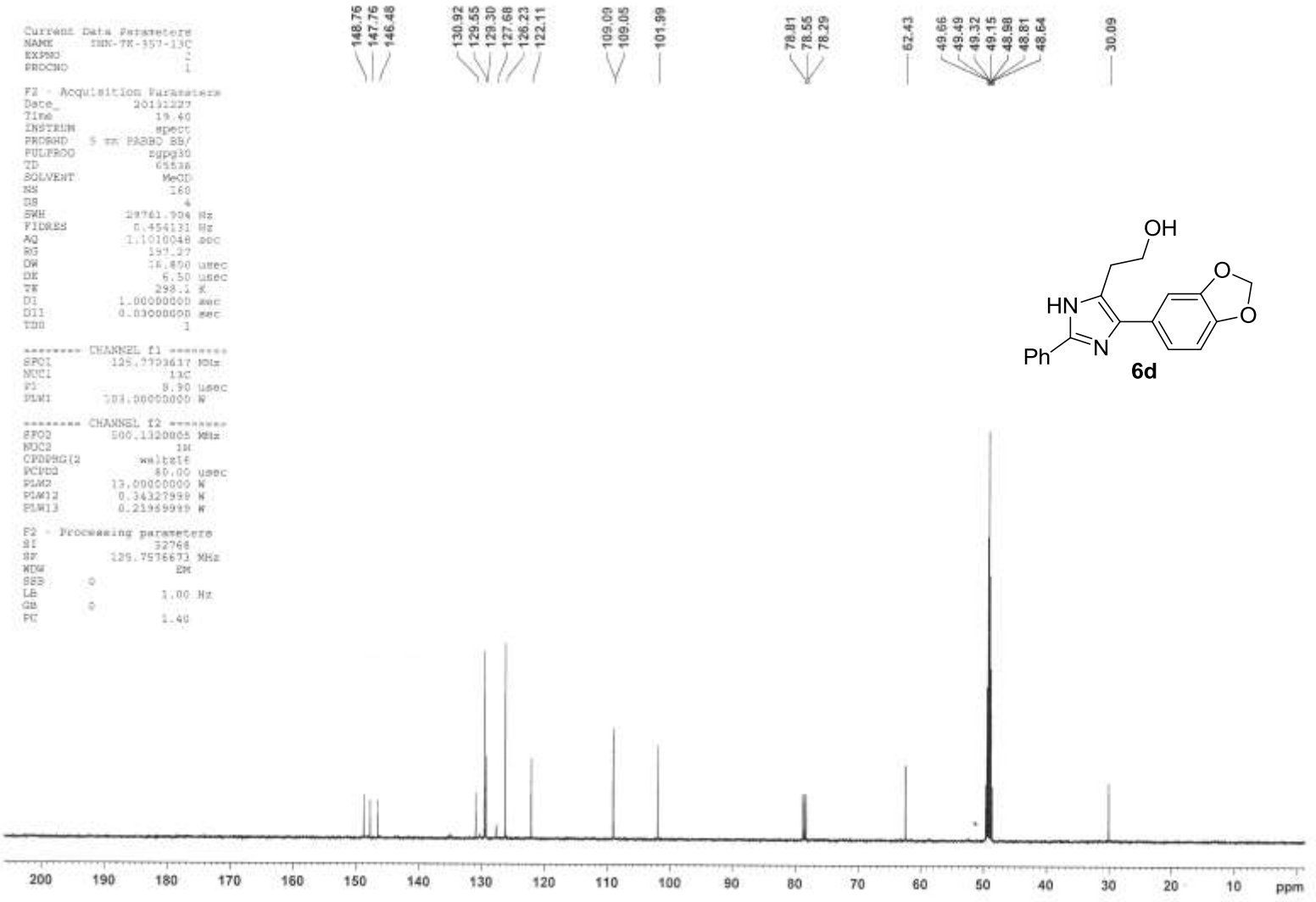


Figure S66. ^{13}C NMR spectrum of **6d**

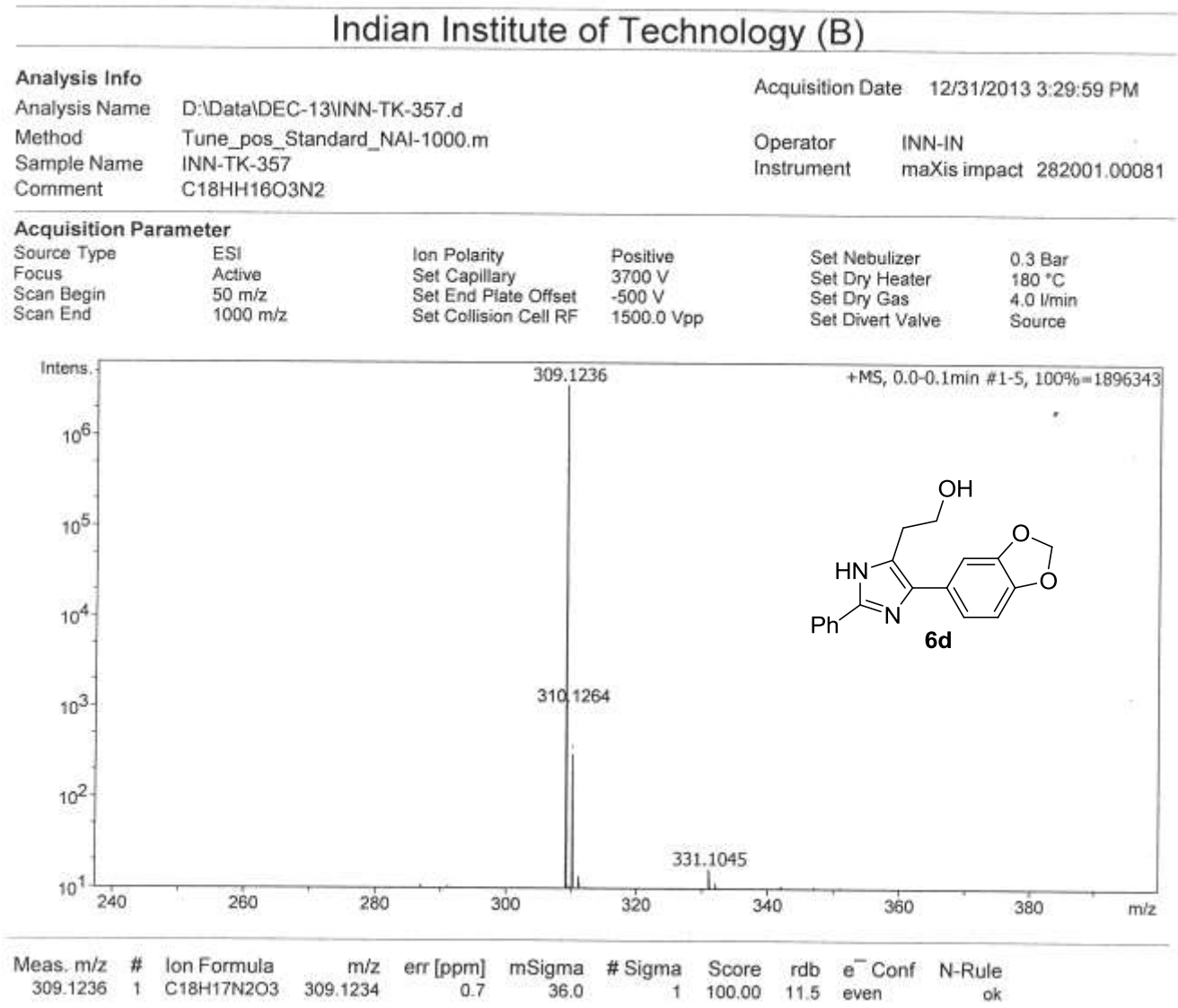


Figure S67. HRMS spectrum of **6d**

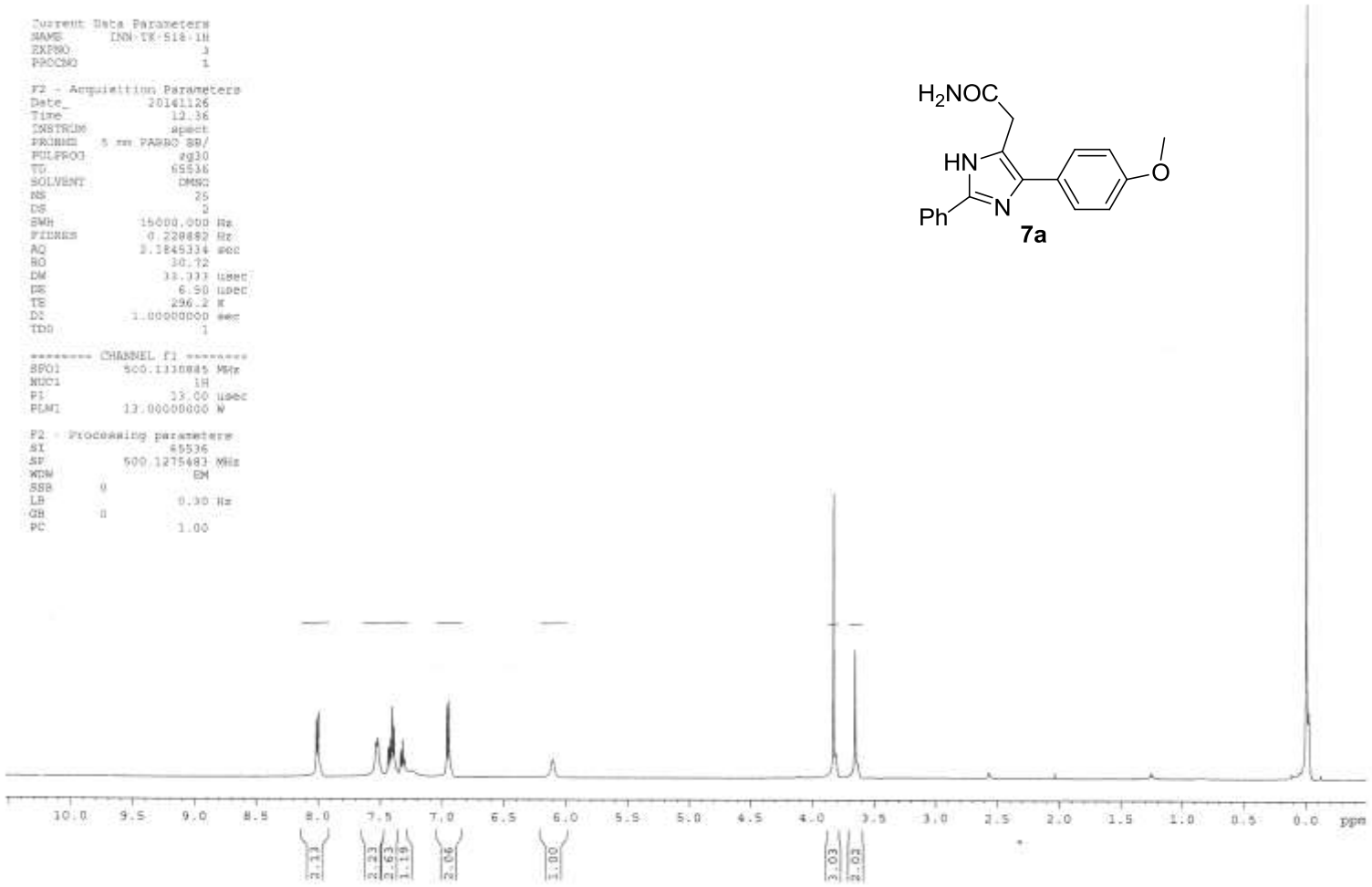


Figure S68. ^{1}H NMR spectrum of **7a**

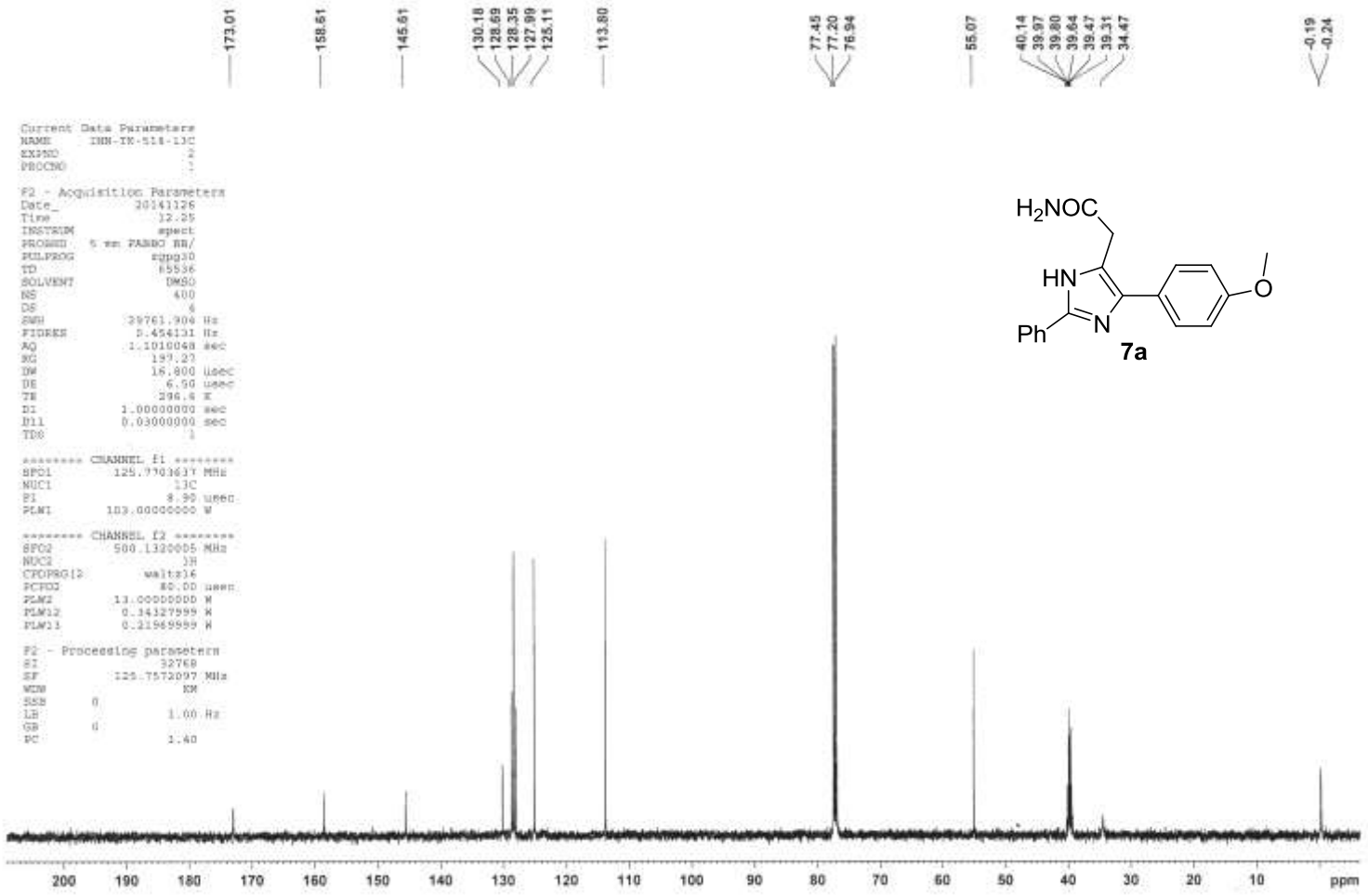


Figure S69. ^{13}C NMR spectrum of **7a**

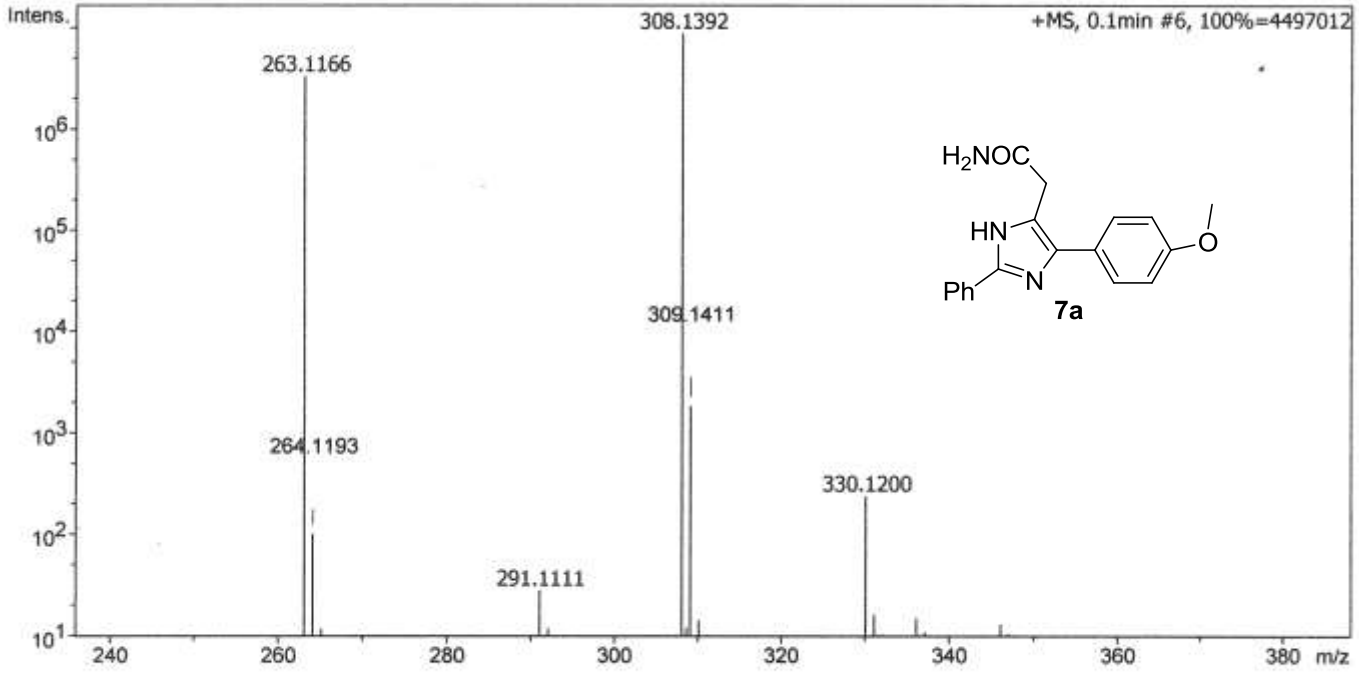
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\NOV-14\INN-TK-518.d	Acquisition Date	11/26/2014 1:26:39 PM
Method	Tune_pos_NAICSI-500.m	Operator	DM OUT
Sample Name	INN-TK-518	Instrument	maXis impact 282001.00081
Comment	C18H17N3O2		

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**

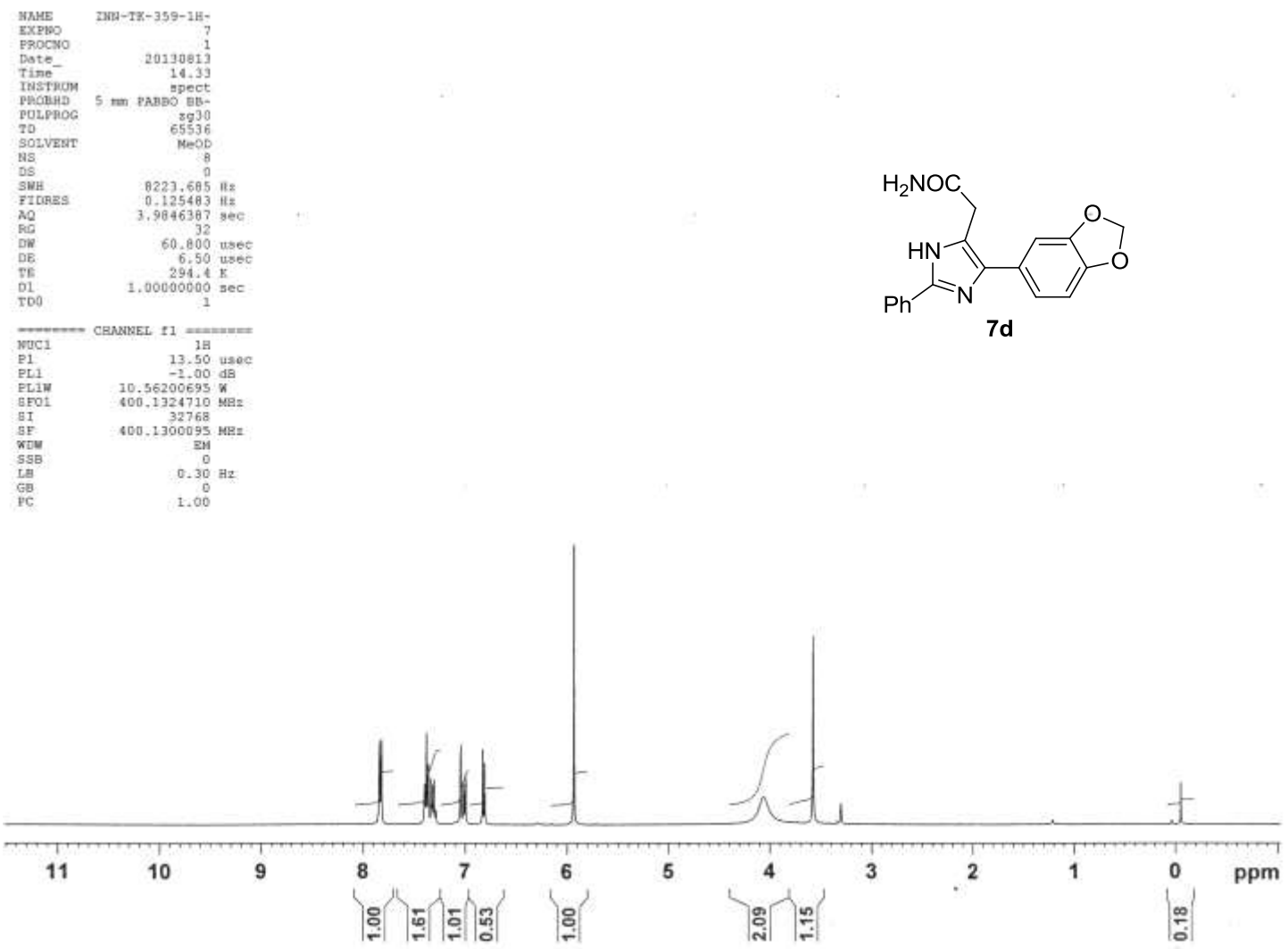


Figure S71. ^{1}H NMR spectrum of **7d**

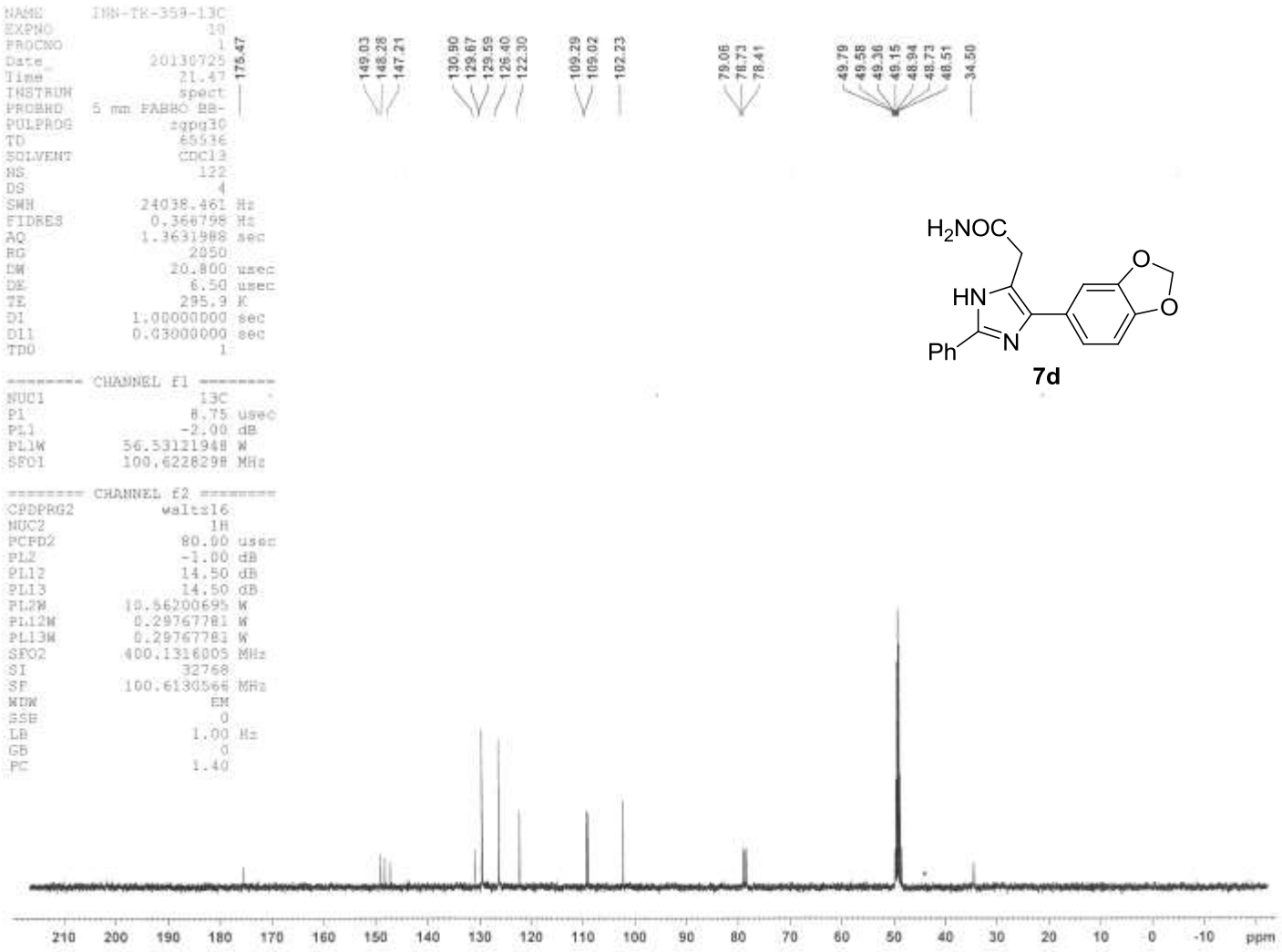


Figure S72. ^{13}C NMR spectrum of **7d**

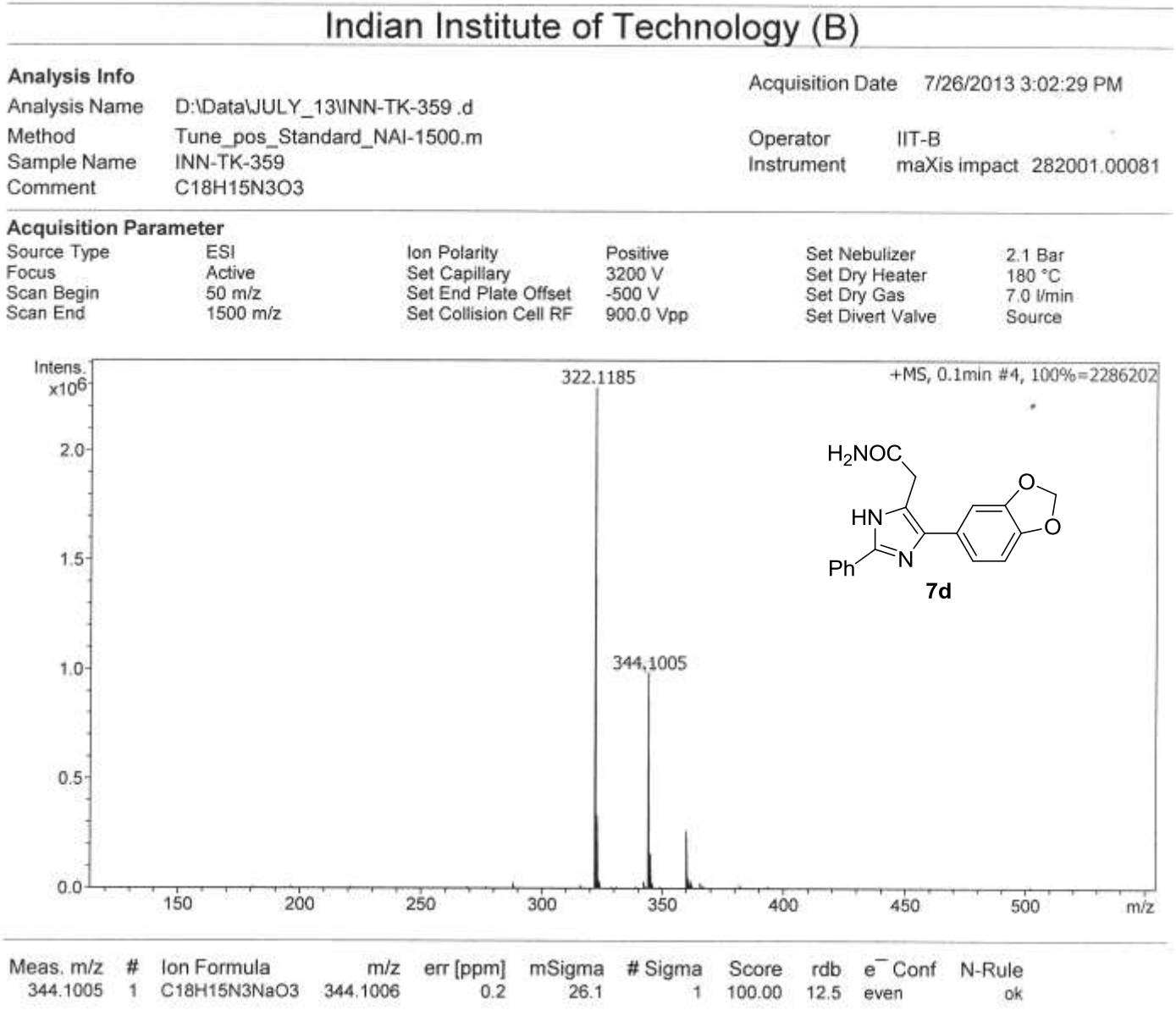


Figure S73. HRMS spectrum of **7d**