

Supporting information

Ligand-free Palladium-catalyzed synthesis of 3-(2,2-dialkyl-2*H*-chromen-4-yl)-2-phenylimidazo[1,2-*a*]pyridine derivatives and evaluation of their antibacterial activity with molecular docking investigation as DNA gyrase inhibitors

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3. **Fig S85-S105:** Molecular docking studies of **16(a-u)** derivatives with *S. aureus* DNA gyrase (PDB ID: 3G7B)

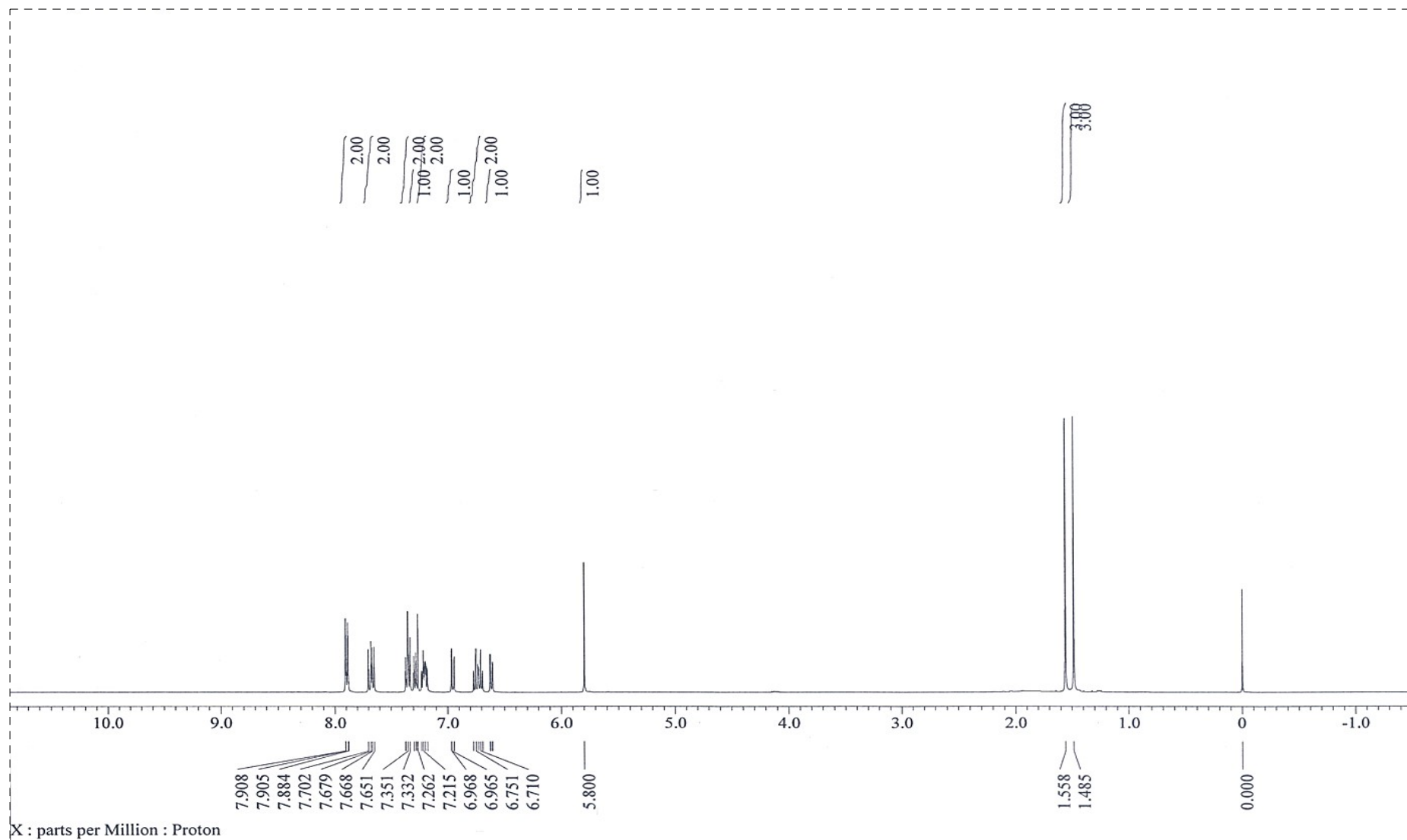


Fig S1: ^1H NMR of 3-(2, 2-dimethyl-2H-chromen-4-yl)-2-phenylimidazo-[1,2-a]pyridine (**16a**)

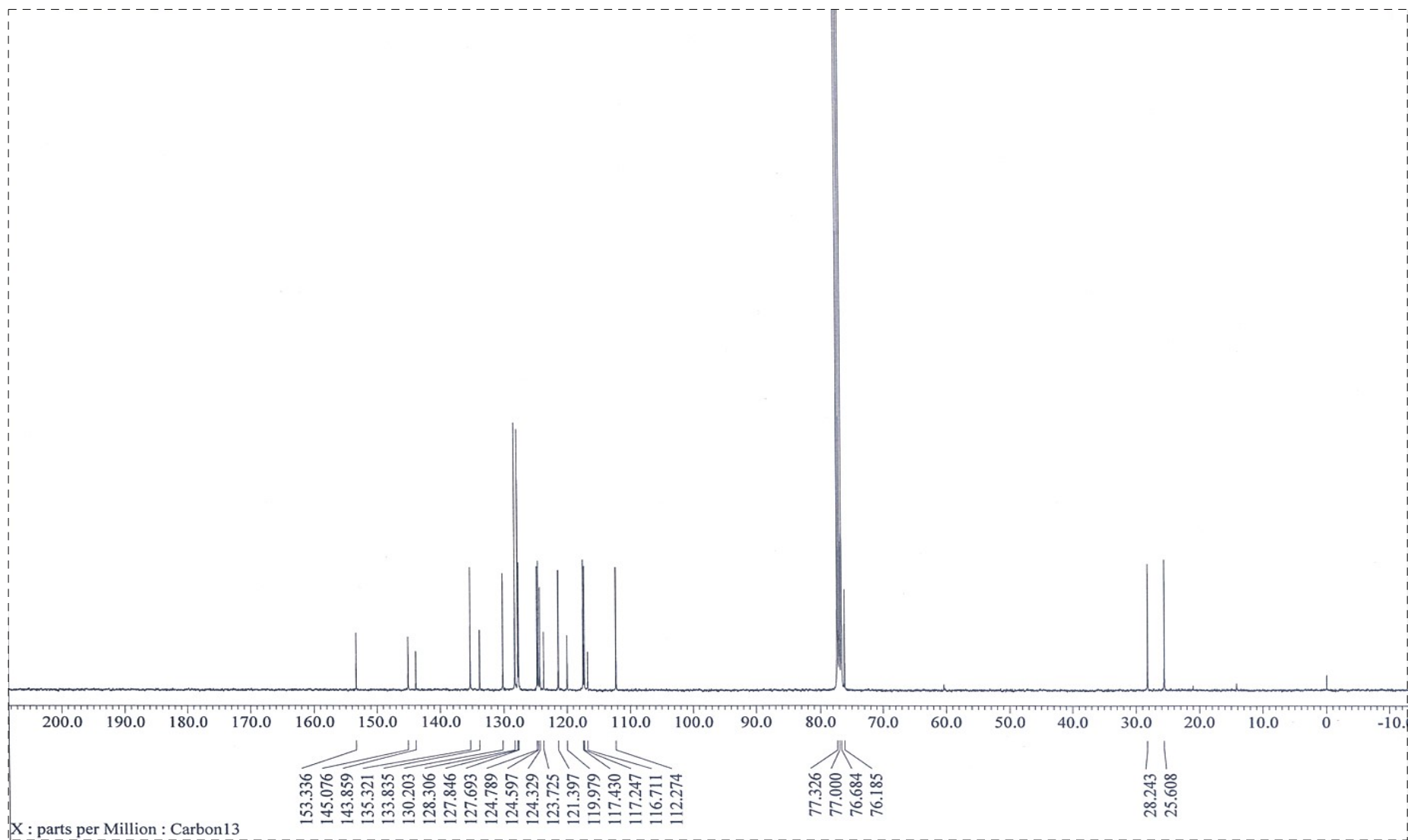


Fig S2: ^{13}C NMR of 3-(2, 2-dimethyl-2H-chromen-4-yl)-2-phenylimidazo-[1,2-a]pyridine (**16a**)

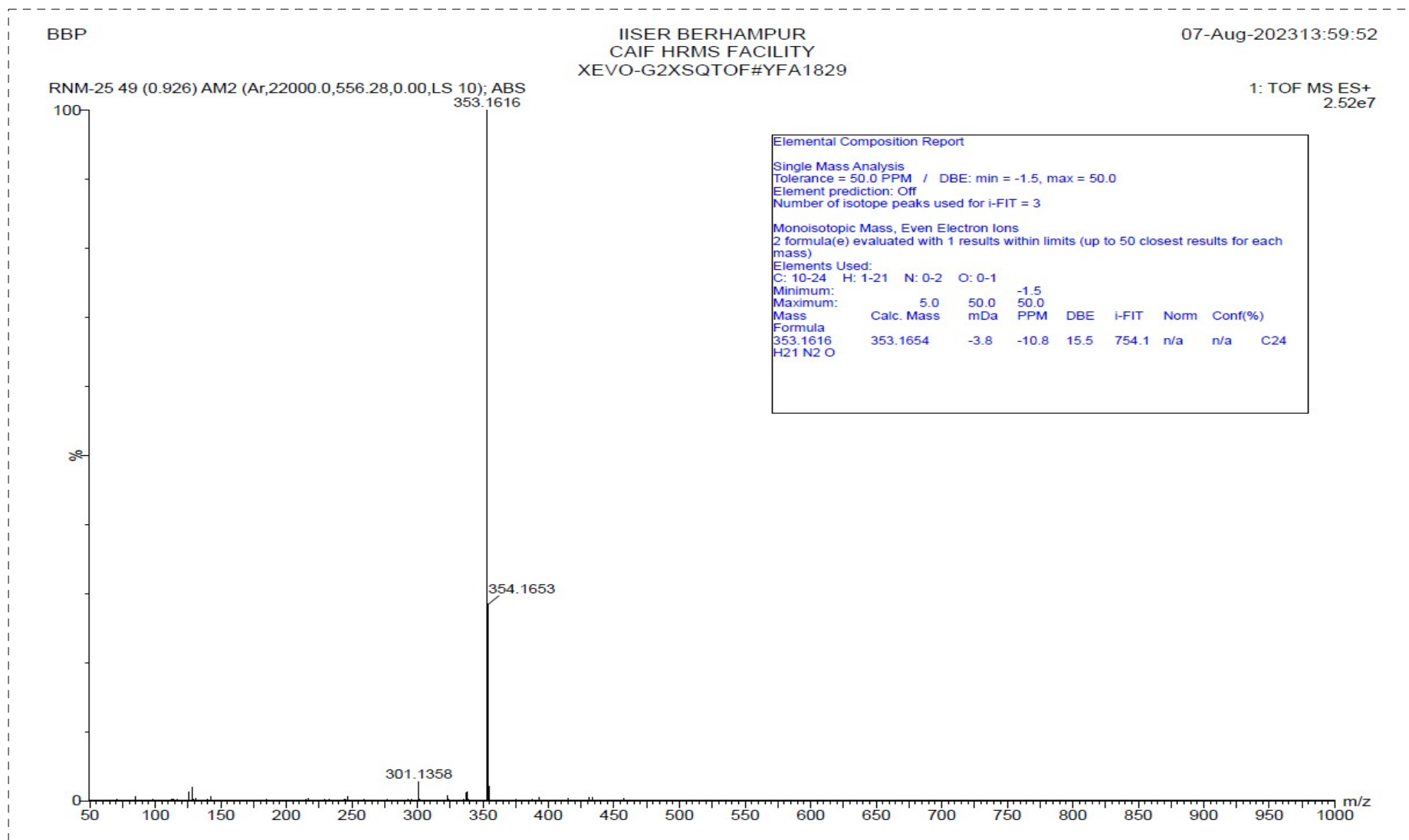


Fig S3: HR-MS of 3-(2, 2-dimethyl-2H-chromen-4-yl)-2-phenylimidazo-[1,2-a]pyridine (**16a**)

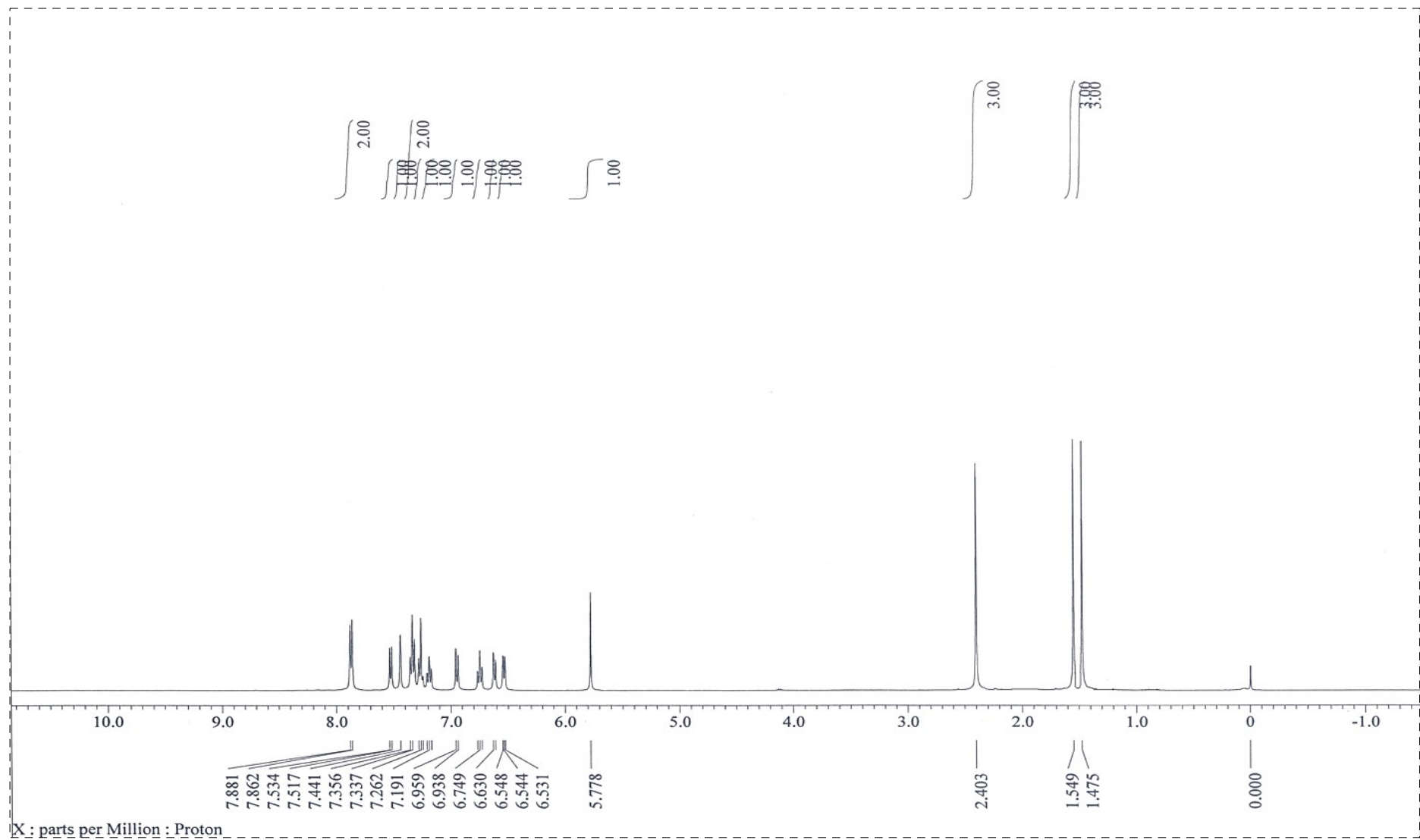


Fig S4: ¹H NMR of 3-(2, 2-dimethyl-2H-chromen-4-yl)-7-methyl-2-phenylimidazo-[1,2-a]pyridine (16b)

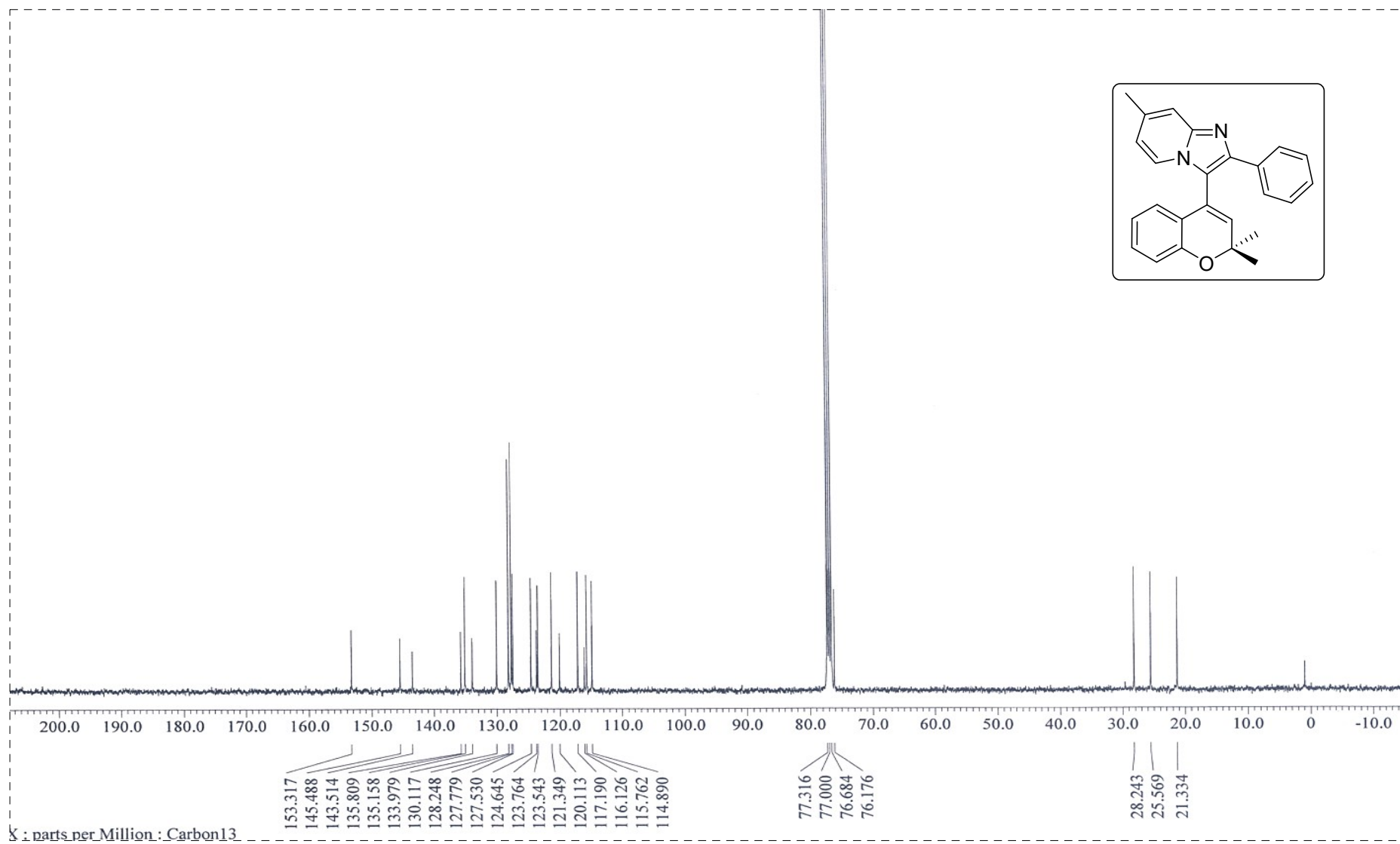


Fig S5: ^{13}C NMR of 3-(2, 2-dimethyl-2H-chromen-4-yl)-7-methyl-2-phenylimidazo-[1,2-a]pyridine (**16b**)

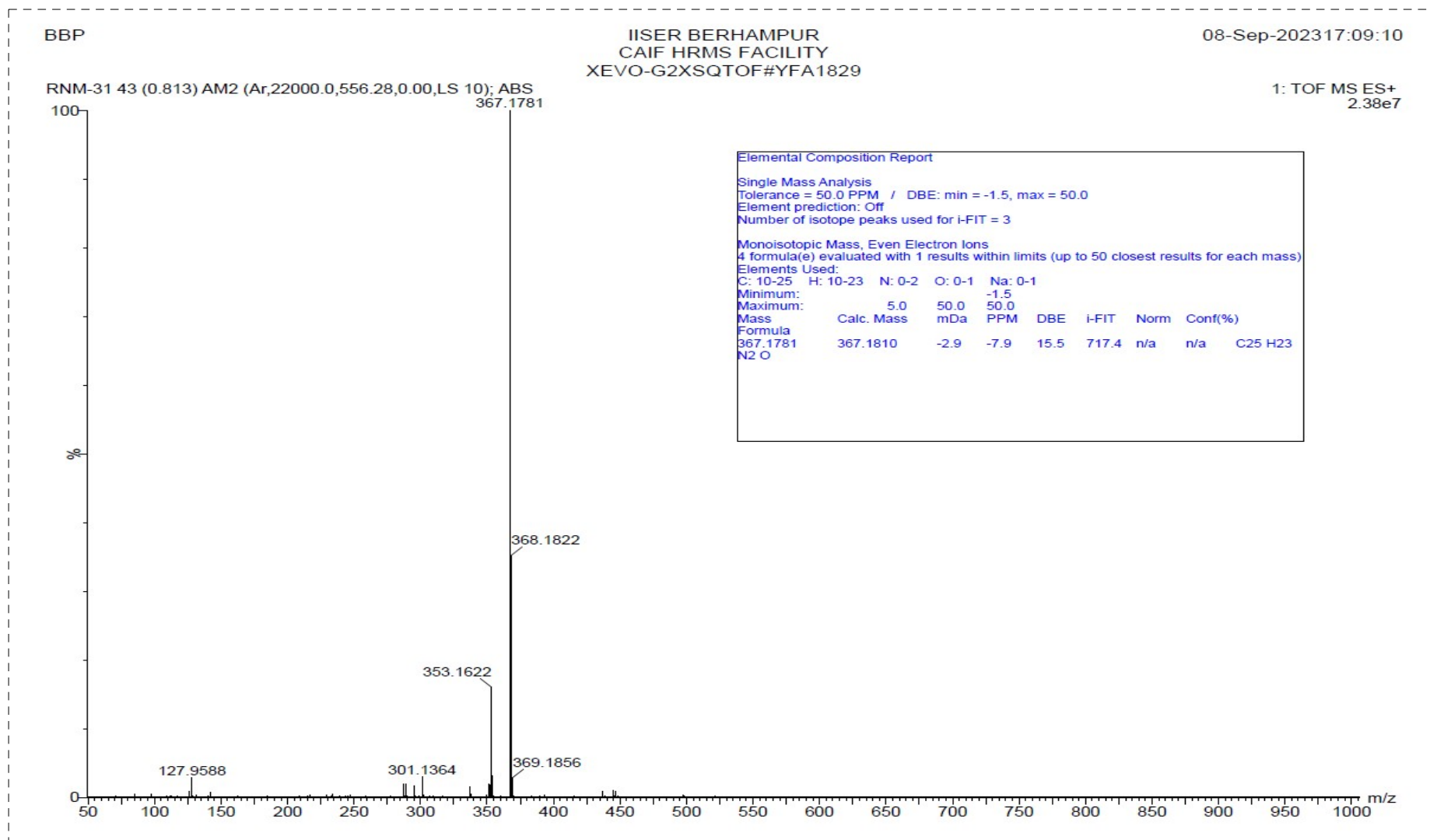


Fig S6: HR-MS of 3-(2, 2-dimethyl-2H-chromen-4-yl)-7-methyl-2-phenylimidazo-[1,2-a]pyridine (**16b**)

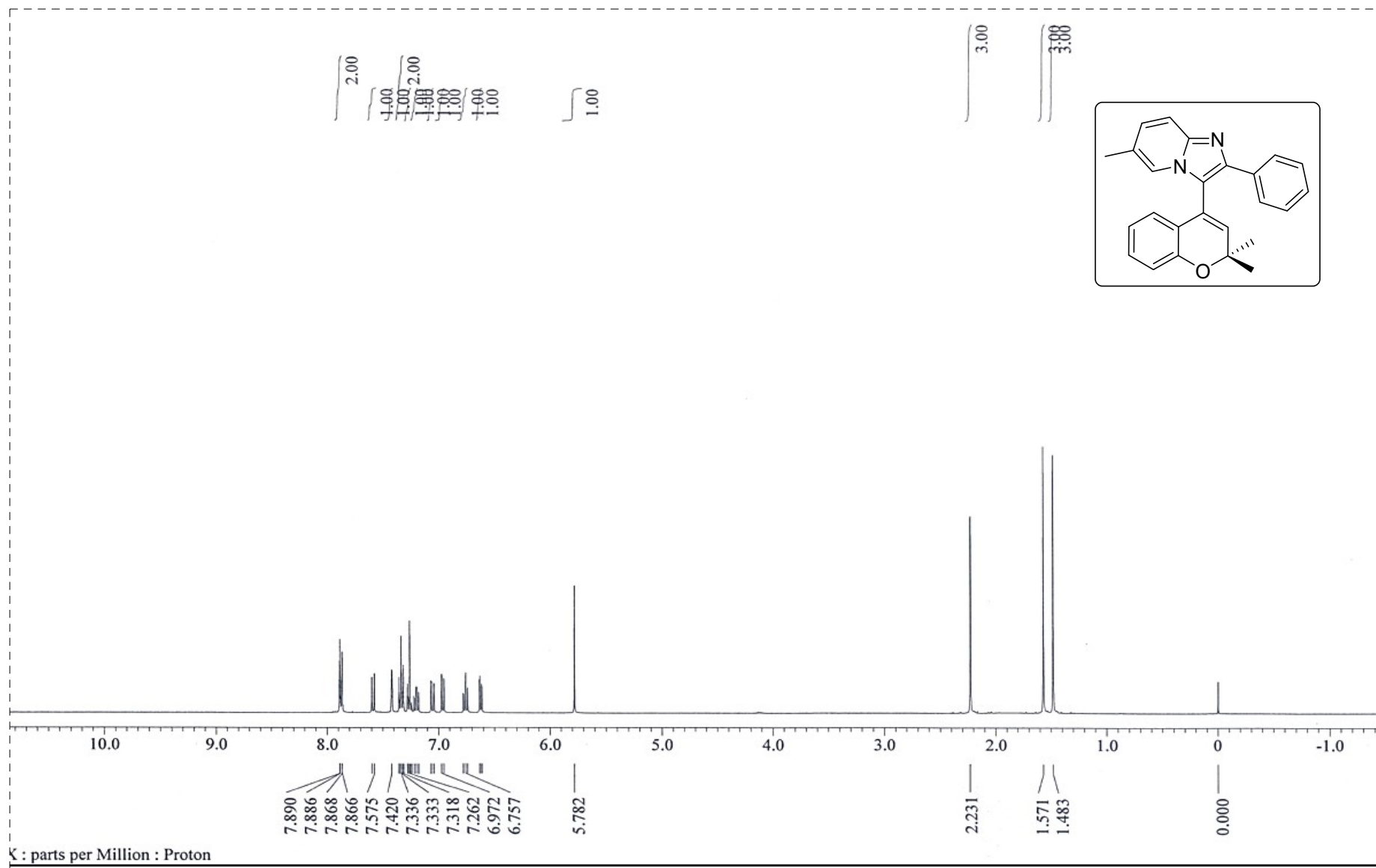


Fig S7: ¹H NMR of 3-(2,2-dimethyl-2H-chromen-4-yl)-6-methyl-2-phenylimidazo-[1,2-a]pyridine (**16c**)

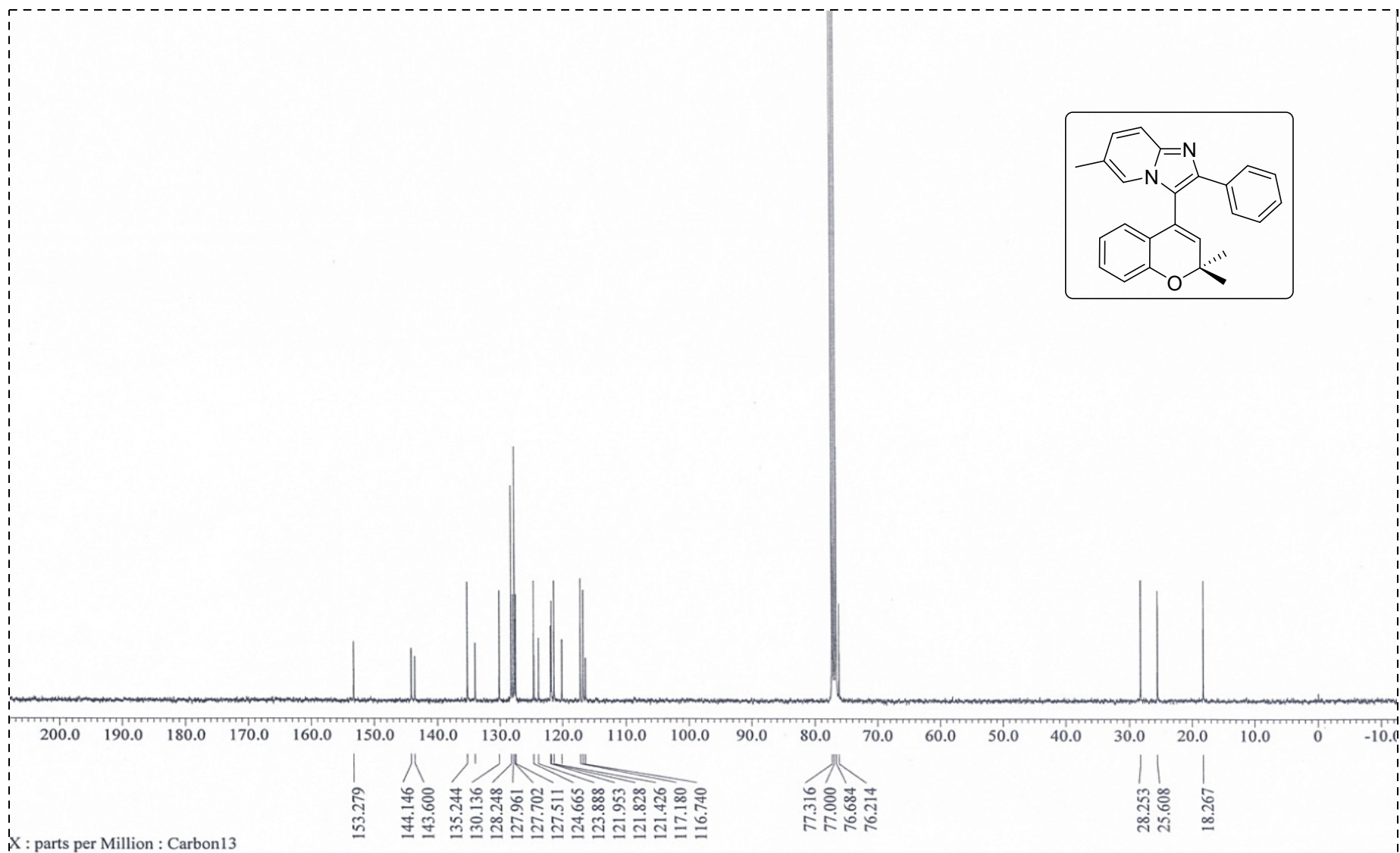


Fig S8: ^{13}C NMR of 3-(2, 2-dimethyl-2H-chromen-4-yl)-6-methyl-2-phenylimidazo-[1,2-a]pyridine (**16c**)

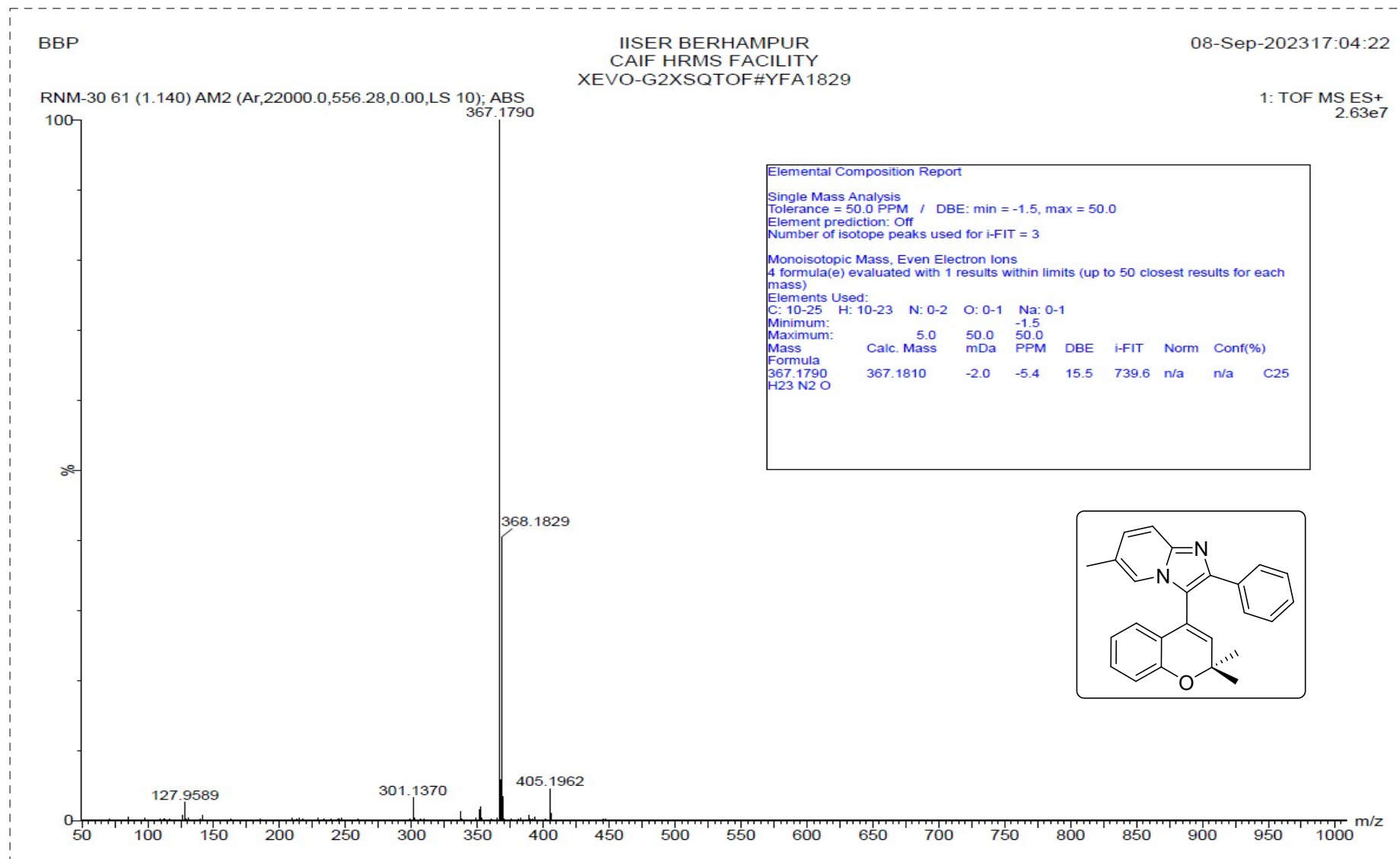


Fig S9: HR-MS of 3-(2,2-dimethyl-2H-chromen-4-yl)-6-methyl-2-phenylimidazo-[1,2-a]pyridine (16c)

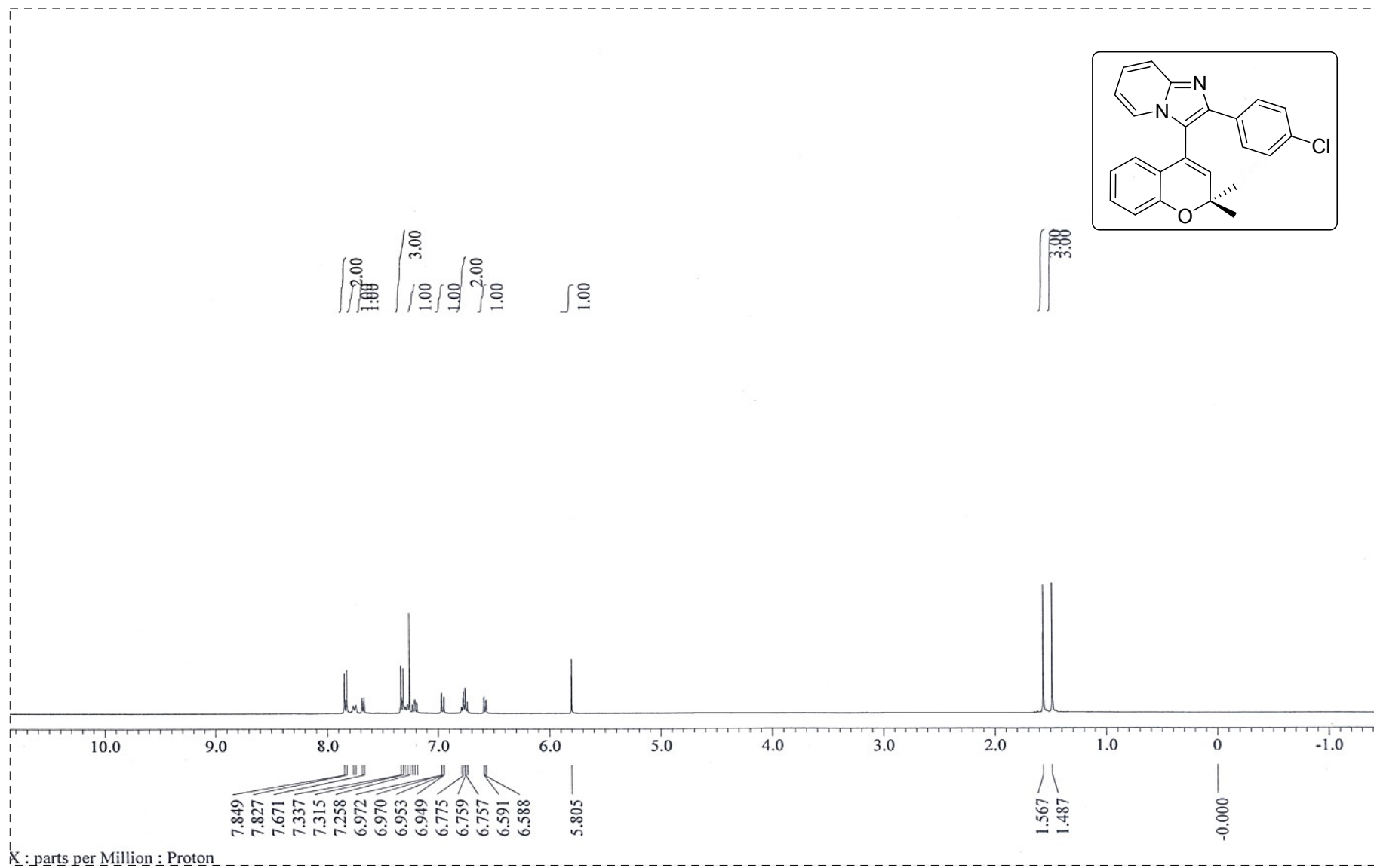


Fig S10: ¹H NMR of 2-(4-Chlorophenyl)-3-(2,2-dimethyl-2H-Chromen-4-yl)-imidazo[1,2-a]pyridine (**16d**)

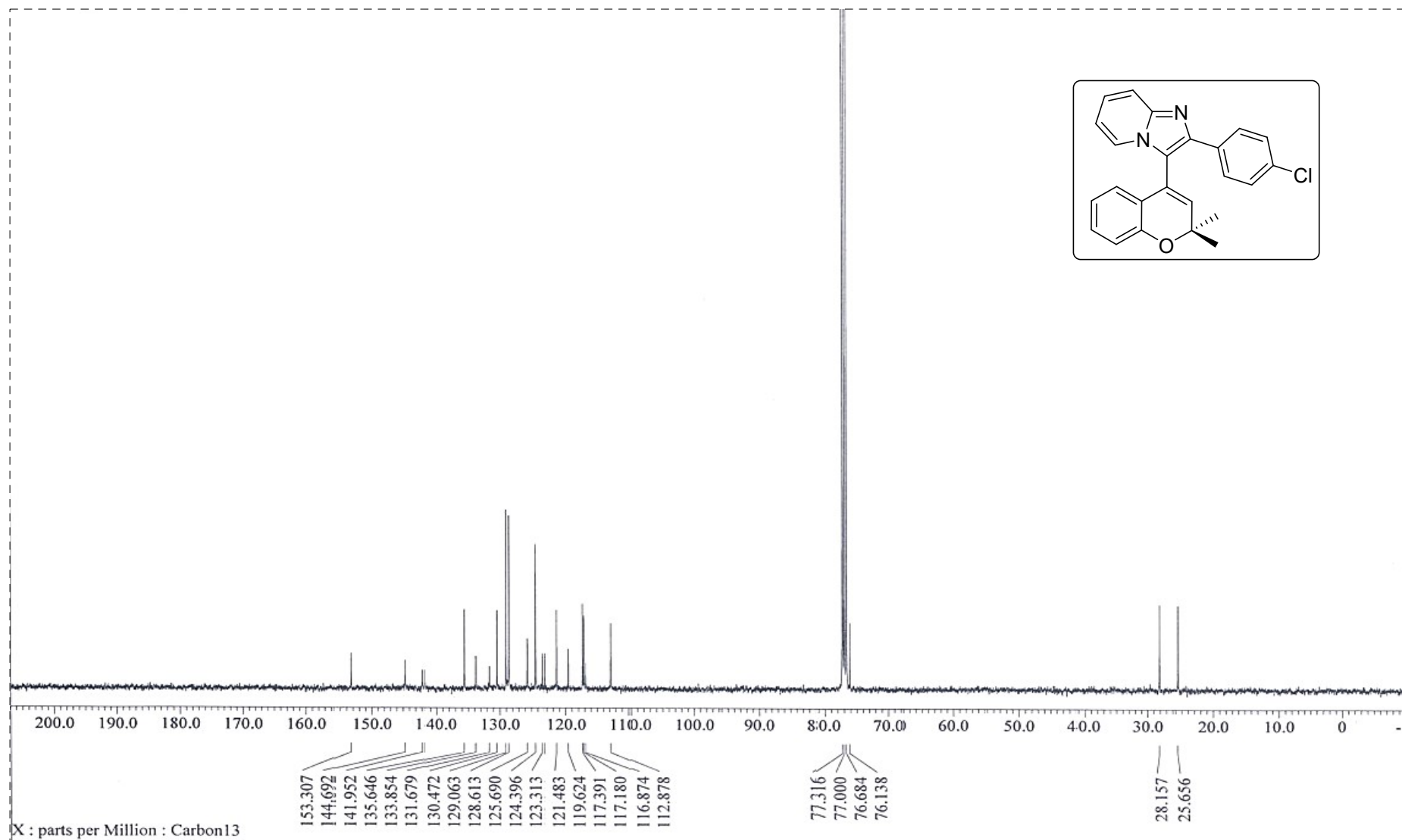


Fig S11: ¹³C NMR of 2-(4-Chlorophenyl)-3-(2,2-dimethyl-2H-Chromen-4-yl)-imidazo[1,2-a]pyridine (**16d**)

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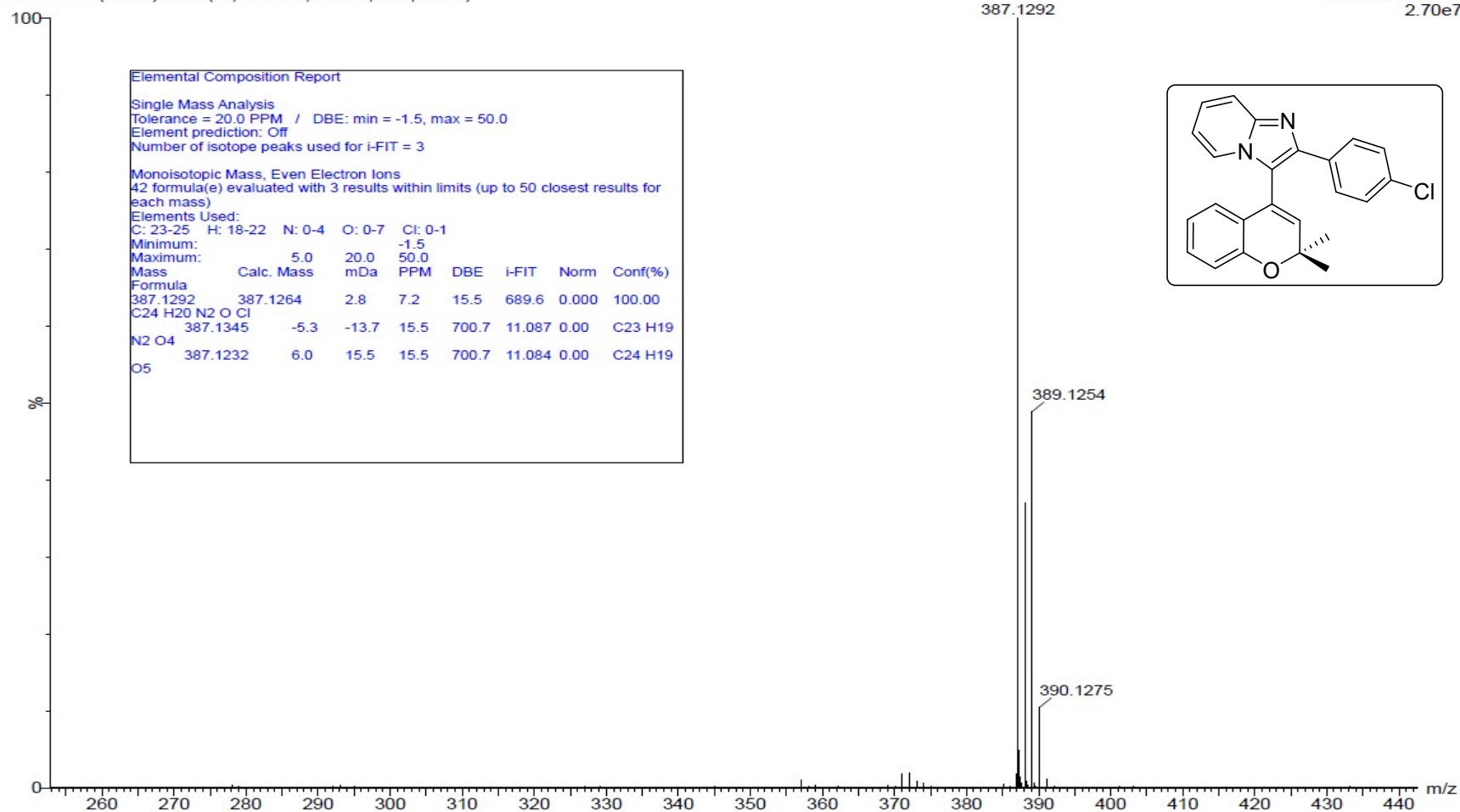
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Fig S12: HR-MS of 2-(4-Chlorophenyl)-3-(2,2-dimethyl-2H-Chromen-4-yl)-imidazo[1,2-a]pyridine (16d)

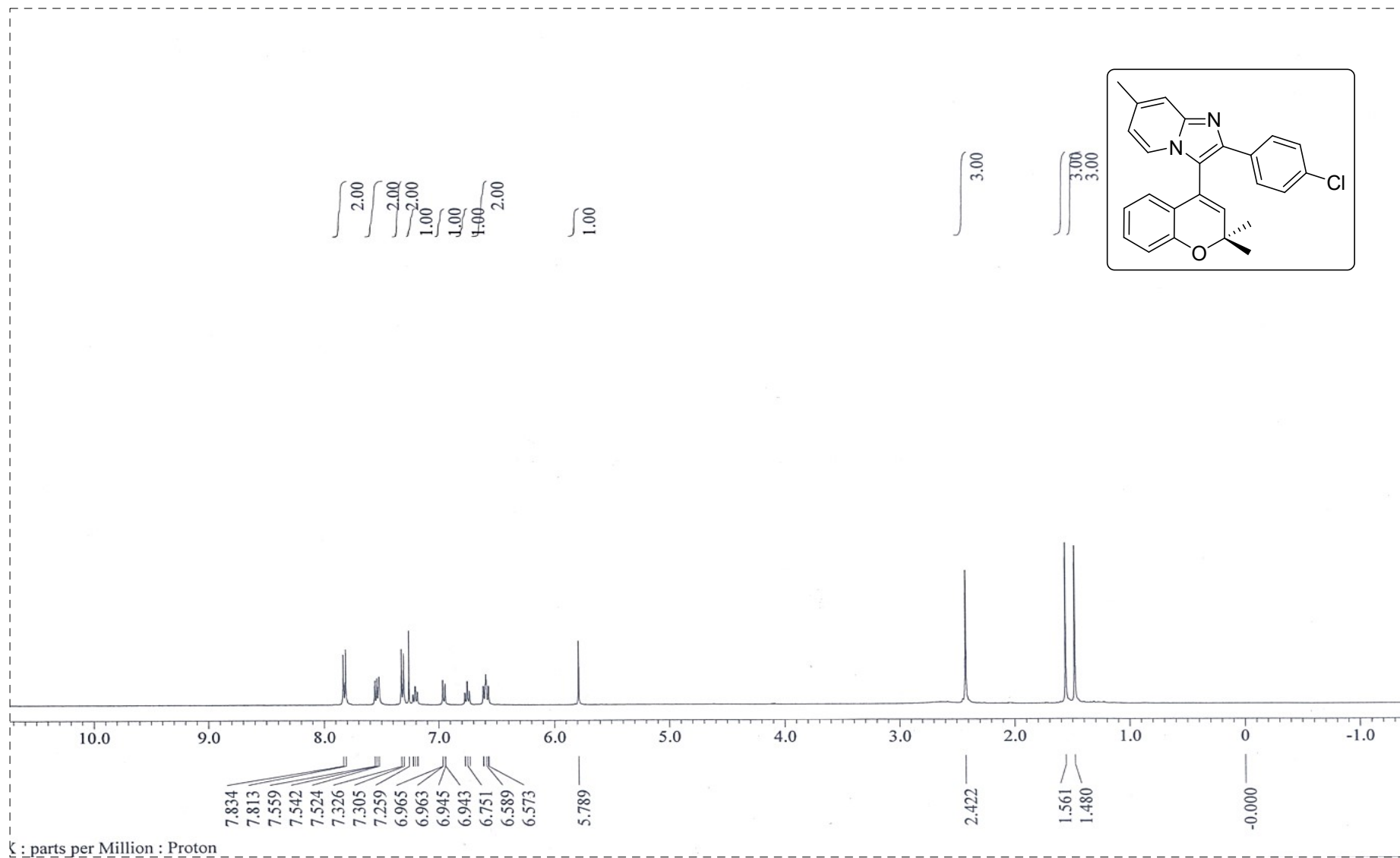


Fig S13: ^1H NMR of 2-(4-chlorophenyl)-3-(2,2-dimethyl-2H-chromen-4-yl)-7-methylimidazo-[1,2-a]pyridine (**16e**)

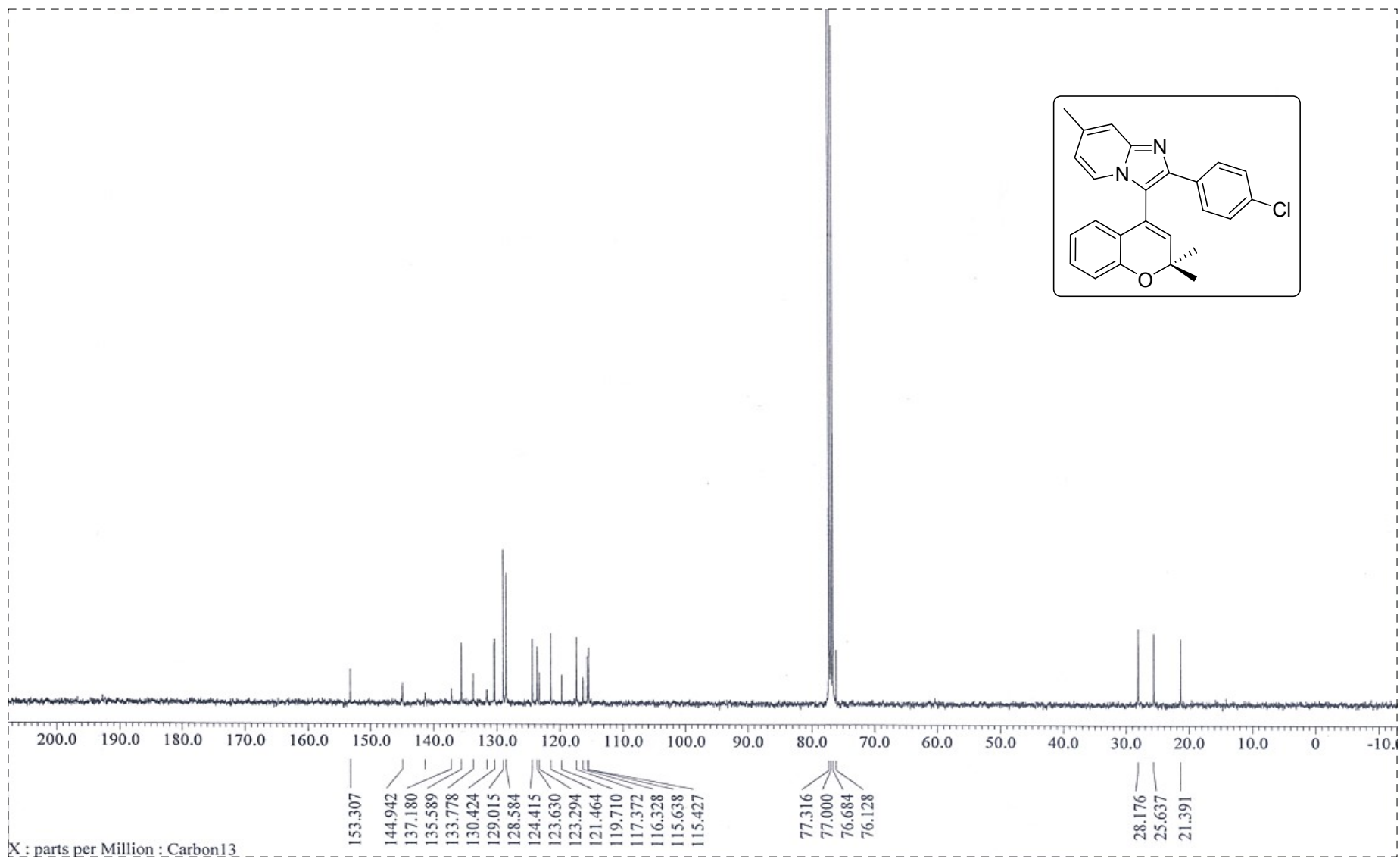


Fig S14: ^{13}C NMR of 2-(4-chlorophenyl)-3-(2,2-dimethyl-2H-chromen-4-yl)-7-methylimidazo-[1,2-a]pyridine (**16e**)

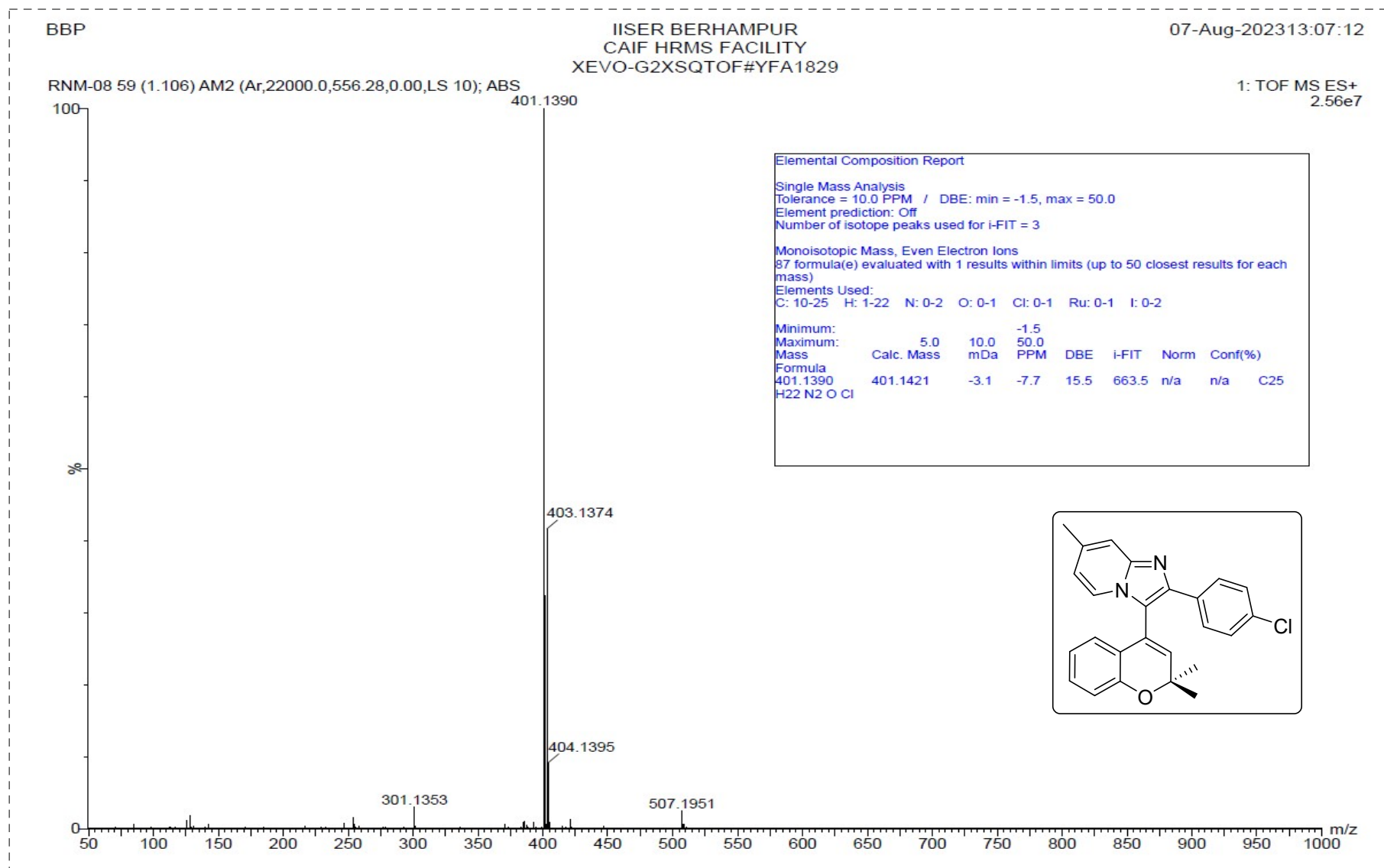


Fig S15: HR-MS of 2-(4-chlorophenyl)-3-(2,2-dimethyl-2H-chromen-4-yl)-7-methylimidazo-[1,2-a]pyridine (16e)

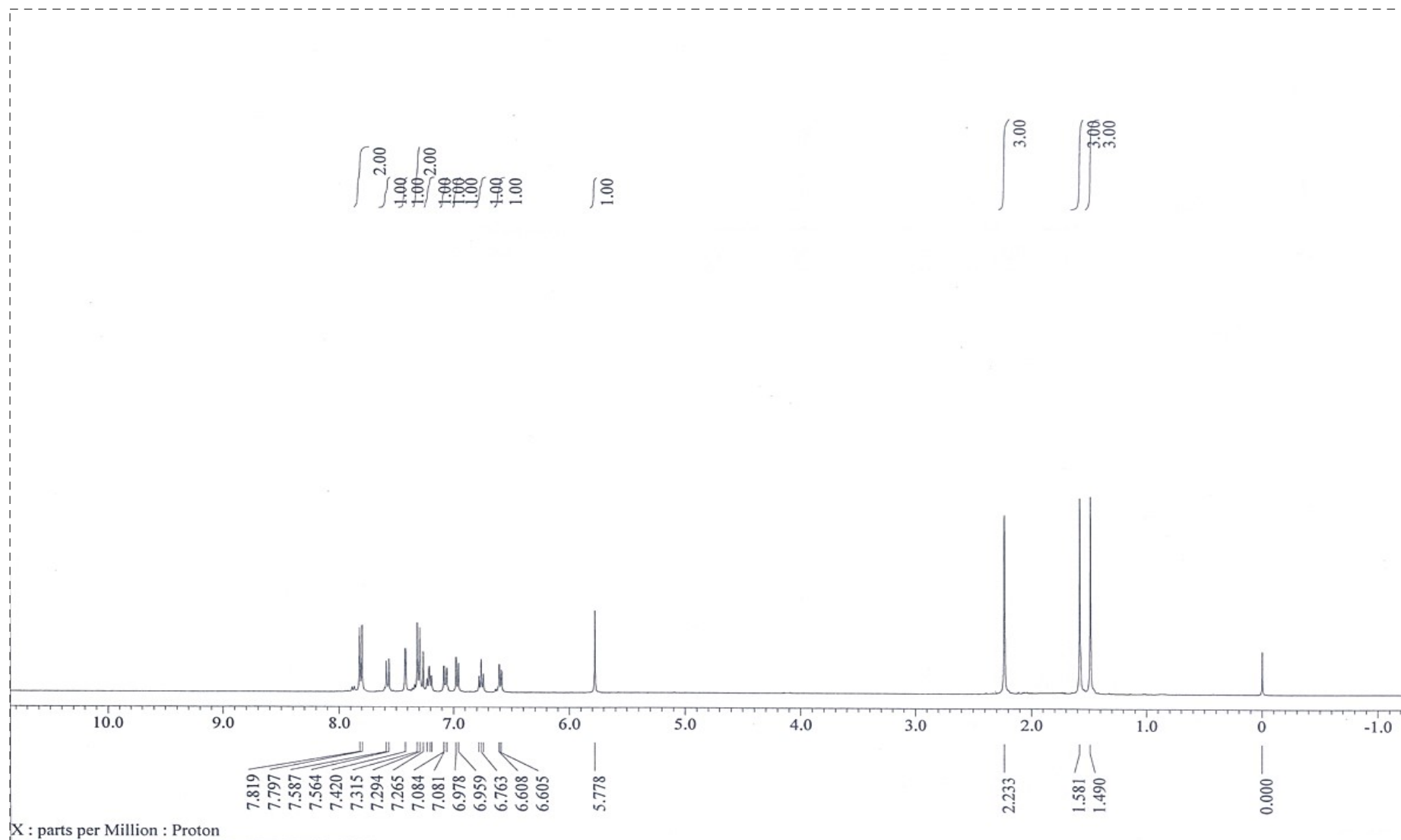


Fig S16: ^1H NMR of 2-(4-chlorophenyl)-3-(2,2-dimethyl-2H-chromen-4-yl)-6-methylimidazo-[1,2-a]pyridine (**16f**)

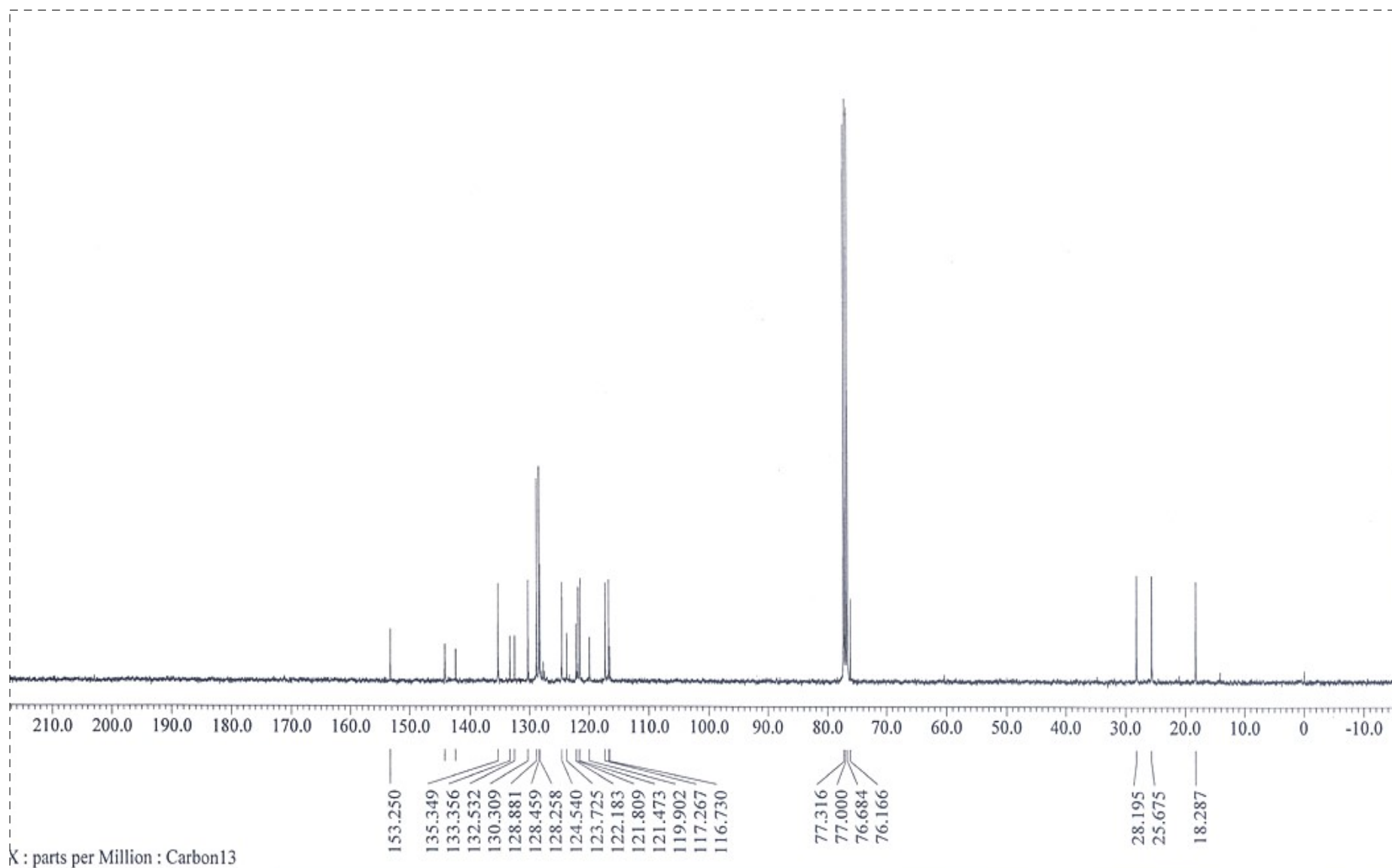


Fig S17: ^{13}C NMR of 2-(4-chlorophenyl)-3-(2,2-dimethyl-2H-chromen-4-yl)-6-methylimidazo-[1,2-a]pyridine (**16f**)

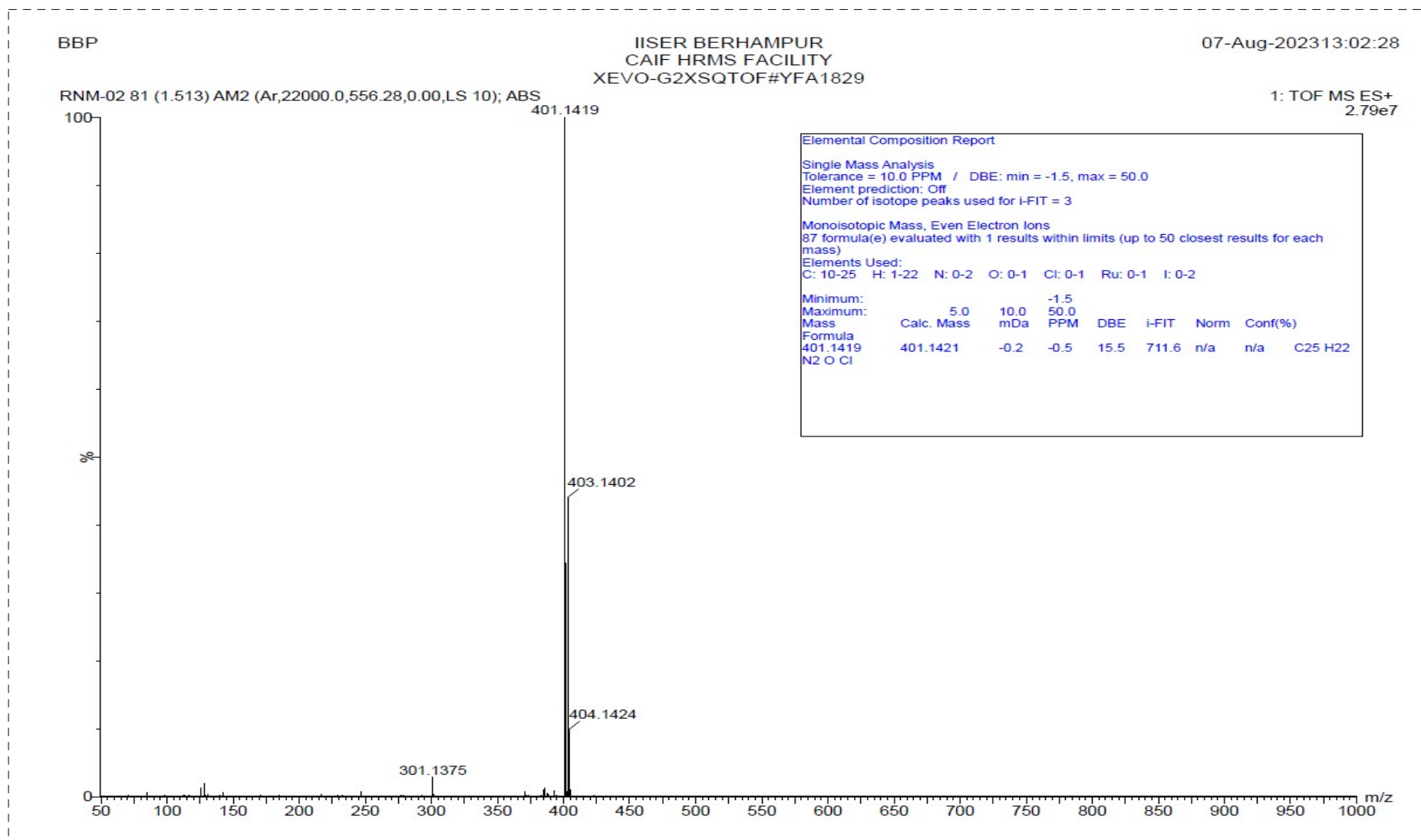


Fig S18: HR-MS of 2-(4-chlorophenyl)-3-(2,2-dimethyl-2H-chromen-4-yl)-6-methylimidazo-[1,2-a]pyridine (**16f**)

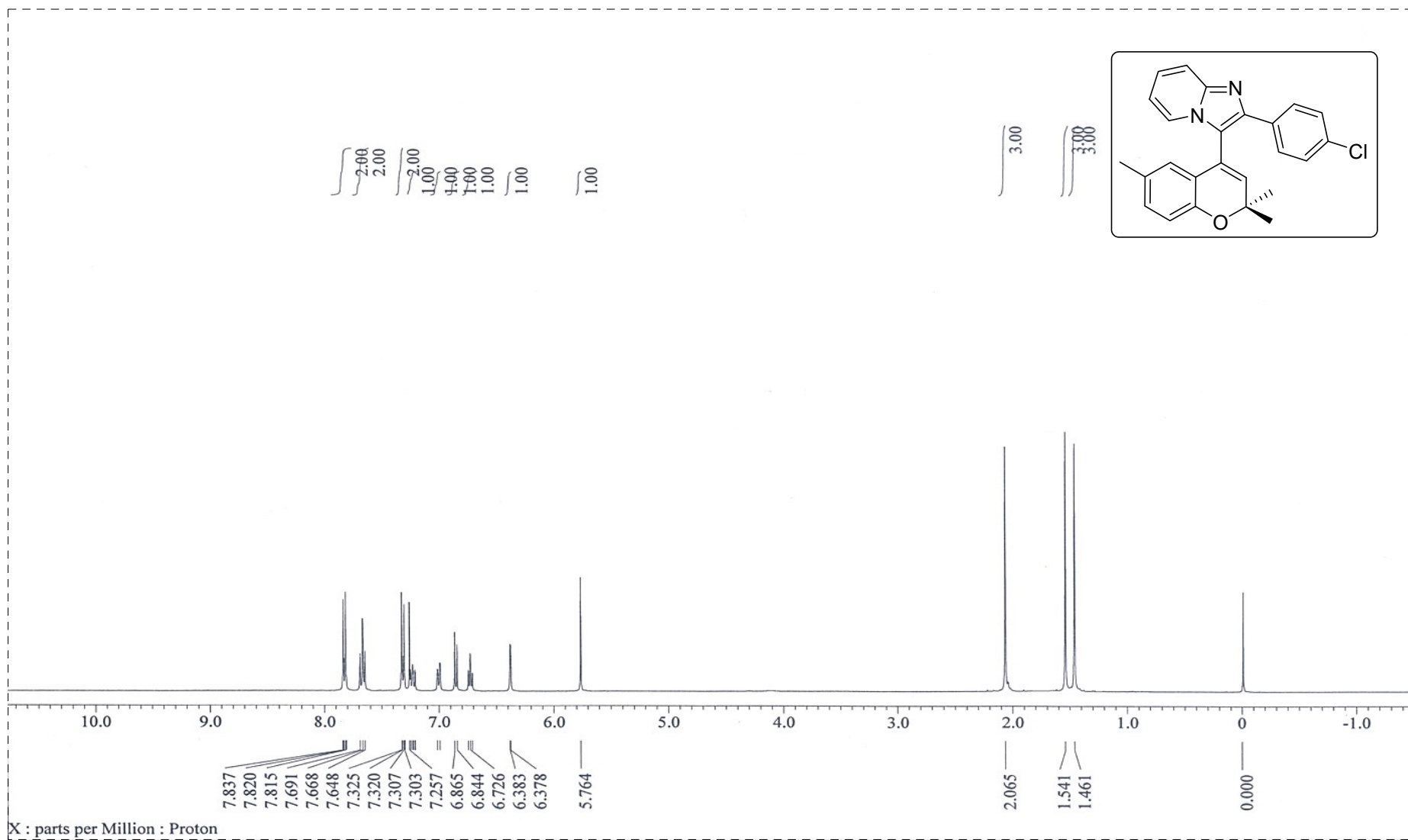


Fig S19: ¹H NMR of 2-(4-chlorophenyl)-3-(2,2,6-trimethyl-2H-chromen-4-yl)-imidazo-[1,2-a]pyridine (16g)

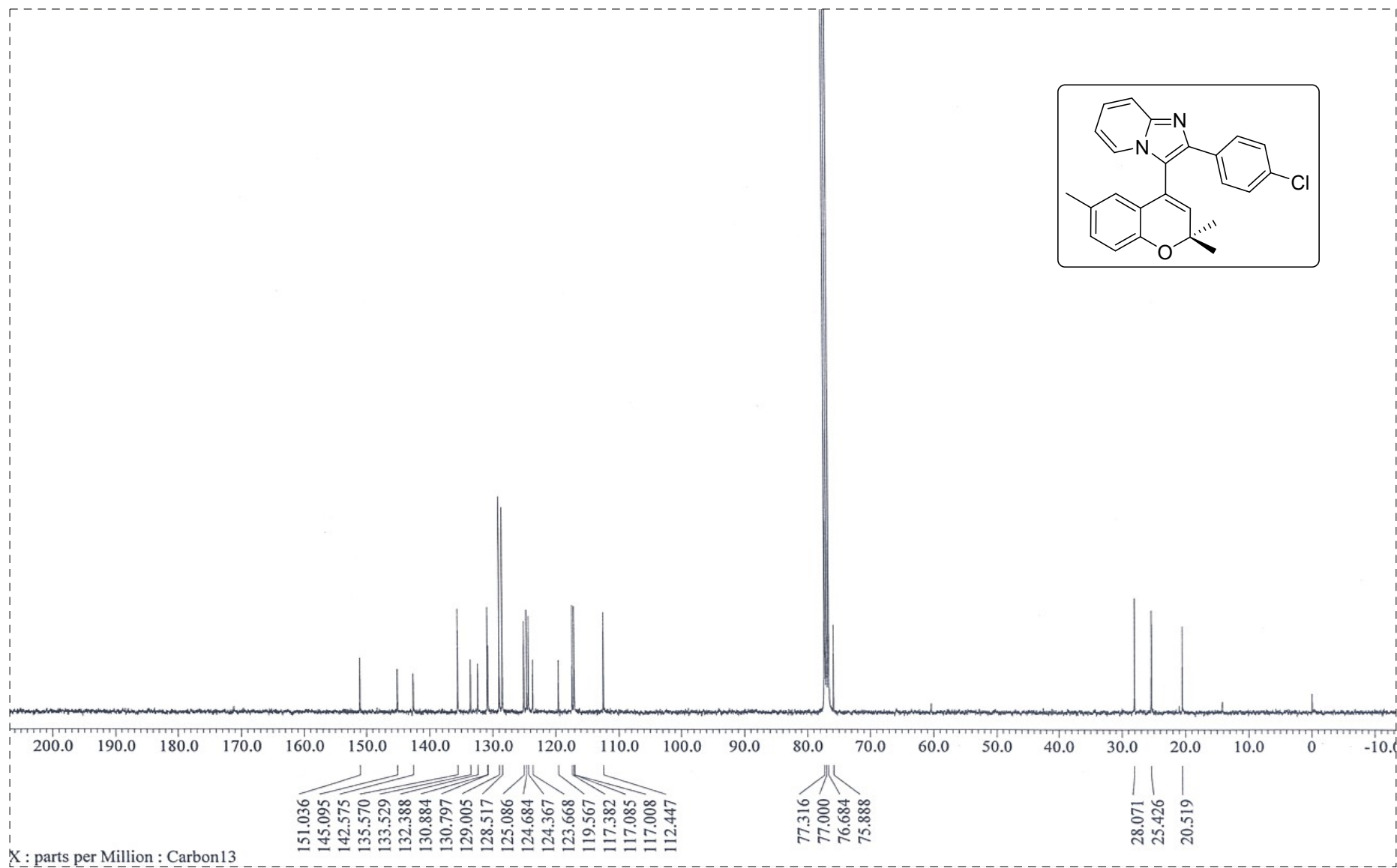


Fig S20: ¹³C NMR of 2-(4-chlorophenyl)-3-(2,2,6-trimethyl-2H-chromen-4-yl)-imidazo-[1,2-a]pyridine (**16g**)

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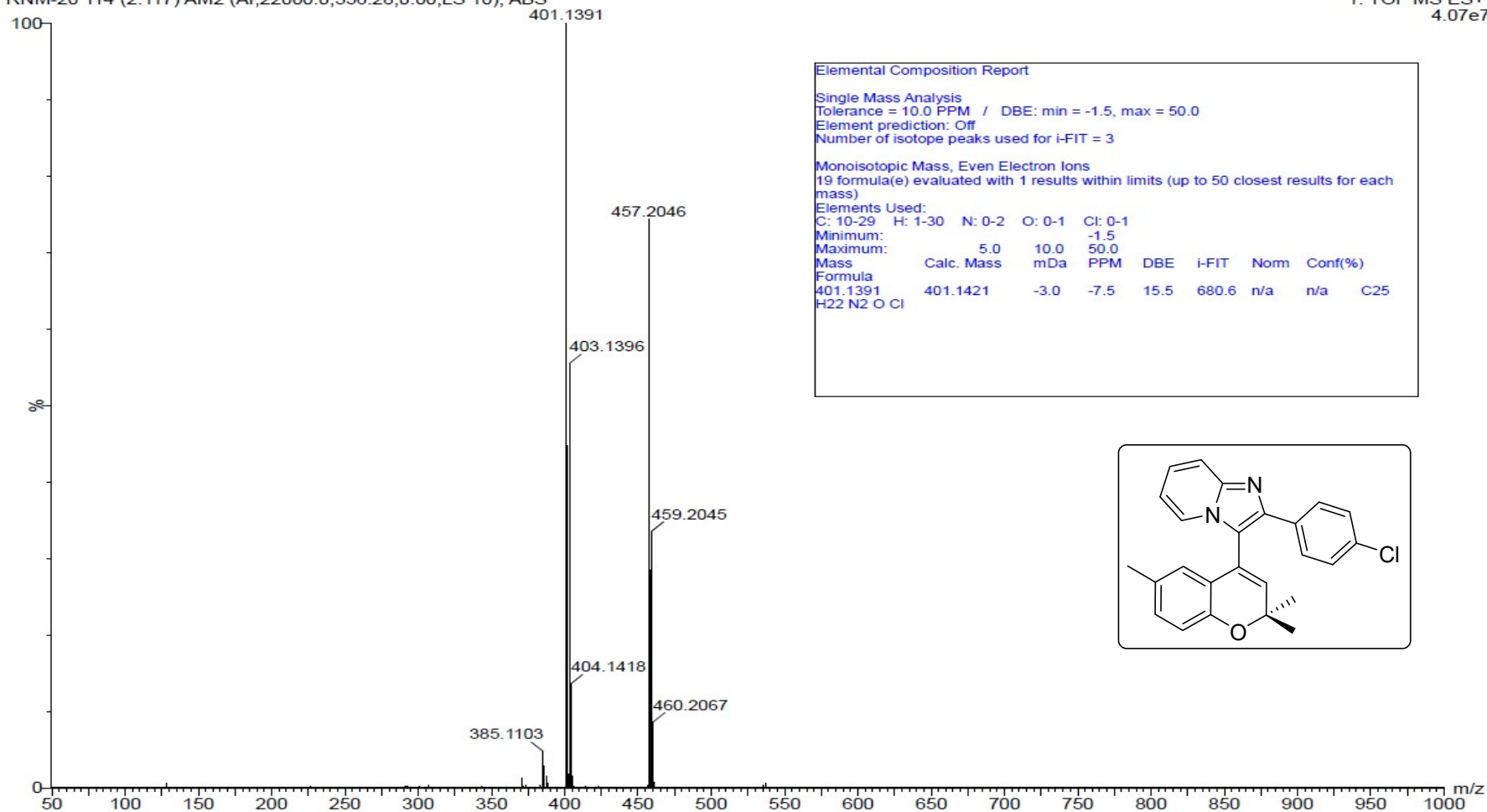
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Fig S21: HR-MS of 2-(4-chlorophenyl)-3-(2,2,6-trimethyl-2H-chromen-4-yl)-imidazo-[1,2-a]pyridine (**16g**)

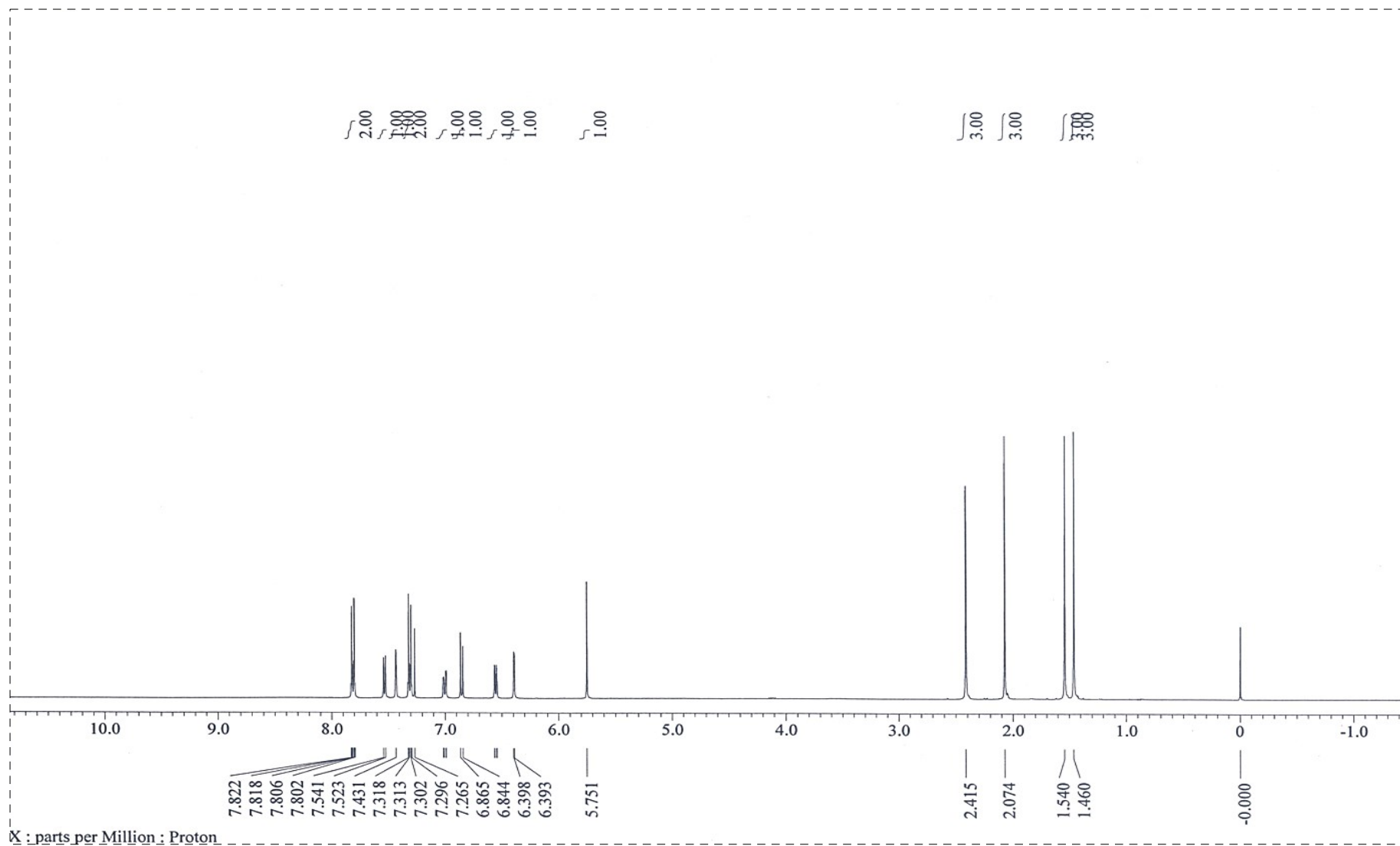


Fig S22: ^1H NMR of 2-(4-chlorophenyl)-7-methyl-3-(2,2,6-trimethyl-2H-chromen-4-yl)-imidazo-[1,2-a]pyridine (**16h**)

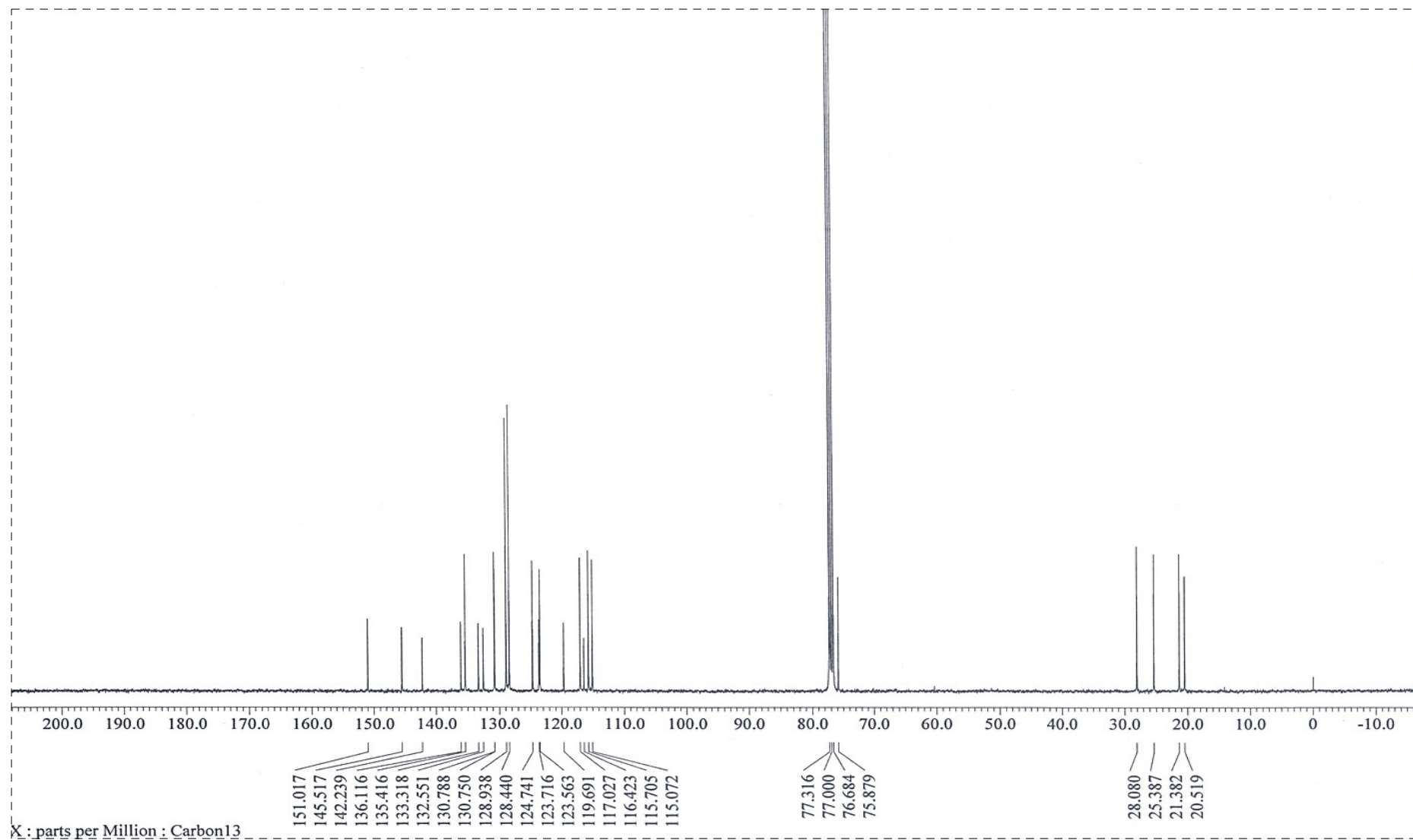


Fig S23: ^{13}C NMR of 2-(4-chlorophenyl)-7-methyl-3-(2,2,6-trimethyl-2H-chromen-4-yl)-imidazo-[1,2-a]pyridine (**16h**)

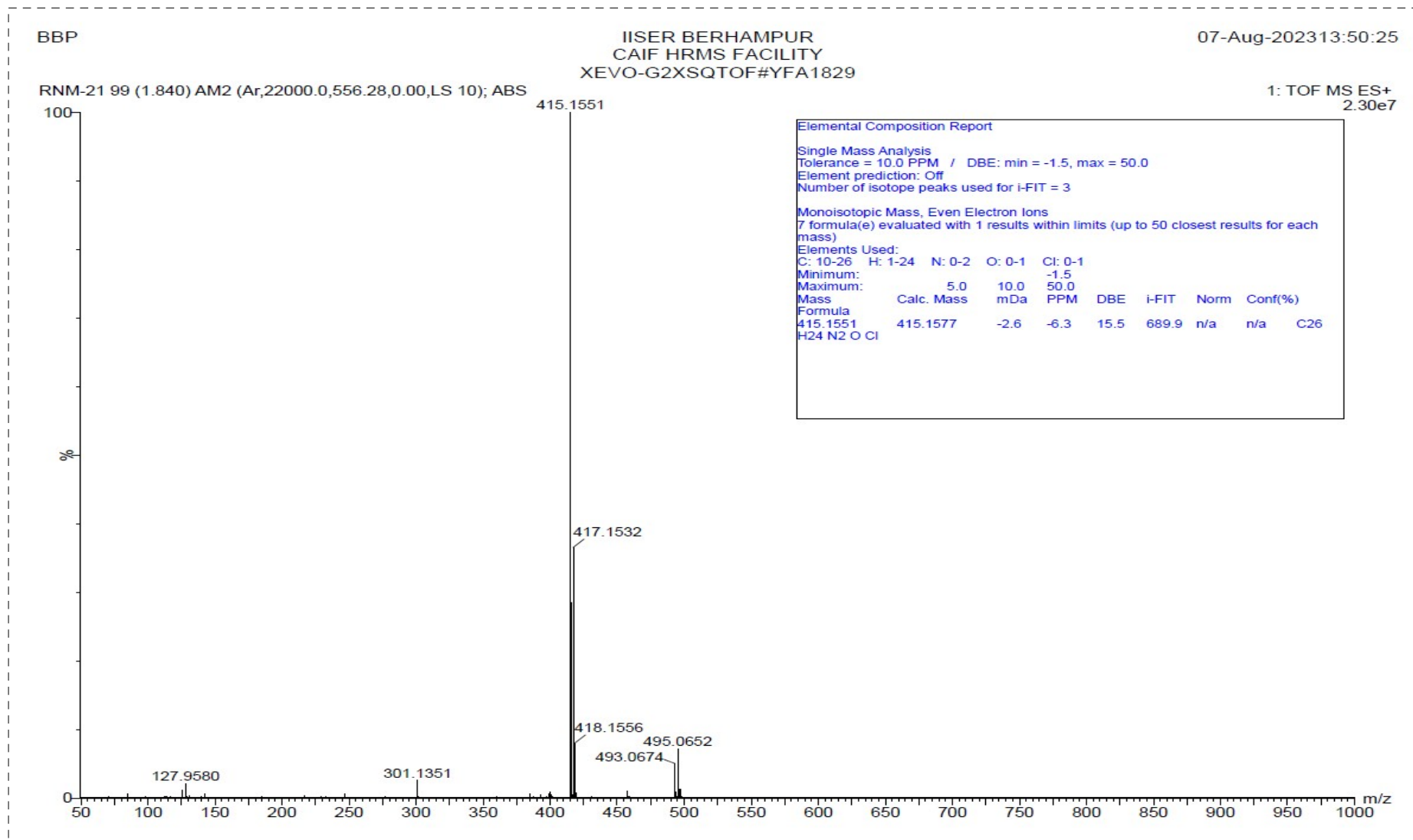


Fig S24: HR-MS of 2-(4-chlorophenyl)-7-methyl-3-(2,2,6-trimethyl-2H-chromen-4-yl)-imidazo-[1,2-a]pyridine (16h)

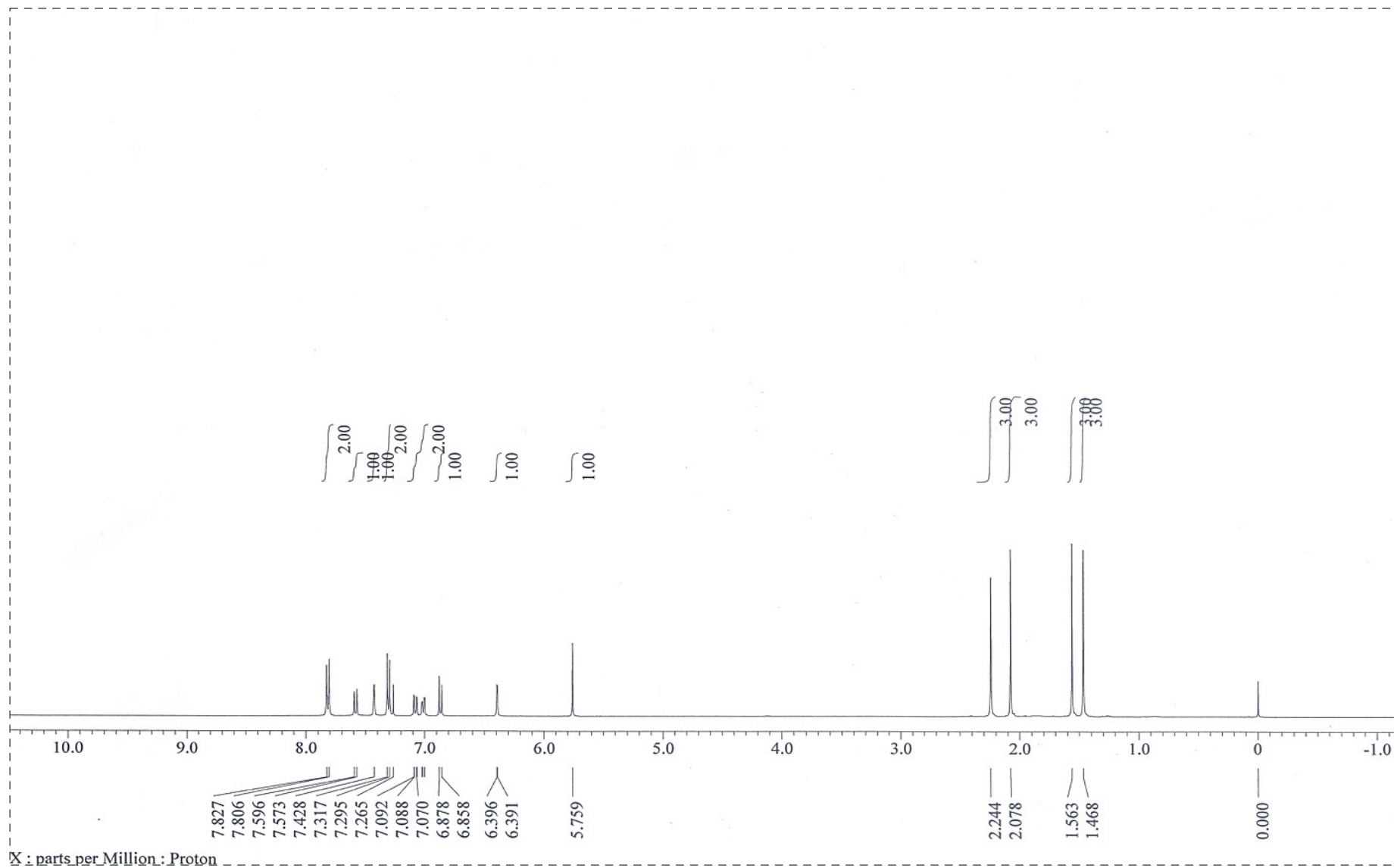


Fig S25: ^1H NMR of 2-(4-chlorophenyl)-6-methyl-3-(2,2,6-trimethyl-2H-chromen-4-yl)-imidazo-[1,2-a]pyridine (**16i**)

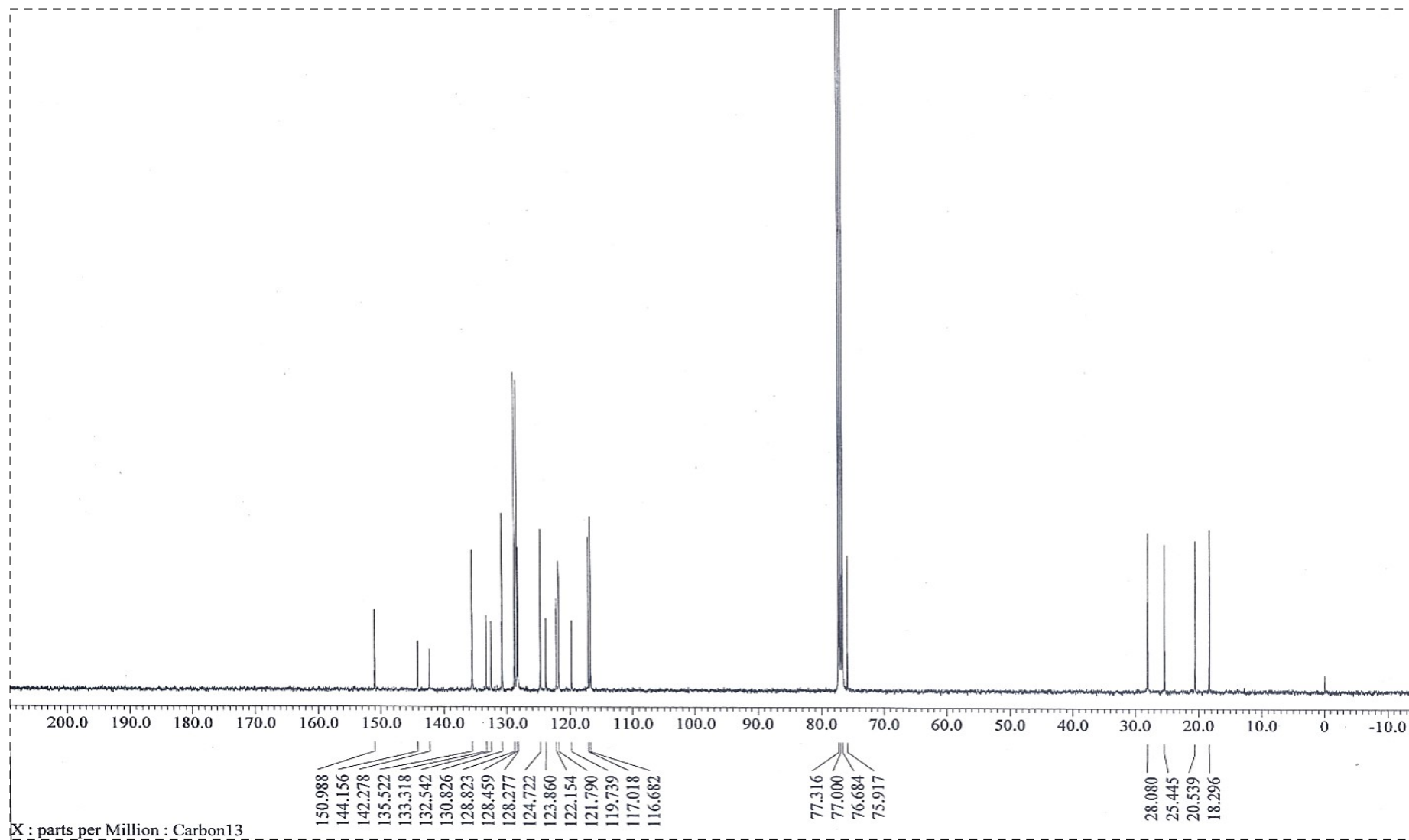


Fig S26: ^{13}C NMR of 2-(4-chlorophenyl)-6-methyl-3-(2,2,6-trimethyl-2H-chromen-4-yl)-imidazo-[1,2-a]pyridine (**16i**)

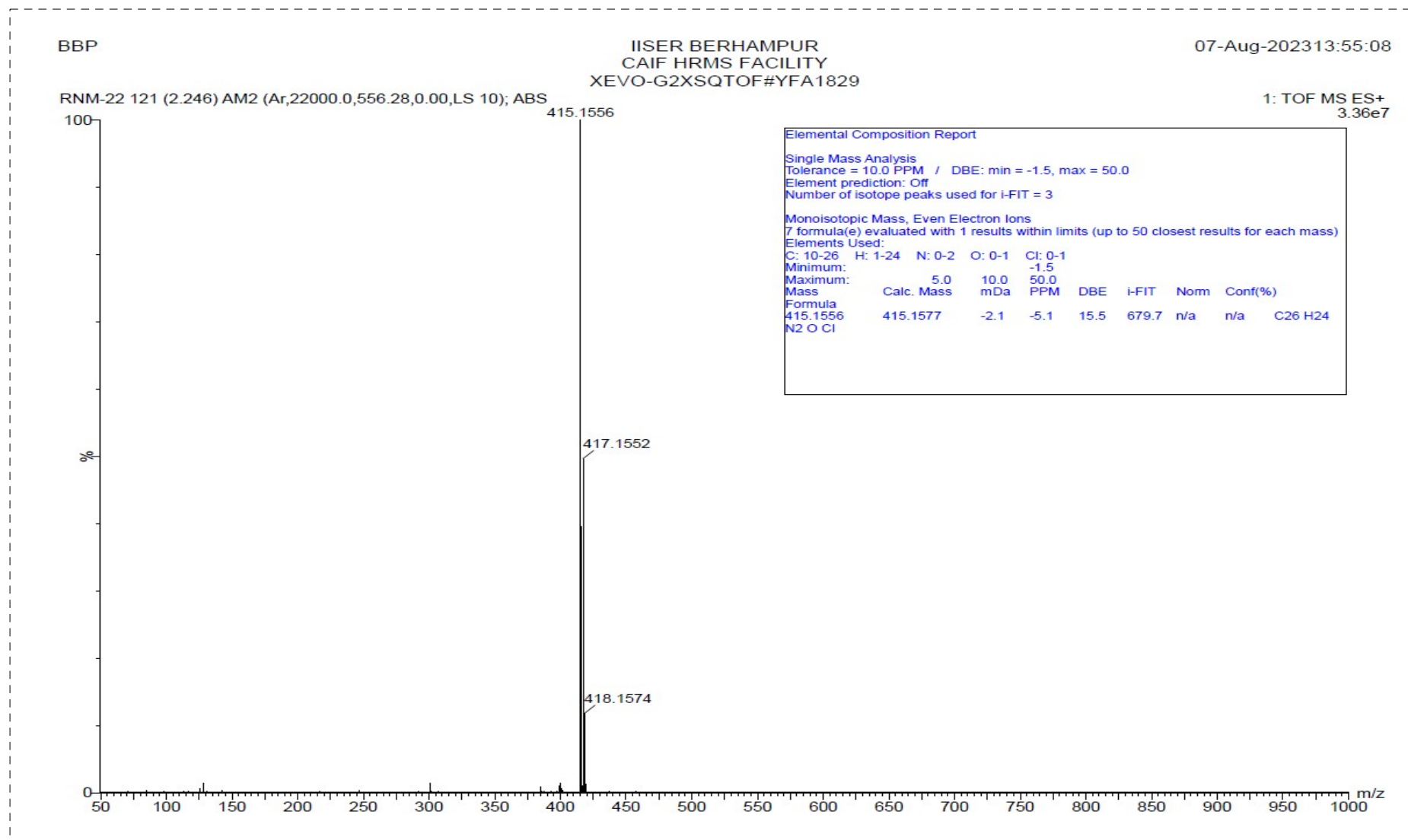


Fig S27: HR-MS of 2-(4-chlorophenyl)-6-methyl-3-(2,2,6-trimethyl-2H-chromen-4-yl)-imidazo-[1,2-a]pyridine (**16i**)

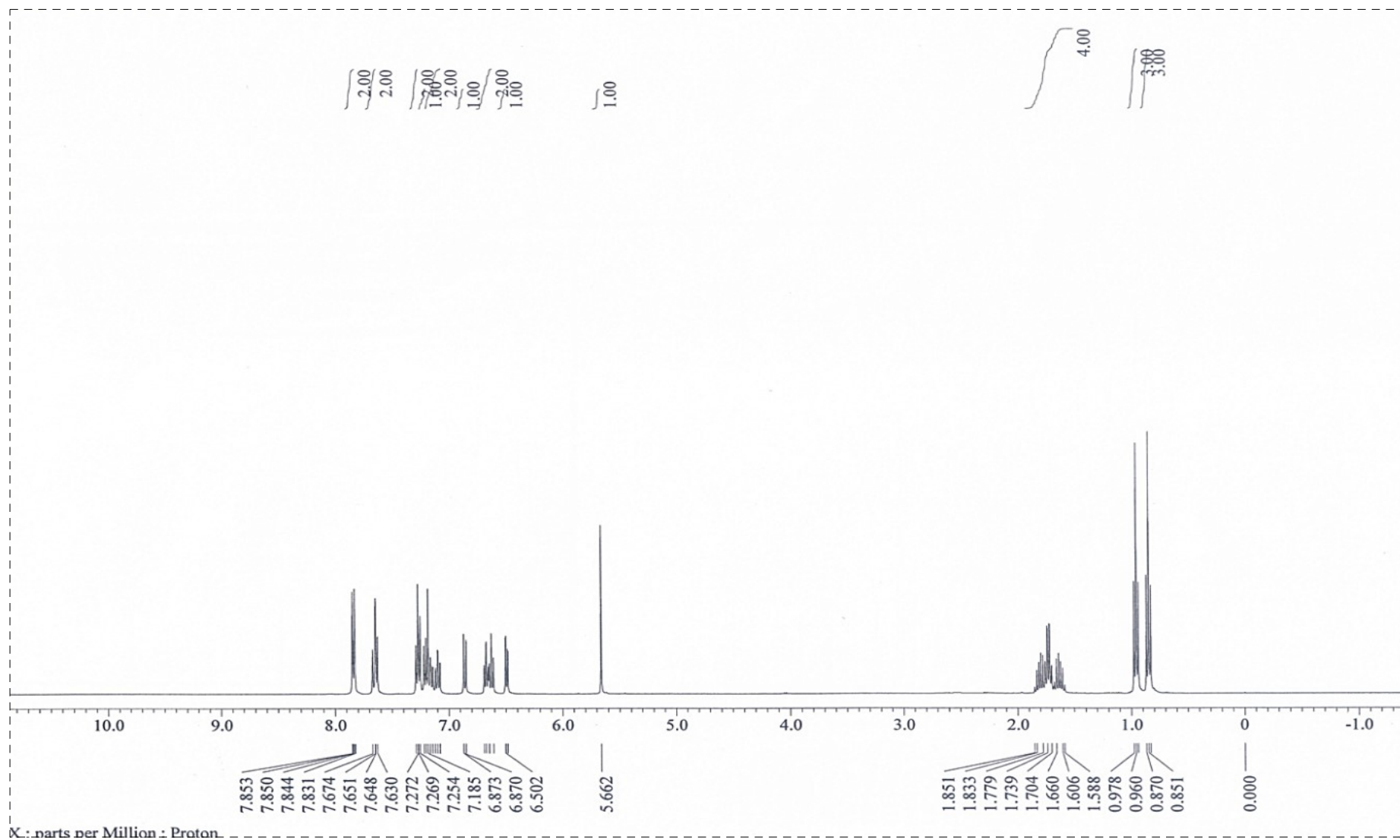


Fig S28: ^1H NMR of 3-(2, 2-diethyl-2H-chromen-4-yl)-2-phenylimidazo-[1,2-a]pyridine (**16j**)

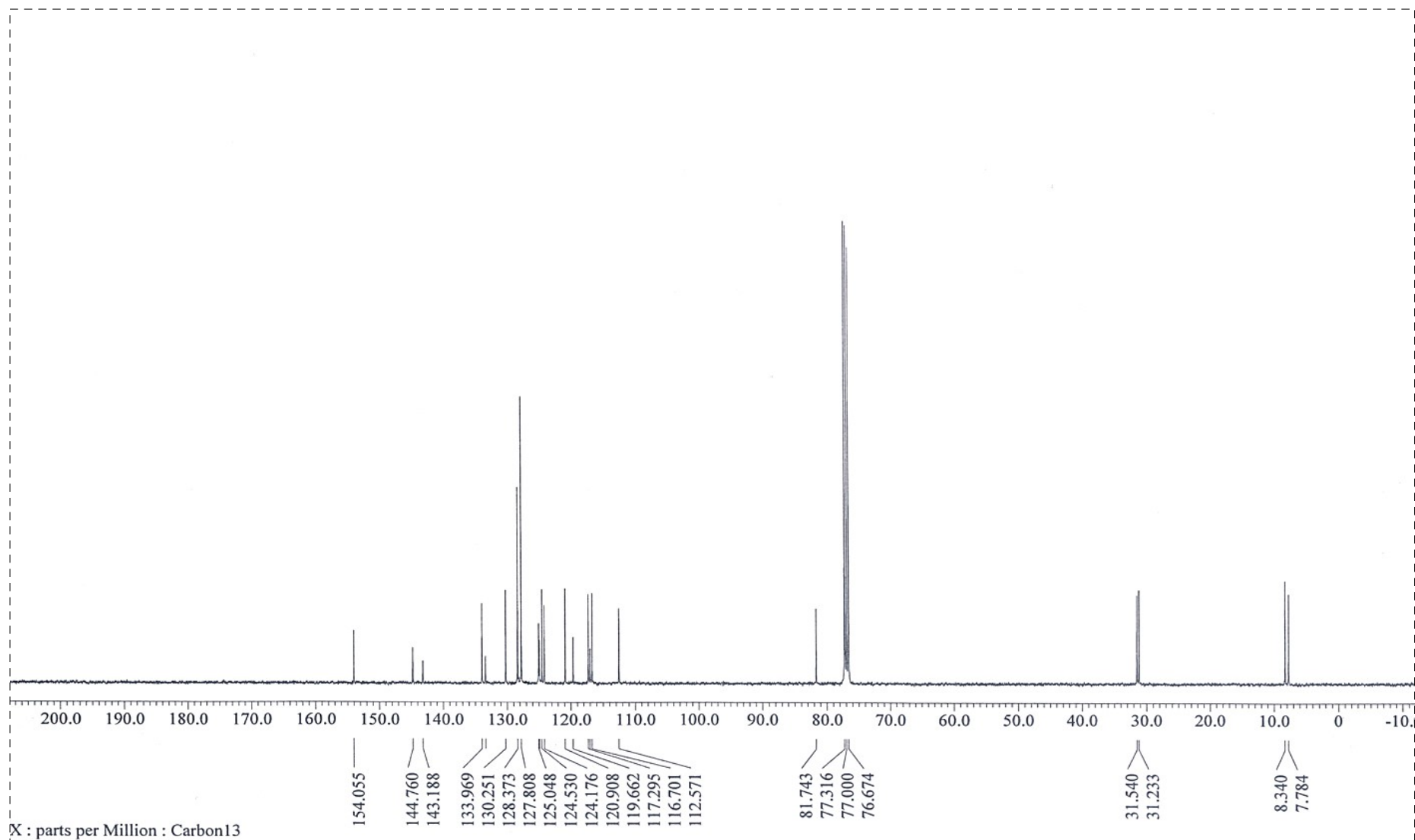


Fig S29: ^{13}C NMR of 3-(2, 2-diethyl-2H-chromen-4-yl)-2-phenylimidazo-[1,2-a]pyridine (**16j**)

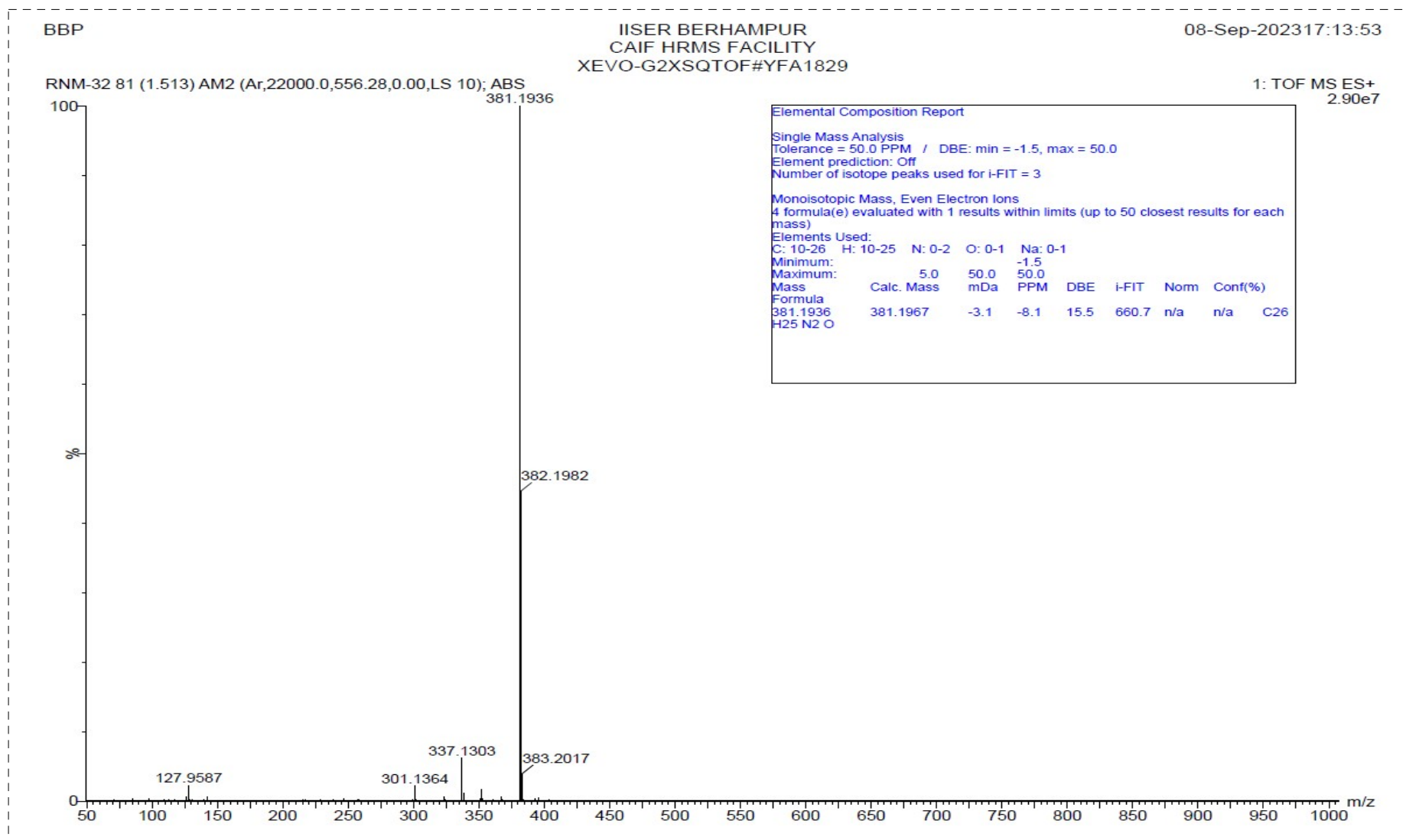


Fig S30: HR-MS of 3-(2, 2-diethyl-2H-chromen-4-yl)-2-phenylimidazo-[1,2-a]pyridine (**16j**)

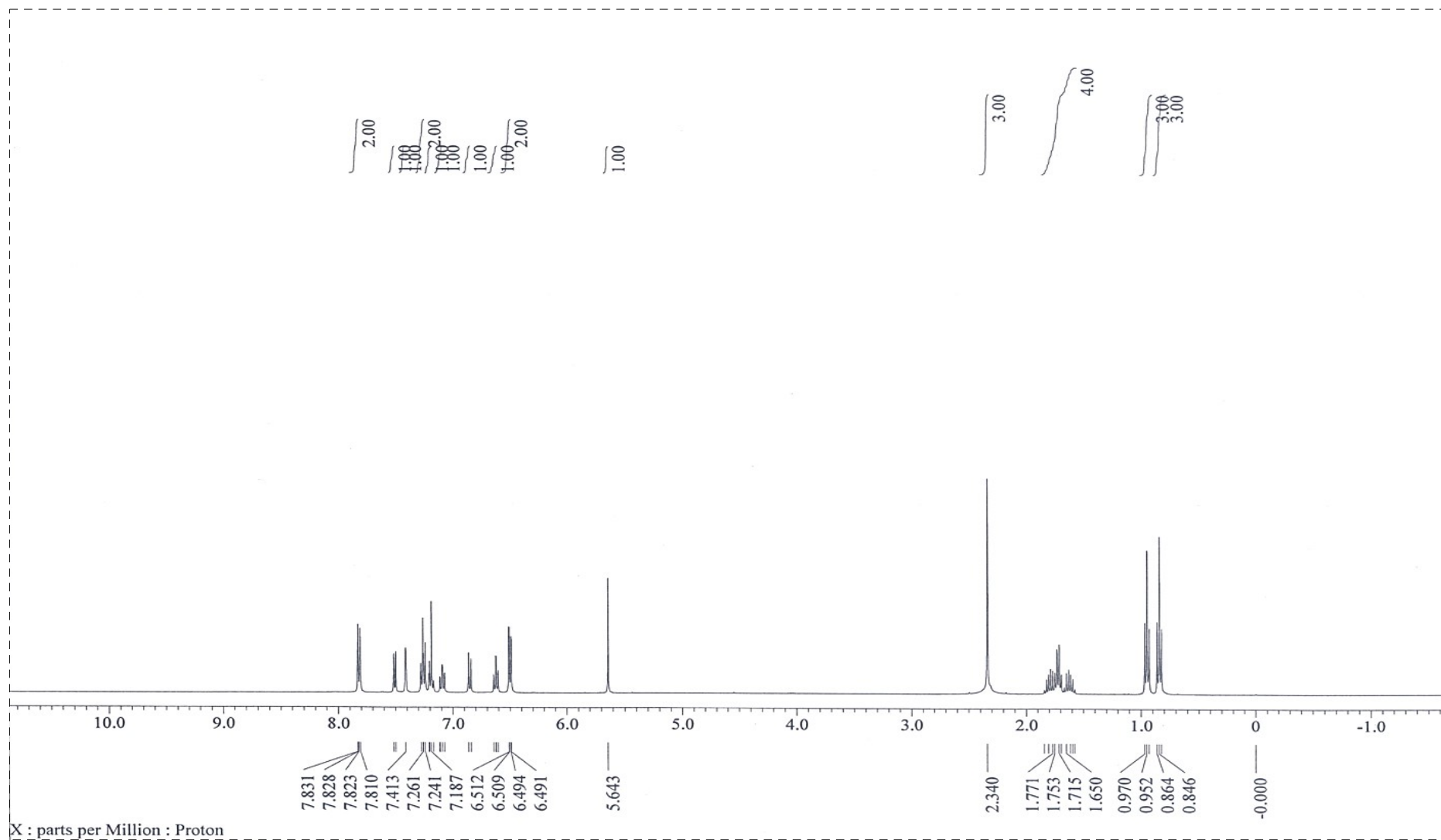


Fig S31: ^1H NMR of 3-(2, 2-diethyl-2H-chromen-4-yl)-7-methyl-2-phenylimidazo-[1,2-a]pyridine (**16k**)

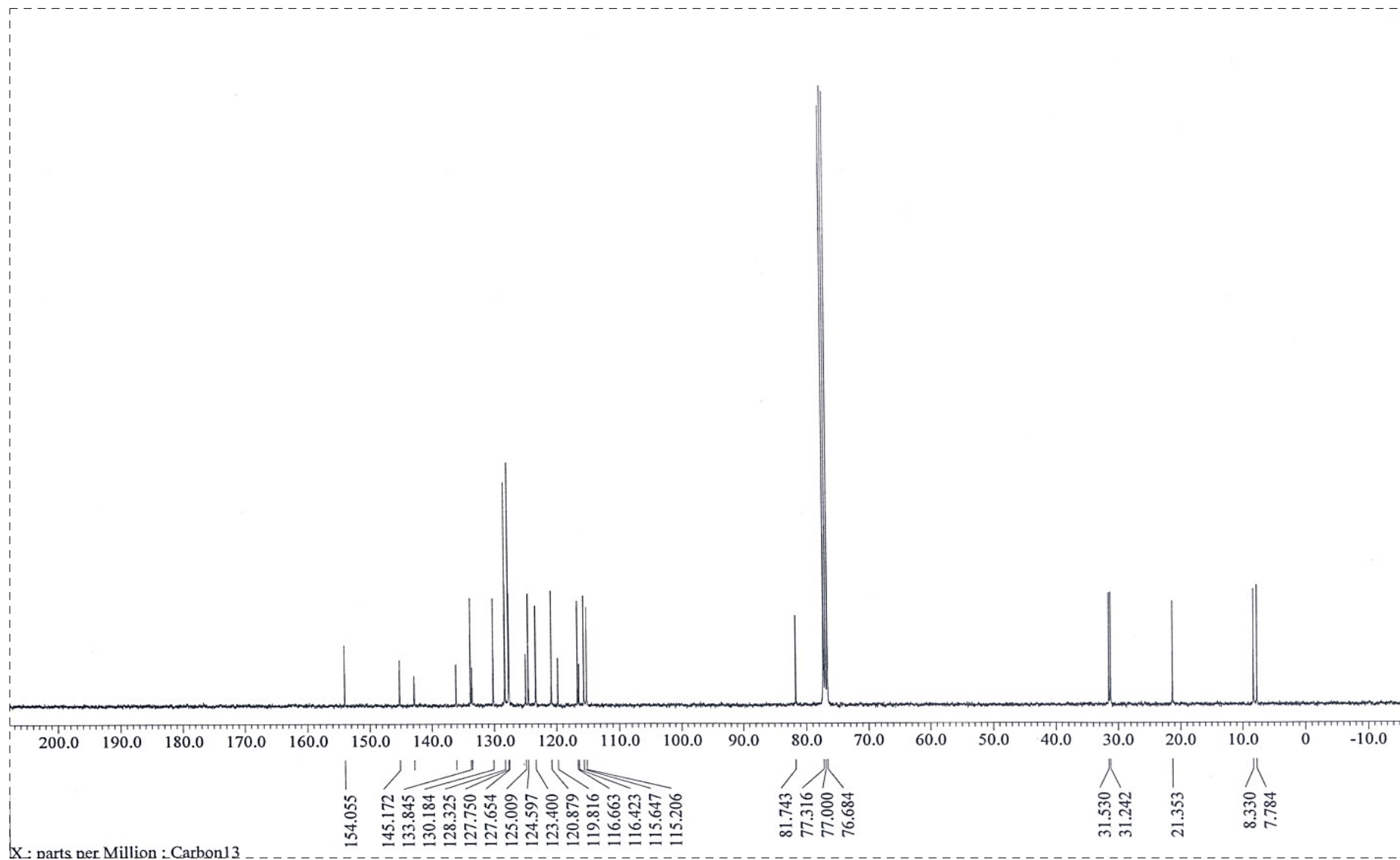


Fig S32: ^{13}C NMR of 3-(2, 2-diethyl-2H-chromen-4-yl)-7-methyl-2-phenylimidazo-[1,2-a]pyridine (**16k**)

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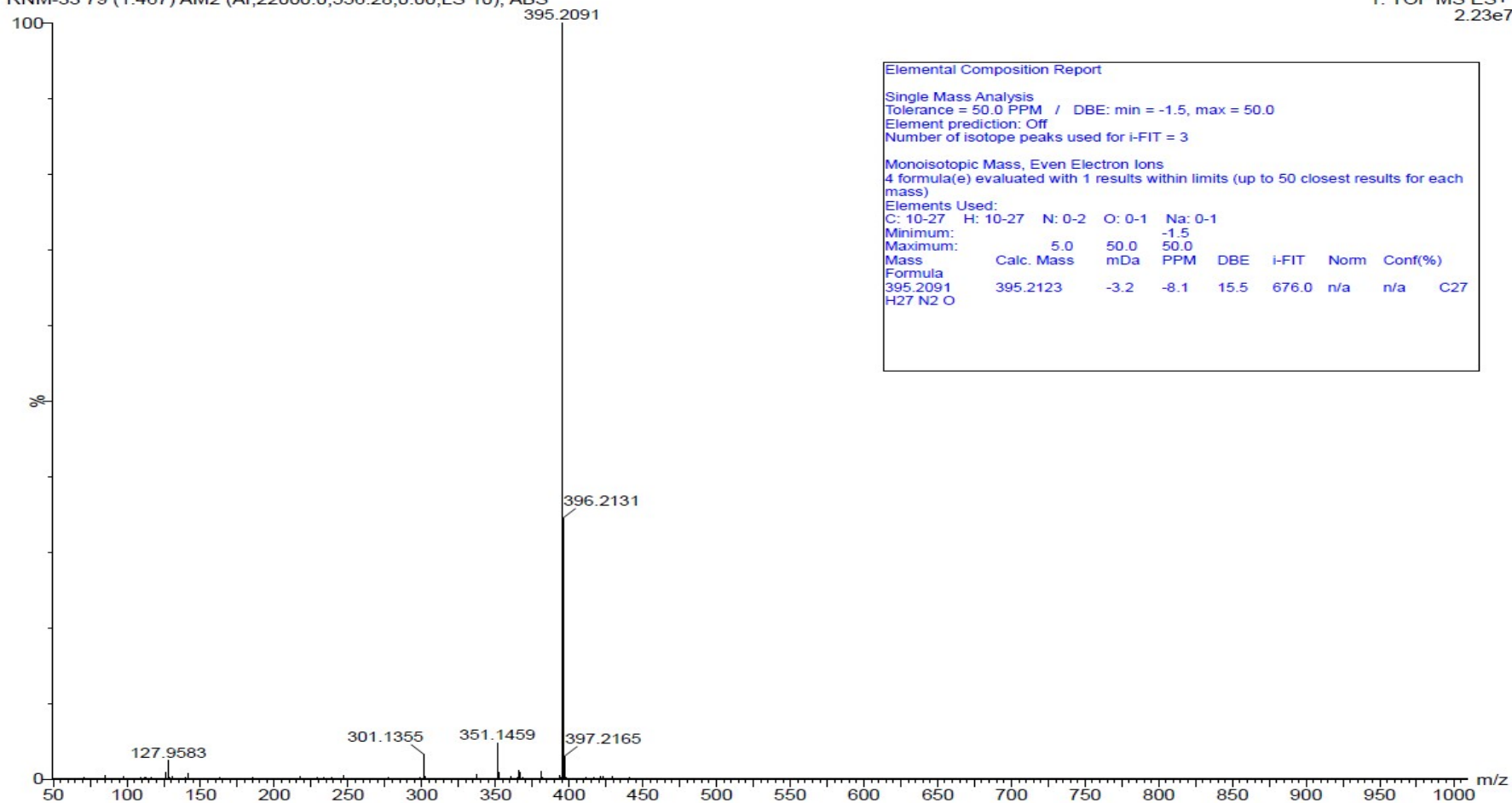
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Fig S33: HR-MS of 3-(2, 2-diethyl-2H-chromen-4-yl)-7-methyl-2-phenylimidazo-[1,2-a]pyridine (16k)

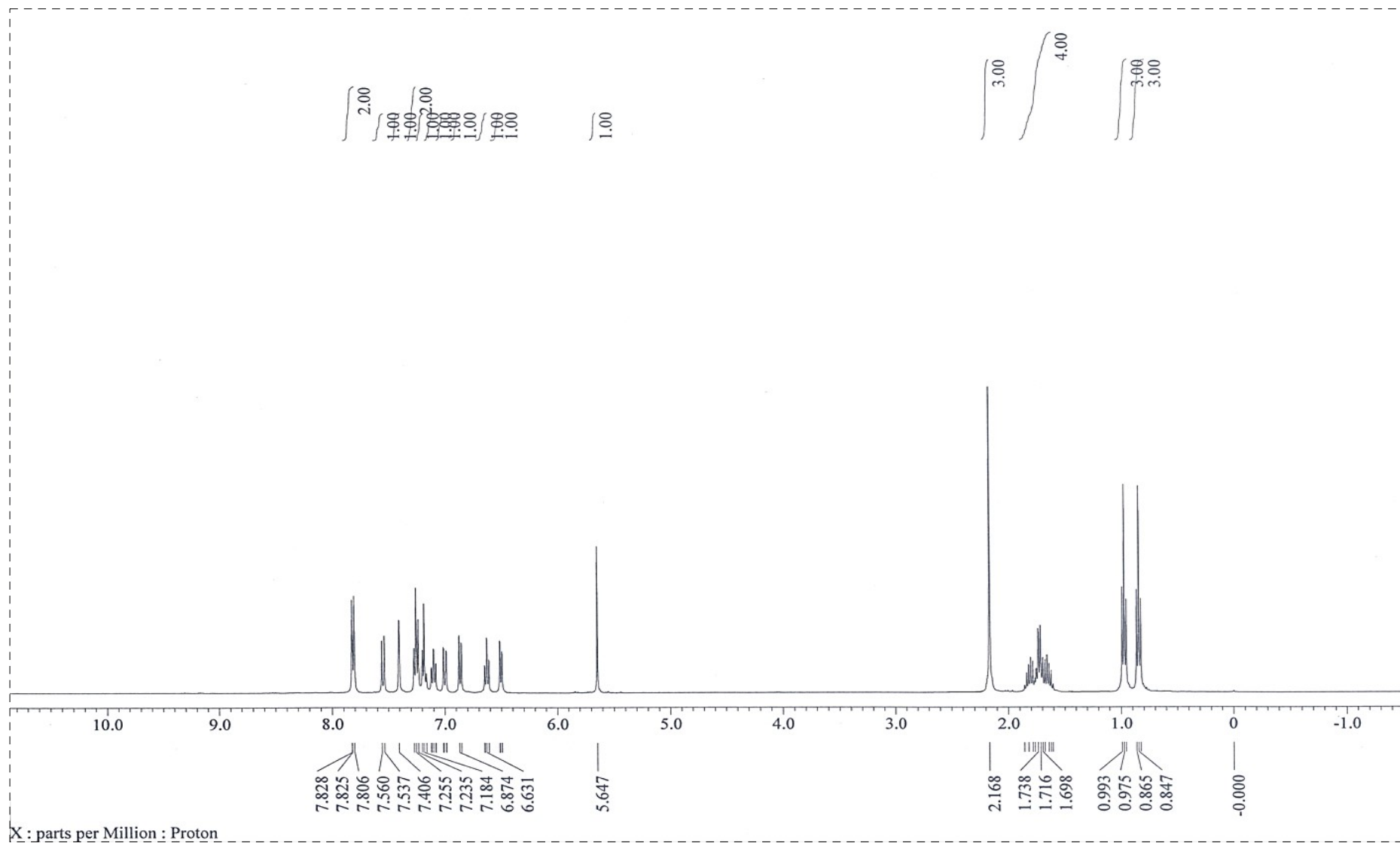


Fig S34: ^1H NMR of 3-(2, 2-diethyl-2H-chromen-4-yl)-6-methyl-2-phenylimidazo-[1,2-a]pyridine (**16l**)

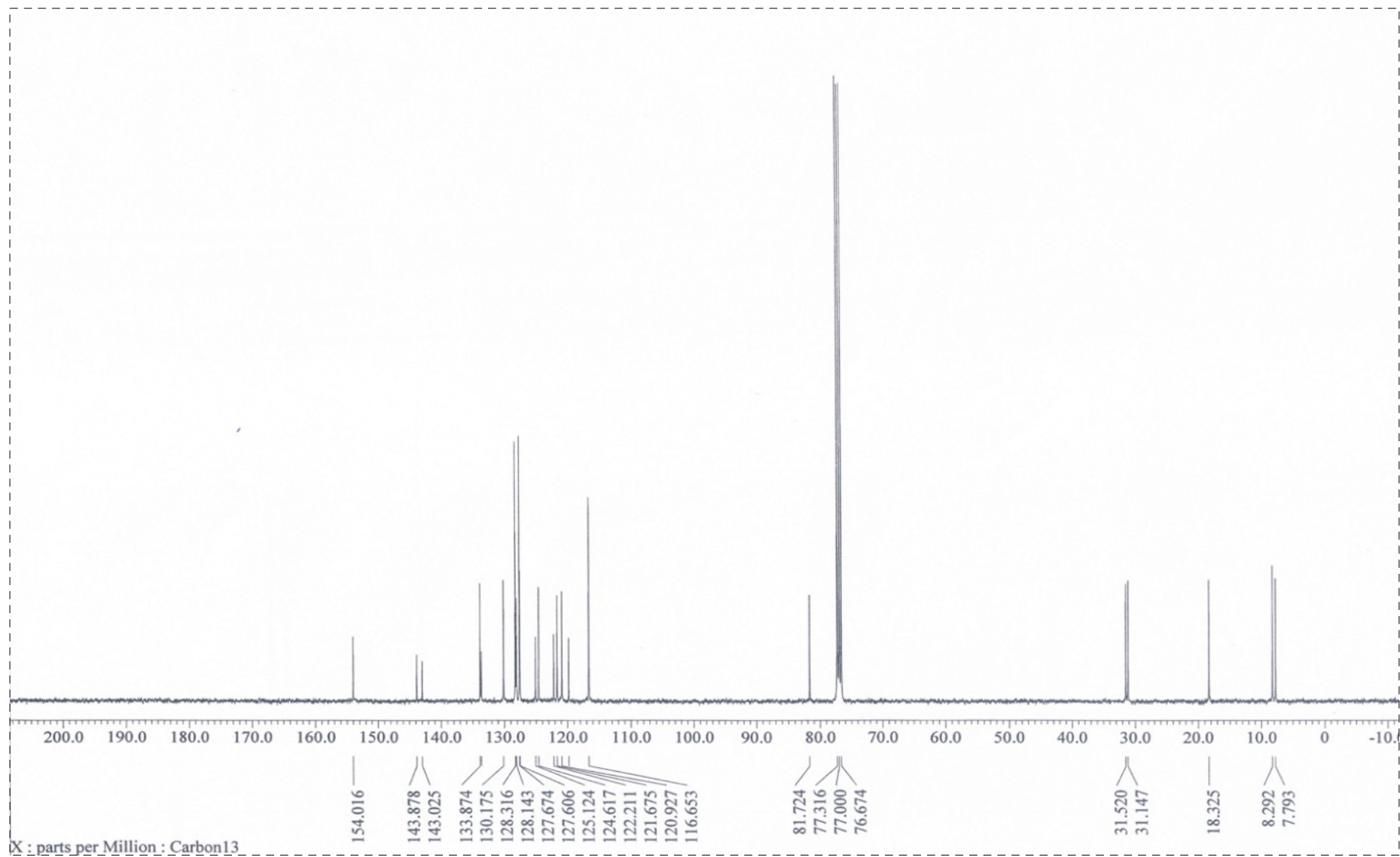


Fig S35: ^{13}C NMR of 3-(2, 2-diethyl-2H-chromen-4-yl)-6-methyl-2-phenylimidazo-[1,2-a]pyridine (**16**)

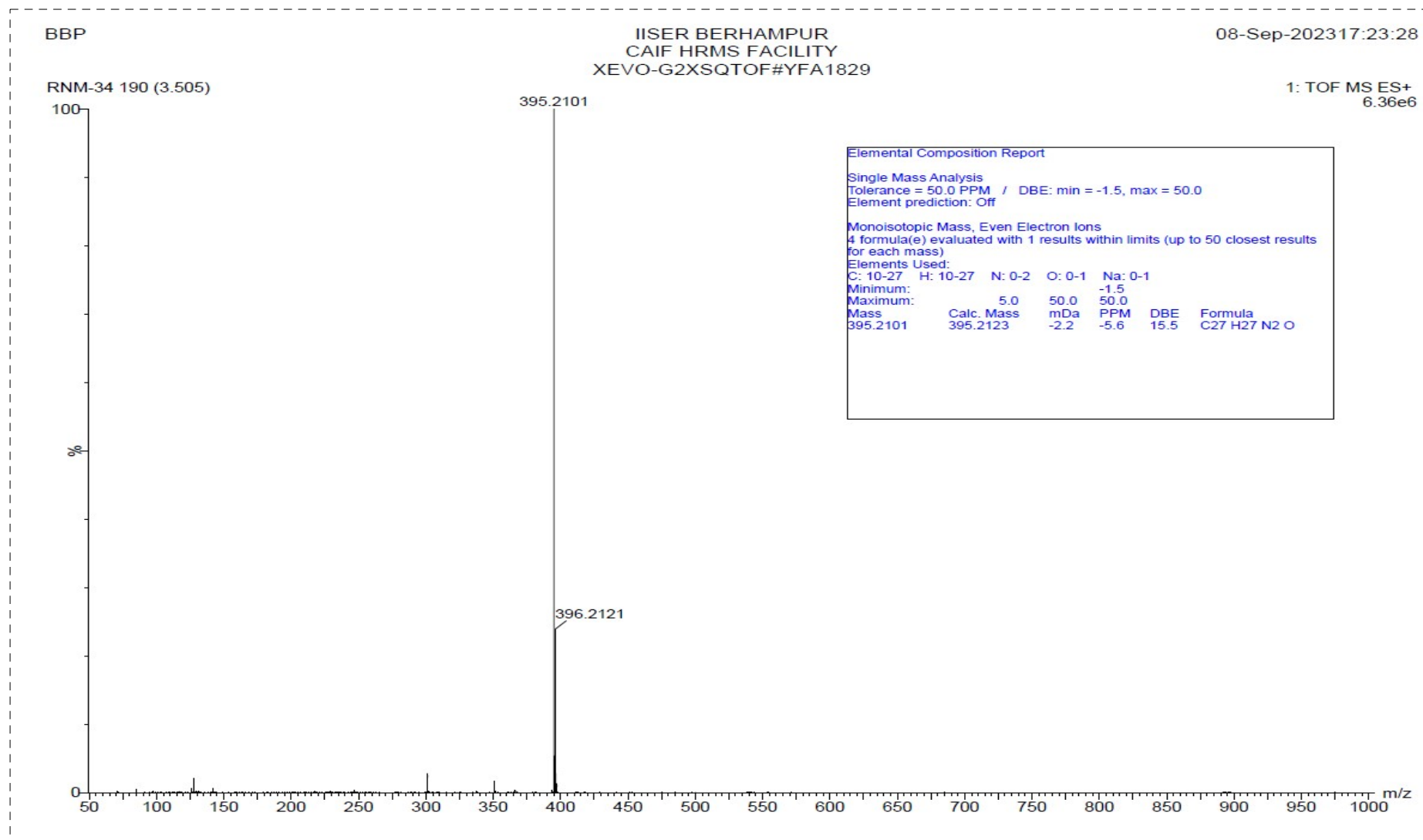


Fig S36: HR-MS of 3-(2, 2-diethyl-2H-chromen-4-yl)-6-methyl-2-phenylimidazo-[1,2-a]pyridine (**16l**)

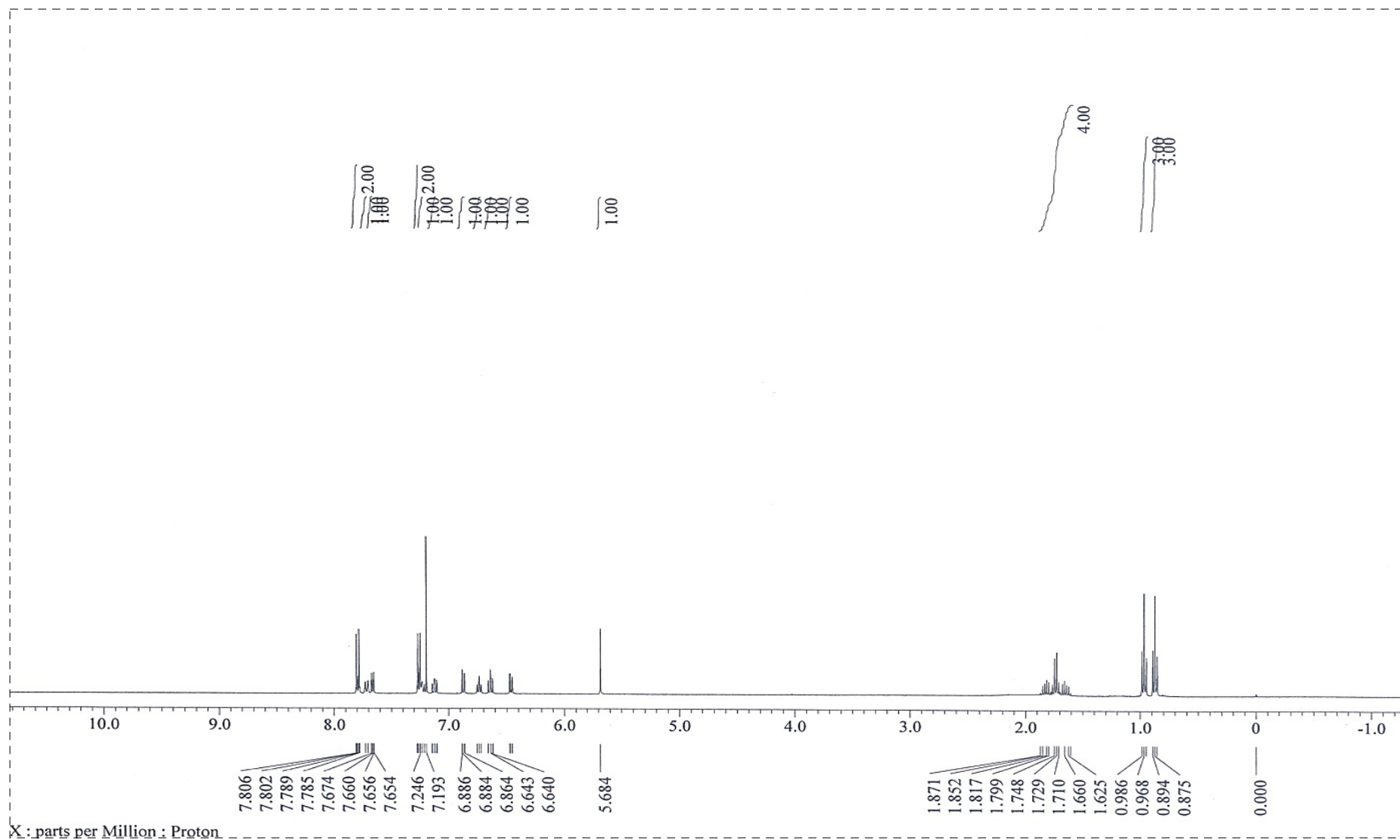


Fig S37: ^1H NMR of 2-(4-Chlorophenyl)-3-(2,2-diethyl-2H-Chromen-4-yl)-imidazo[1,2-a]pyridine (**16m**)

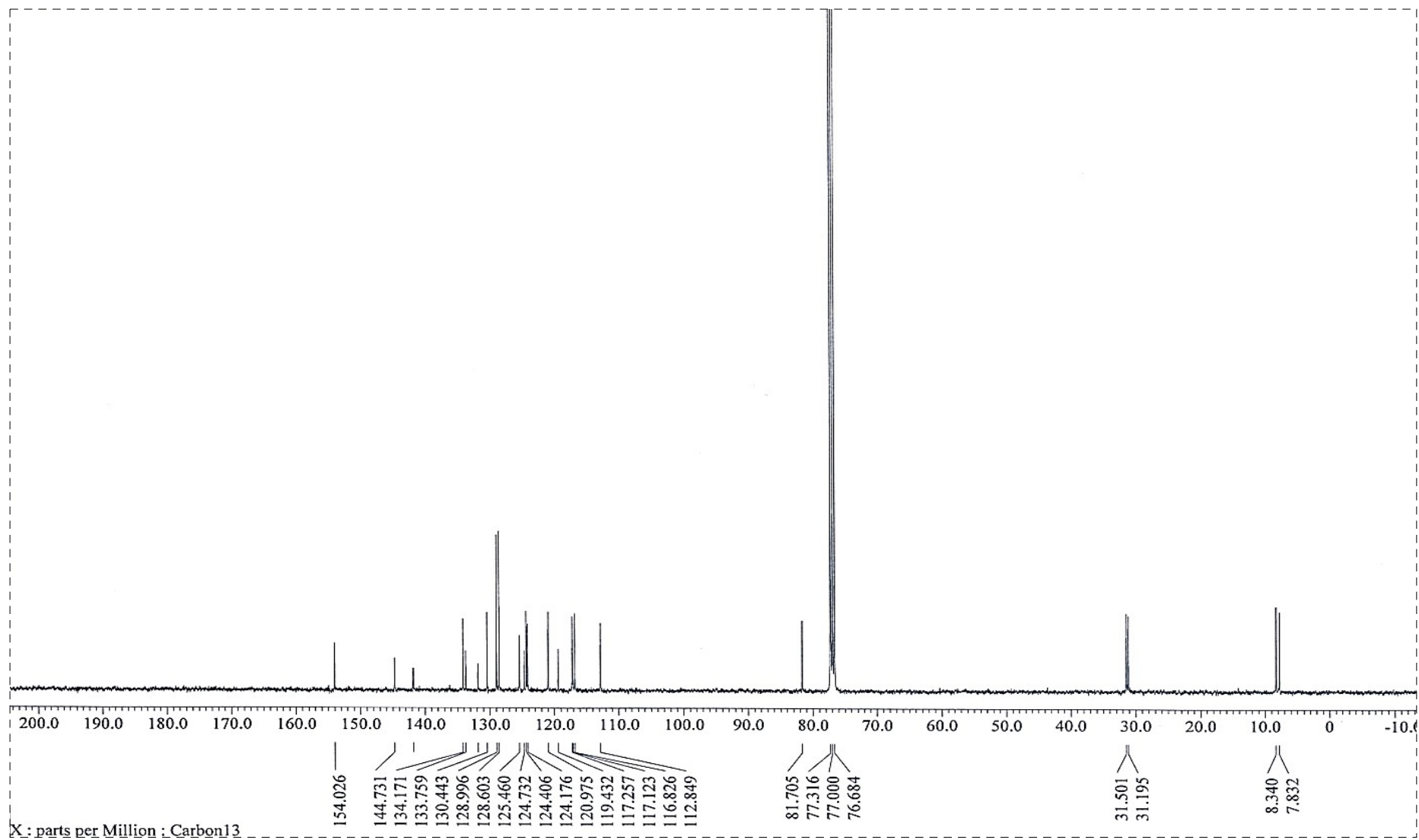


Fig S38: ^{13}C NMR of 2-(4-Chlorophenyl)-3-(2,2-diethyl-2H-Chromen-4-yl)-imidazo[1,2-a]pyridine (**16m**)

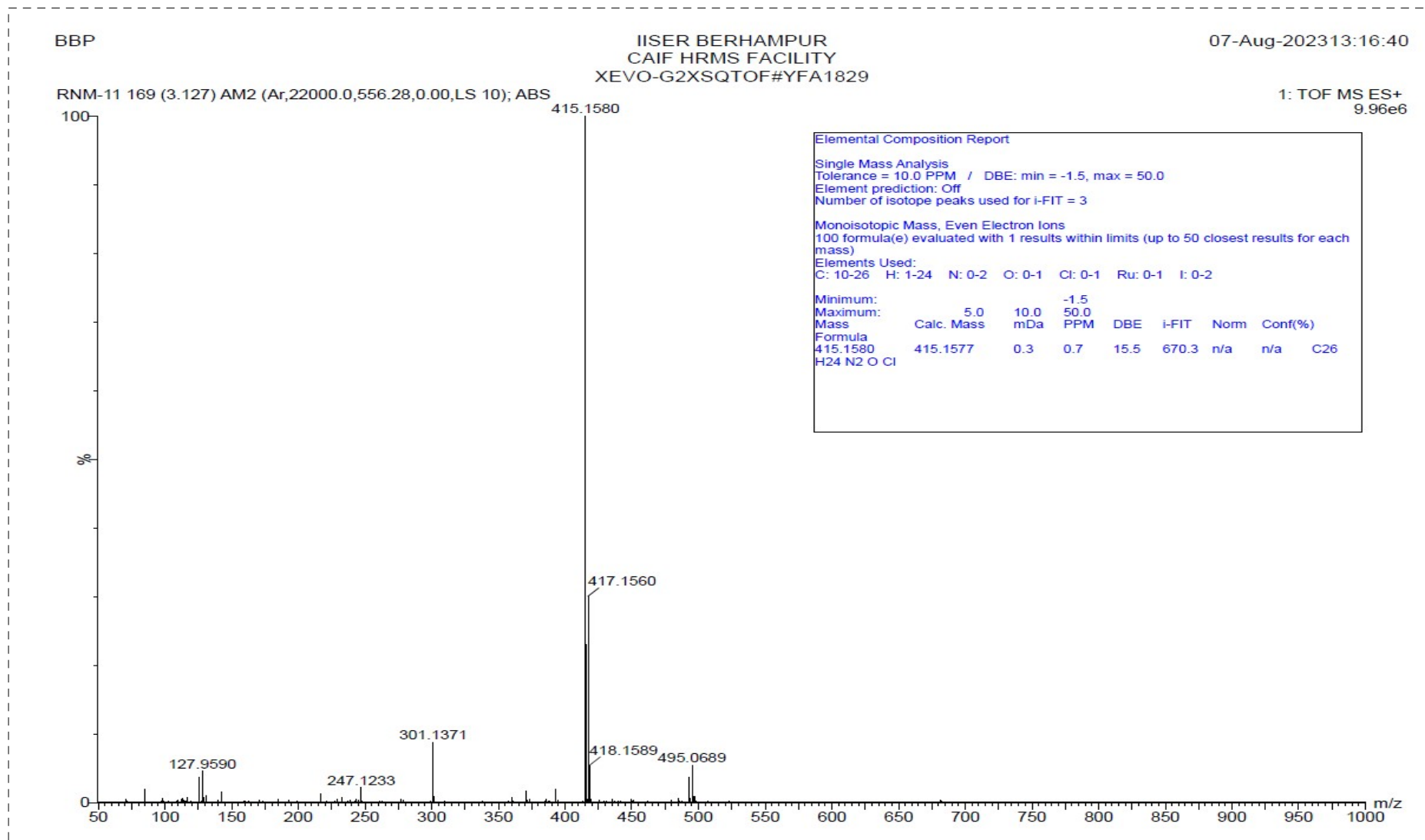


Fig S39: HR-MS of 2-(4-Chlorophenyl)-3-(2,2-diethyl-2H-Chromen-4-yl)-imidazo[1,2-a]pyridine (**16m**)

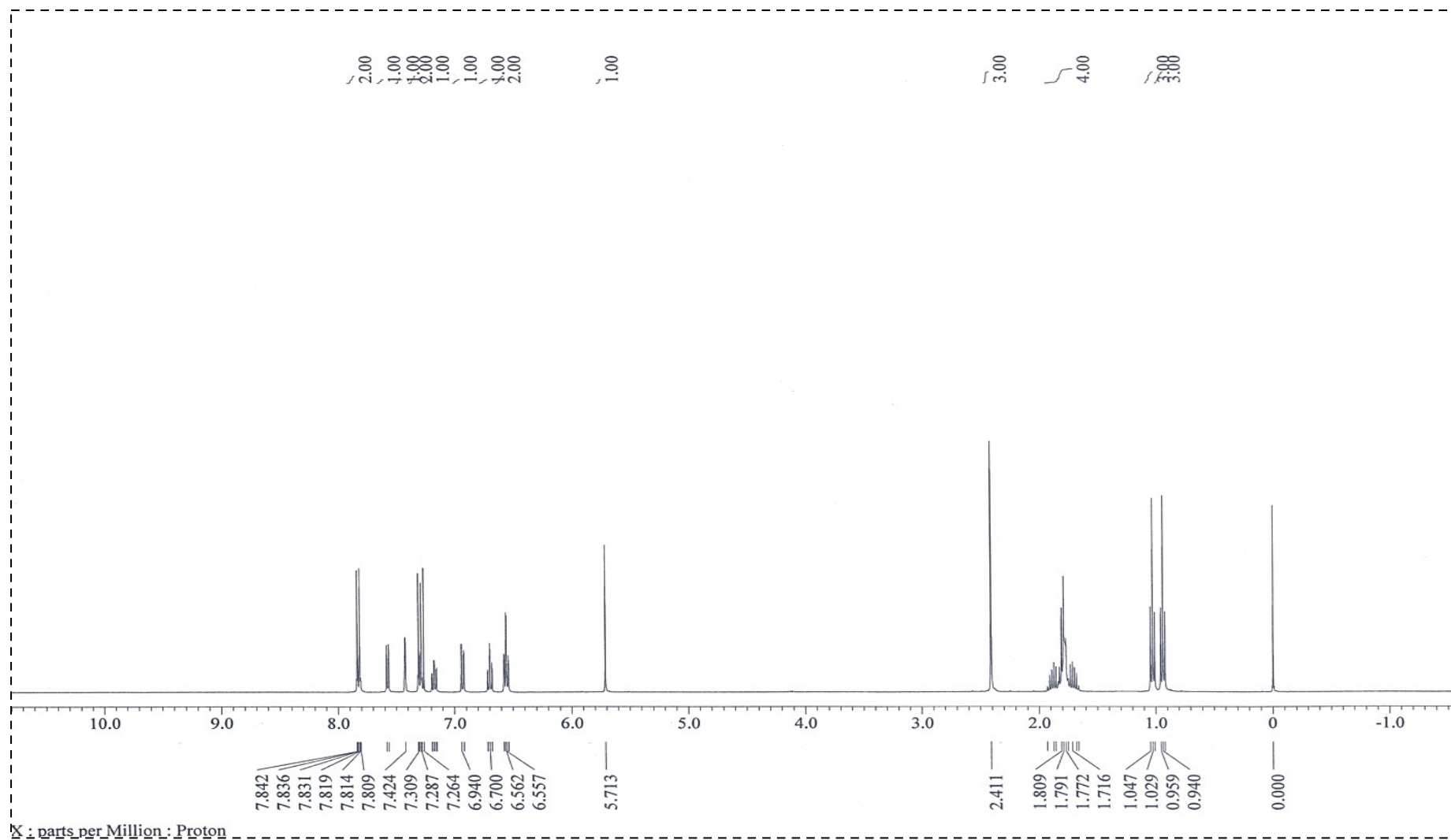


Fig S40: ^1H NMR of 2-(4-chlorophenyl)-3-(2,2-diethyl-2H-chromen-4-yl)-7-methylimidazo[1,2-a]pyridine (**16n**)

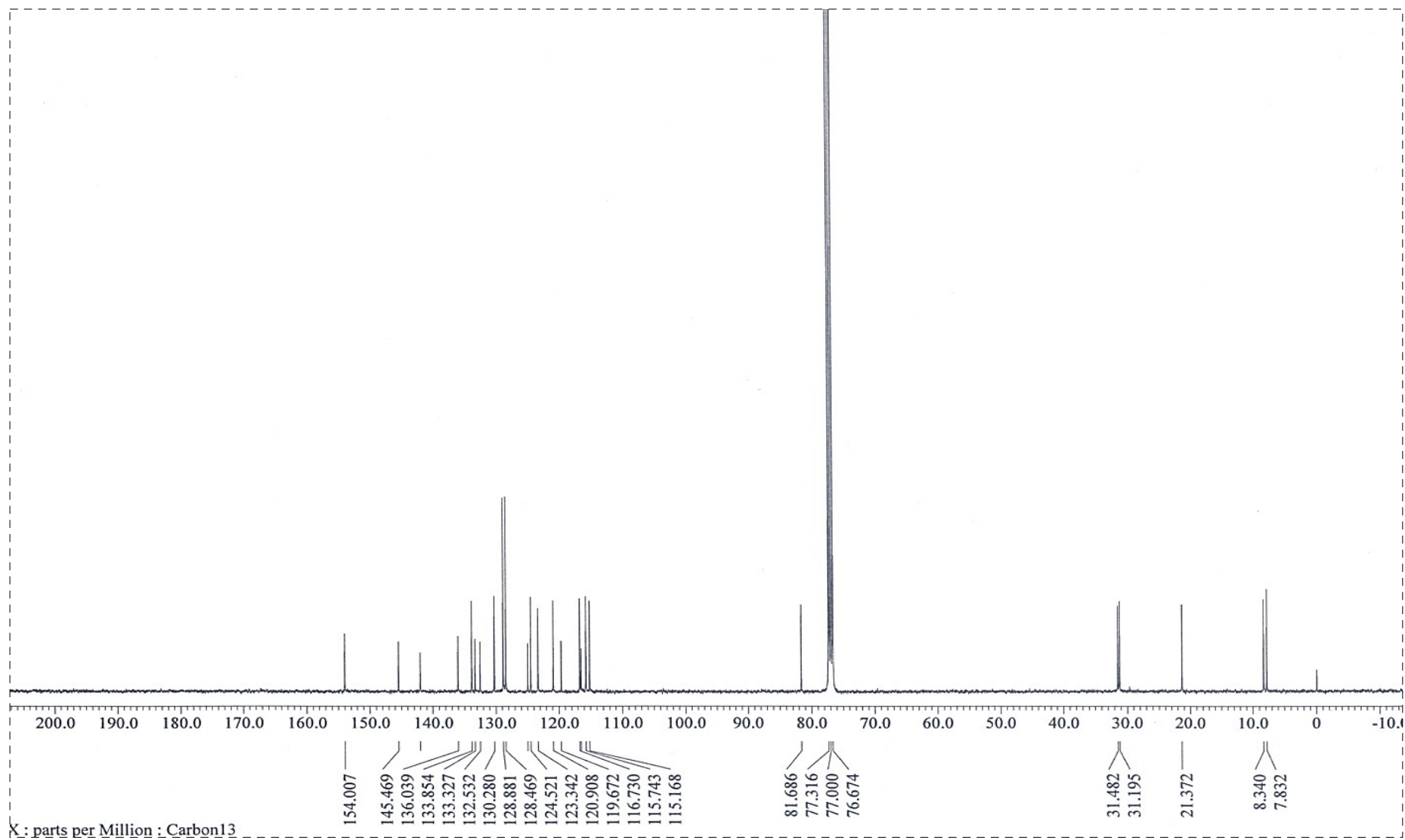


Fig S41: ^{13}C NMR of 2-(4-chlorophenyl)-3-(2,2-diethyl-2H-chromen-4-yl)-7-methylimidazo[1,2-a]pyridine (**16n**)

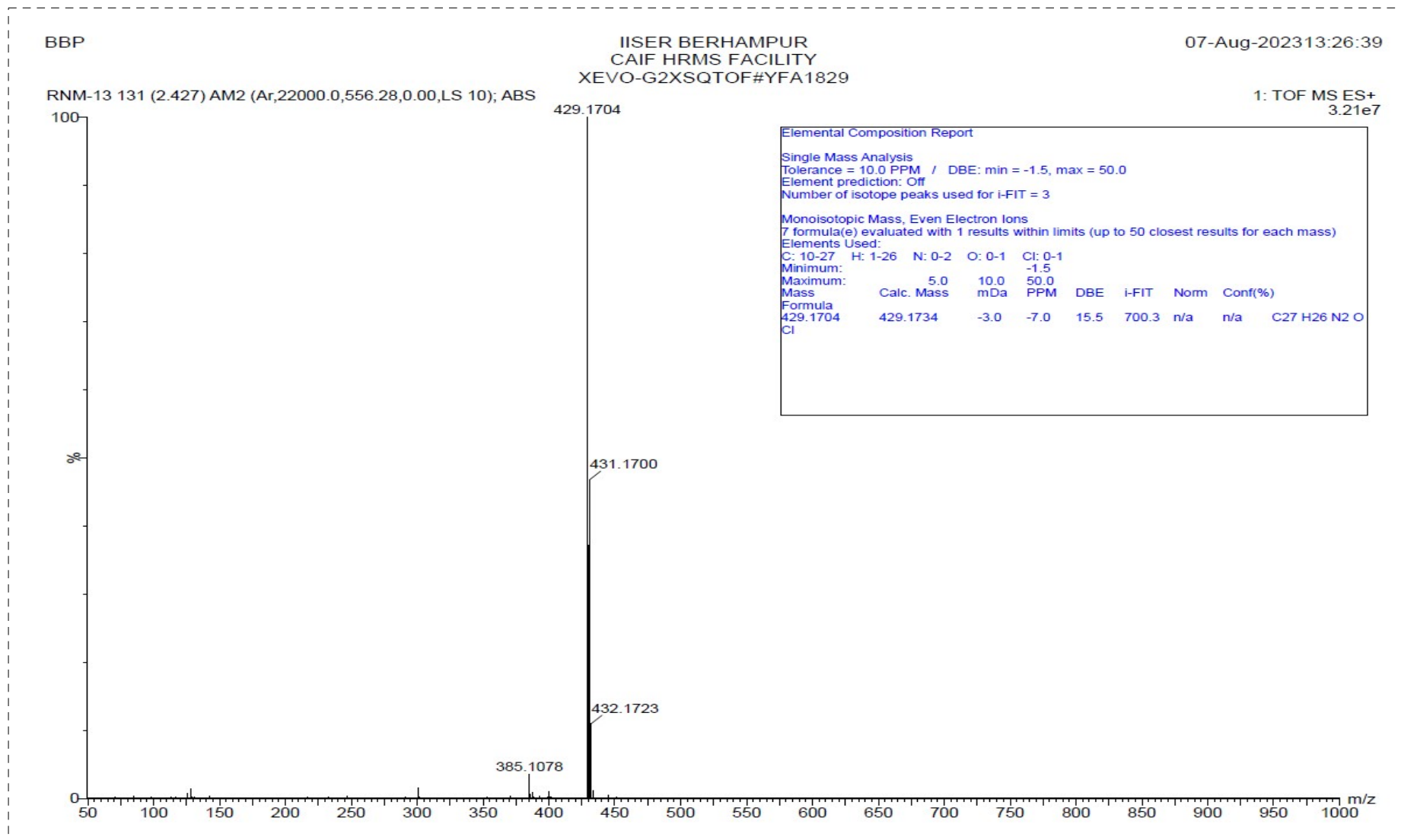


Fig S42: HRMS of 2-(4-chlorophenyl)-3-(2,2-diethyl-2H-chromen-4-yl)-7-methylimidazo[1,2-a]pyridine (**16n**)

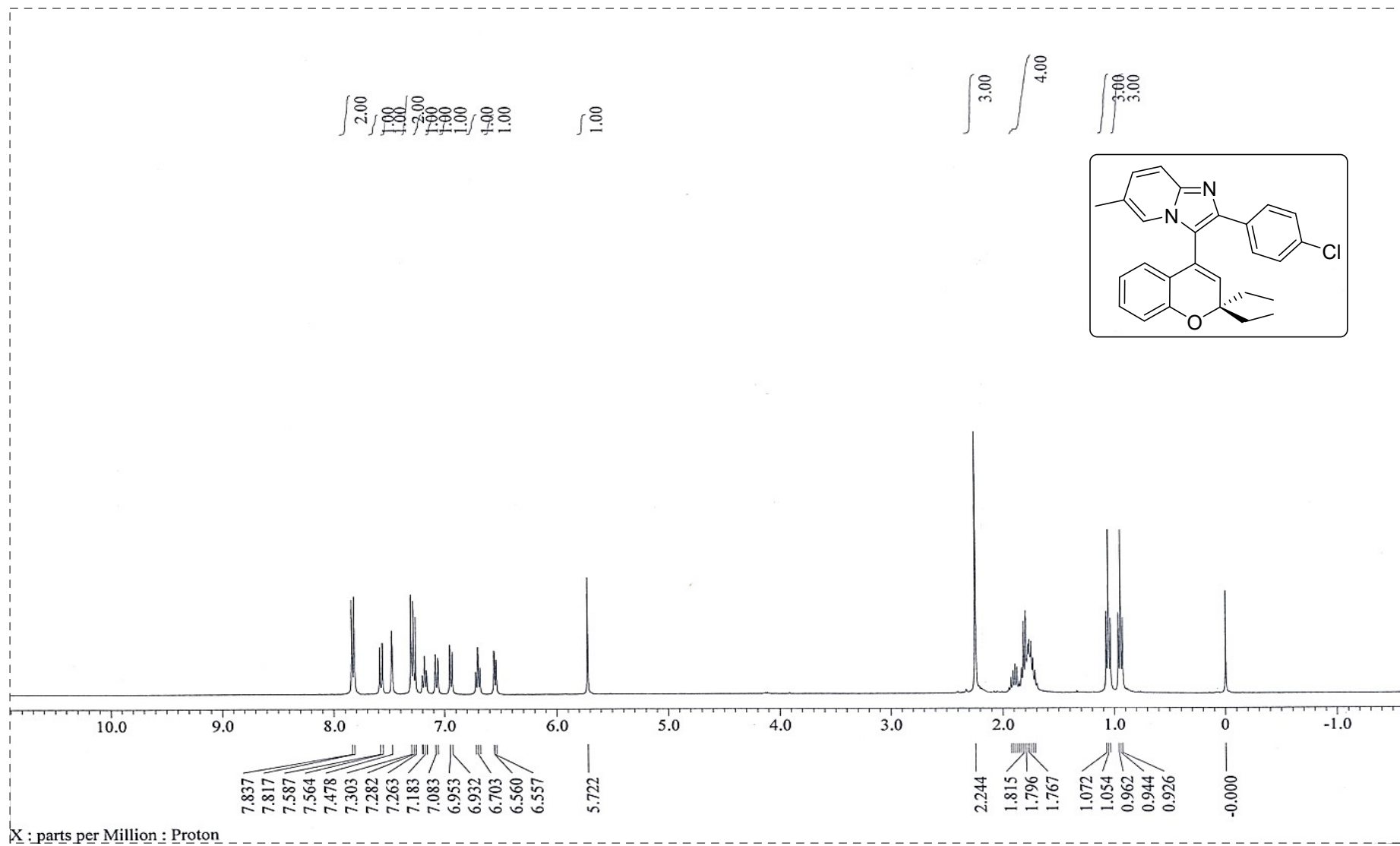


Fig S43: ^1H NMR of 2-(4-chlorophenyl)-3-(2,2-diethyl-2H-chromen-4-yl)-6-methylimidazo[1,2-a]pyridine (**160**)

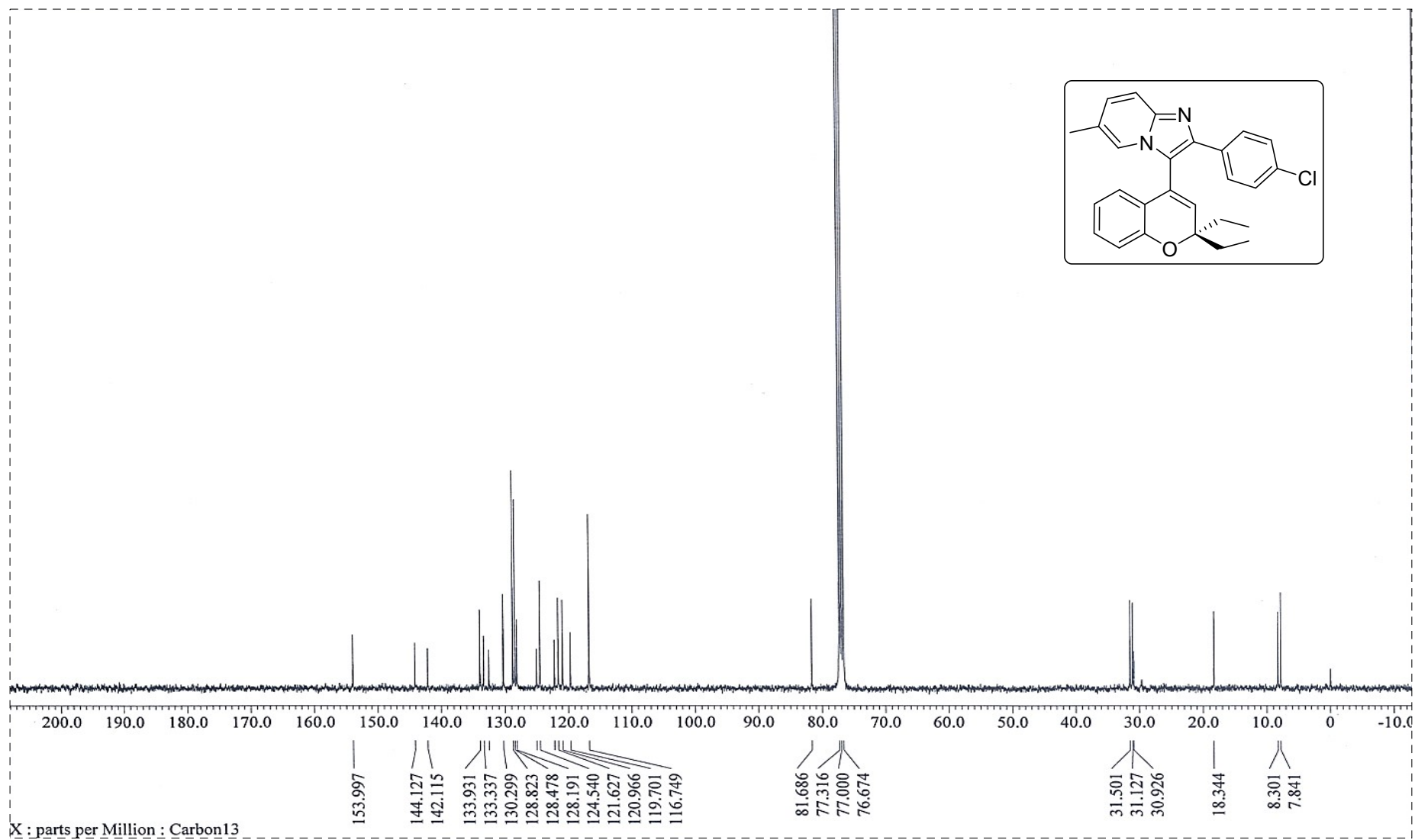


Fig S44: ^{13}C NMR of 2-(4-chlorophenyl)-3-(2,2-diethyl-2H-chromen-4-yl)-6-methylimidazo[1,2-a]pyridine (**160**)

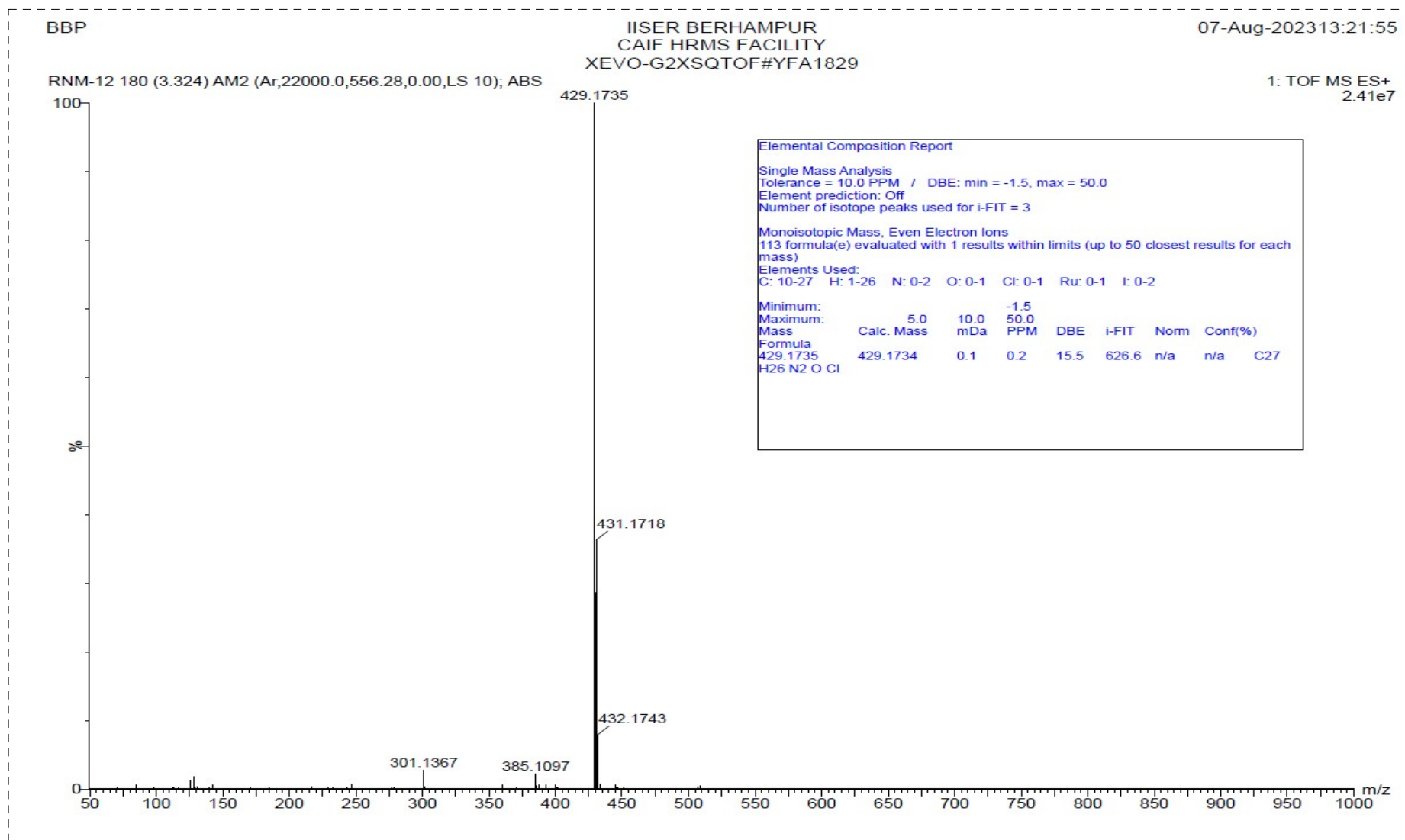


Fig S45: HR-MS of 2-(4-chlorophenyl)-3-(2,2-diethyl-2H-chromen-4-yl)-6-methylimidazo[1,2-a]pyridine (**16o**)

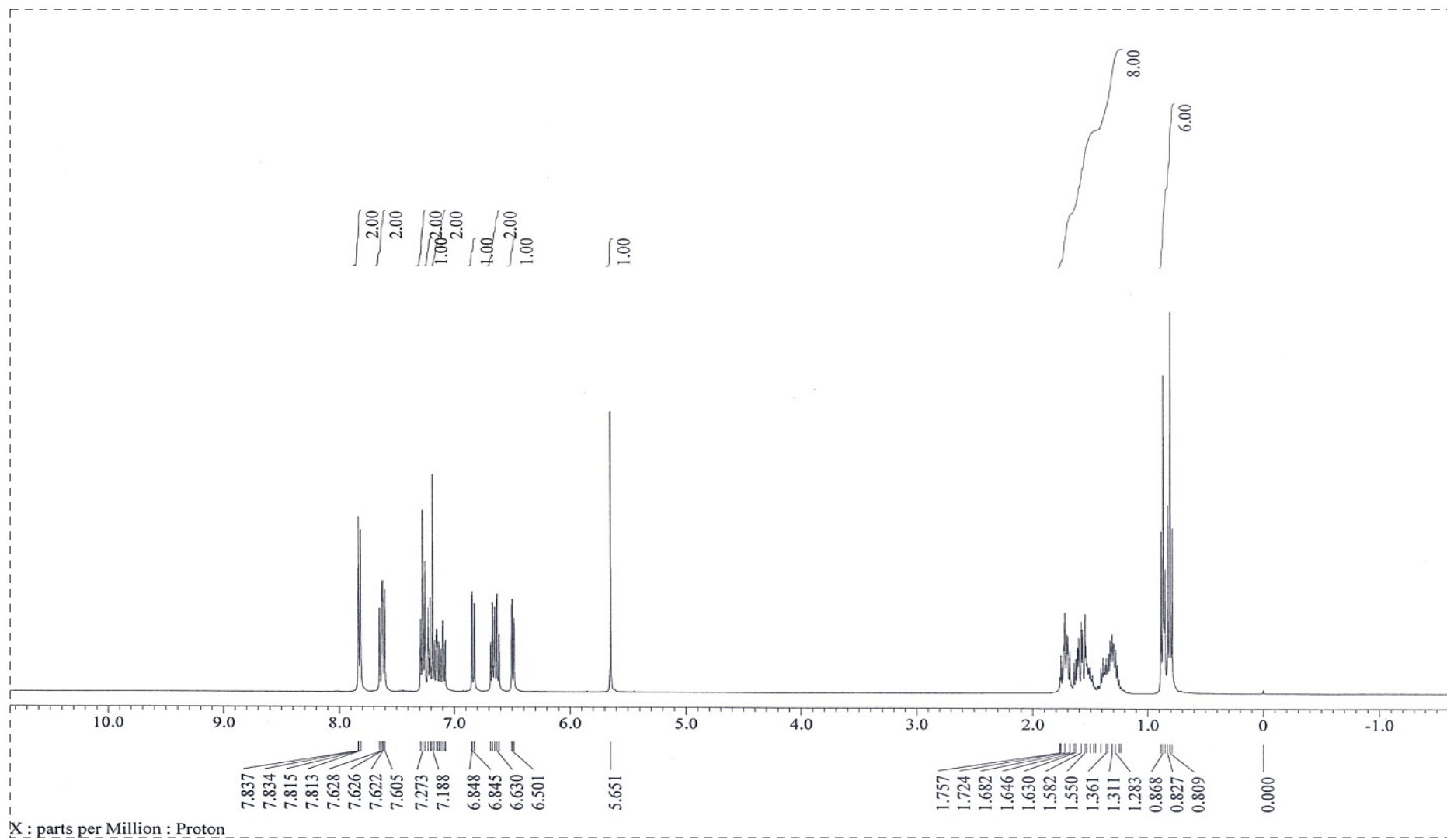


Fig S46: ^1H NMR of 3-(2, 2-dipropyl-2H-chromen-4-yl)-2-phenylimidazo-[1,2-a]pyridine (**16p**)

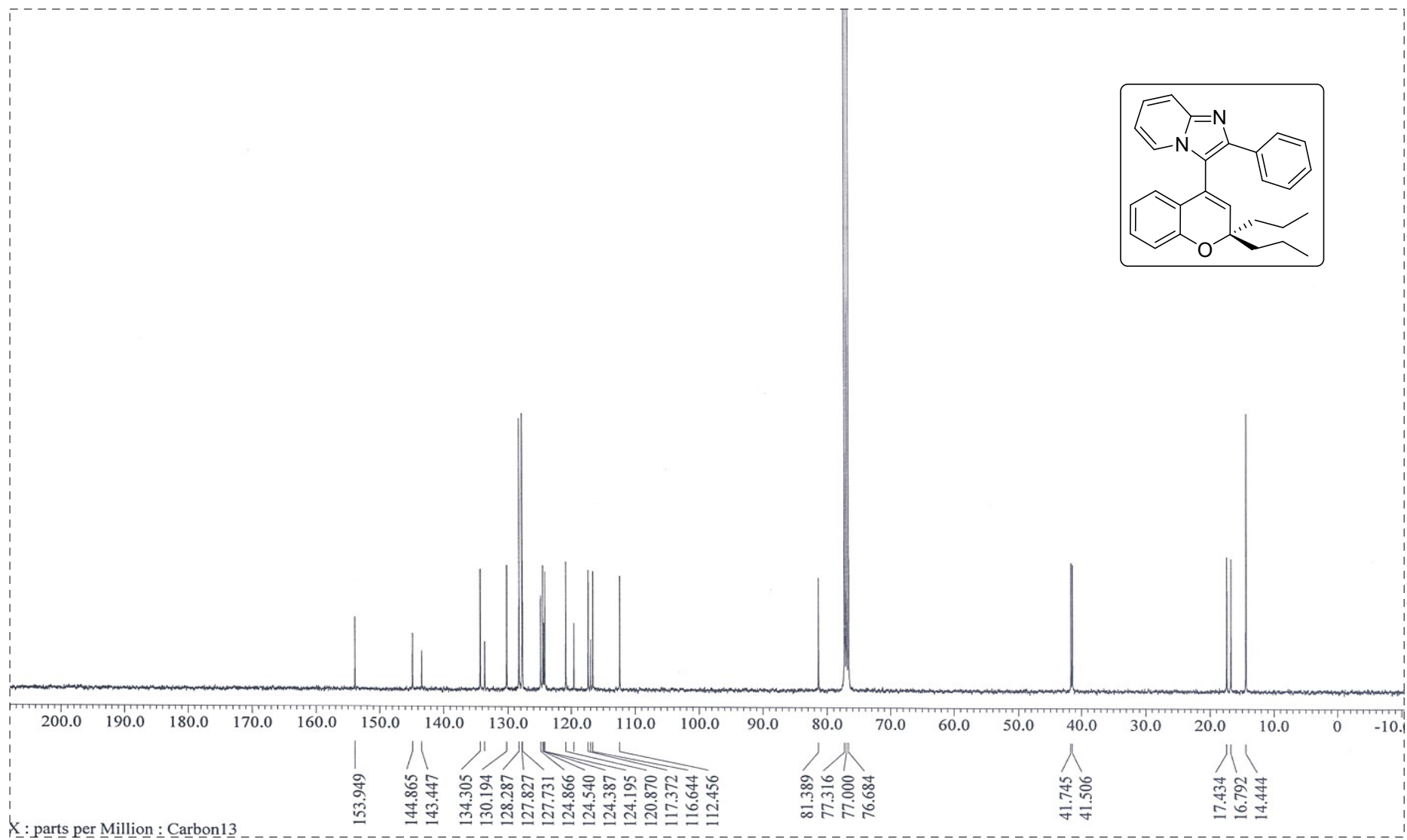


Fig S47: ¹³C NMR of 3-(2, 2-dipropyl-2H-chromen-4-yl)-2-phenylimidazo-[1,2-a]pyridine (**16p**)

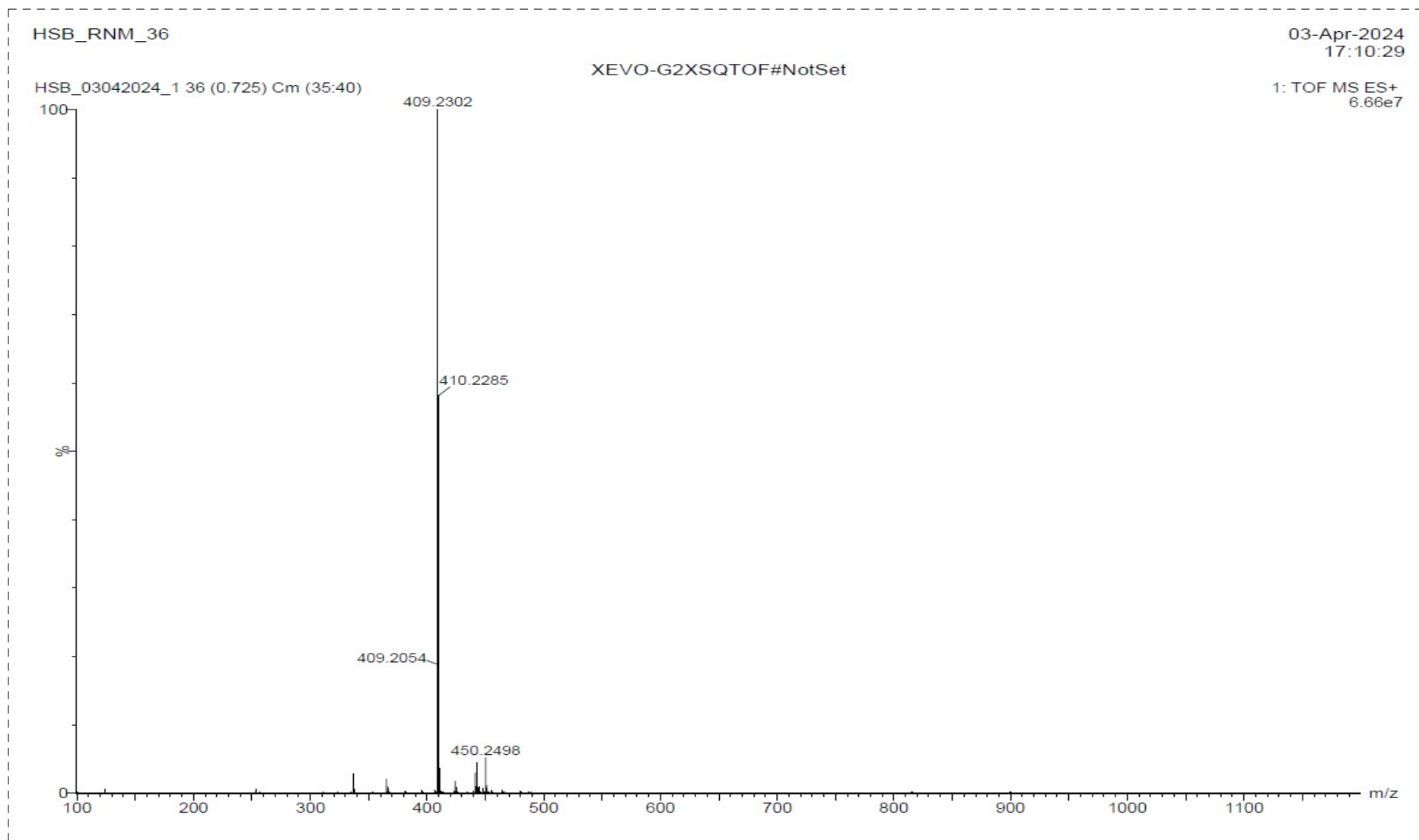


Fig S48: HR-MS of 3-(2, 2-dipropyl-2H-chromen-4-yl)-2-phenylimidazo-[1,2-a]pyridine (**16p**)

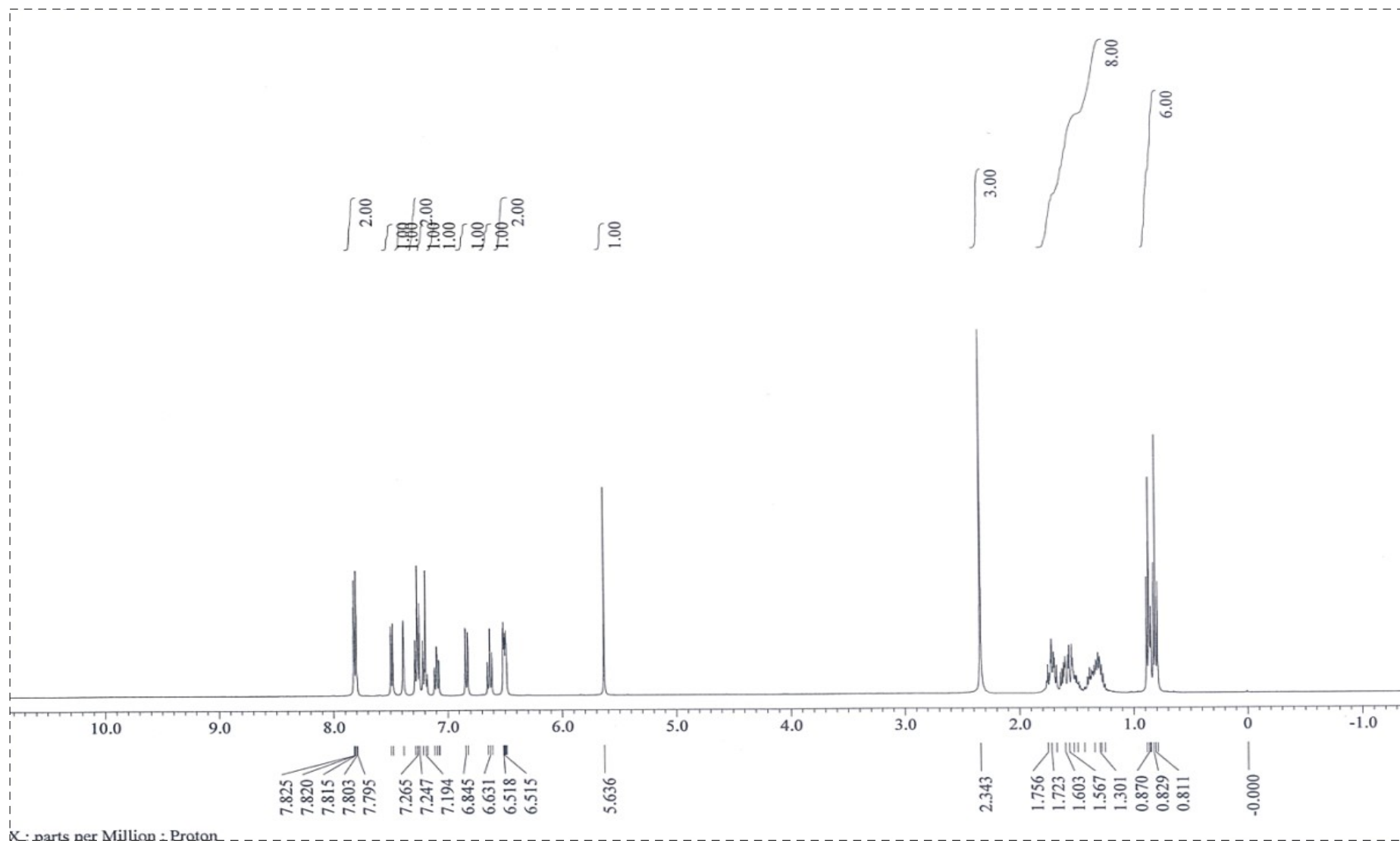


Fig S49: ^1H NMR of 3-(2,2-dipropyl-2H-chromen-4-yl)-7-methyl-2-phenylimidazo[1,2-a]pyridine (**16q**)

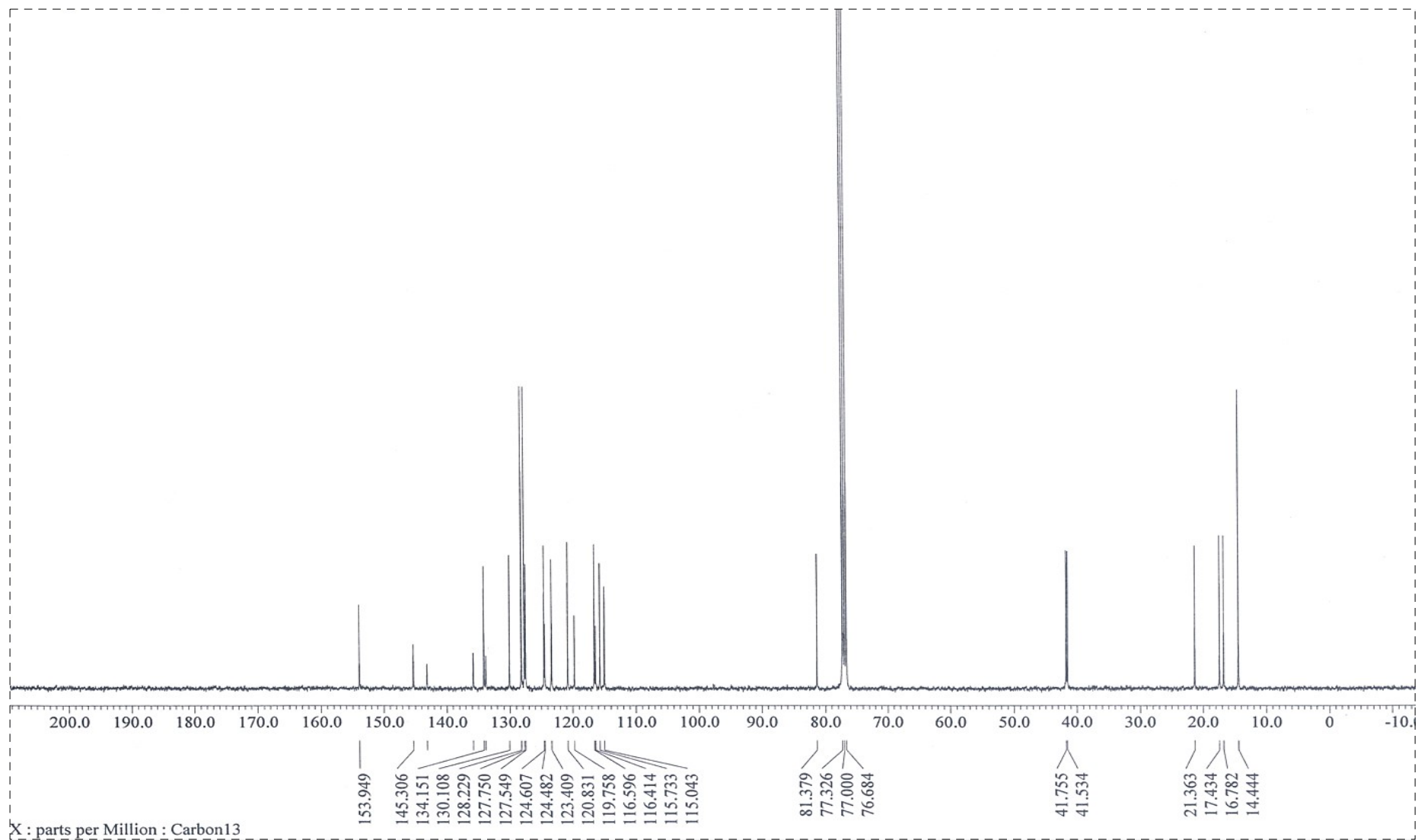


Fig S50: ^{13}C NMR of 3-(2,2-dipropyl-2H-chromen-4-yl)-7-methyl-2-phenylimidazo[1,2-a]pyridine (**16q**)

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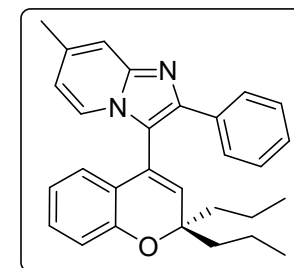
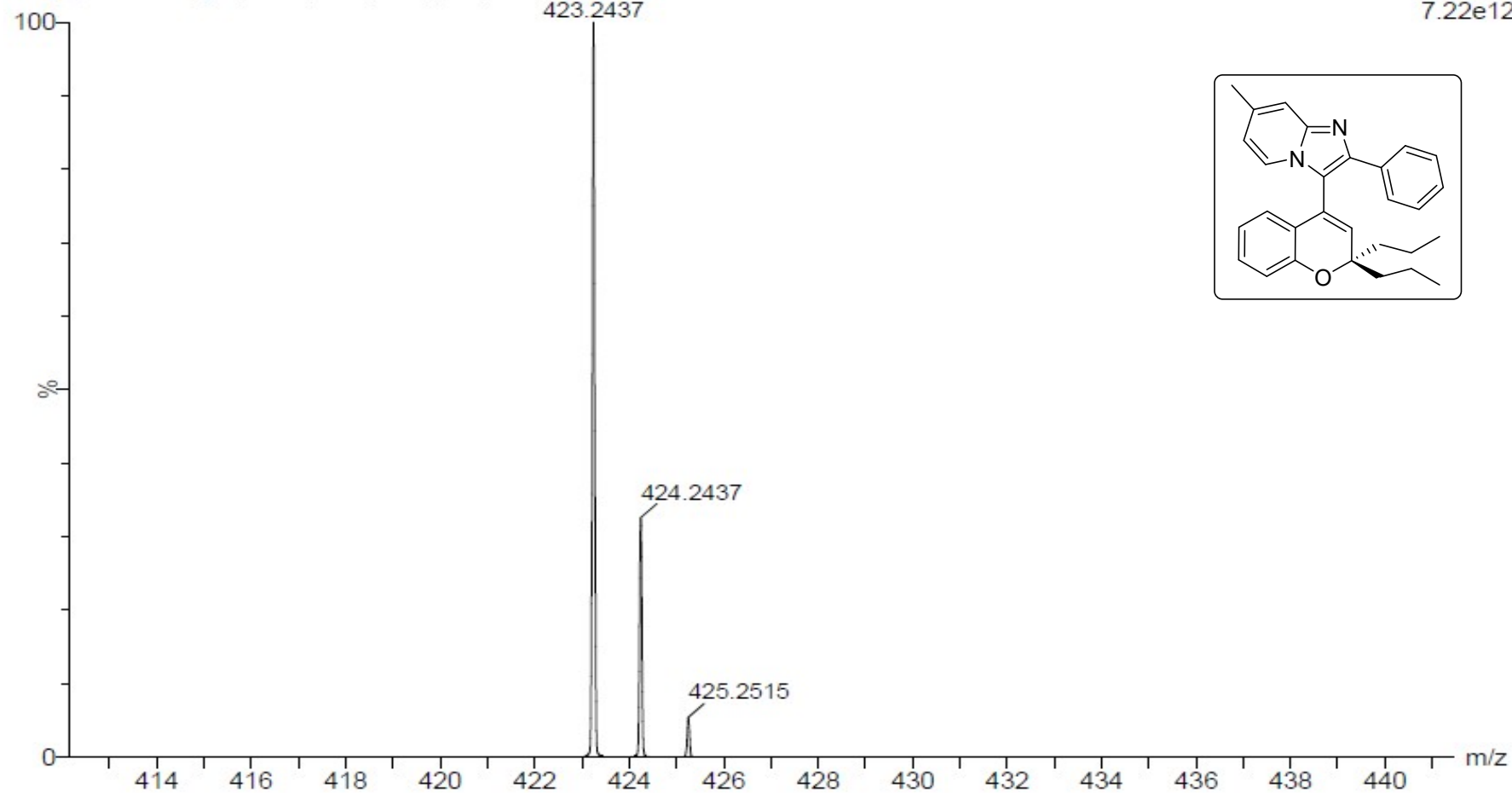


Fig S51: HR-MS of 3-(2,2-dipropyl-2H-chromen-4-yl)-7-methyl-2-phenylimidazo[1,2-a]pyridine (**16q**)

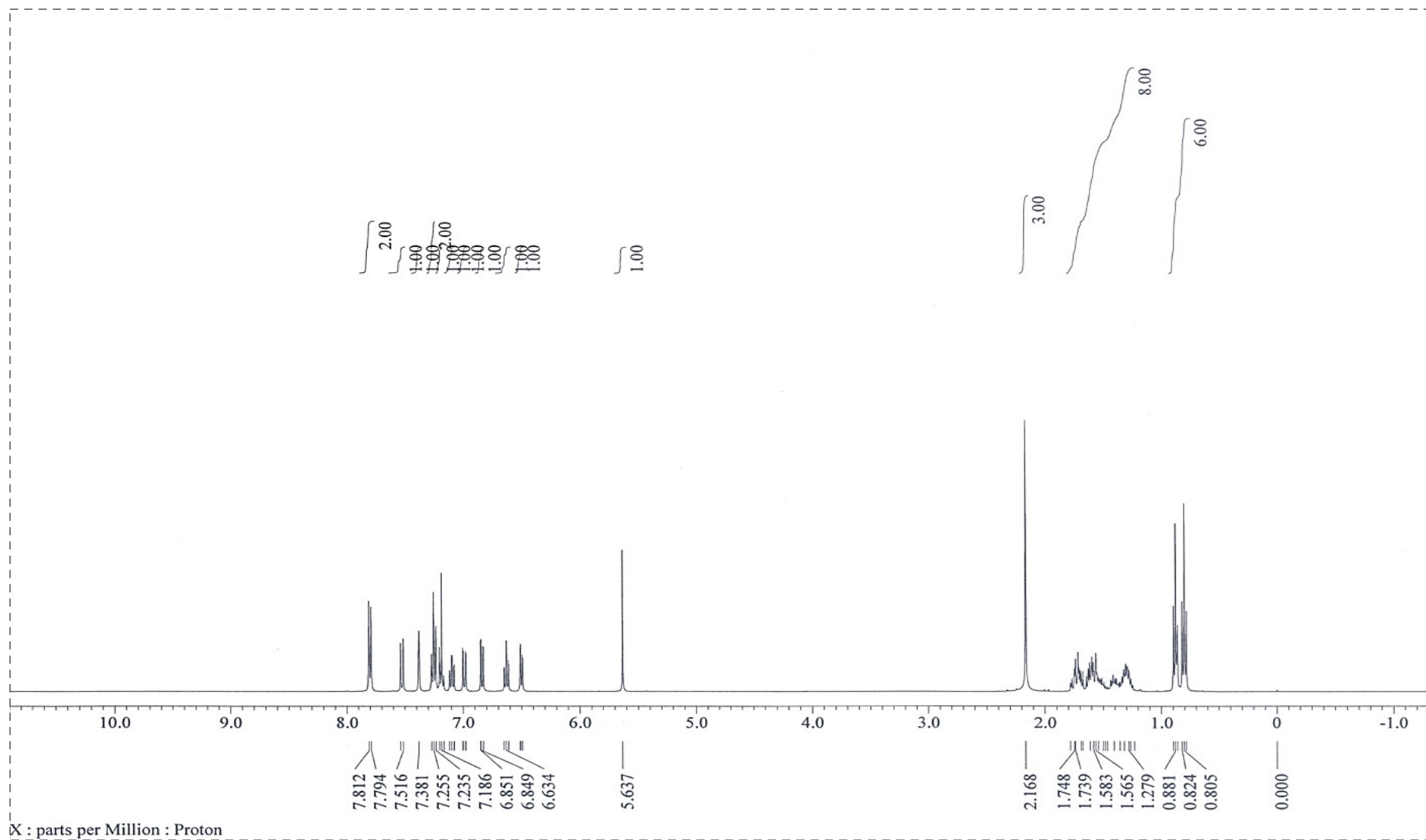


Fig S52: ^1H NMR of 3-(2,2-dipropyl-2H-chromen-4-yl)-6-methyl-2-phenylimidazo-[1,2-a]pyridine (**16r**)

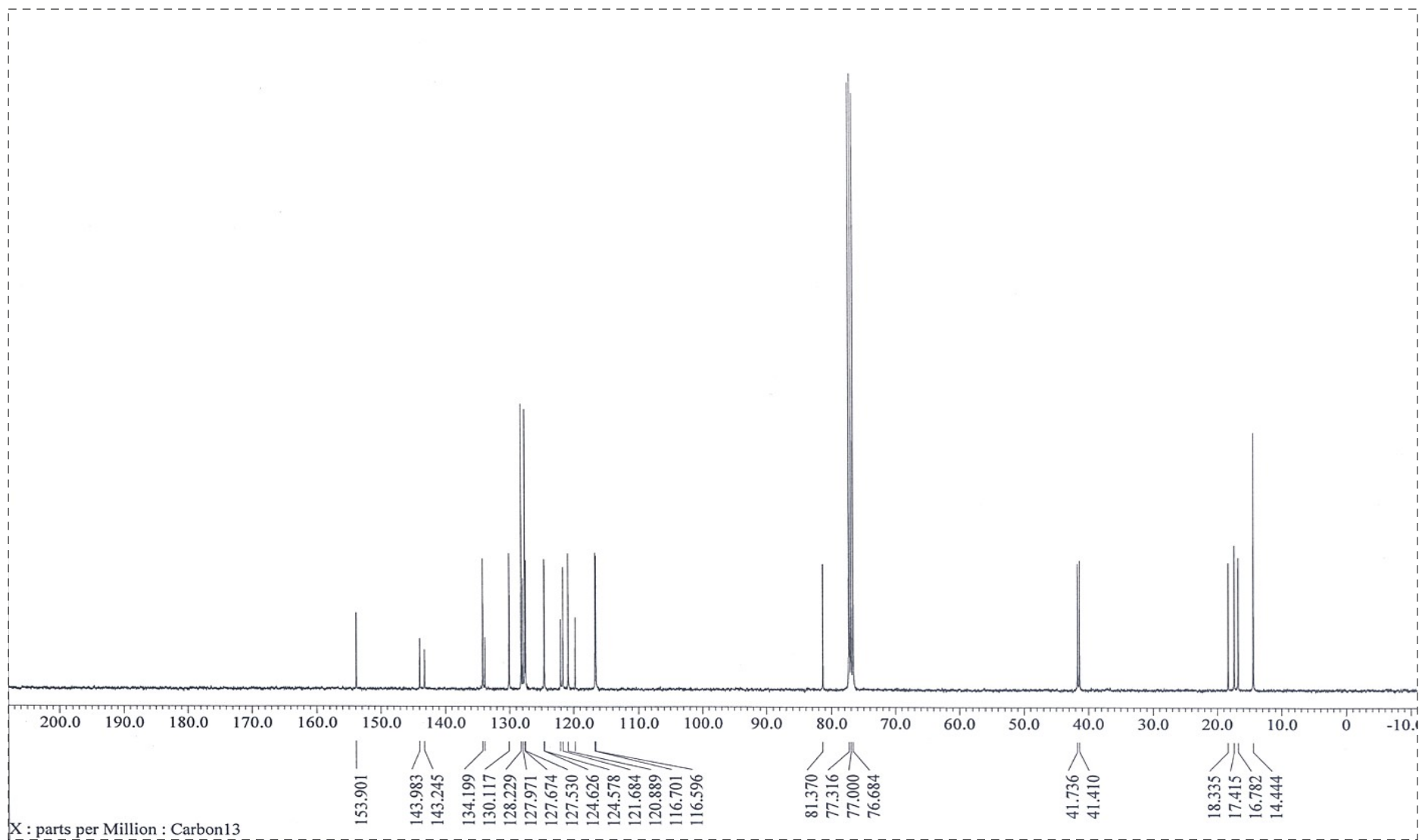


Fig S53: ^{13}C NMR of 3-(2,2-dipropyl-2H-chromen-4-yl)-6-methyl-2-phenylimidazo-[1,2-a]pyridine (**16r**)

HSB_RNM_37_R

03-Apr-2024
17:49:48

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7.22e12

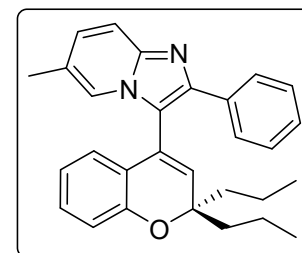
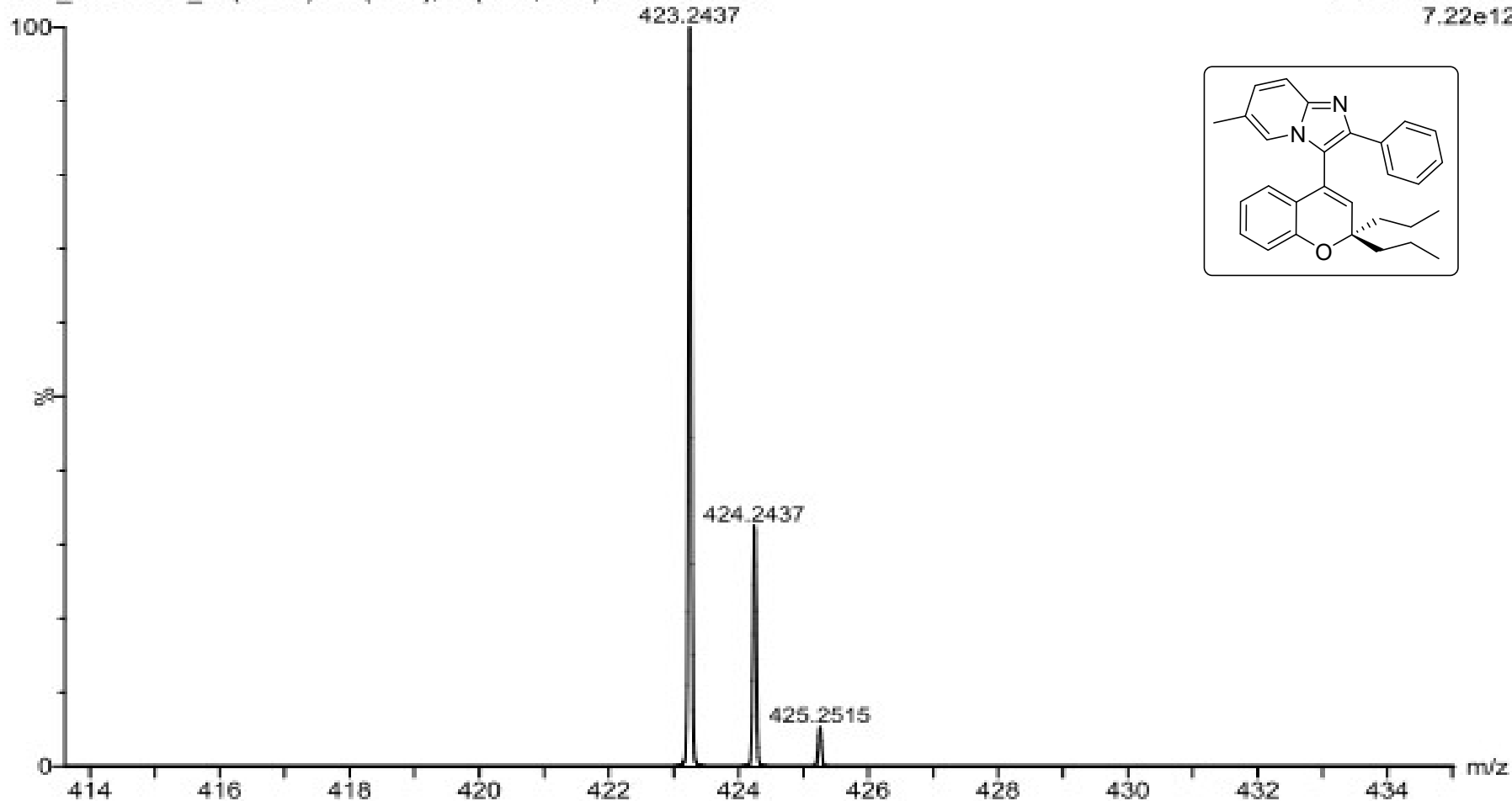


Fig S54: HR-MS of 3-(2,2-dipropyl-2H-chromen-4-yl)-6-methyl-2-phenylimidazo-[1,2-a]pyridine (**16r**)

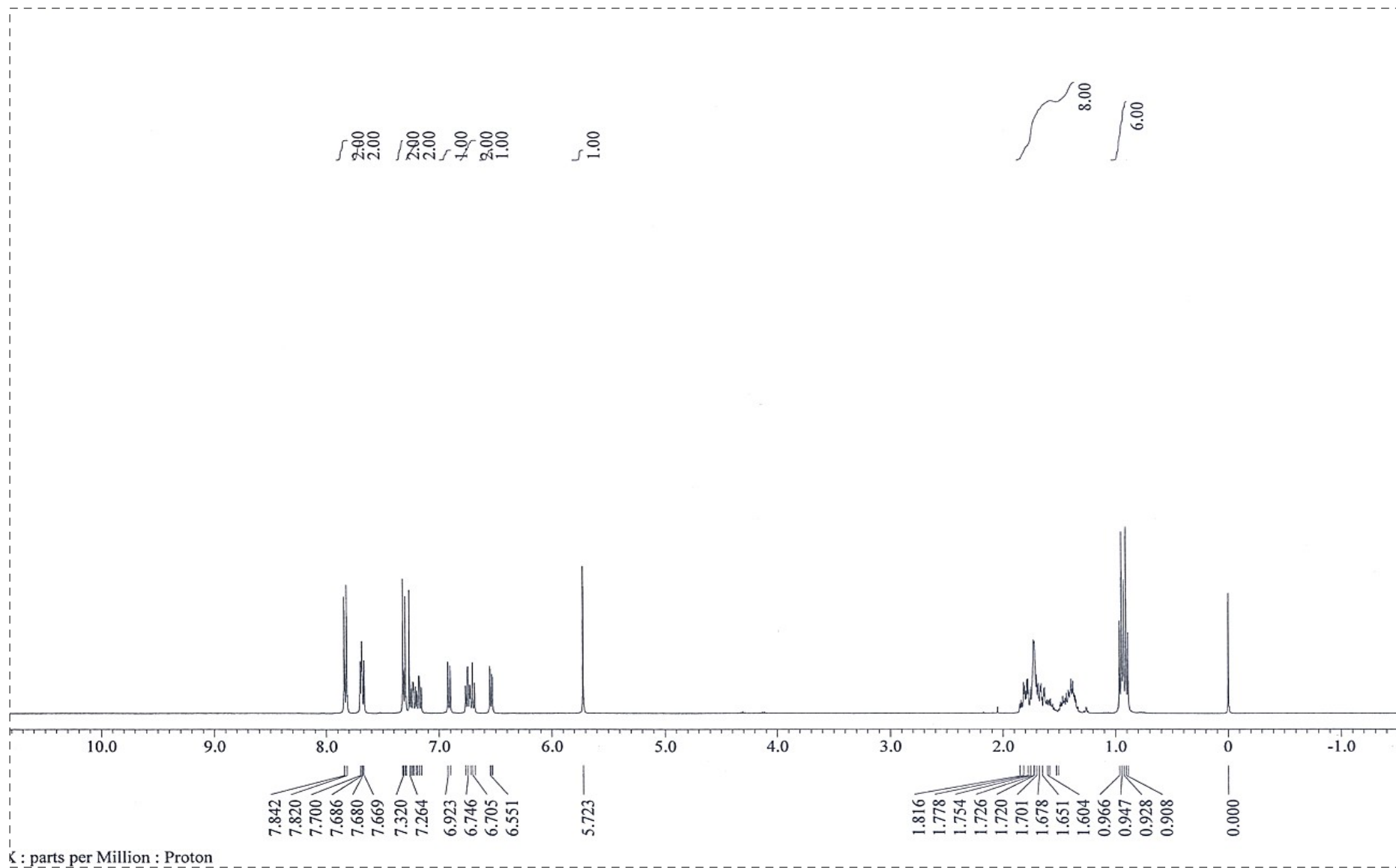


Fig S55: ^1H NMR of 2-(4-chlorophenyl)-3-(2,2-dipropyl-2H-chromen-4-yl)-imidazo-[1,2-a]pyridine (**16s**)

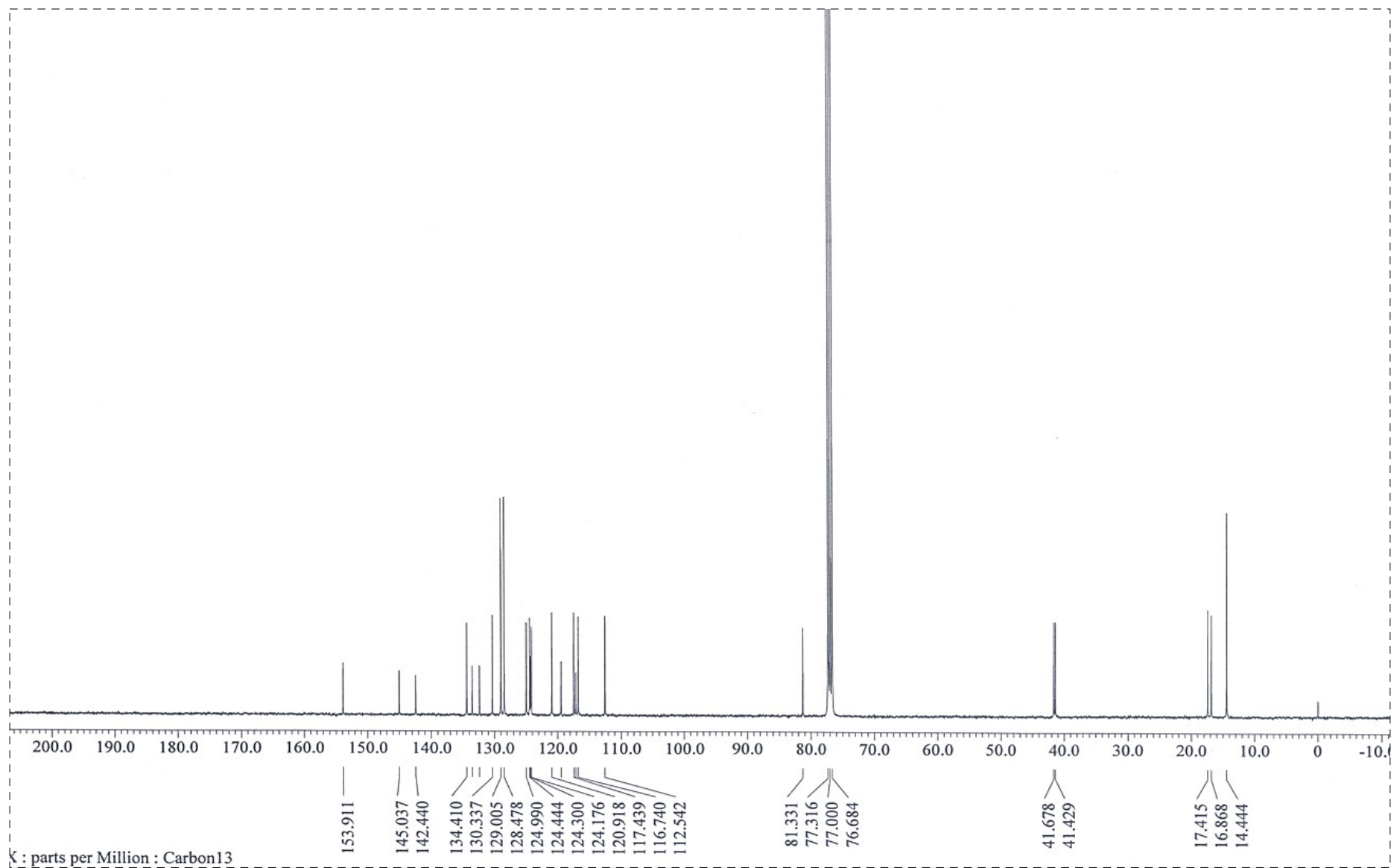


Fig S56: ^{13}C NMR of 2-(4-chlorophenyl)-3-(2,2-dipropyl-2H-chromen-4-yl)-imidazo-[1,2-a]pyridine (**16s**)

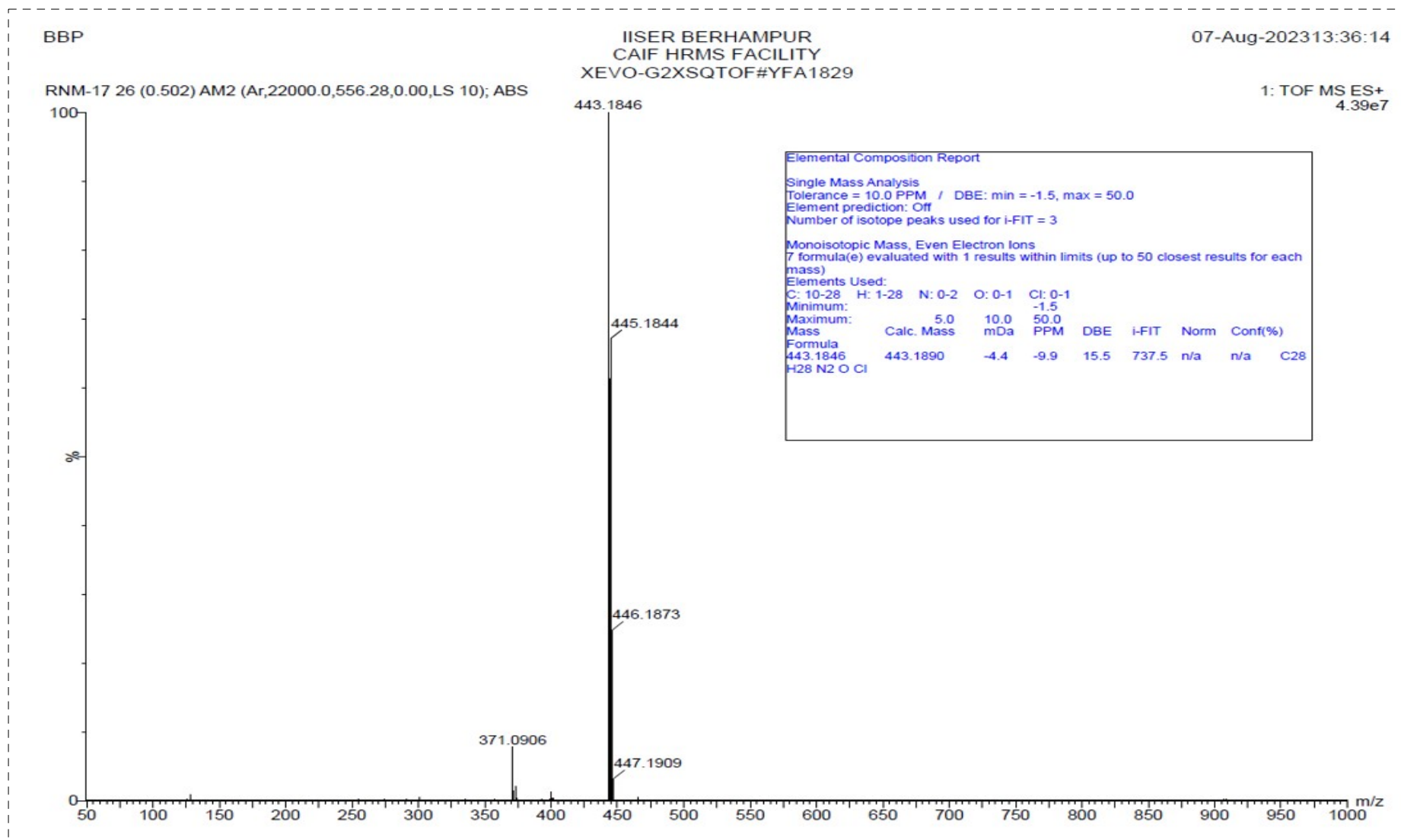


Fig S57: HR-MS of 2-(4-chlorophenyl)-3-(2, 2-dipropyl-2H-chromen-4-yl)-imidazo-[1,2-a]pyridine (16s)

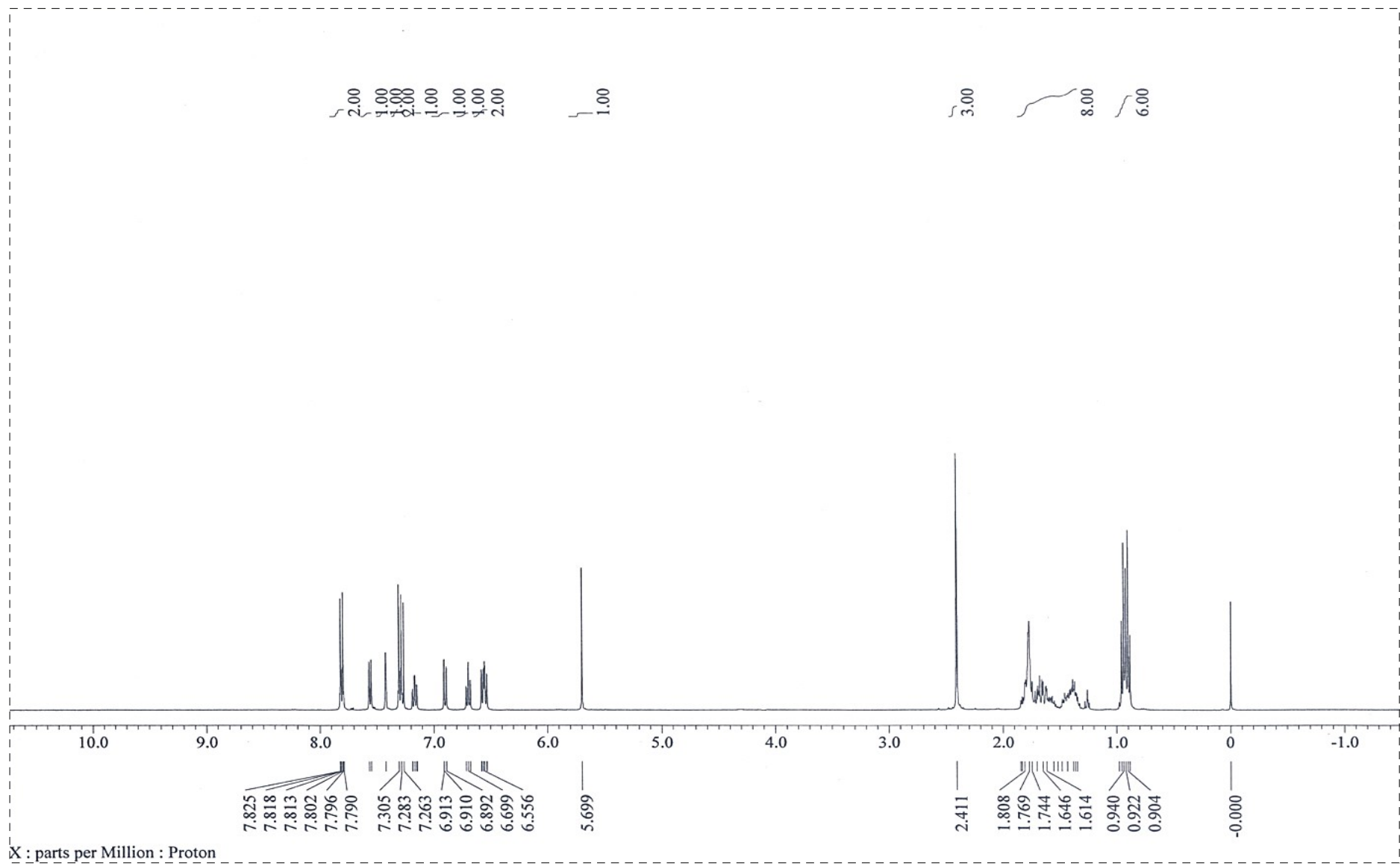


Fig S58: ^1H NMR of 2-(4-chlorophenyl)-3-(2,2-dipropyl-2H-chromen-4-yl)-7-methylimidazo[1,2-a]pyridine (**16t**)

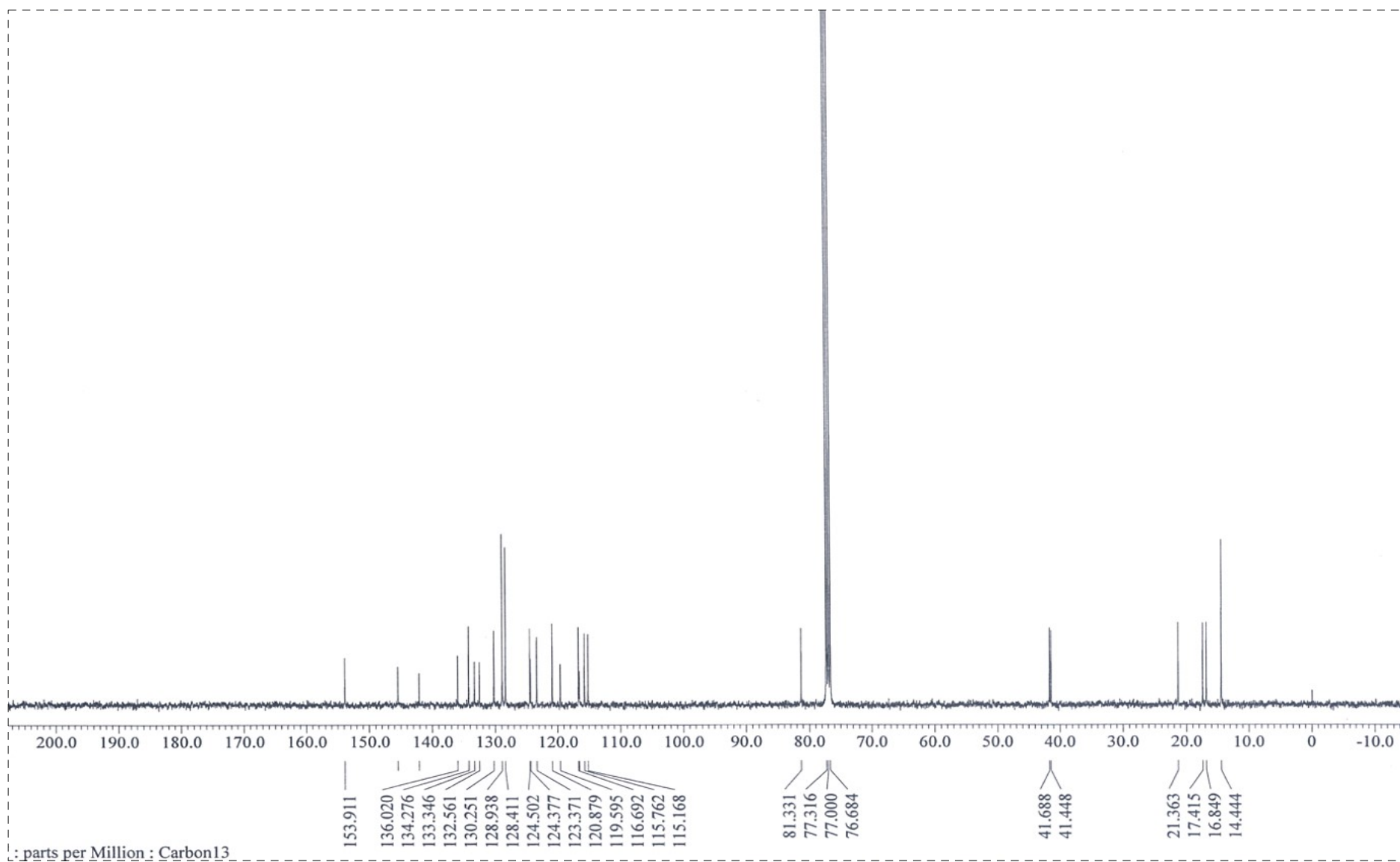


Fig S59: ¹³C NMR of 2-(4-chlorophenyl)-3-(2,2-dipropyl-2H-chromen-4-yl)-7-methylimidazo[1,2-a]pyridine (**16t**)

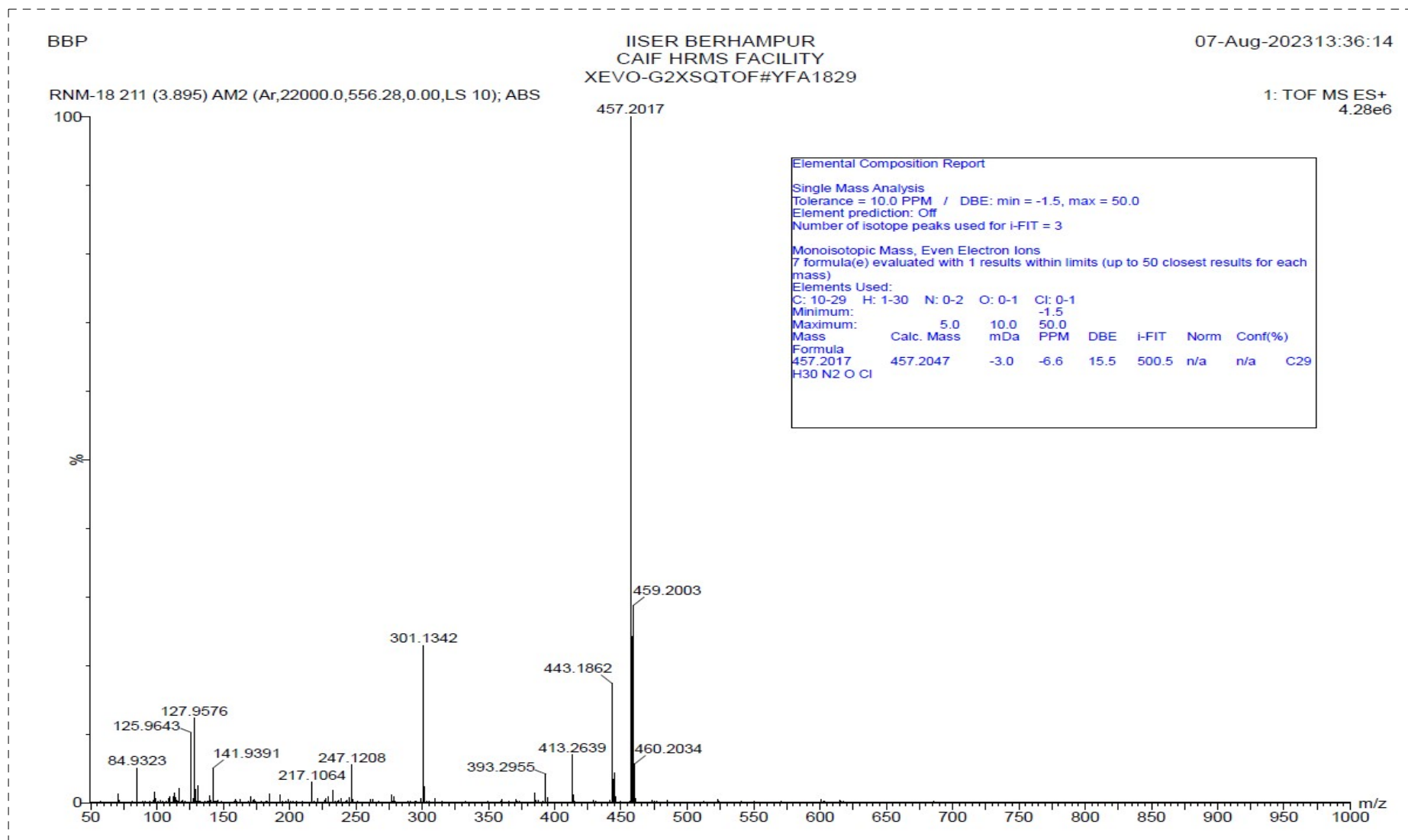


Fig S60: HR-MS of 2-(4-chlorophenyl)-3-(2,2-dipropyl-2H-chromen-4-yl)-7-methylimidazo[1,2-a]pyridine (**16t**)

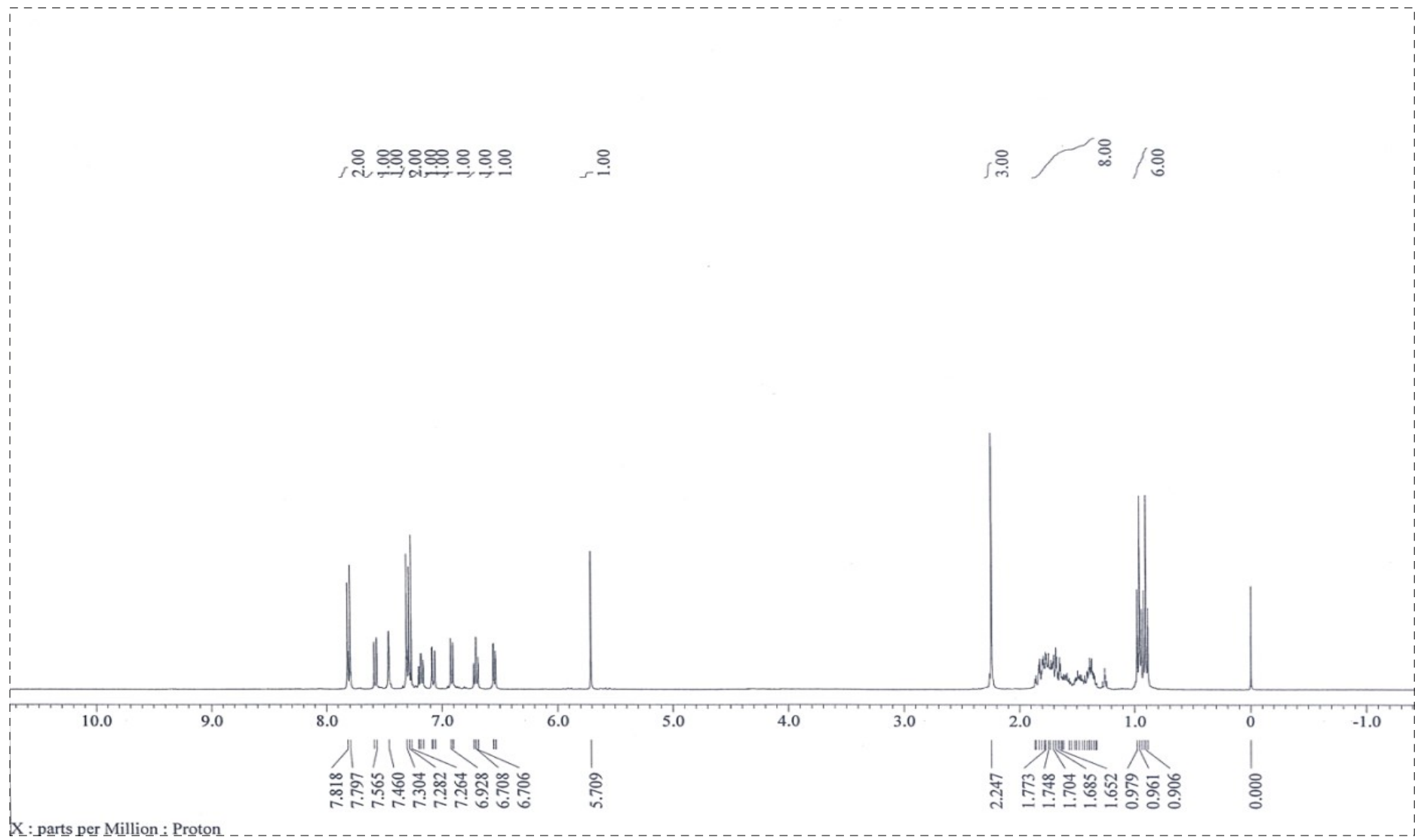


Fig S61: ¹H NMR of 2-(4-chlorophenyl)-3-(2,2-dipropyl-2H-chromen-4-yl)-7,6-methylimidazo-[1,2-a]pyridine (**16u**)

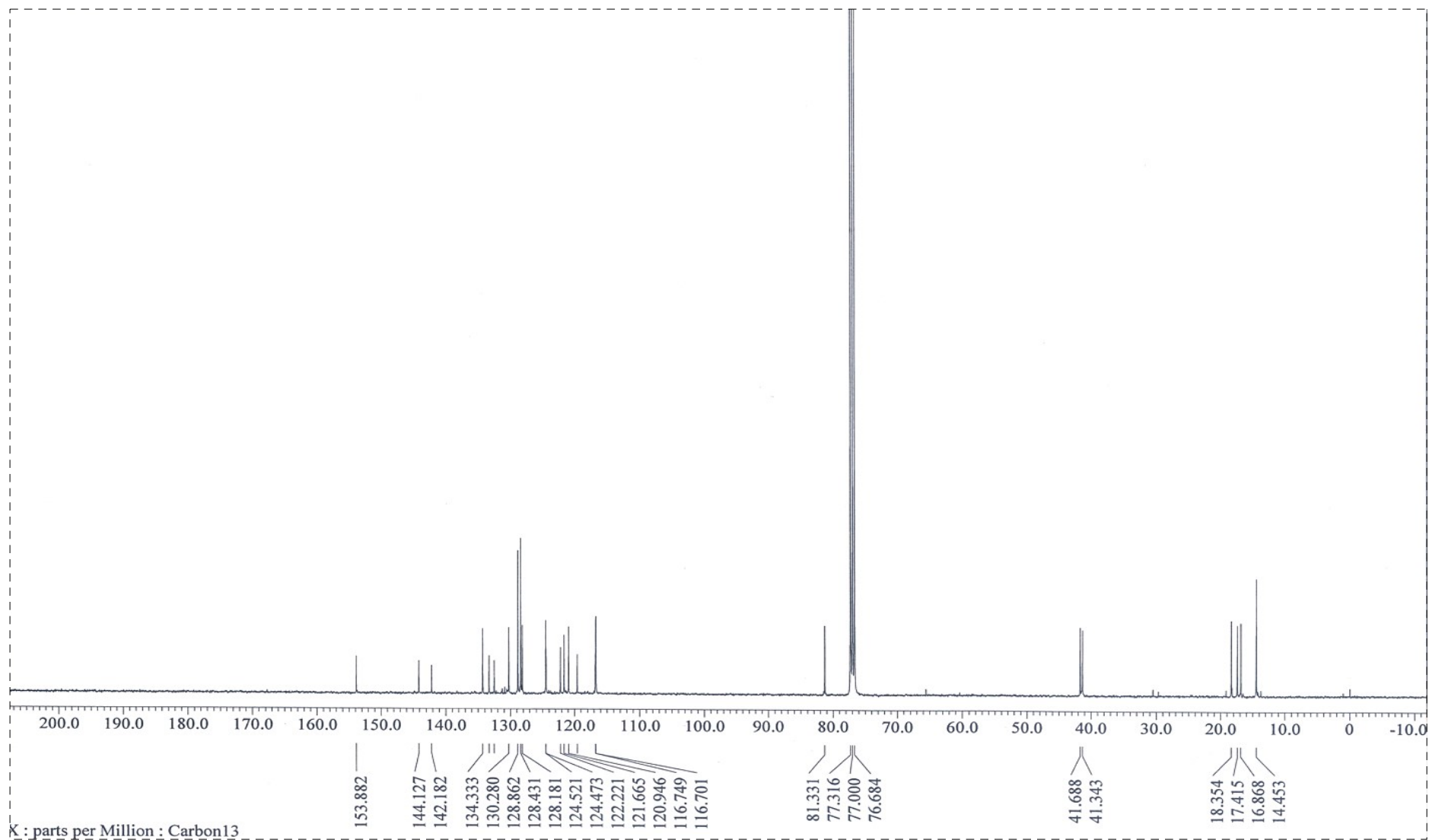


Fig S62: ^{13}C NMR of 2-(4-chlorophenyl)-3-(2,2-dipropyl-2H-chromen-4-yl)-7,6-methylimidazo-[1,2-a]pyridine (**16u**)

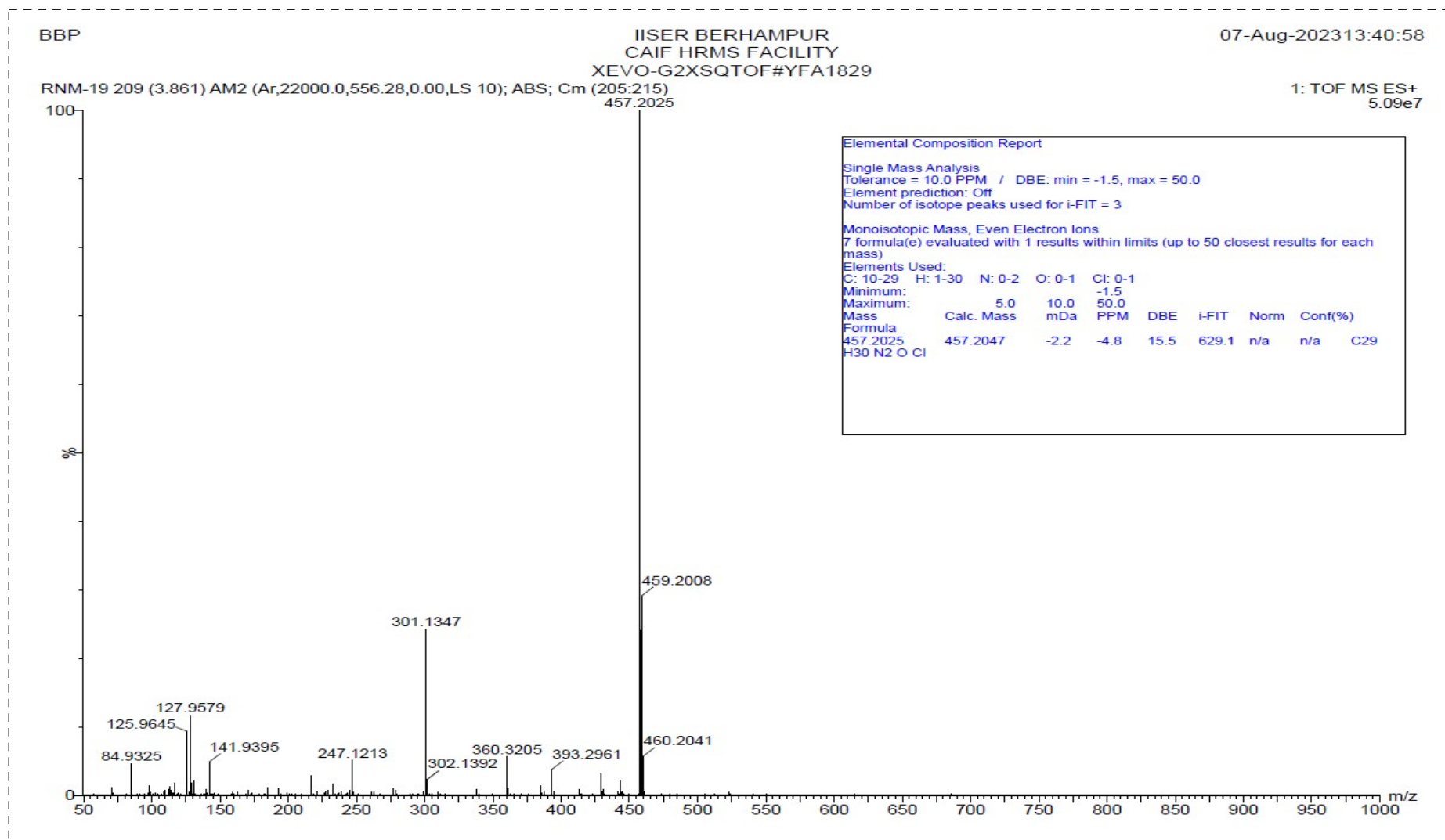


Fig S63: HR-MS of 2-(4-chlorophenyl)-3-(2,2-dipropyl-2H-chromen-4-yl)-7-6-methylimidazo-[1,2-a]pyridine (**16u**)

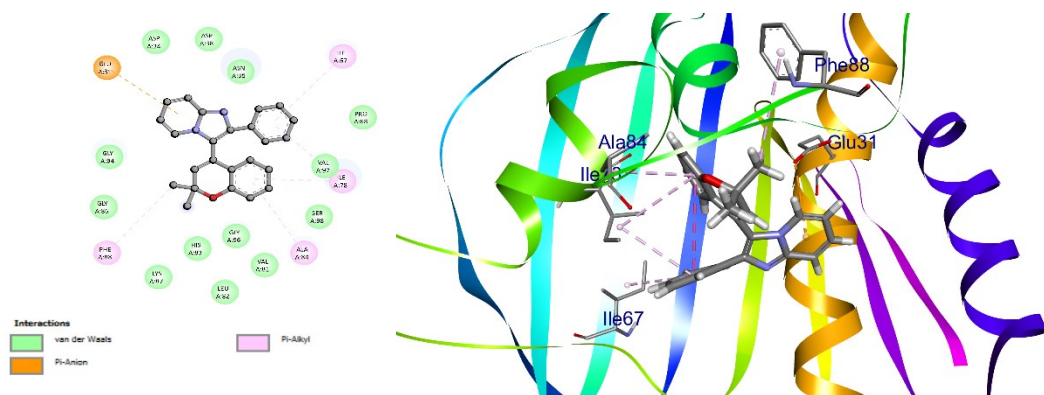


Fig. S64. Docking interaction and 3D binding image of compound **16a** with *E. coli* DNA gyrase (PDBID: 1AJ6)

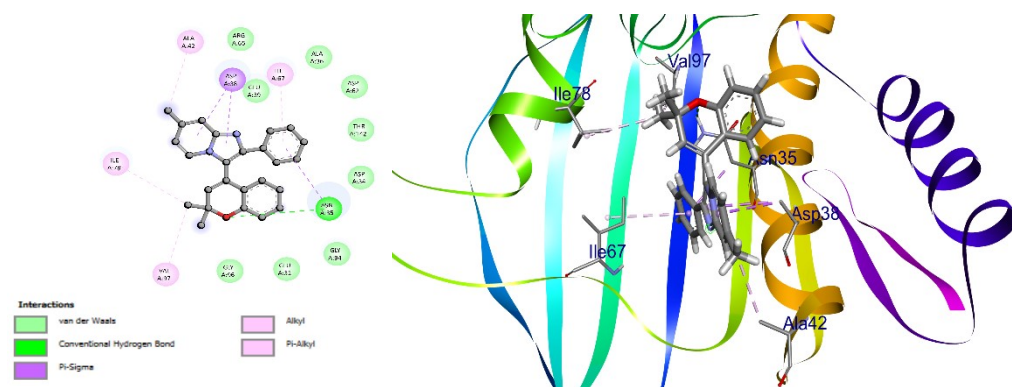


Fig. S65. Docking interaction and 3D binding image of compound **16b** with *E. coli* DNA gyrase (PDBID: 1AJ6)

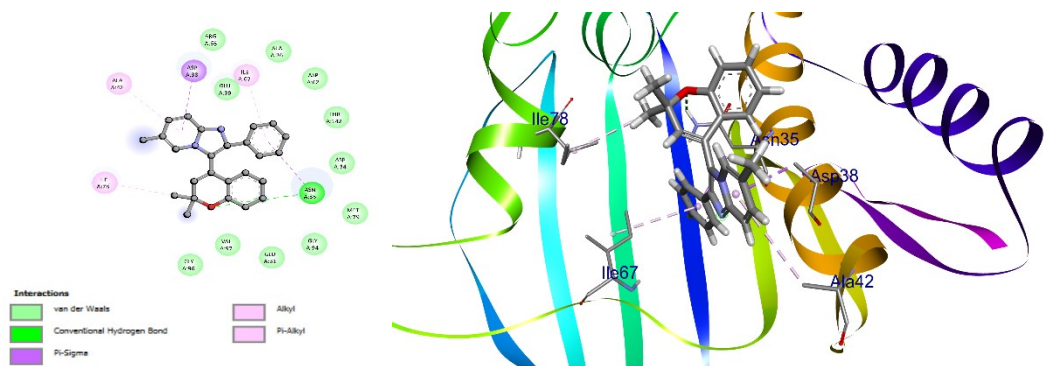


Fig. S66. Docking interaction and 3D binding image of compound **16c** with *E. coli* DNA gyrase (PDBID: 1AJ6)

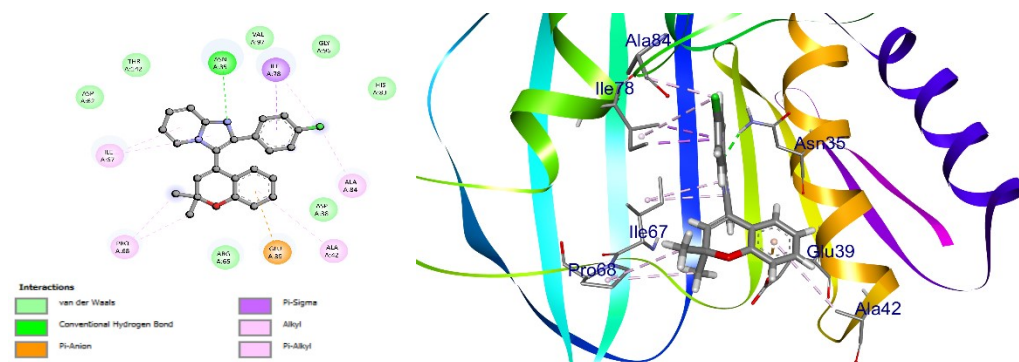


Fig. S67. Docking interaction and 3D binding image of compound **16d** with *E. coli* DNA gyrase (PDBID: 1AJ6)

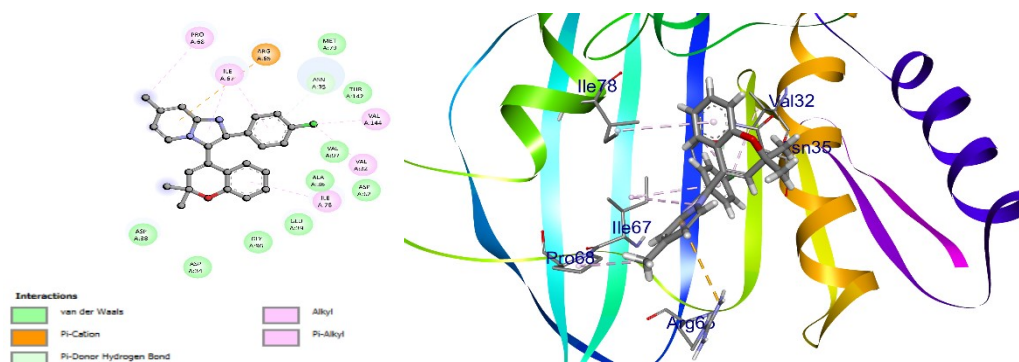


Fig. S68. Docking interaction and 3D binding image of compound **16e** with *E. coli* DNA gyrase (PDBID: 1AJ6)

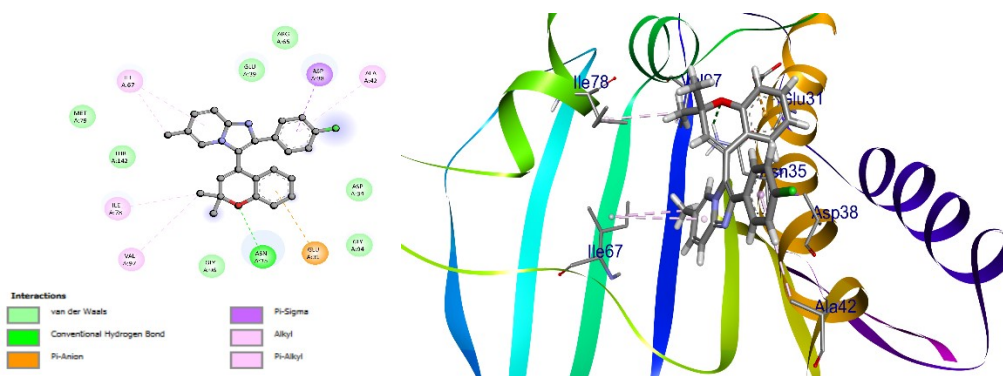


Fig. S69. Docking interaction and 3D binding image of compound **16f** with *E. coli* DNA gyrase (PDBID: 1AJ6)

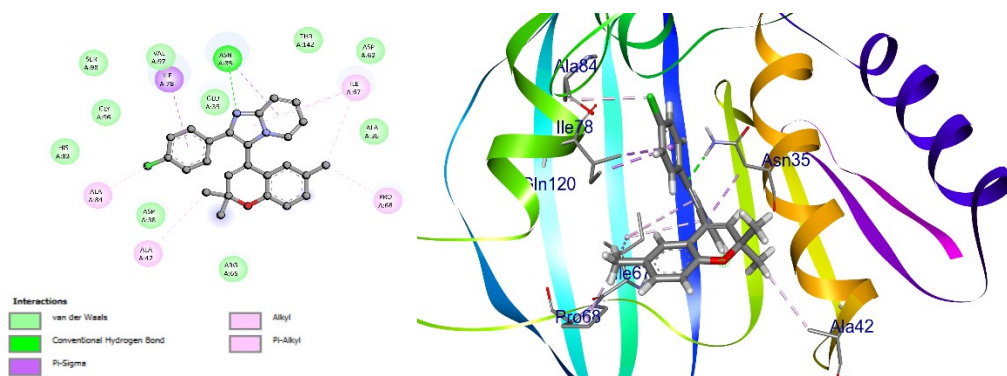


Fig. S70. Docking interaction and 3D binding image of compound **16g** with *E. coli* DNA gyrase (PDBID: 1AJ6)

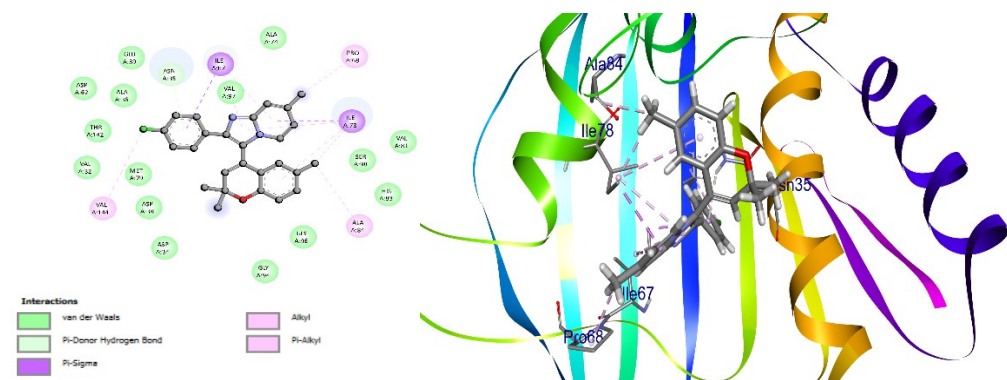


Fig. S71. Docking interaction and 3D binding image of compound **16h** with *E. coli* DNA gyrase (PDBID: 1AJ6)

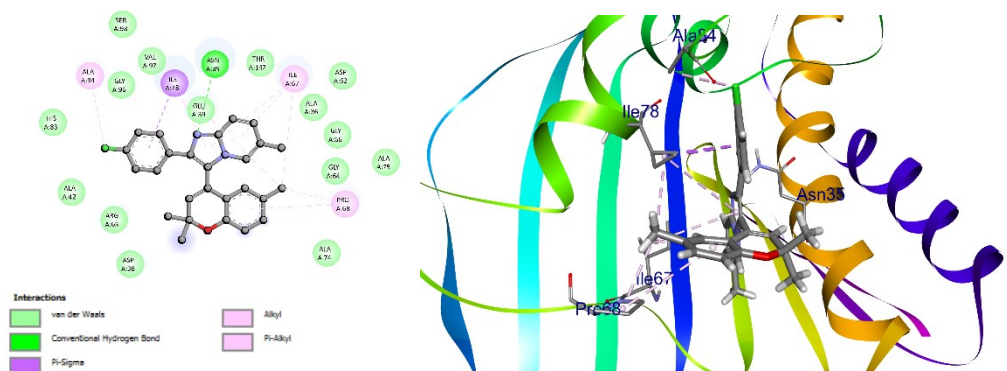


Fig. S72. Docking interaction and 3D binding image of compound **16i** with *E. coli* DNA gyrase (PDBID: 1AJ6)

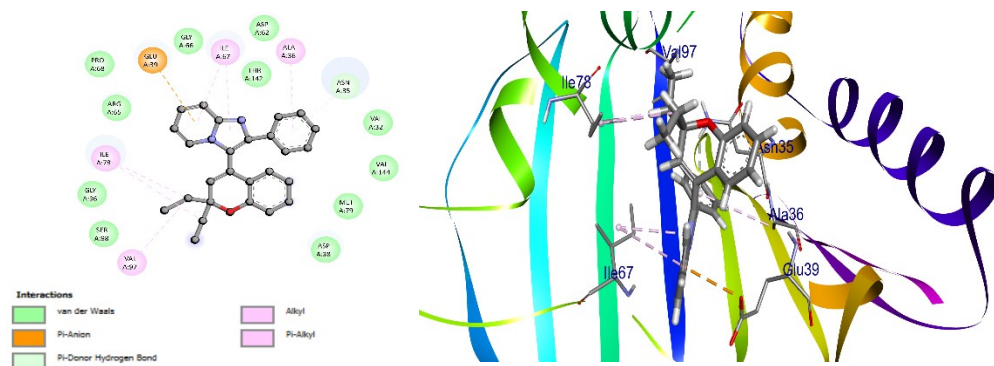


Fig. S73. Docking interaction and 3D binding image of compound **16j** with *E. coli* DNA gyrase (PDBID: 1AJ6)

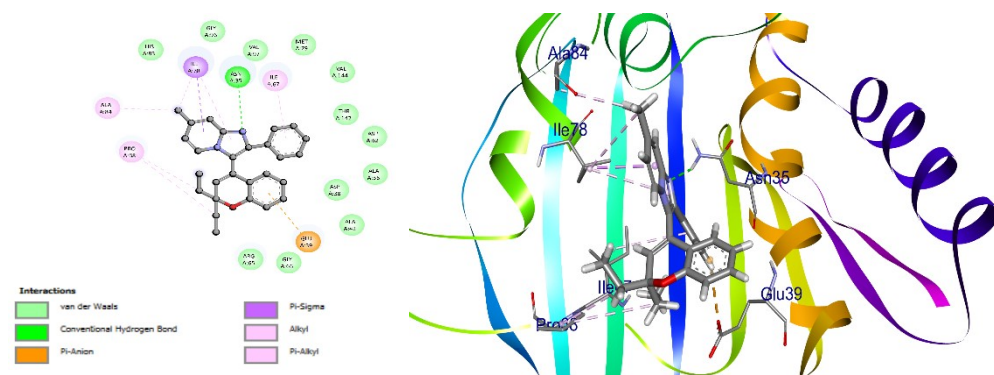


Fig. S74. Docking interaction and 3D binding image of compound **16k** with *E. coli* DNA gyrase (PDBID: 1AJ6)

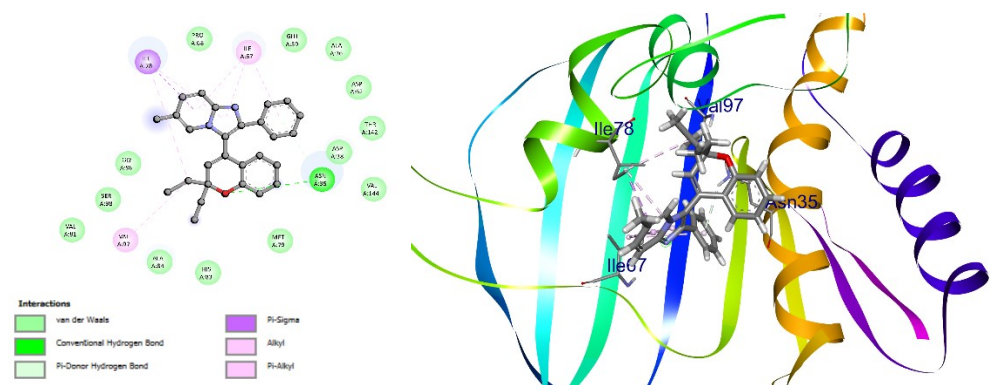


Fig. S75. Docking interaction and 3D binding image of compound **16l** with *E. coli* DNA gyrase (PDBID: 1AJ6)

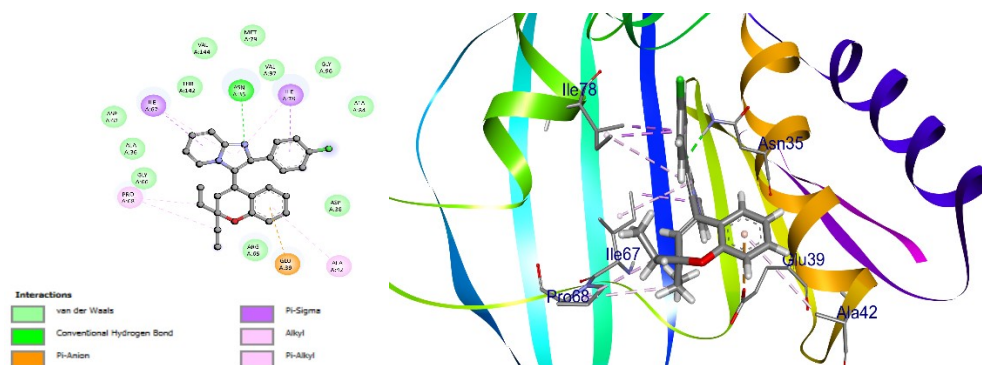


Fig. S76. Docking interaction and 3D binding image of compound **16m** with *E. coli* DNA gyrase (PDBID: 1AJ6)

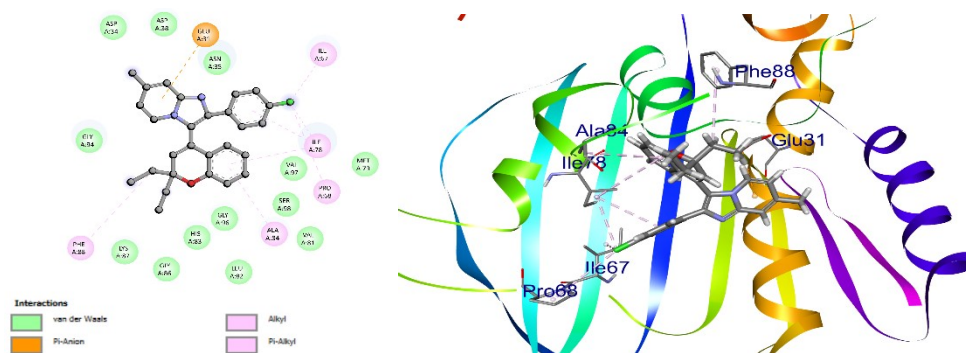


Fig. S77. Docking interaction and 3D binding image of compound **16n** with *E. coli* DNA gyrase (PDBID: 1AJ6)

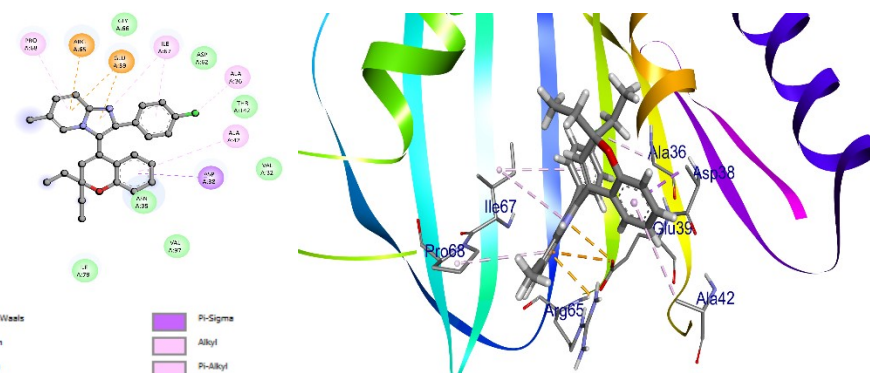


Fig. S78. Docking interaction and 3D binding image of compound **16o** with *E. coli* DNA gyrase (PDBID: 1AJ6)

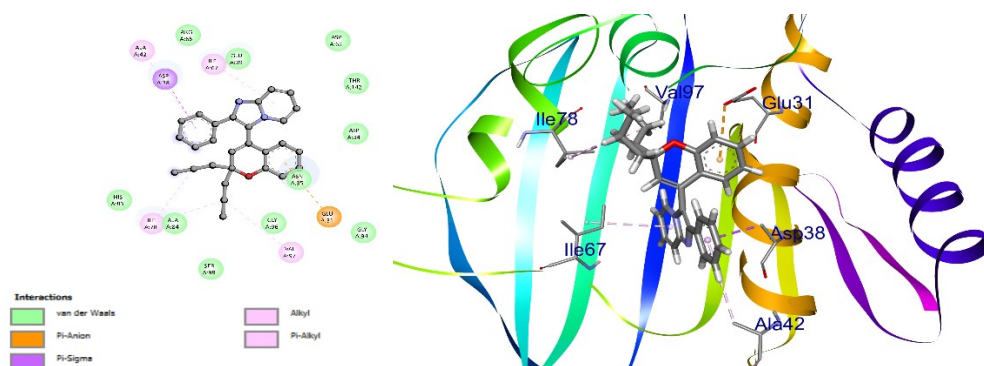


Fig. S79. Docking interaction and 3D binding image of compound **16p** with *E. coli* DNA gyrase (PDBID: 1AJ6)

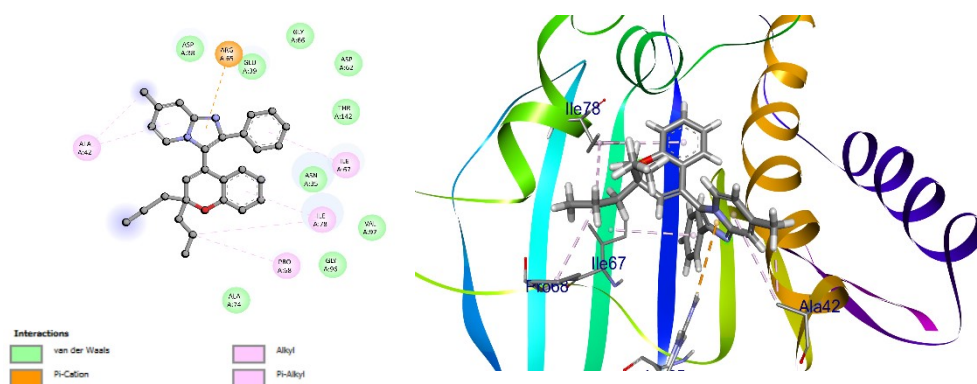


Fig. S80. Docking interaction and 3D binding image of compound **16q** with *E. coli* DNA gyrase (PDBID: 1AJ6)

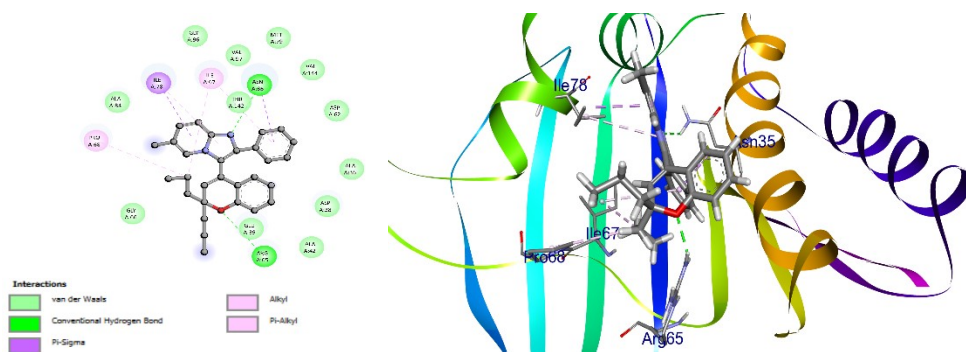


Fig. S81. Docking interaction and 3D binding image of compound **16r** with *E. coli* DNA gyrase (PDBID: 1AJ6)

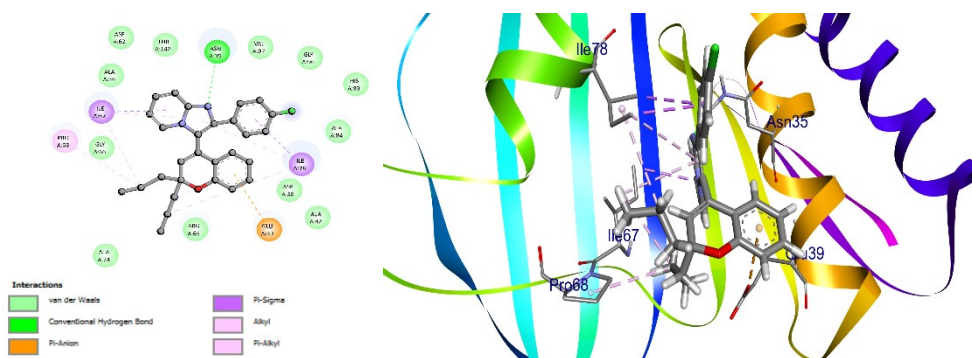


Fig. S82. Docking interaction and 3D binding image of compound **16s** with *E. coli* DNA gyrase (PDBID: 1AJ6)

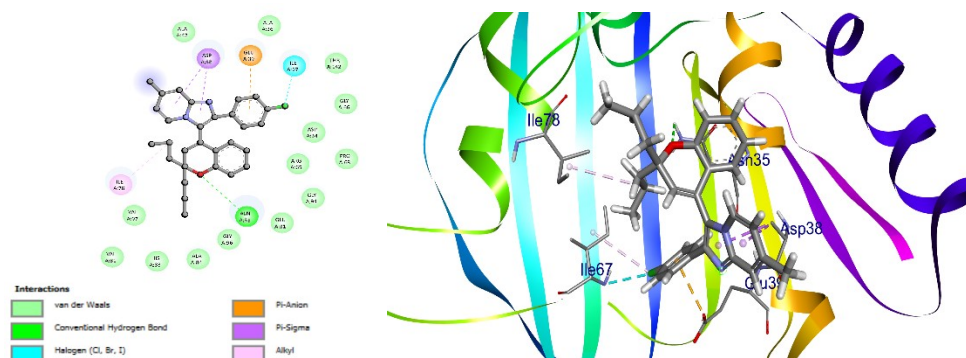


Fig. S83. Docking interaction and 3D binding image of compound **16t** with *E. coli* DNA gyrase (PDBID: 1AJ6)

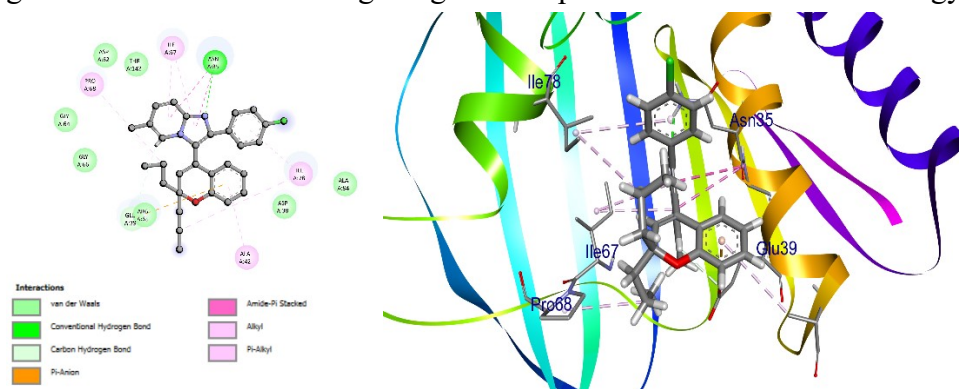


Fig. S84. Docking interaction and 3D binding image of compound **16u** with *E. coli* DNA gyrase (PDBID: 1AJ6)

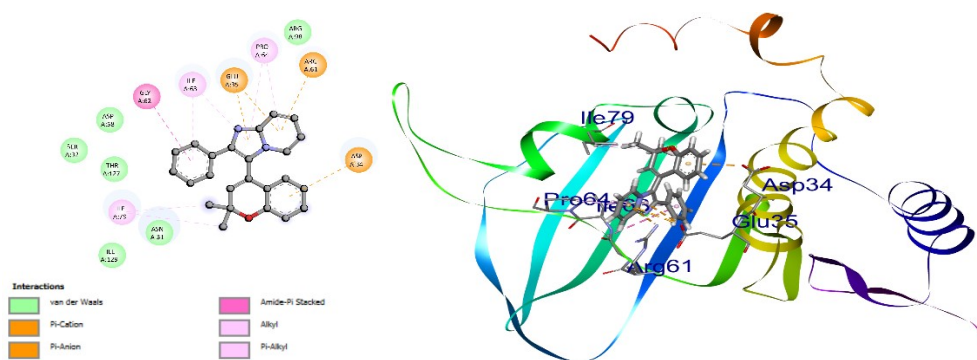


Fig. S85. Docking interaction and 3D binding image of compound **16a** with *S. aureus* DNA gyrase (PDBID: 3G7B)

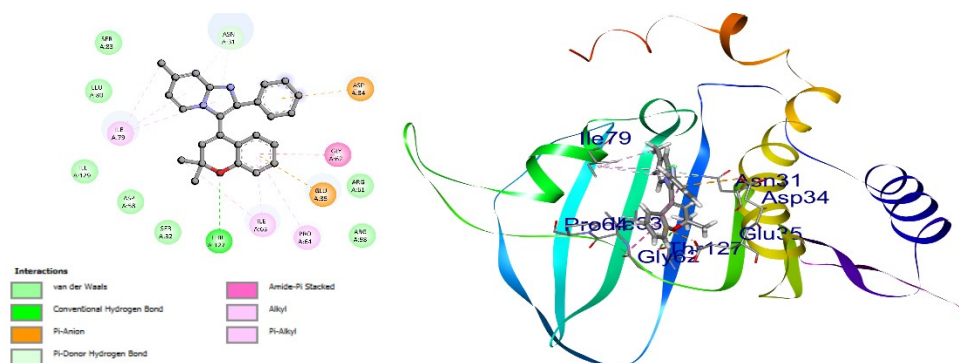


Fig. S86. Docking interaction and 3D binding image of compound **16b** with *S. aureus* DNA gyrase (PDBID: 3G7B)

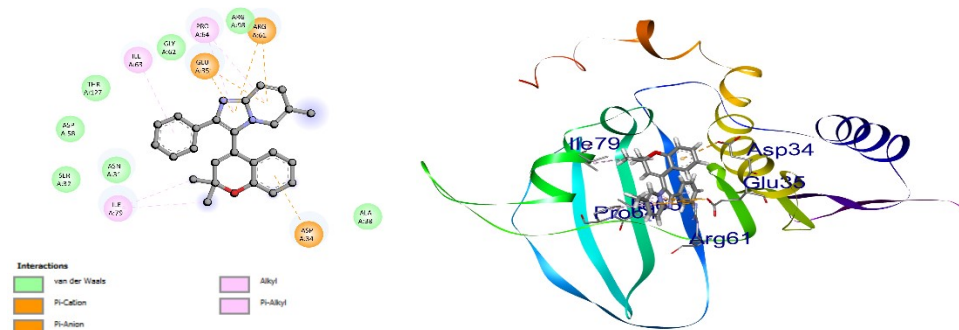


Fig. S87. Docking interaction and 3D binding image of compound **16c** with *S. aureus* DNA gyrase (PDBID: 3G7B)

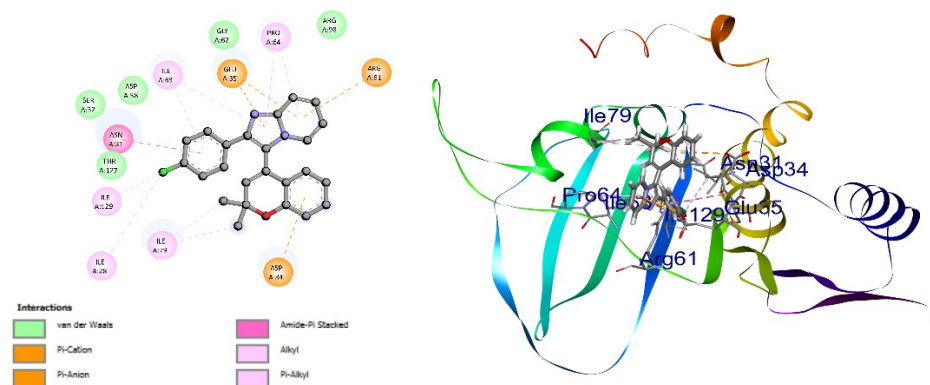


Fig. S88. Docking interaction and 3D binding image of compound **16d** with *S. aureus* DNA gyrase (PDBID: 3G7B)

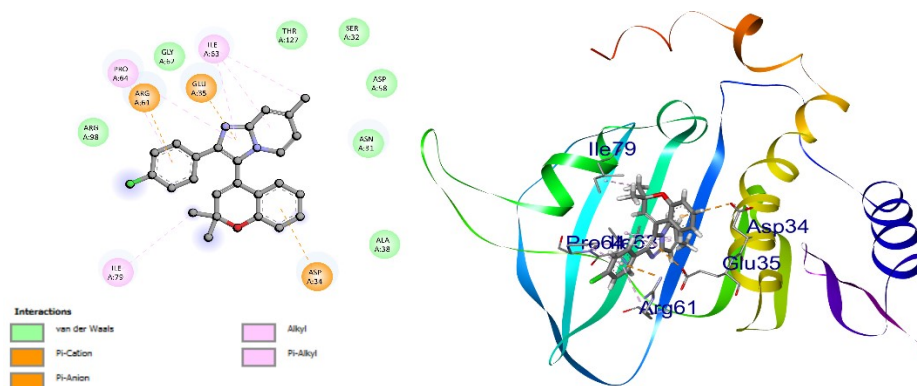


Fig. S89. Docking interaction and 3D binding image of compound **16e** with *S. aureus* DNA gyrase (PDBID: 3G7B)

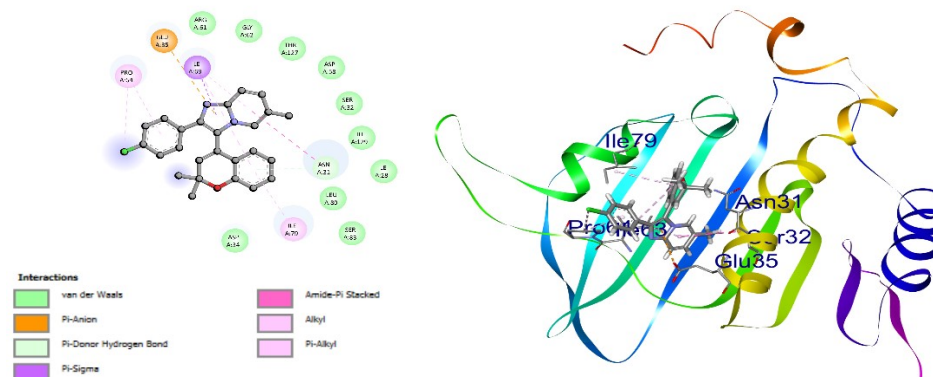


Fig. S90. Docking interaction and 3D binding image of compound **16f** with *S. aureus* DNA gyrase (PDBID: 3G7B)

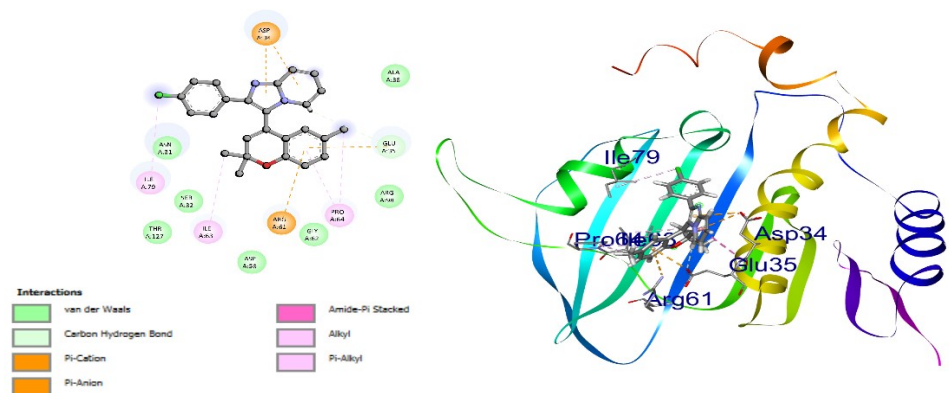


Fig. S91. Docking interaction and 3D binding image of compound **16g** with *S. aureus* DNA gyrase (PDBID: 3G7B)

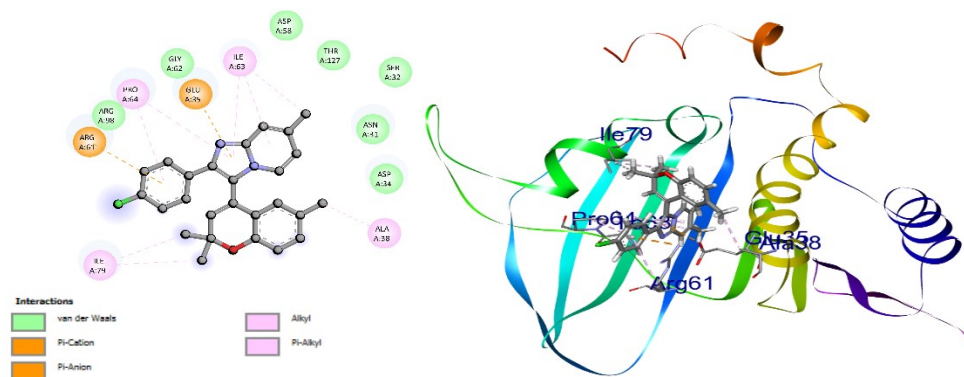


Fig. S92. Docking interaction and 3D binding image of compound **16h** with *S. aureus* DNA gyrase (PDBID: 3G7B)

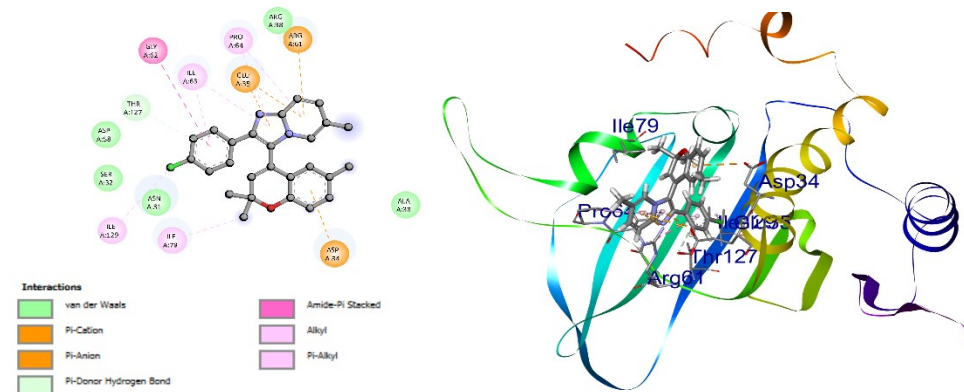


Fig. S93. Docking interaction and 3D binding image of compound **16i** with *S. aureus* DNA gyrase (PDBID: 3G7B)

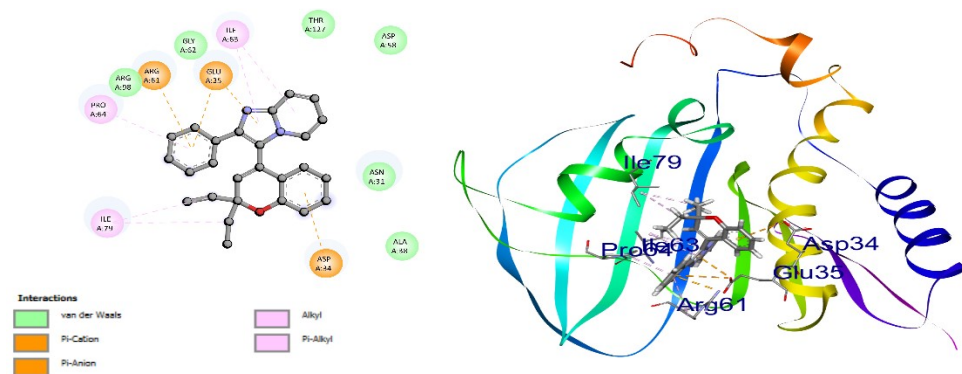


Fig. S94. Docking interaction and 3D binding image of compound **16j** with *S. aureus* DNA gyrase (PDBID: 3G7B)

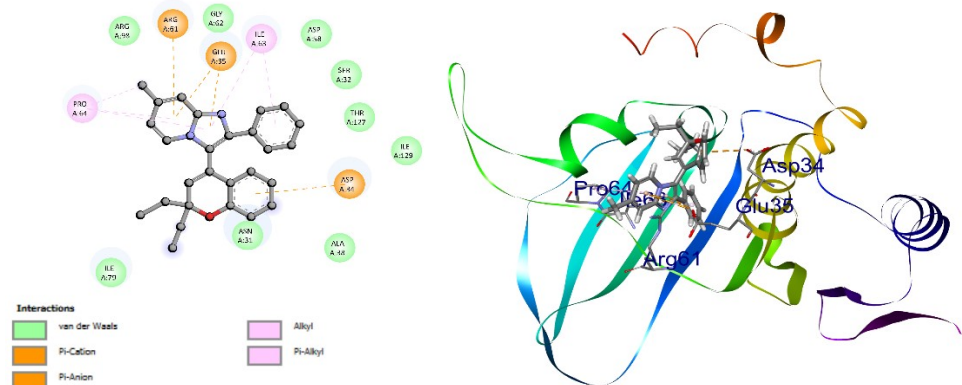


Fig. S95. Docking interaction and 3D binding image of compound **16k** with *S. aureus* DNA gyrase (PDBID: 3G7B)

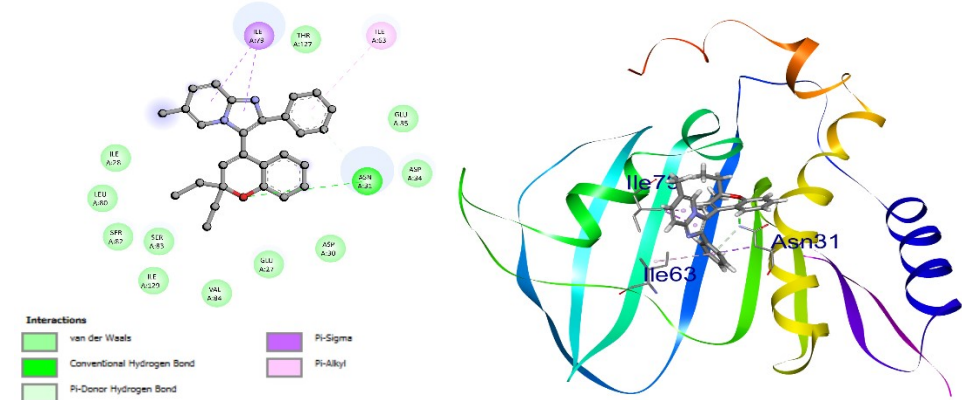


Fig. S99. Docking interaction and 3D binding image of compound **16o** with *S. aureus* DNA gyrase (PDBID: 3G7B)

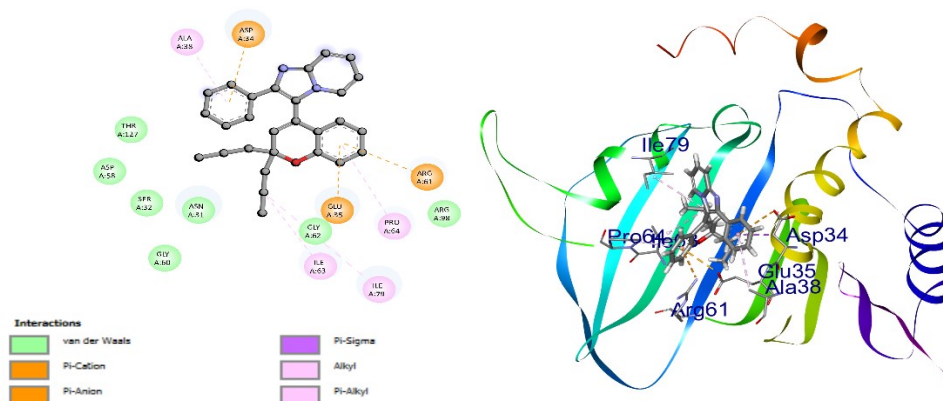


Fig. S100. Docking interaction and 3D binding image of compound **16p** with *S. aureus* DNA gyrase (PDBID: 3G7B)

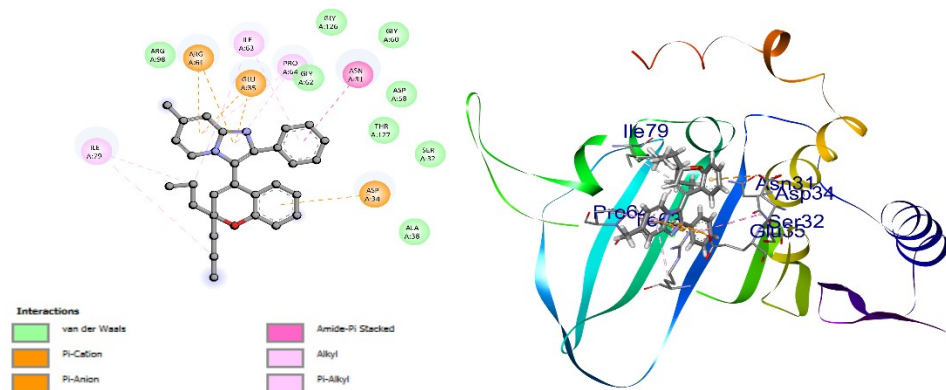


Fig. S101. Docking interaction and 3D binding image of compound **16q** with *S. aureus* DNA gyrase (PDBID: 3G7B)

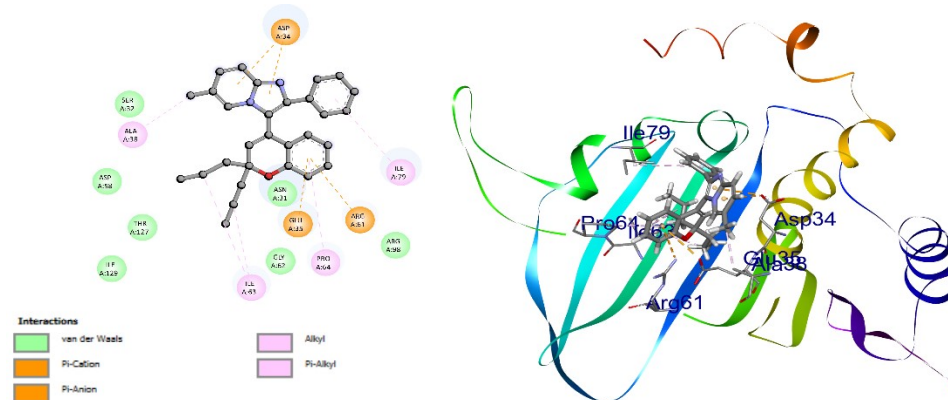


Fig. S102. Docking interaction and 3D binding image of compound **16r** with *S. aureus* DNA gyrase (PDBID: 3G7B)

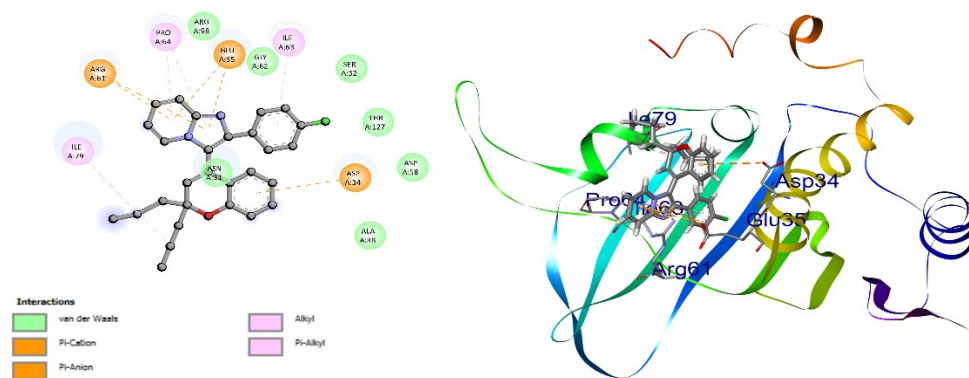


Fig. S103. Docking interaction and 3D binding image of compound **16s** with *S. aureus* DNA gyrase (PDBID: 3G7B)

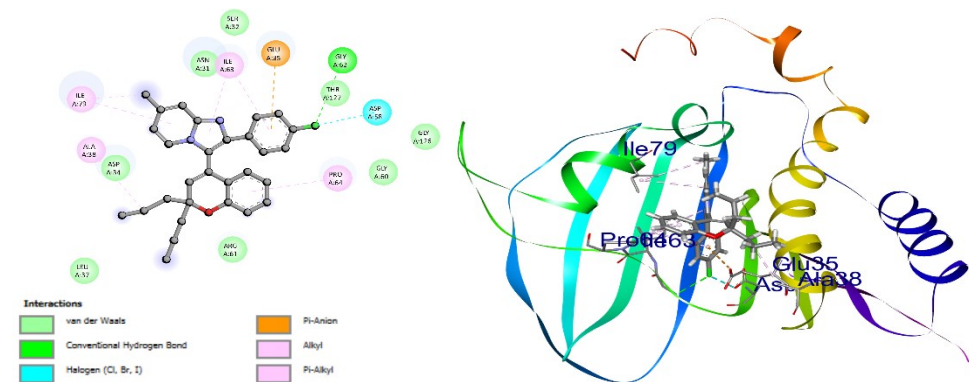


Fig. S104. Docking interaction and 3D binding image of compound **16t** with *S. aureus* DNA gyrase (PDBID: 3G7B)

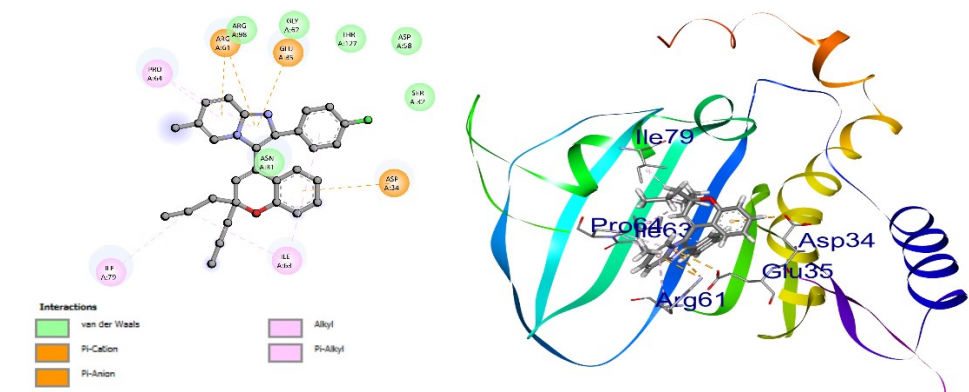


Fig. S105. Docking interaction and 3D binding image of compound **16u** with *S. aureus* DNA gyrase (PDBID: 3G7B)