

Supporting Information

One-pot synthesis of *N*-arylated benzotriazoles and benzotriazinones via *in situ* diazotization and aryne trapping

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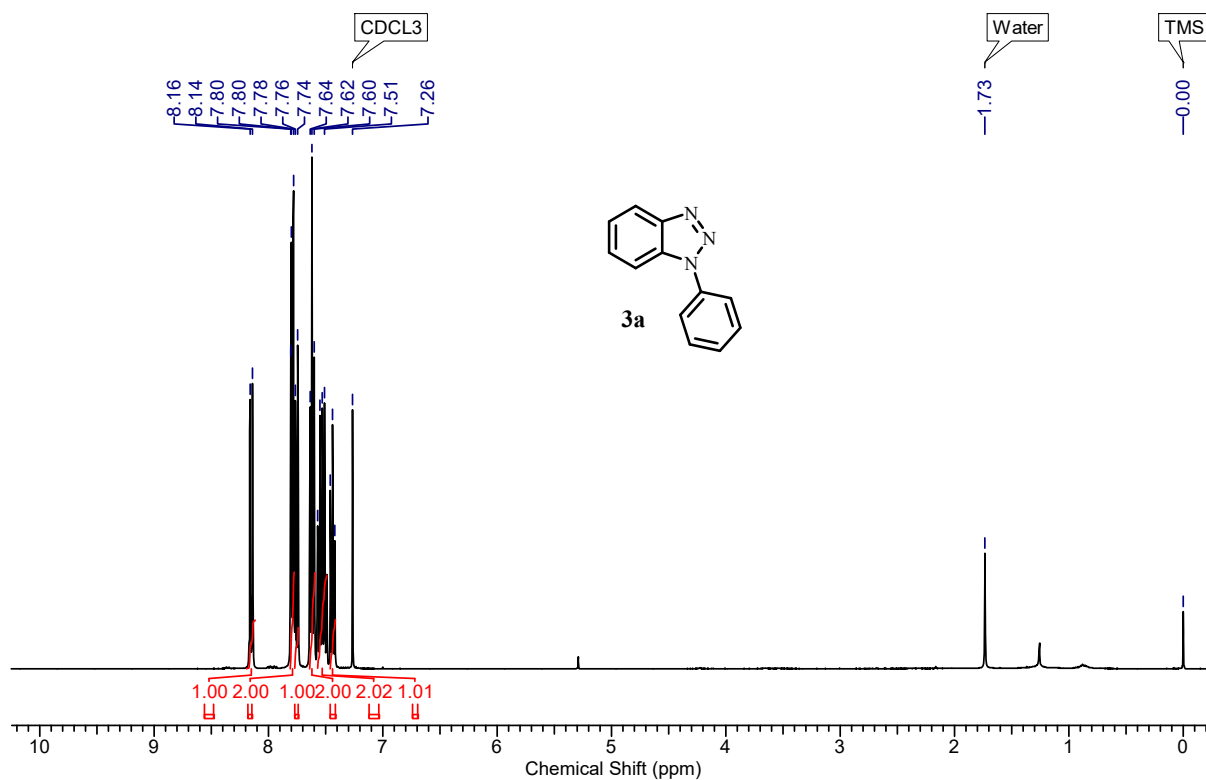
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^bAcademy of Scientific and Innovative Research (AcSIR), CSIR-HRDC Campus, Sector 19, Kamla Nehru Nagar, Ghaziabad, UP, 201 002, India.

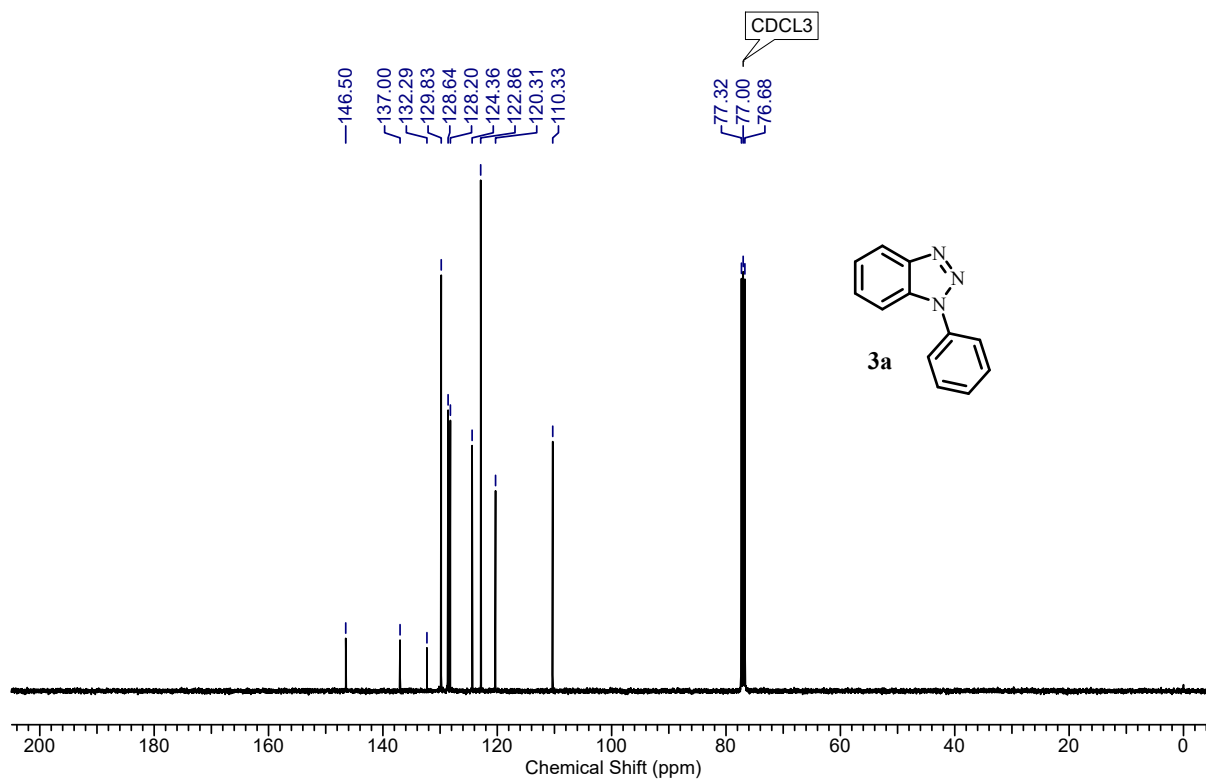
Content

1. Copies of NMR Spectra and HRMS of all the Synthesized Compounds

1. Copies of ^1H , ^{13}C , ^{19}F NMR Spectra and HRMS of all the Synthesized Compounds:

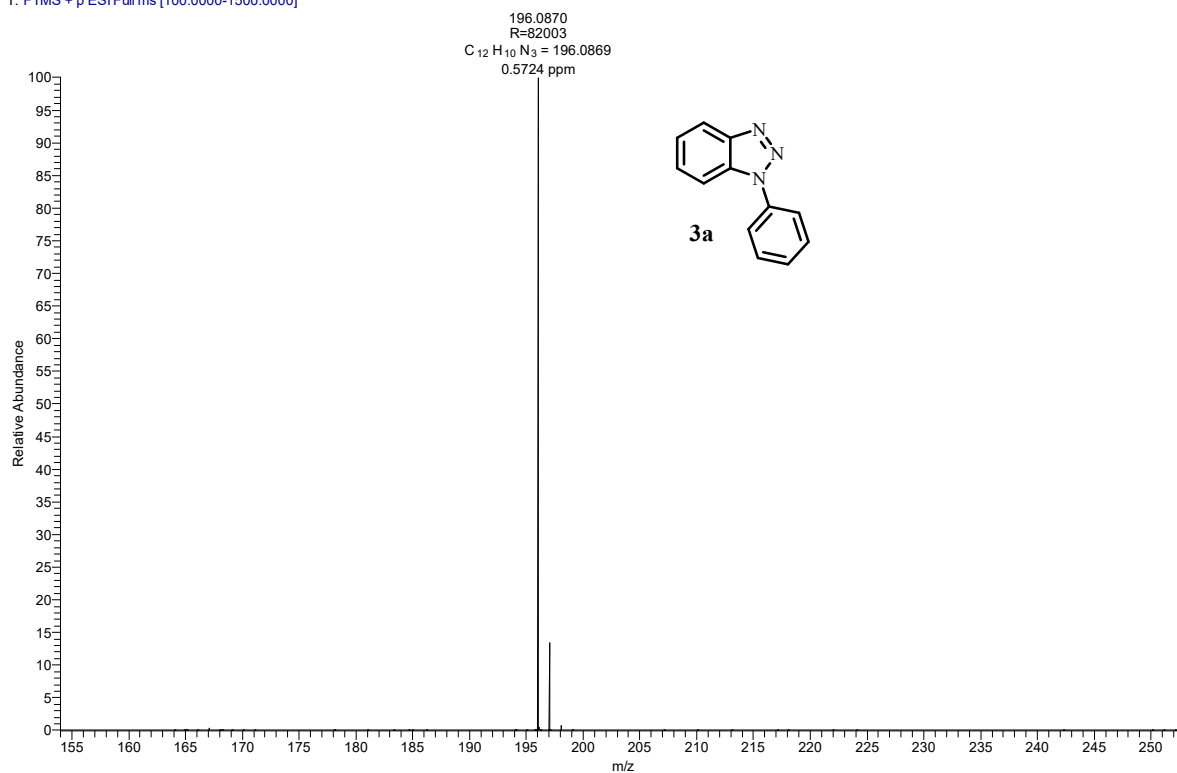


^1H NMR (CDCl_3 , 400 MHz) of Compound 3a

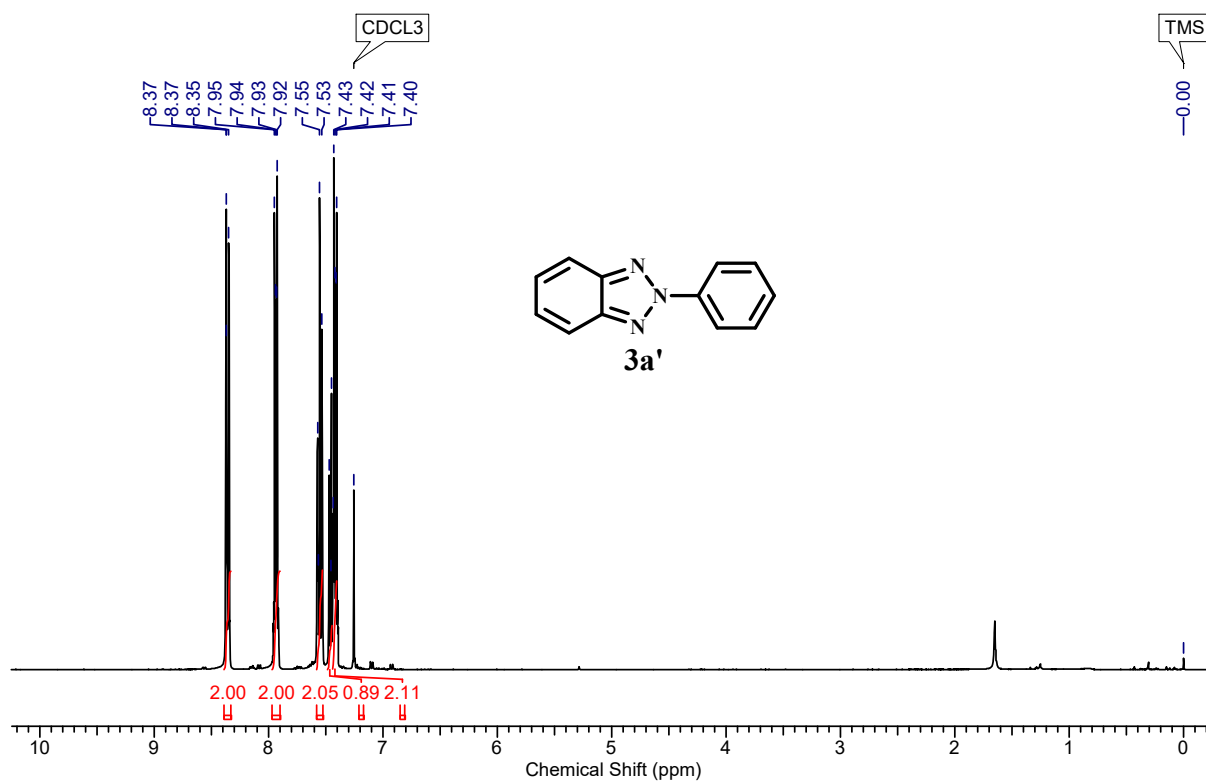


^{13}C NMR (CDCl_3 , 100 MHz) of Compound 3a

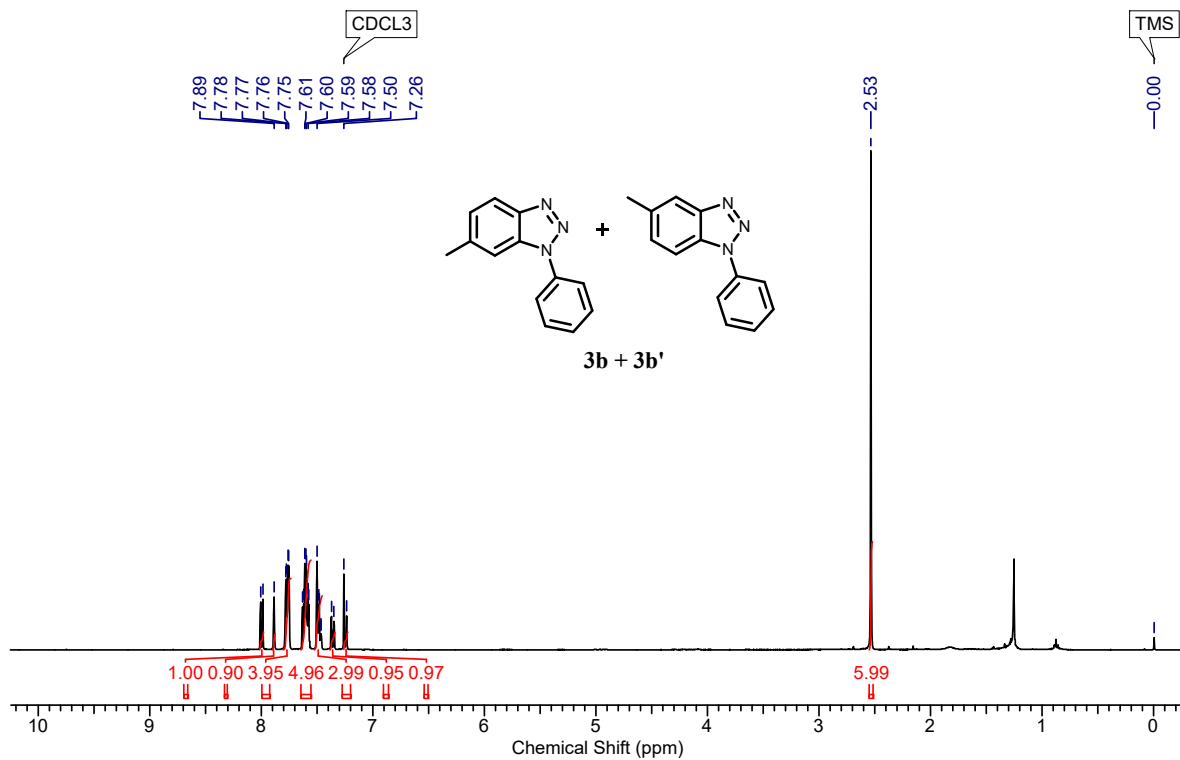
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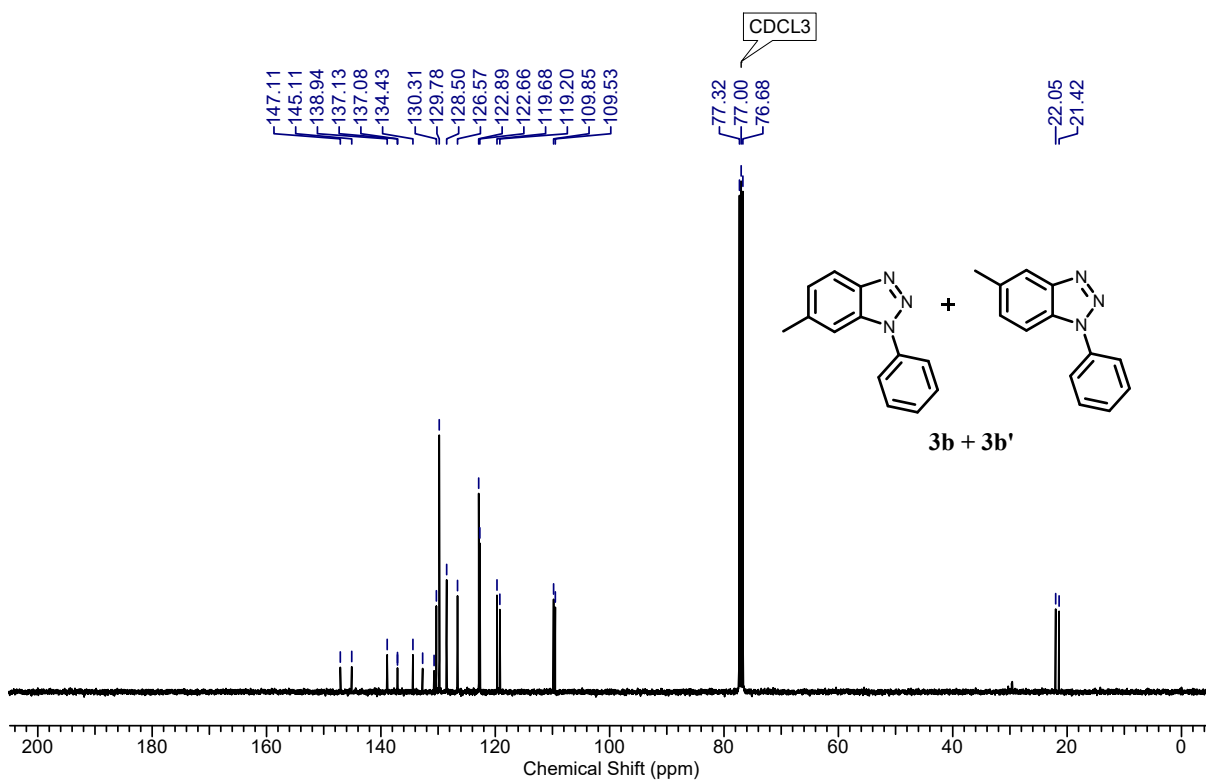
HRMS of Compound 3a



¹H NMR (CDCl₃, 400 MHz) of Compound 3a'

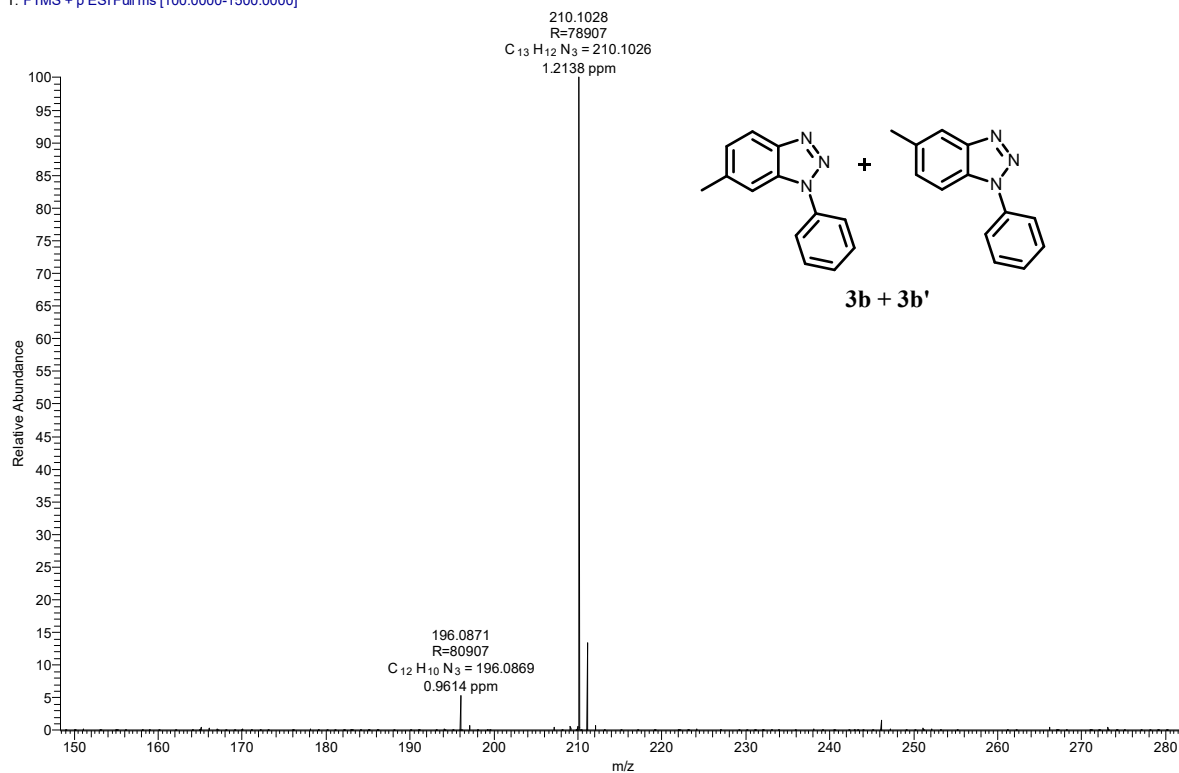


¹H NMR (CDCl₃, 400 MHz) of Compound **3b** + **3b'**

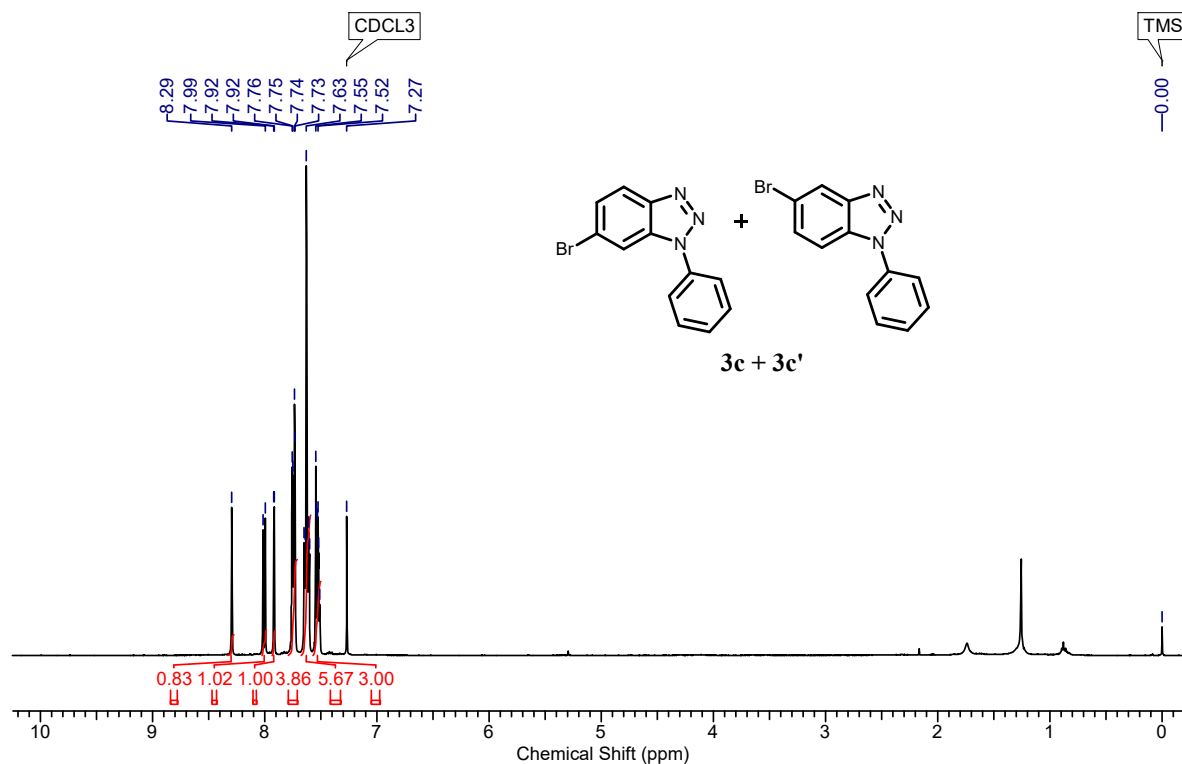


¹³C NMR (CDCl₃, 100 MHz) of Compound **3b** + **3b'**

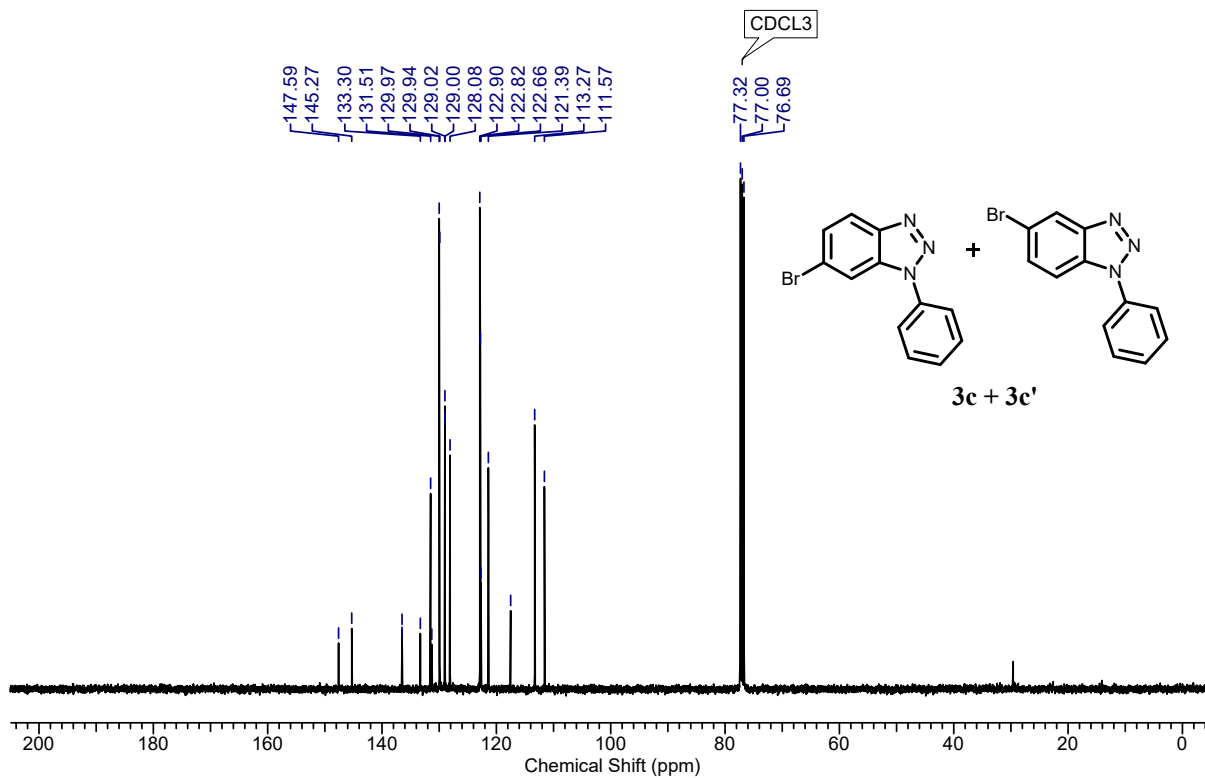
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HRMS of Compound 3b + 3b'

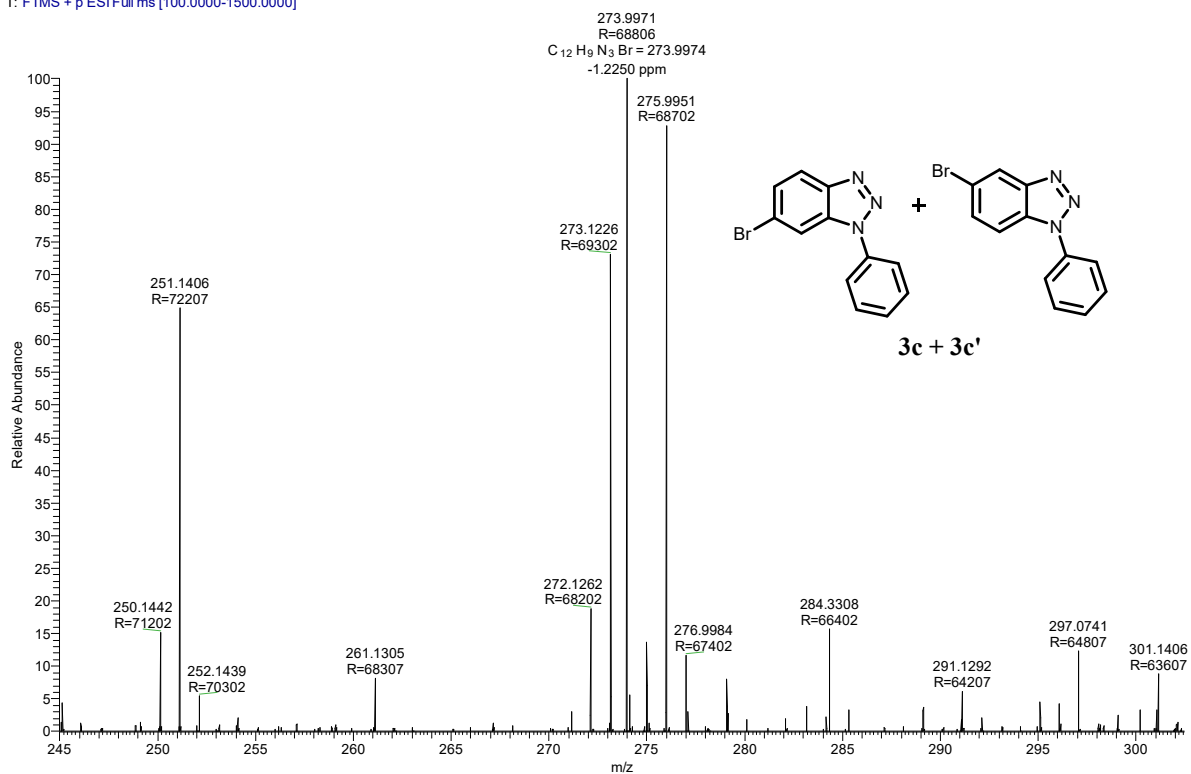


¹H NMR (CDCl₃, 400 MHz) of Compound 3c + 3c'

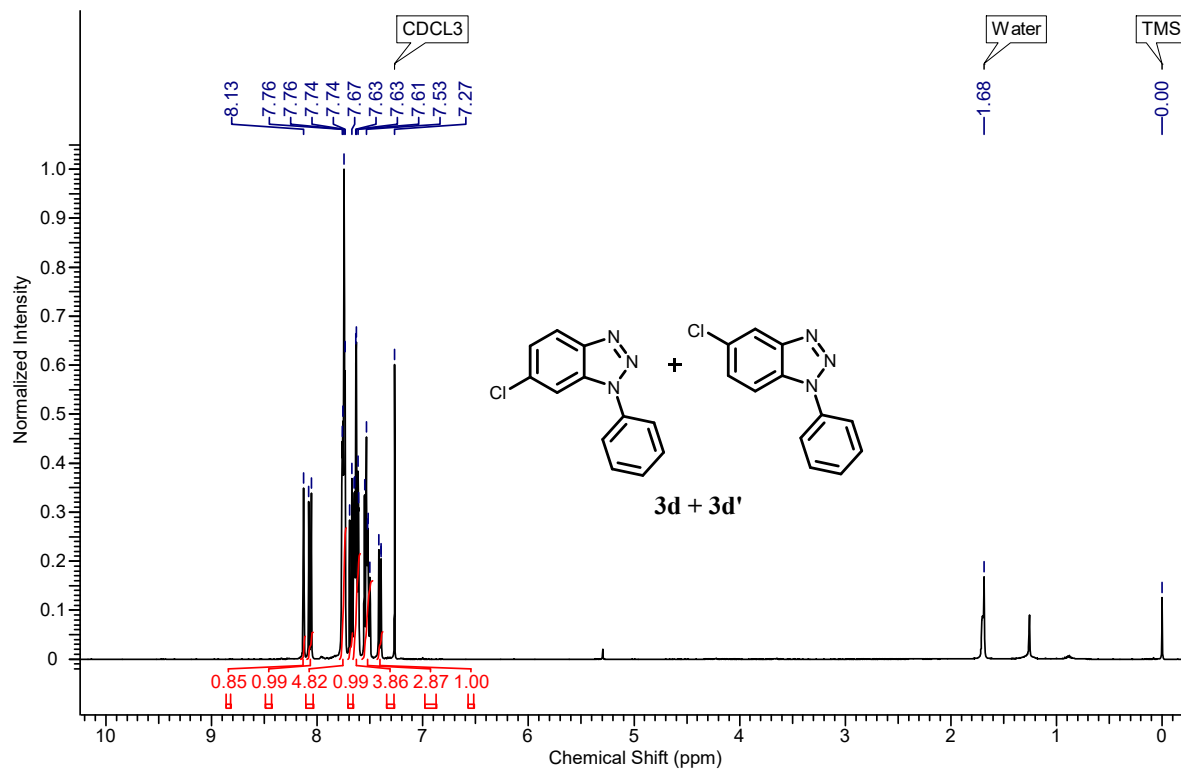


¹³C NMR (CDCl₃, 100 MHz) of Compound 3c + 3c'

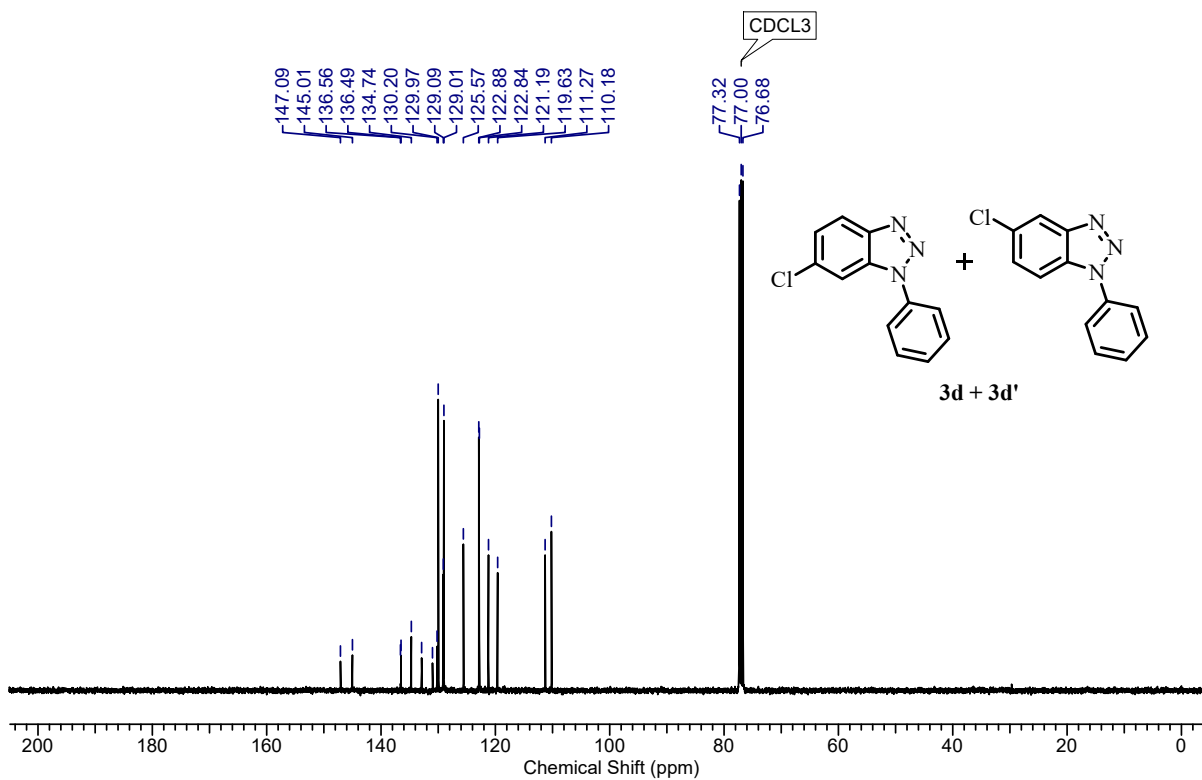
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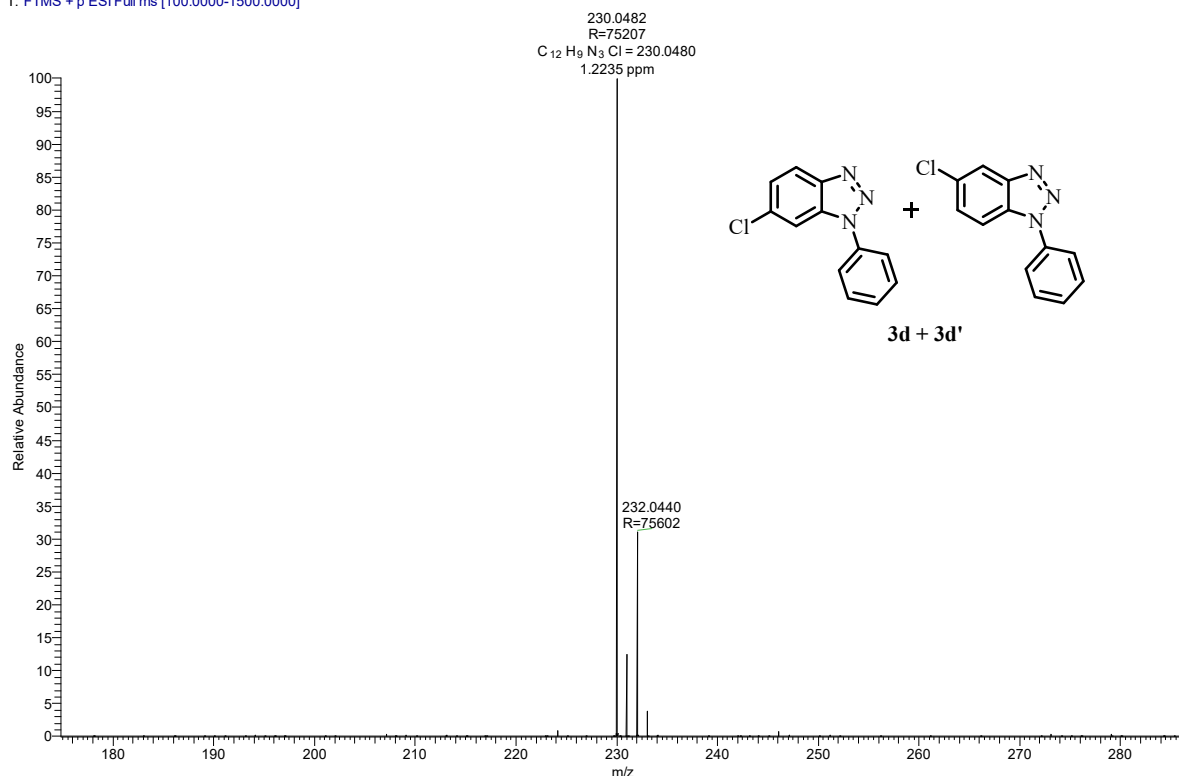
HRMS of Compound 3c + 3c'



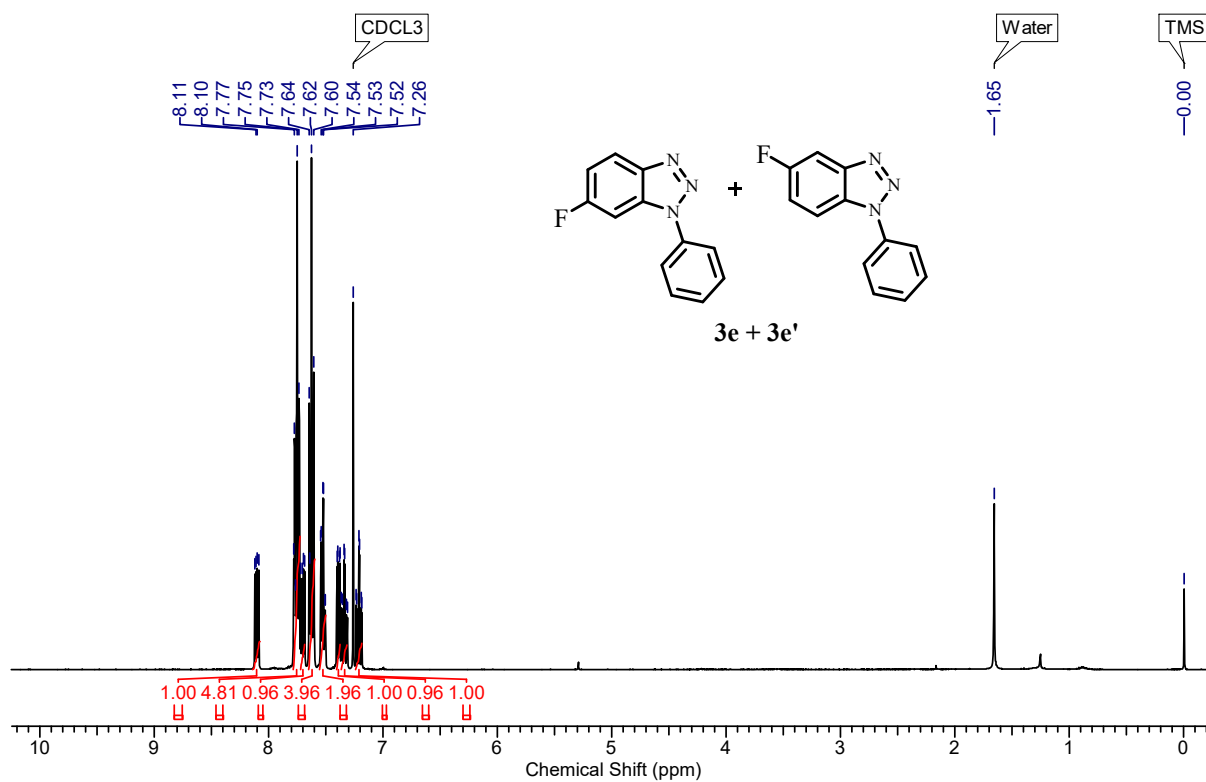
¹H NMR (CDCl₃, 400 MHz) of Compound 3d + 3d'



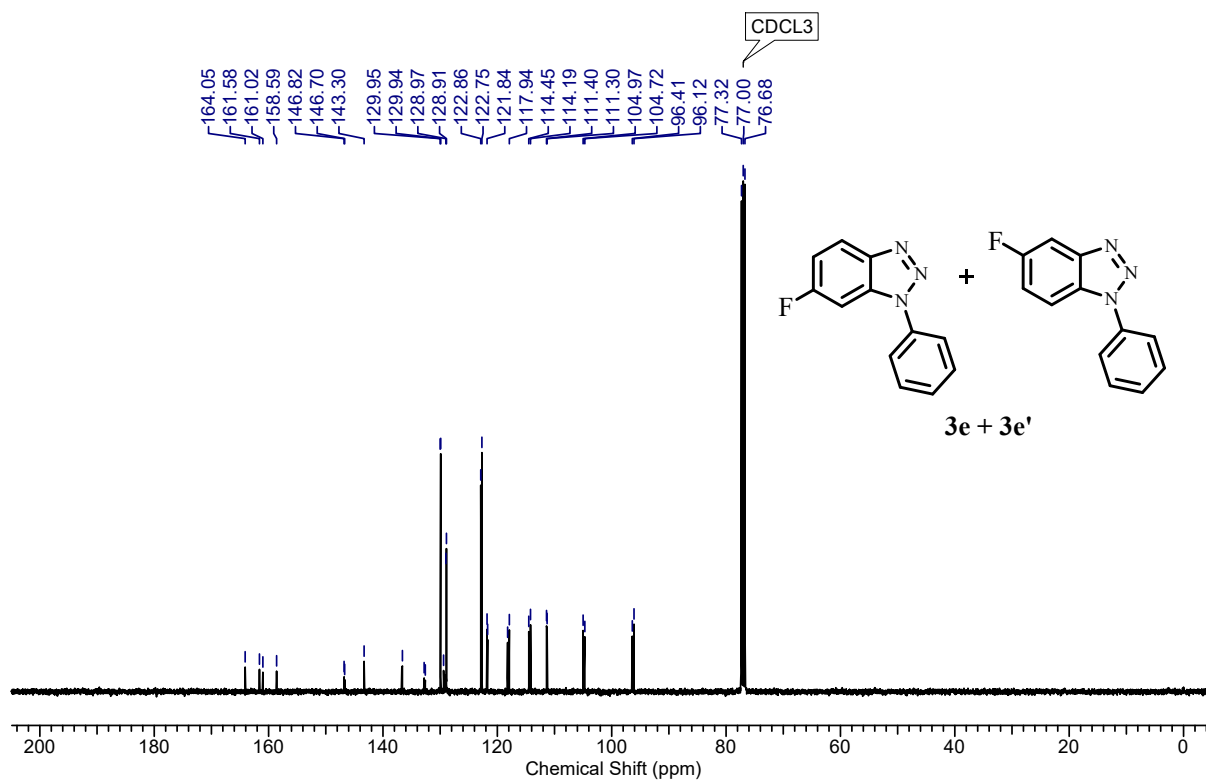
¹³C NMR (CDCl₃, 100 MHz) of Compound 3d + 3d'



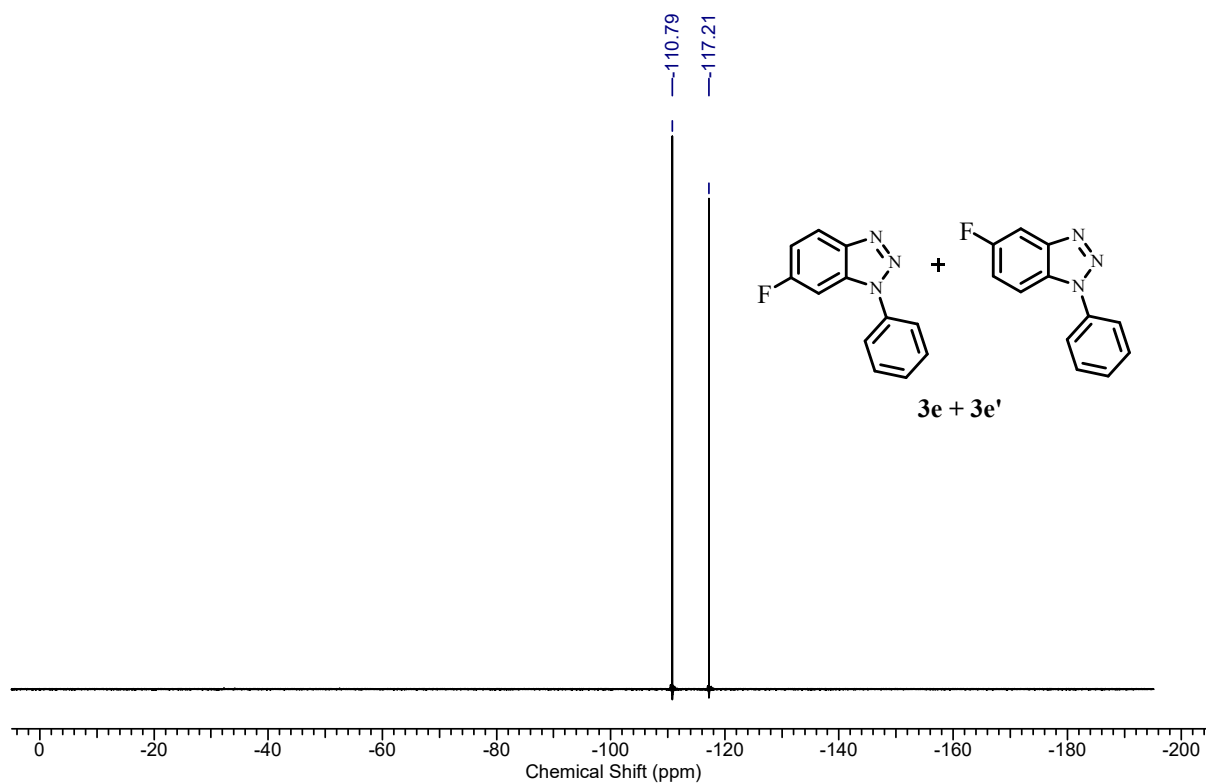
HRMS of Compound 3d + 3d'



¹H NMR (CDCl₃, 400 MHz) of Compound 3e + 3e'

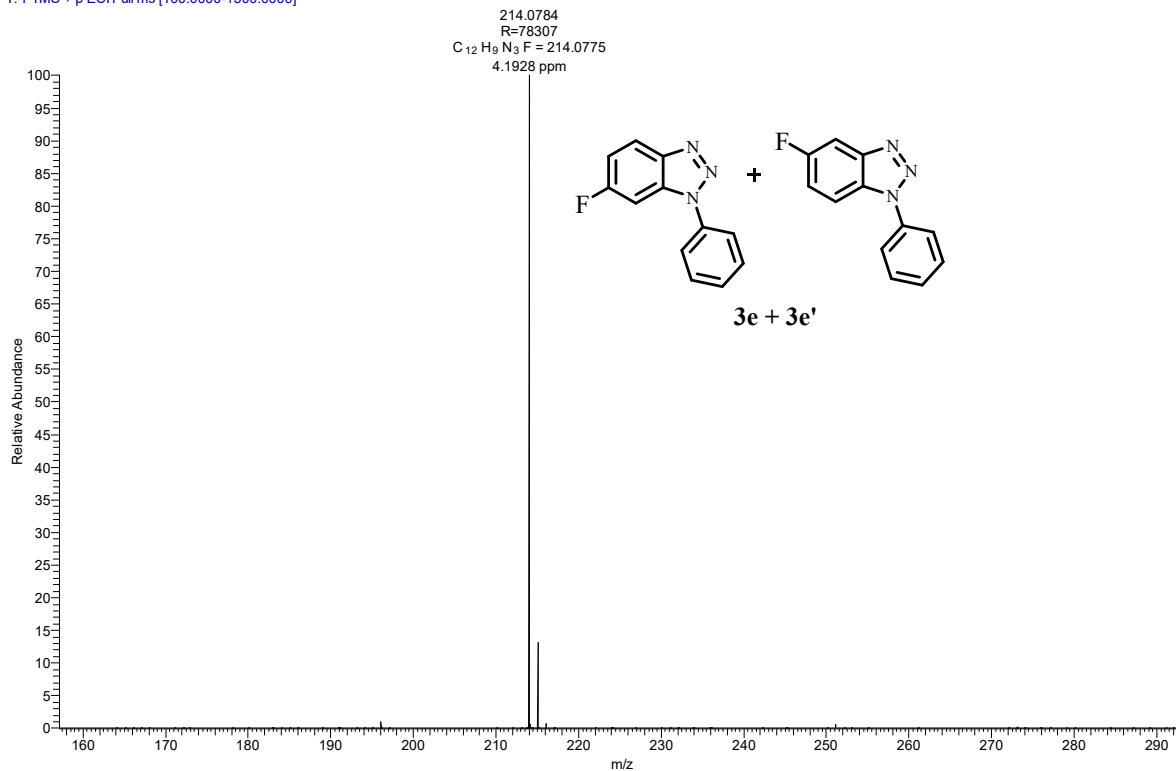


¹³C NMR (CDCl₃, 100 MHz) of Compound 3e + 3e'

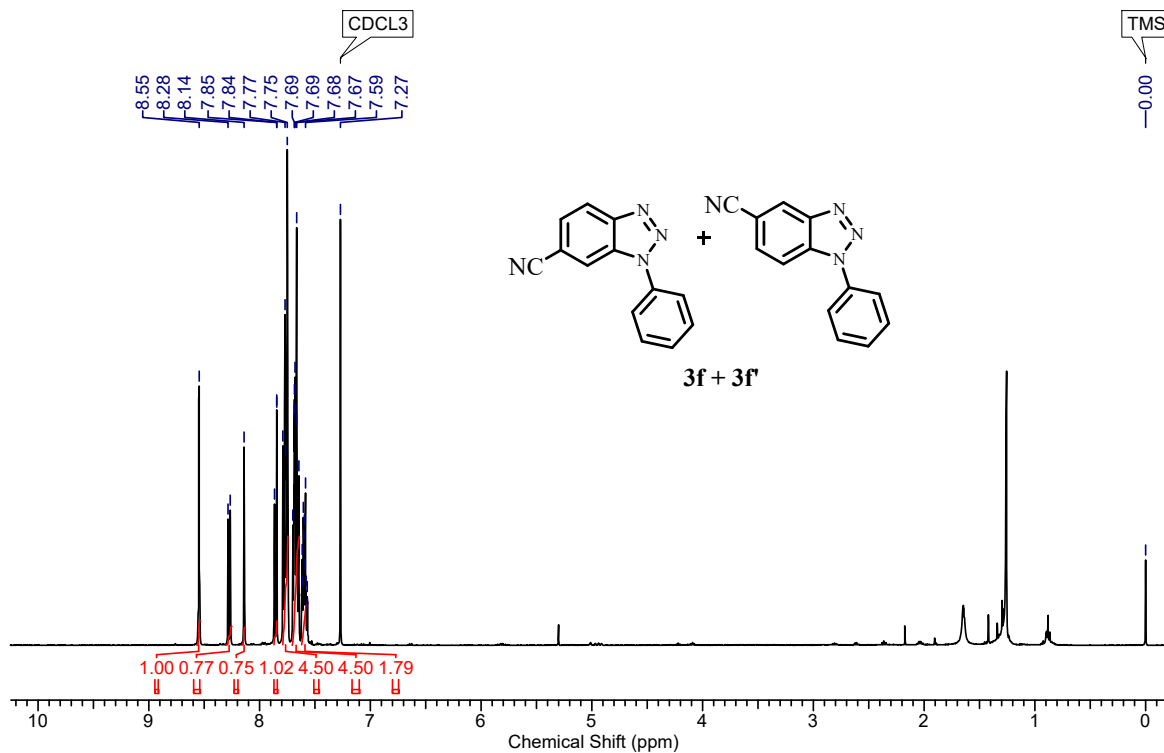


¹⁹F NMR (CDCl₃, 376 MHz) of Compound 3e + 3e'

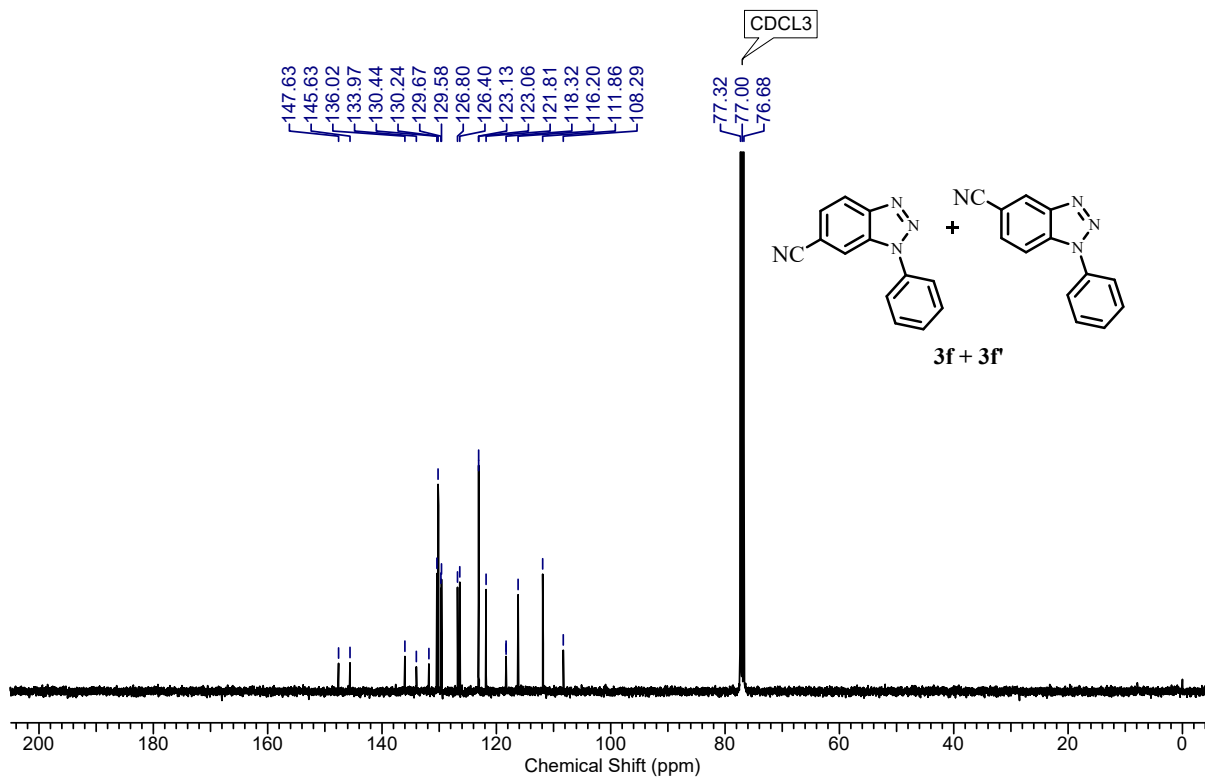
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HRMS of Compound 3e + 3e'

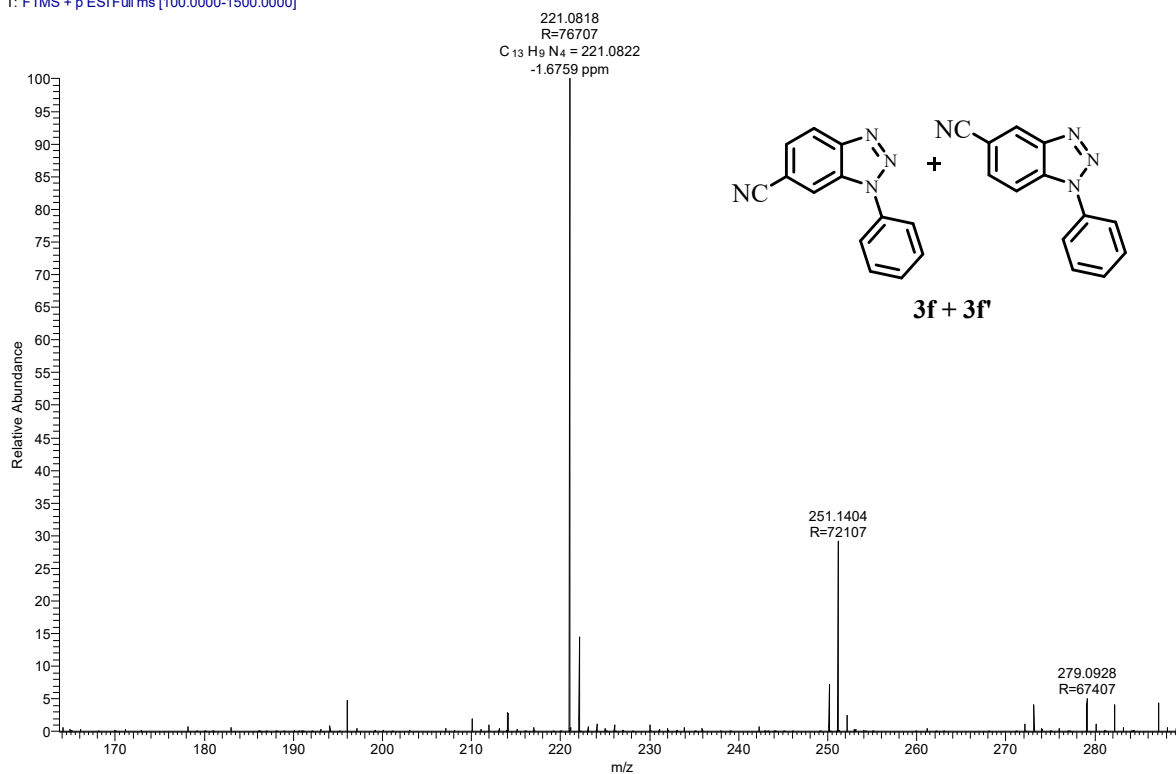


¹H NMR (CDCl₃, 400 MHz) of Compound 3f + 3f'

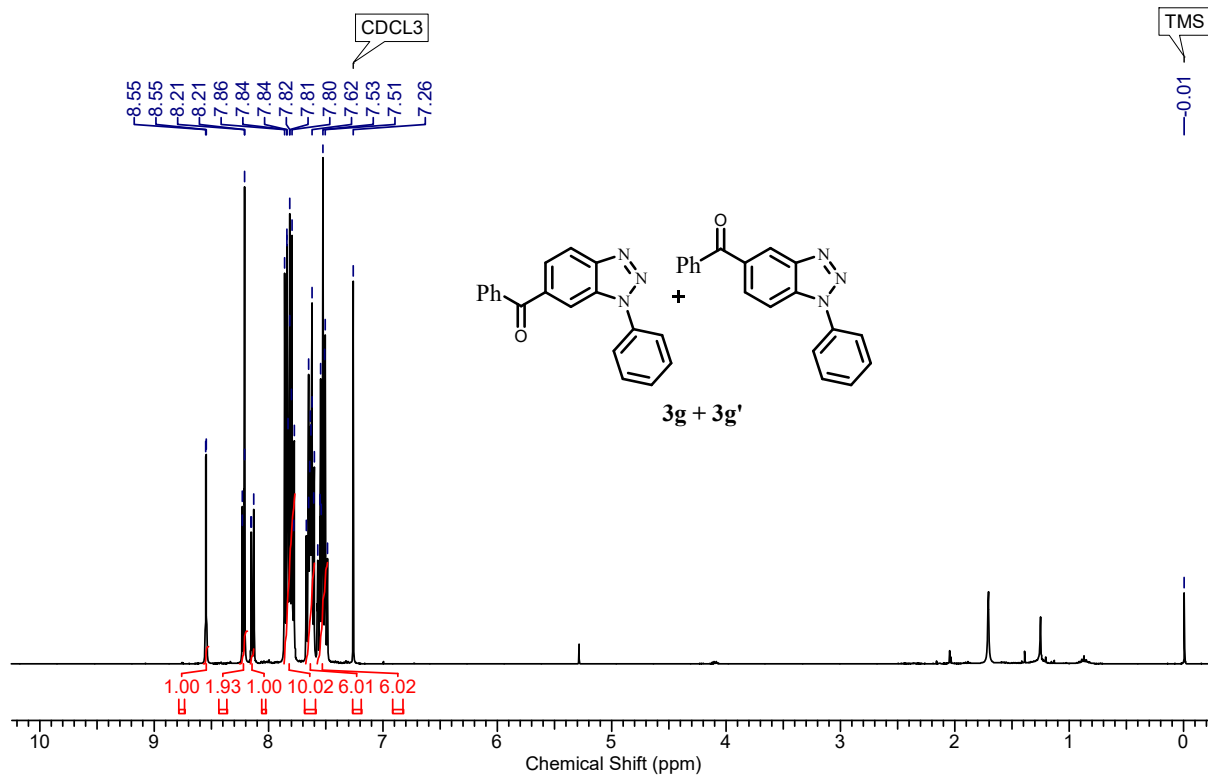


¹³C NMR (CDCl₃, 100 MHz) of Compound 3f + 3f'

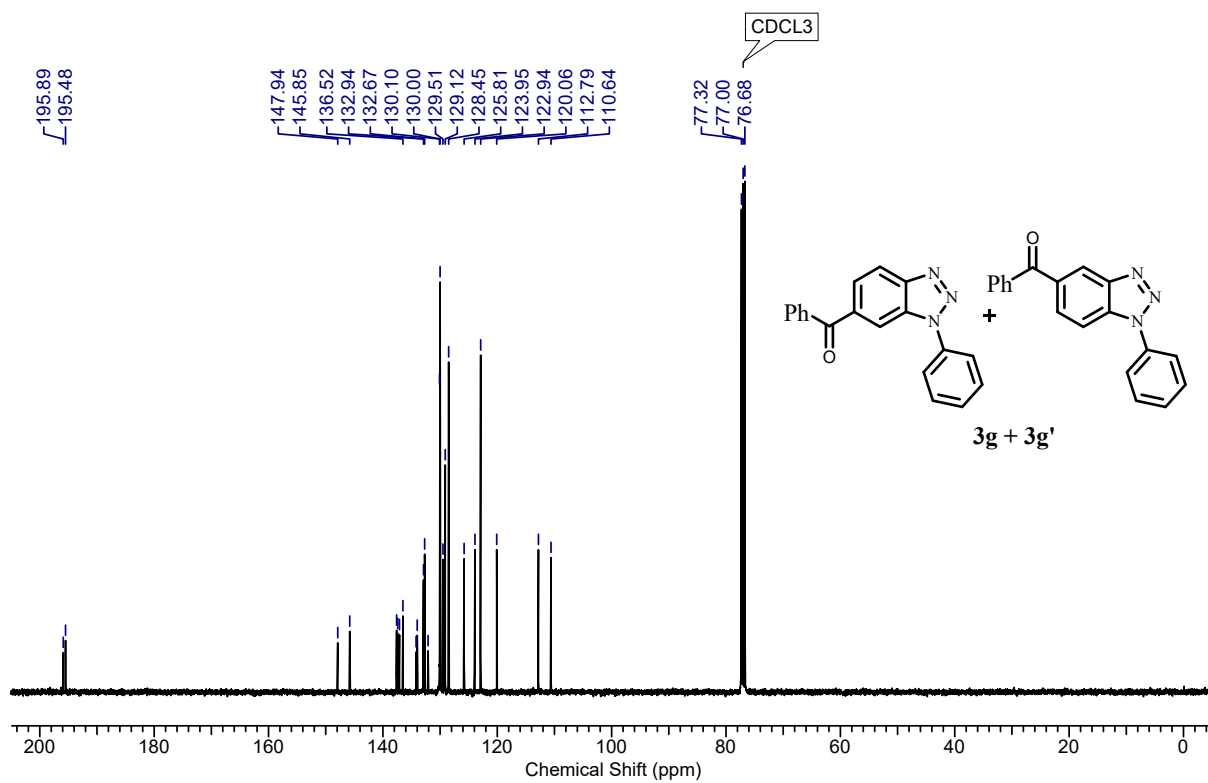
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HRMS of Compound 3f + 3f'

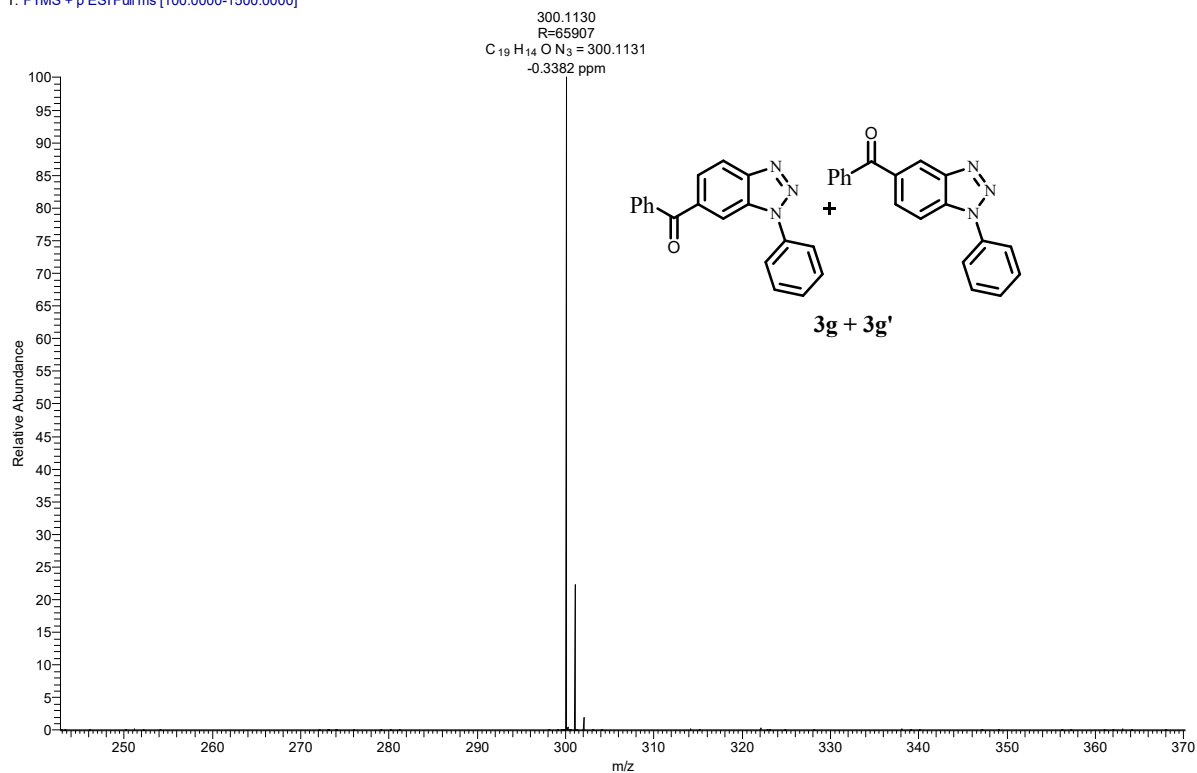


¹H NMR (CDCl₃, 400 MHz) of Compound 3g + 3g'

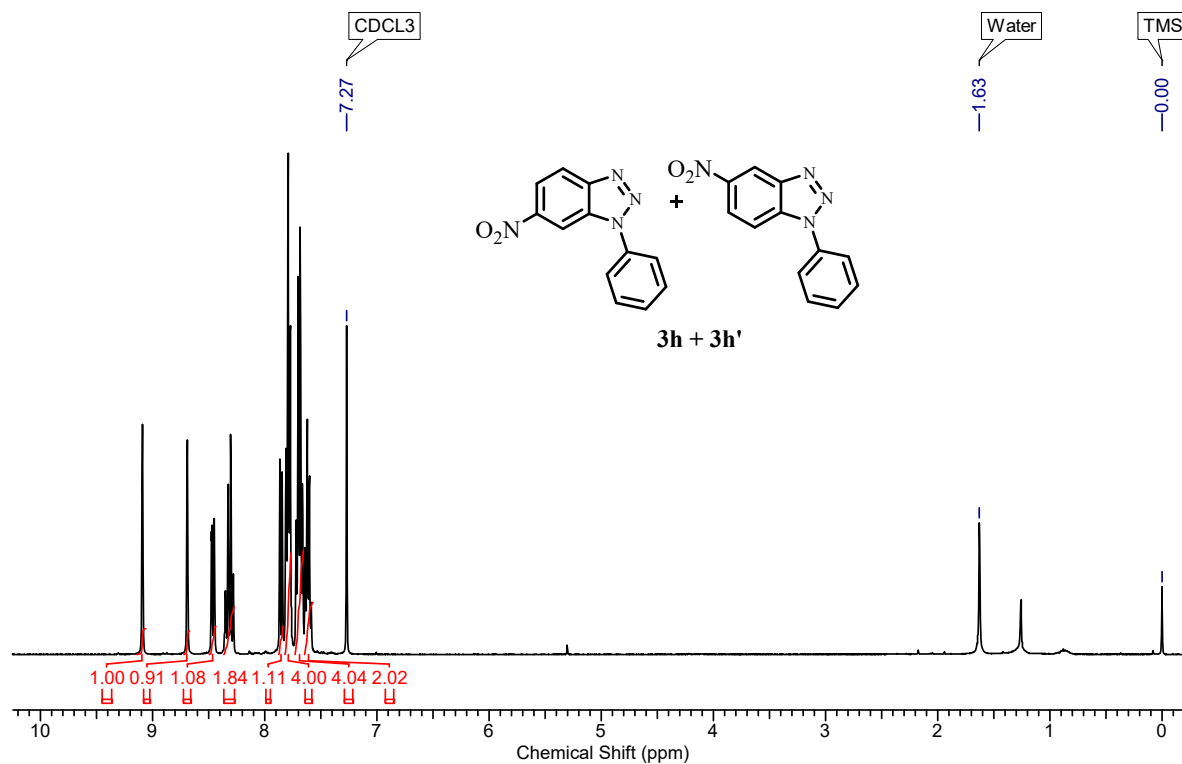


¹³C NMR (CDCl₃, 100 MHz) of Compound 3g + 3g'

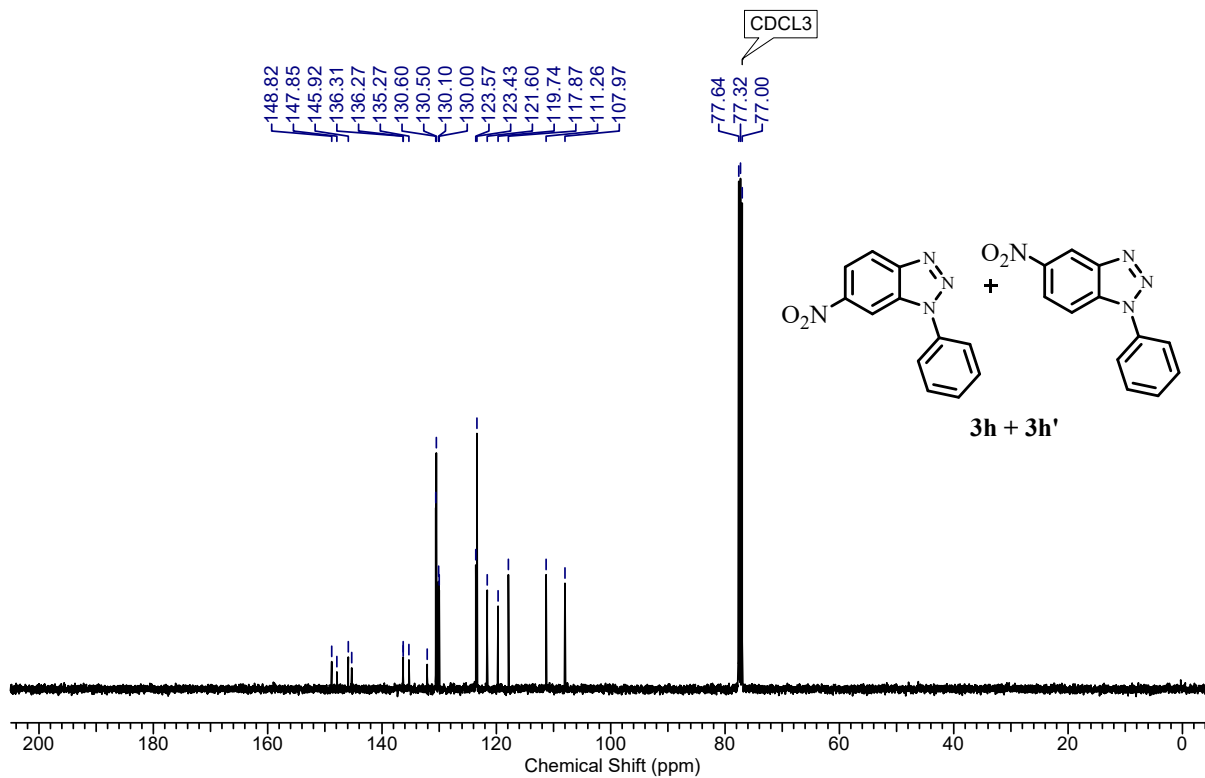
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HRMS of Compound 3g + 3g'

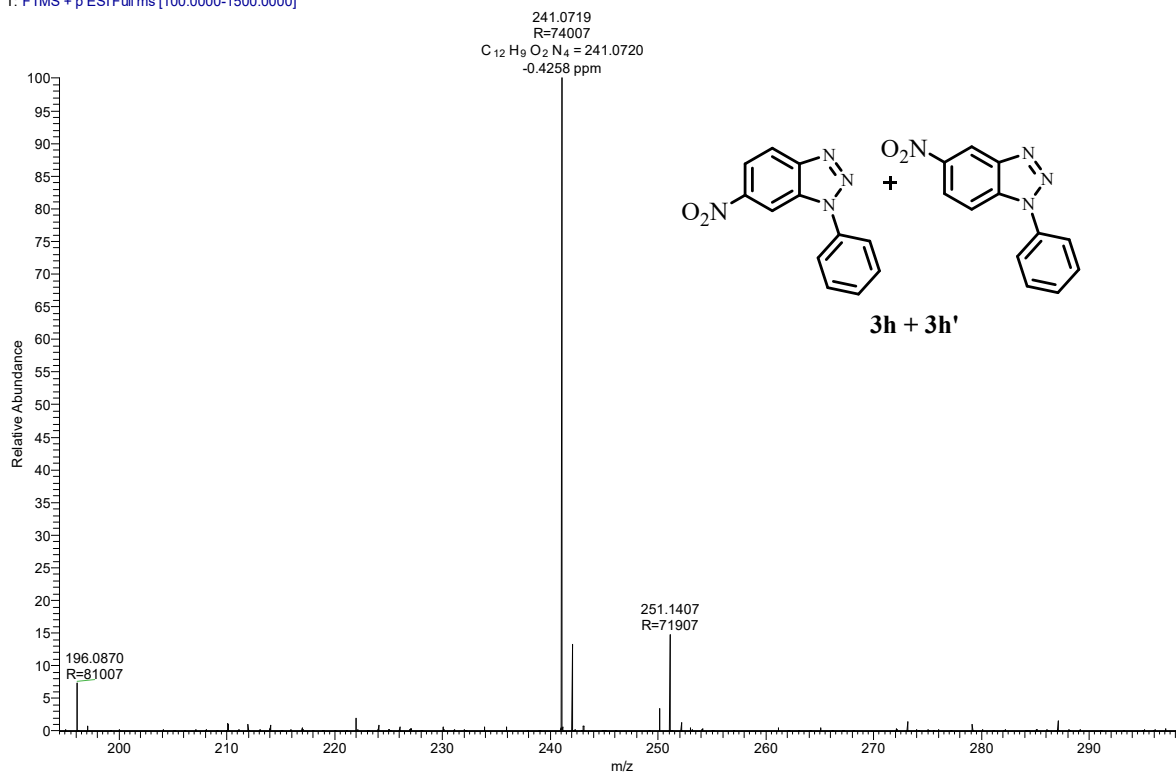


¹H NMR (CDCl₃, 400 MHz) of Compound 3h + 3h'

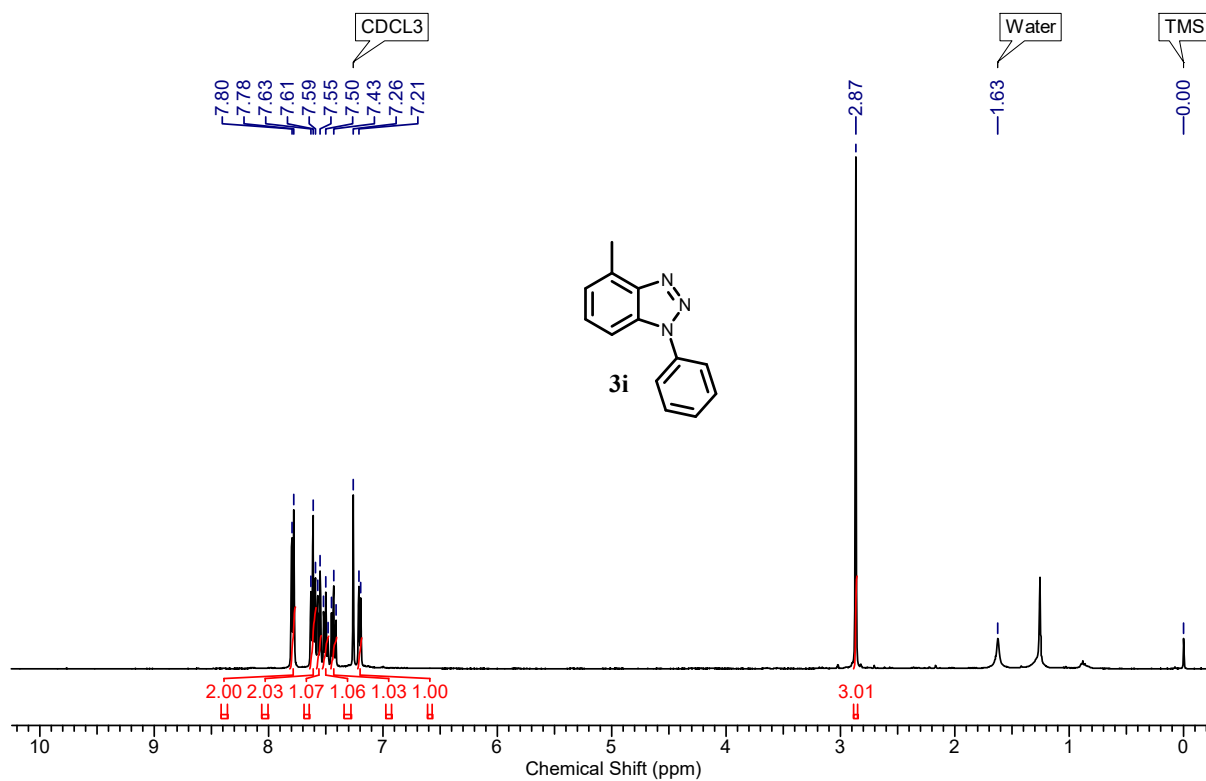


¹³C NMR (CDCl₃, 100 MHz) of Compound 3h + 3h'

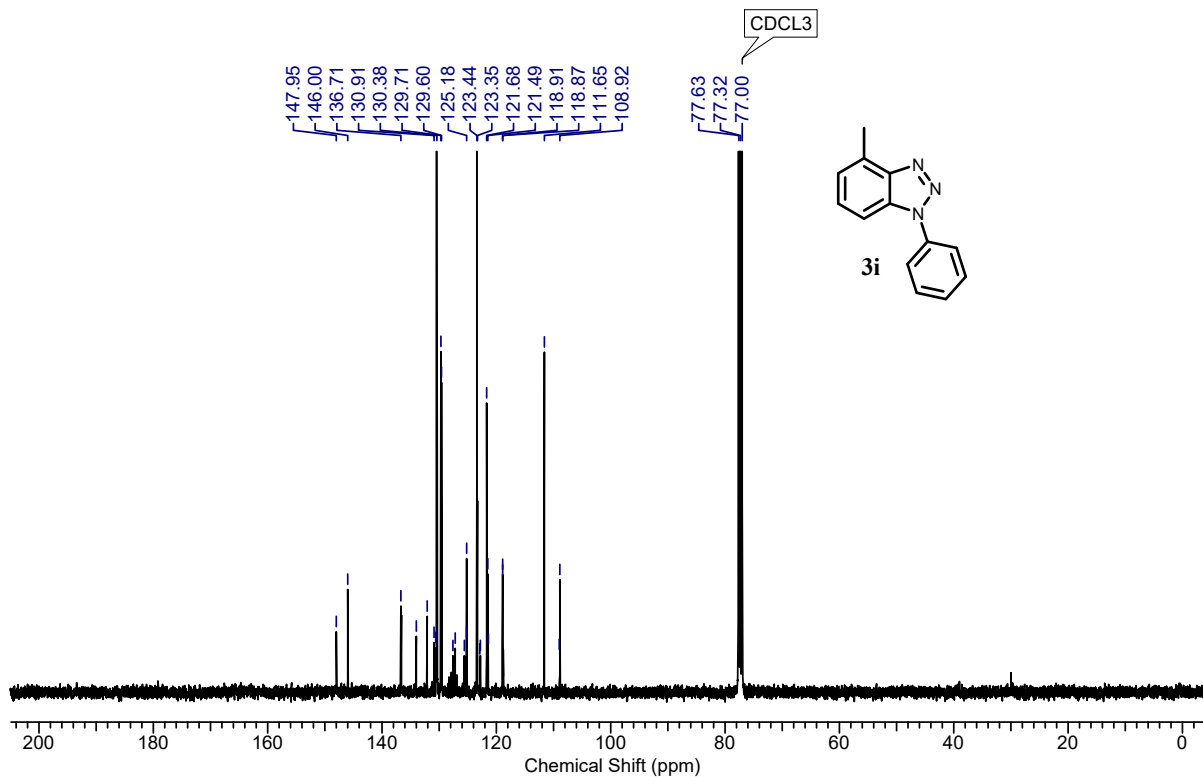
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HRMS of Compound 3h + 3h'

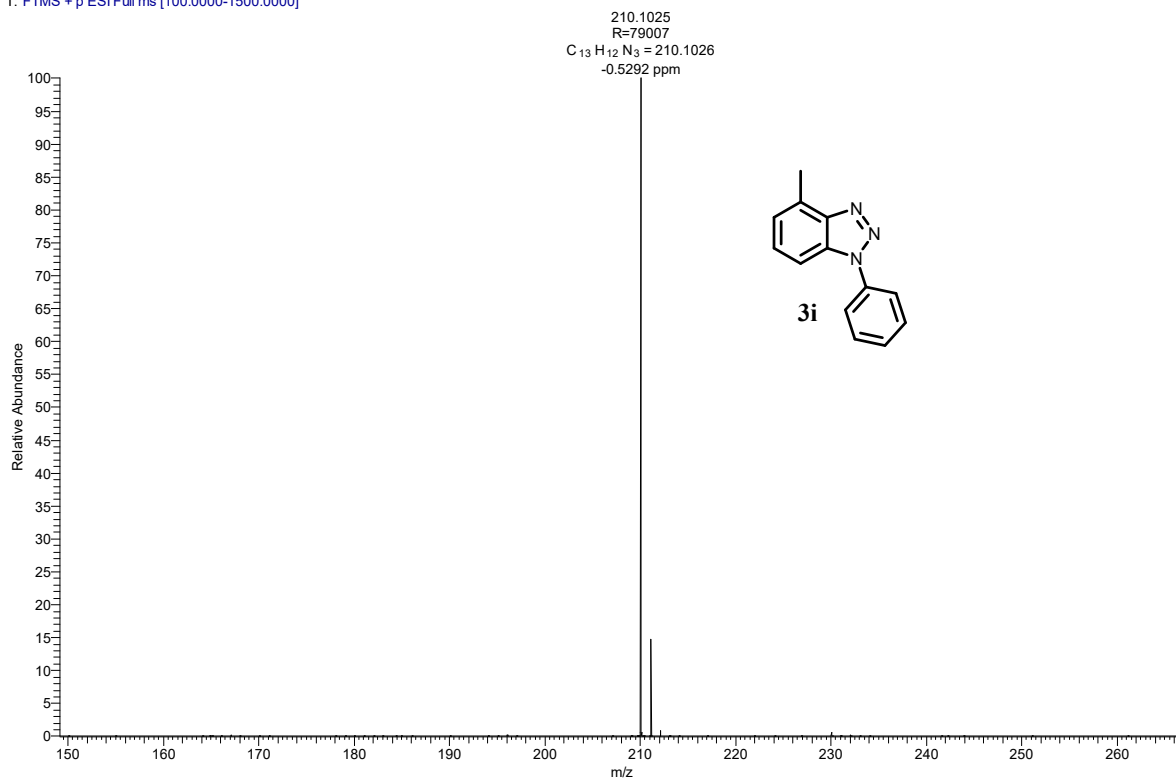


¹H NMR (CDCl₃, 400 MHz) of Compound 3i

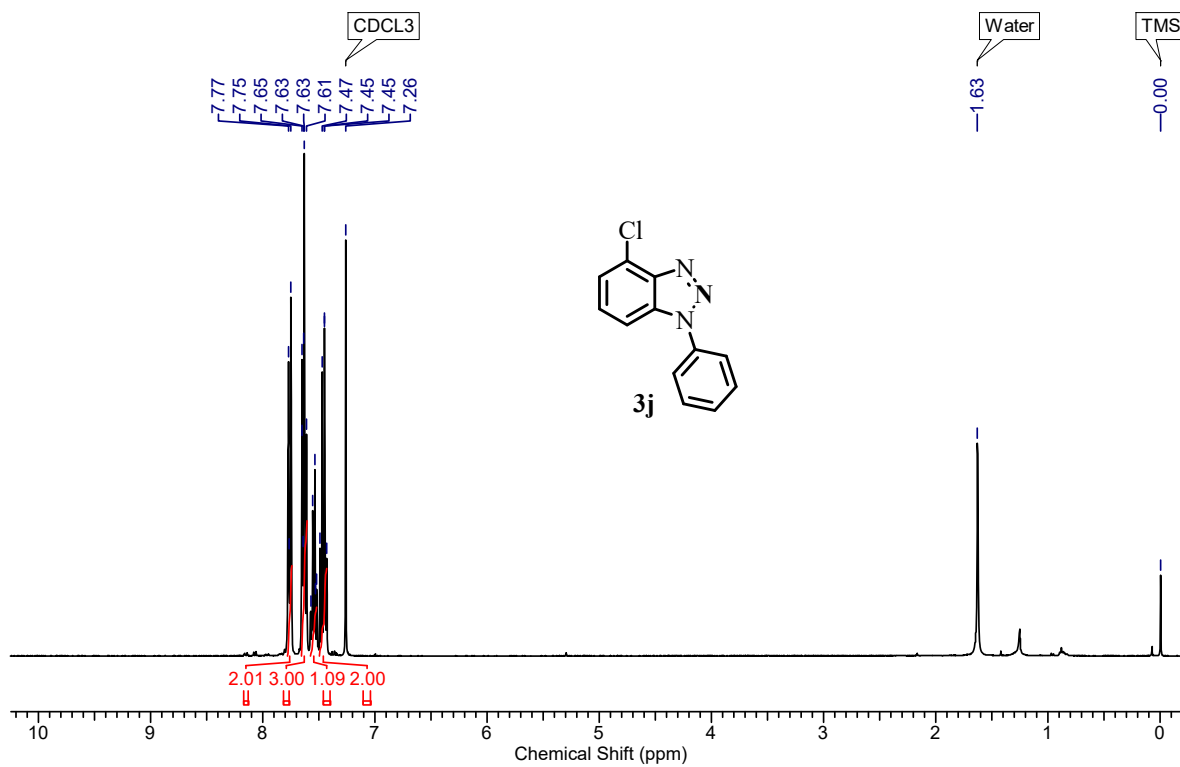


¹³C NMR (CDCl₃, 100 MHz) of Compound 3i

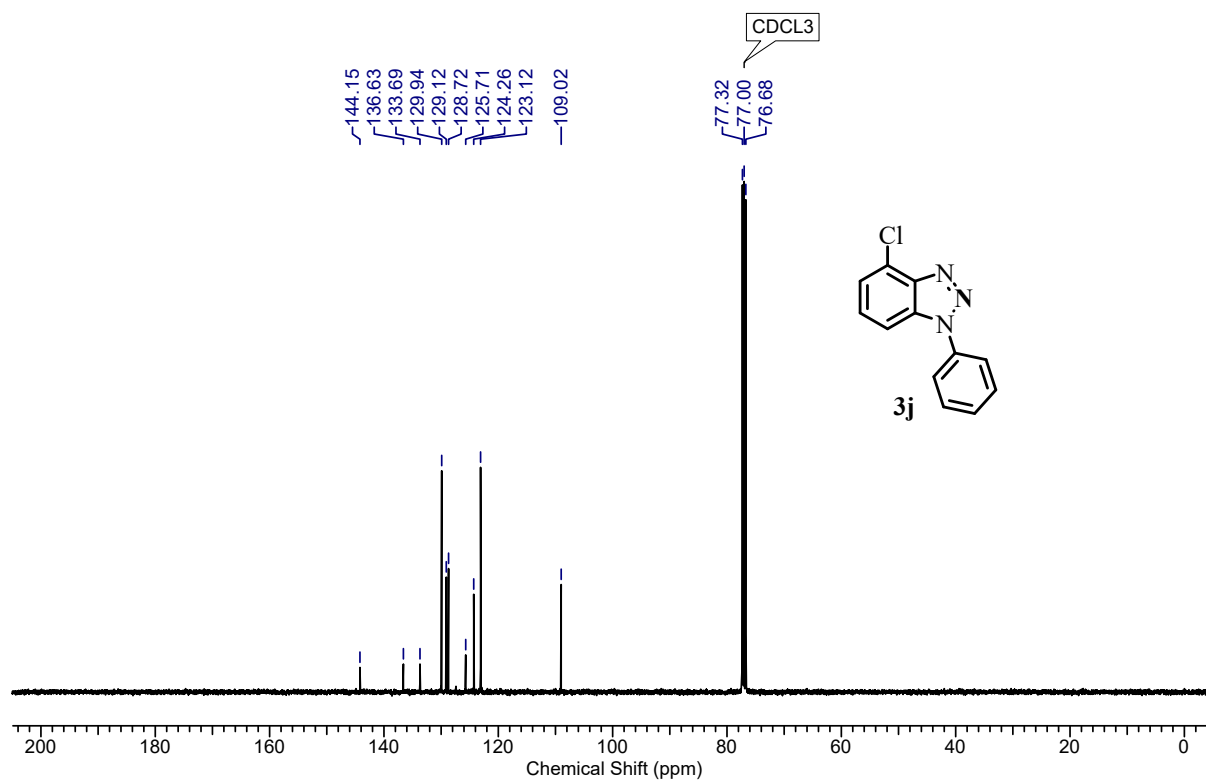
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HRMS of Compound 3i

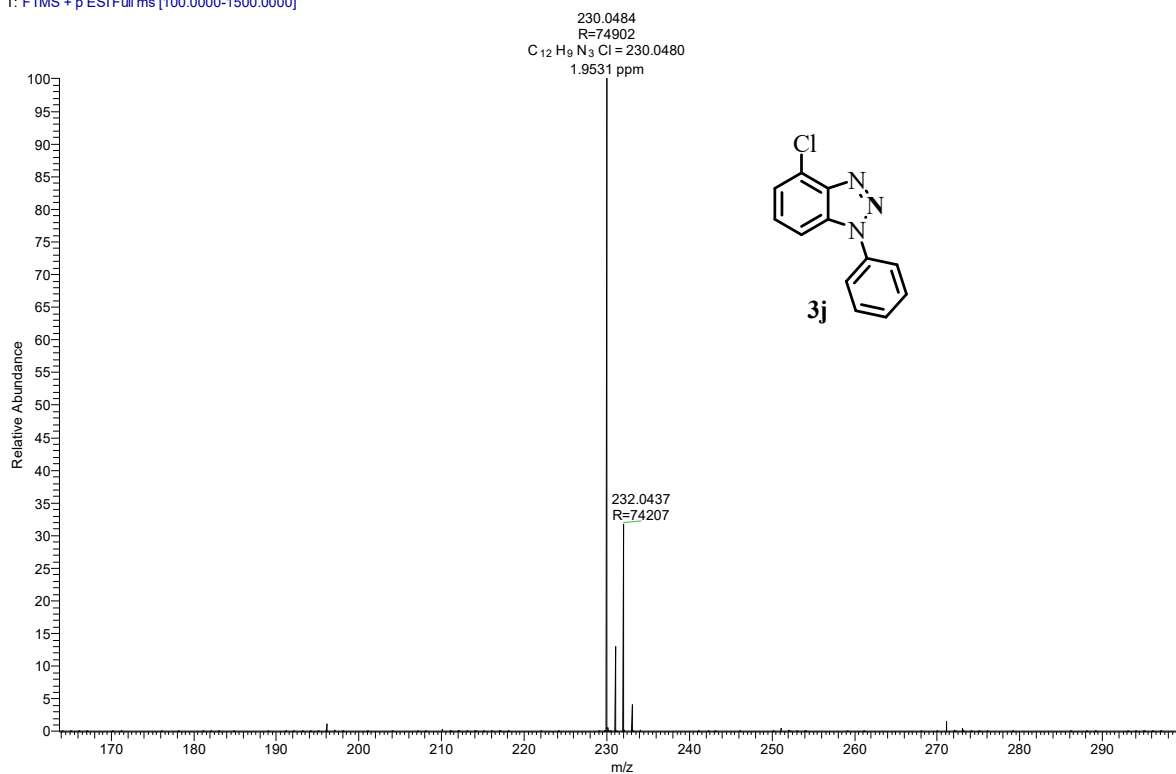


¹H NMR (CDCl₃, 400 MHz) of Compound 3j

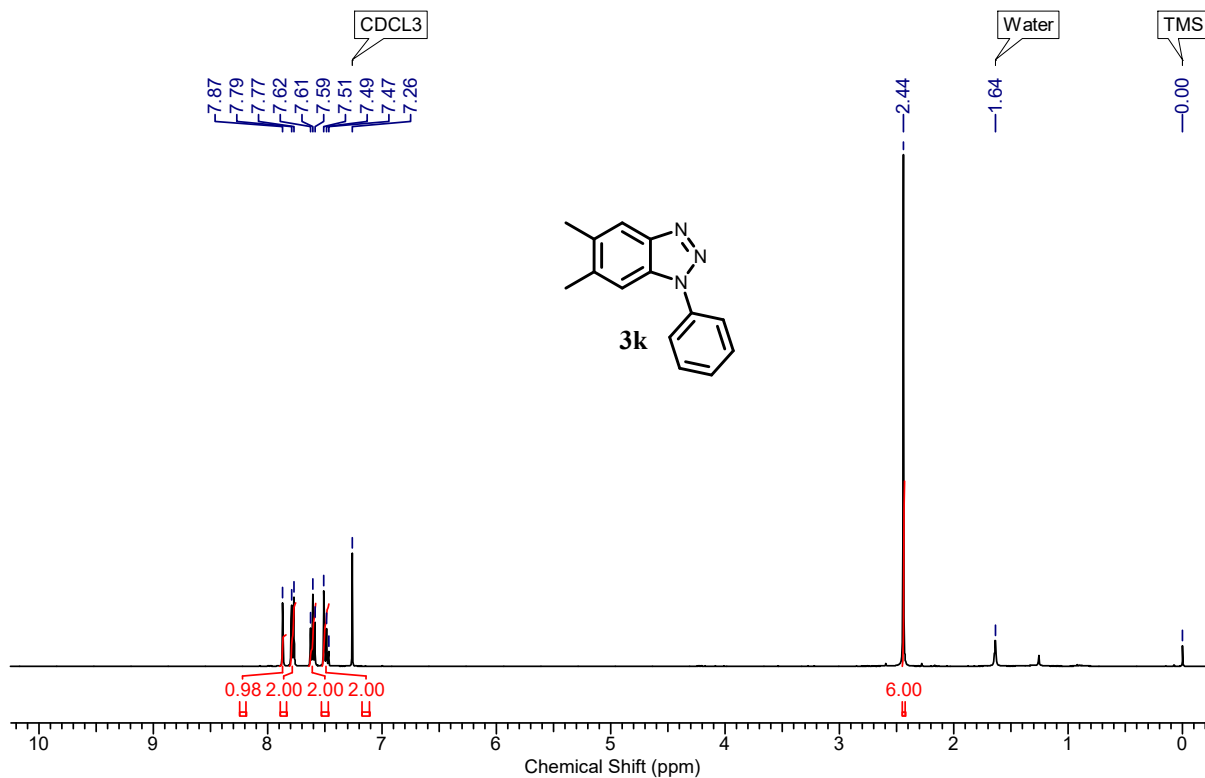


¹³C NMR (CDCl₃, 100 MHz) of Compound 3j

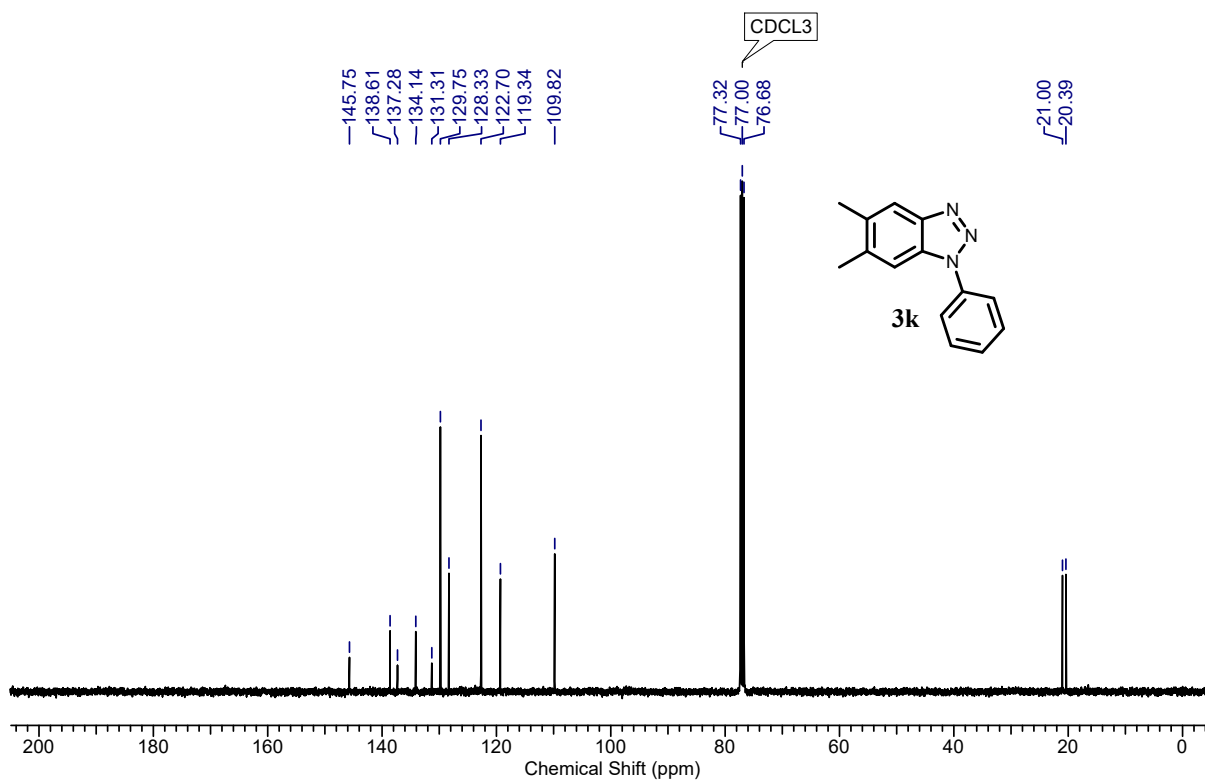
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HRMS of Compound 3j

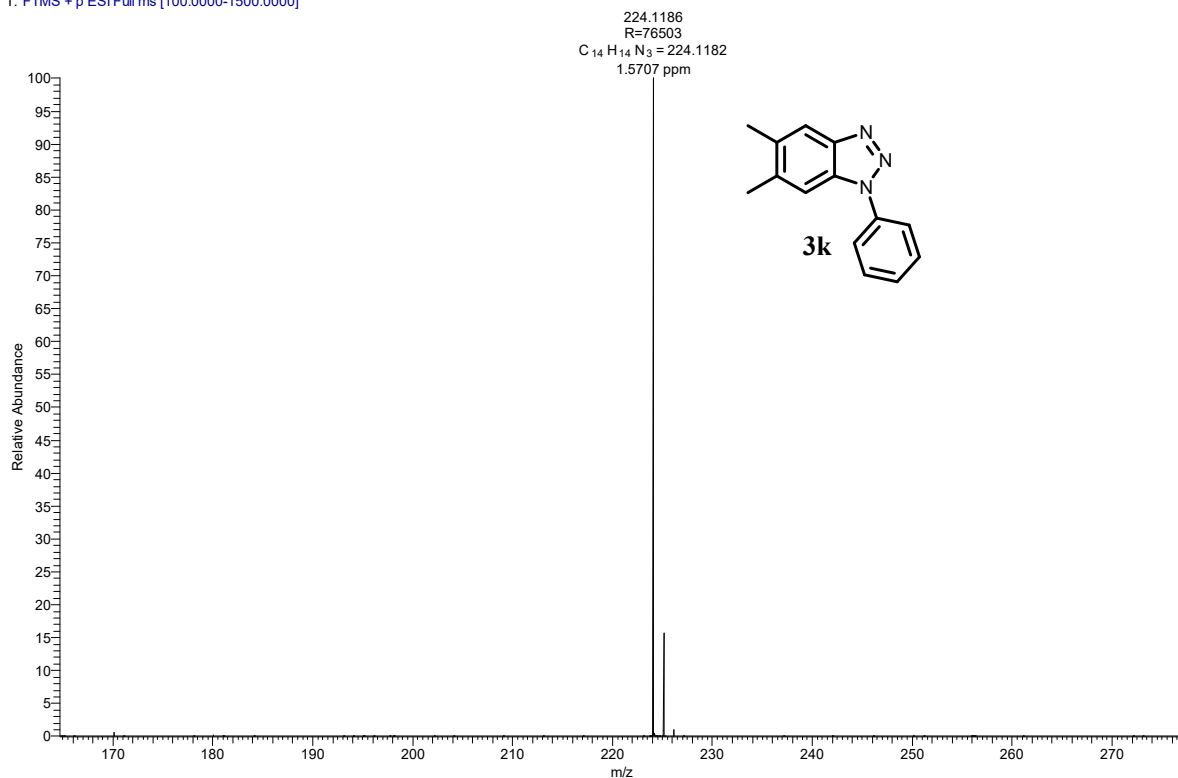


¹H NMR (CDCl₃, 400 MHz) of Compound 3k

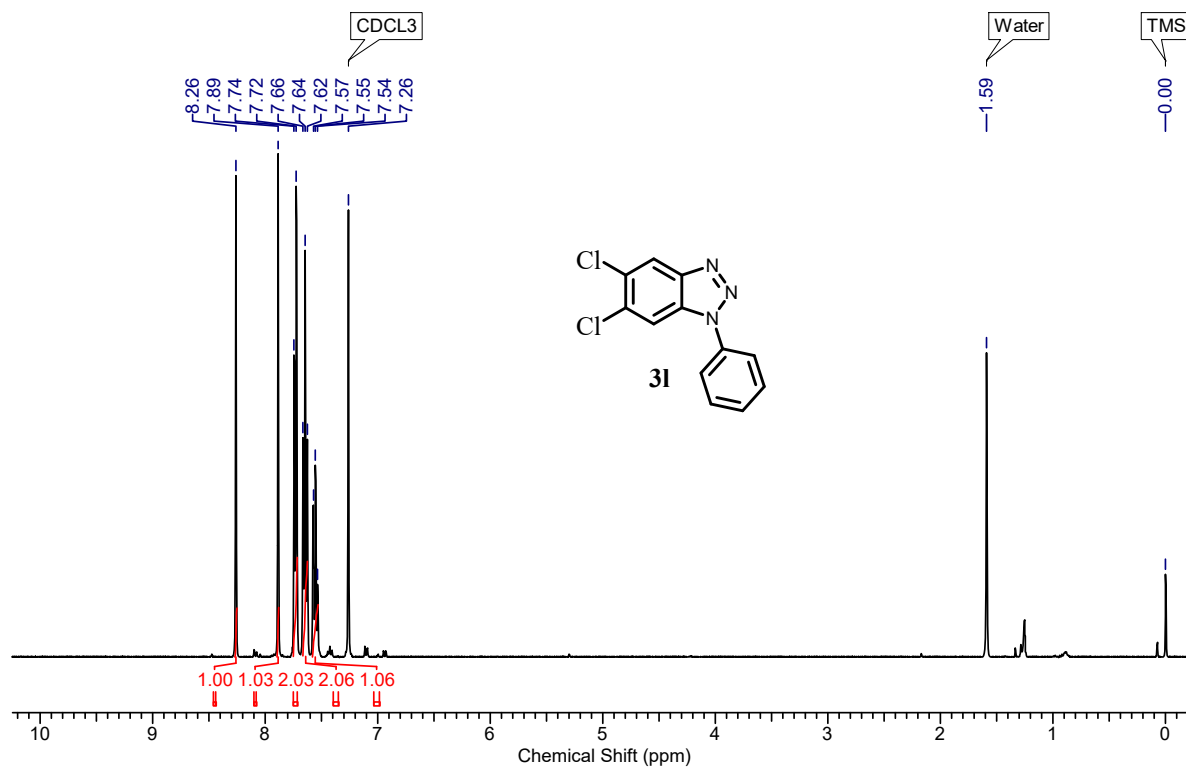


¹³C NMR (CDCl₃, 100 MHz) of Compound 3k

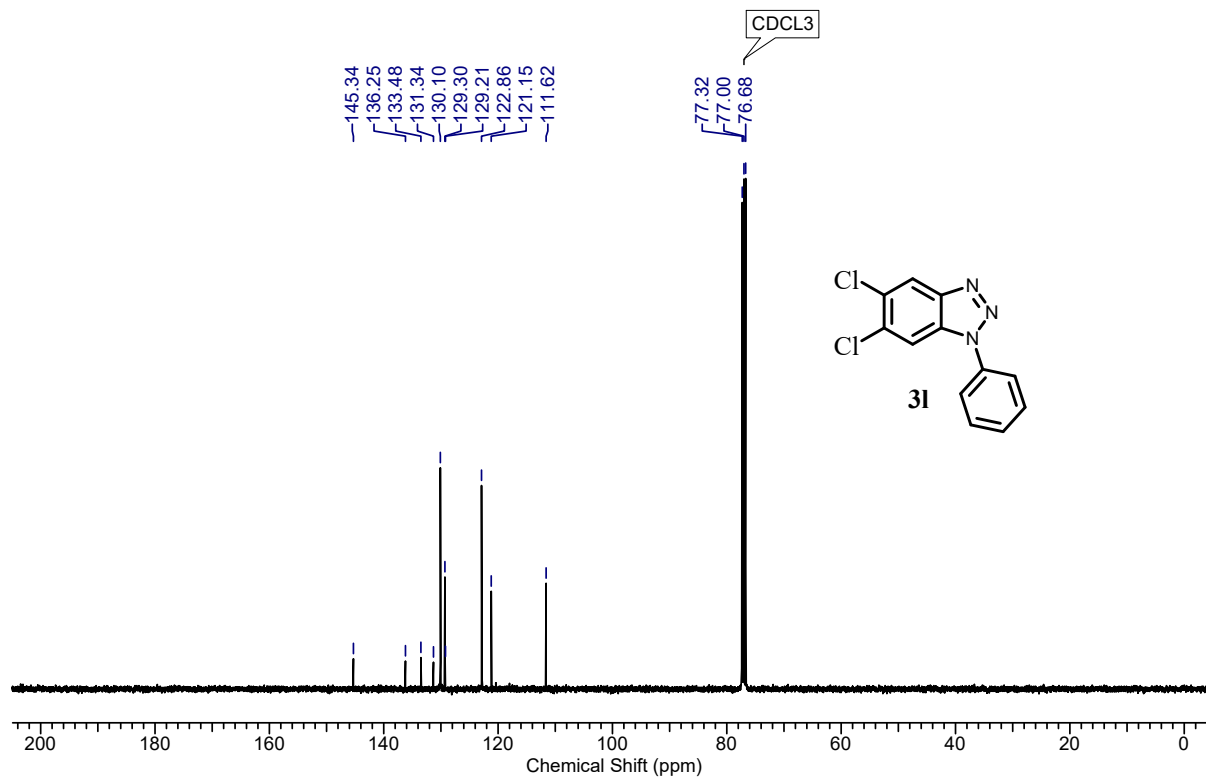
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HRMS of Compound 3k

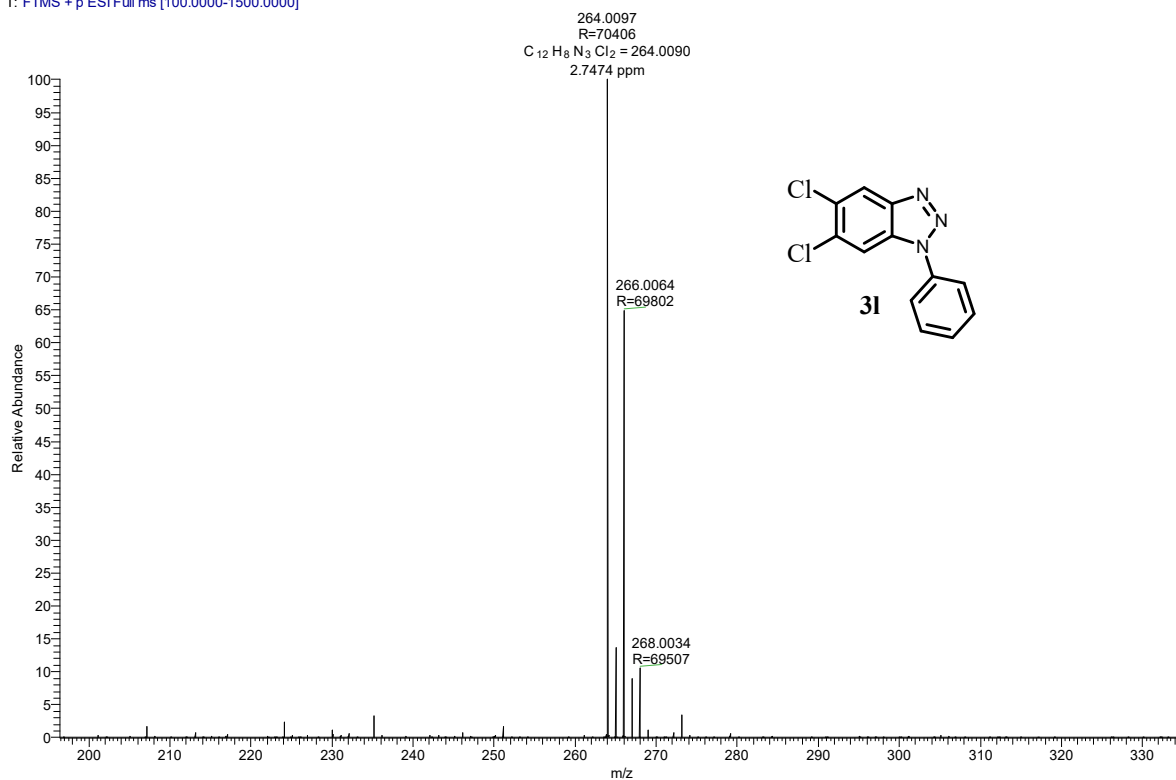


¹H NMR (CDCl₃, 400 MHz) of Compound 31

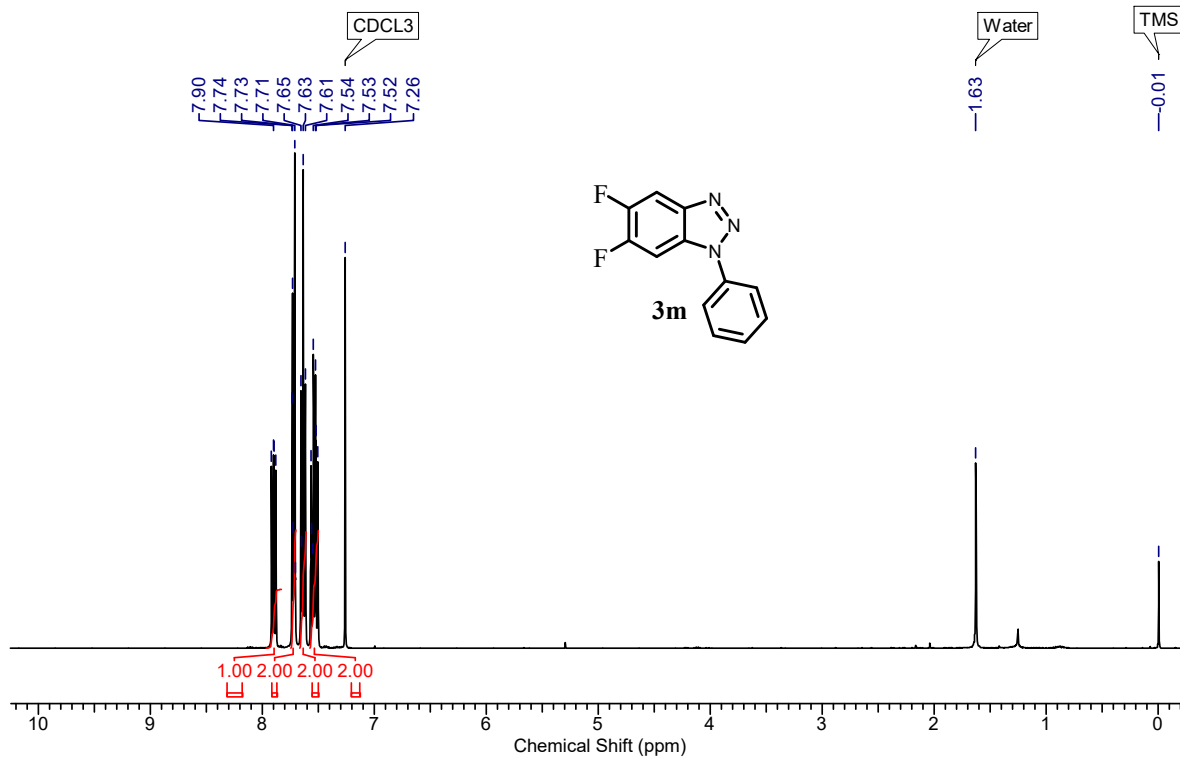


¹³C NMR (CDCl₃, 100 MHz) of Compound 31

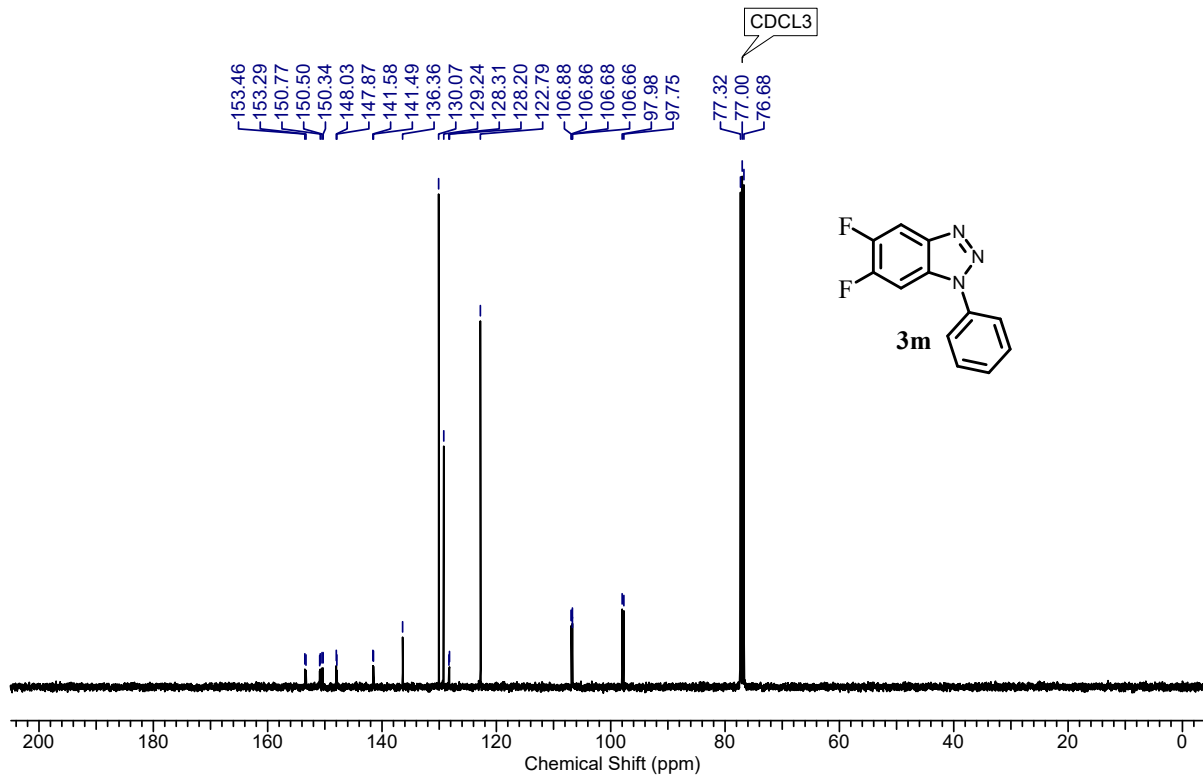
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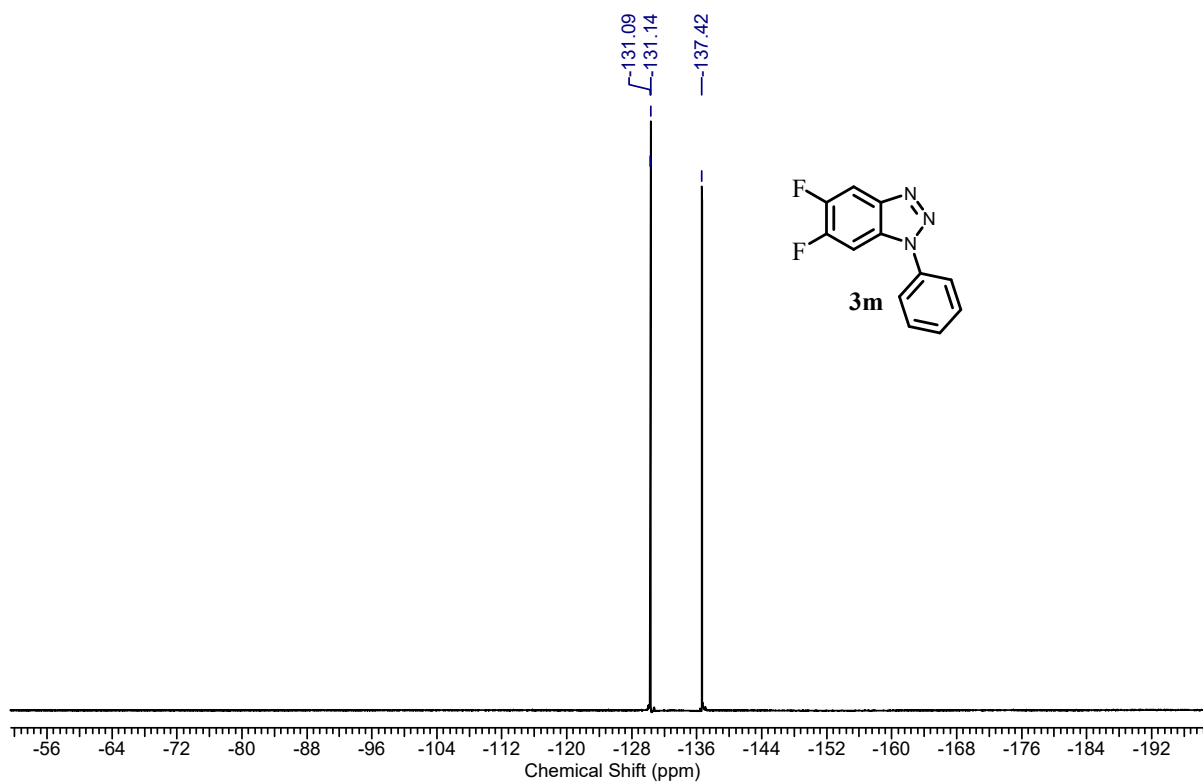
HRMS of Compound 31



¹H NMR (CDCl₃, 400 MHz) of Compound 3m

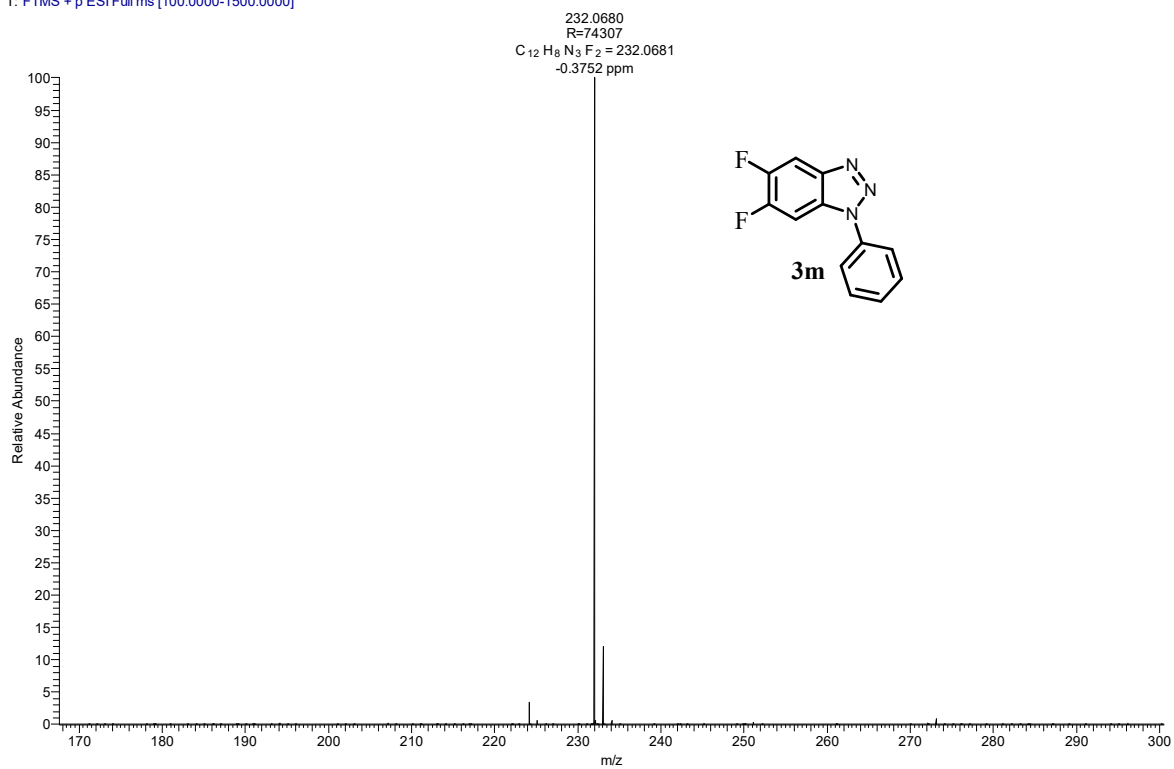


¹³C NMR (CDCl₃, 100 MHz) of Compound 3m

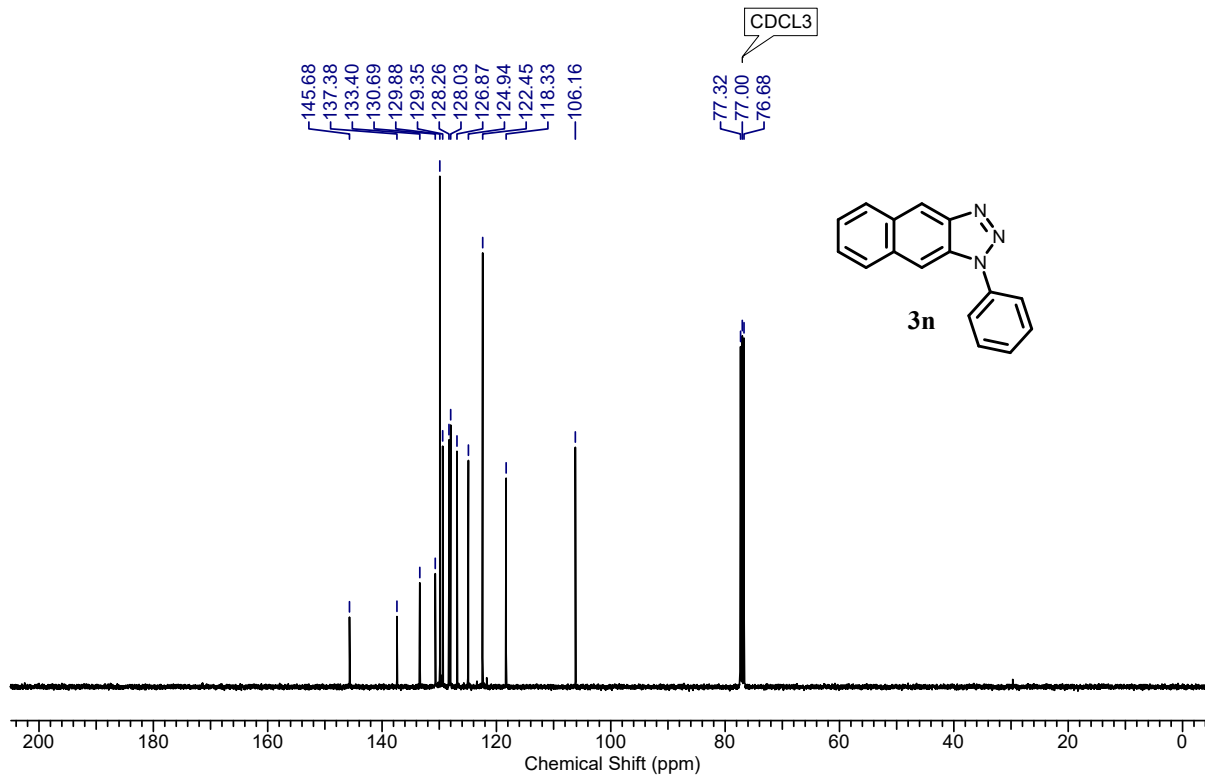
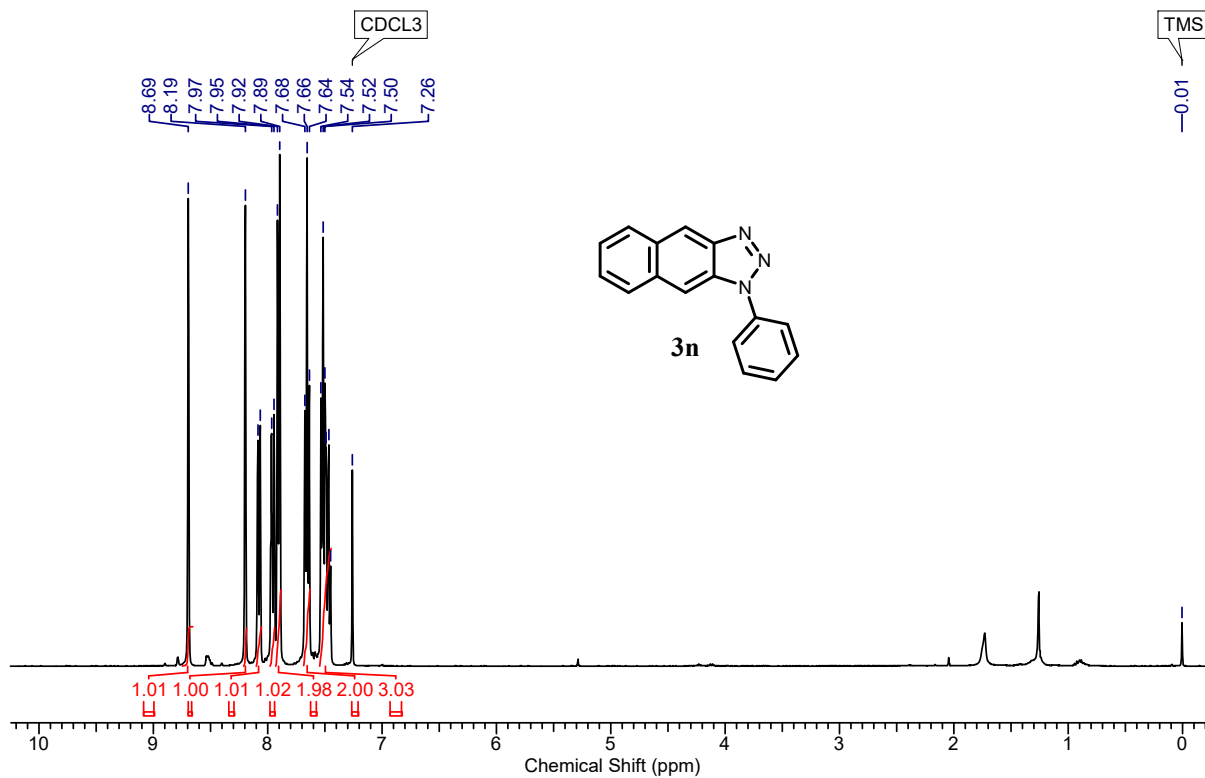


^{19}F NMR (CDCl_3 , 376 MHz) of Compound 3m

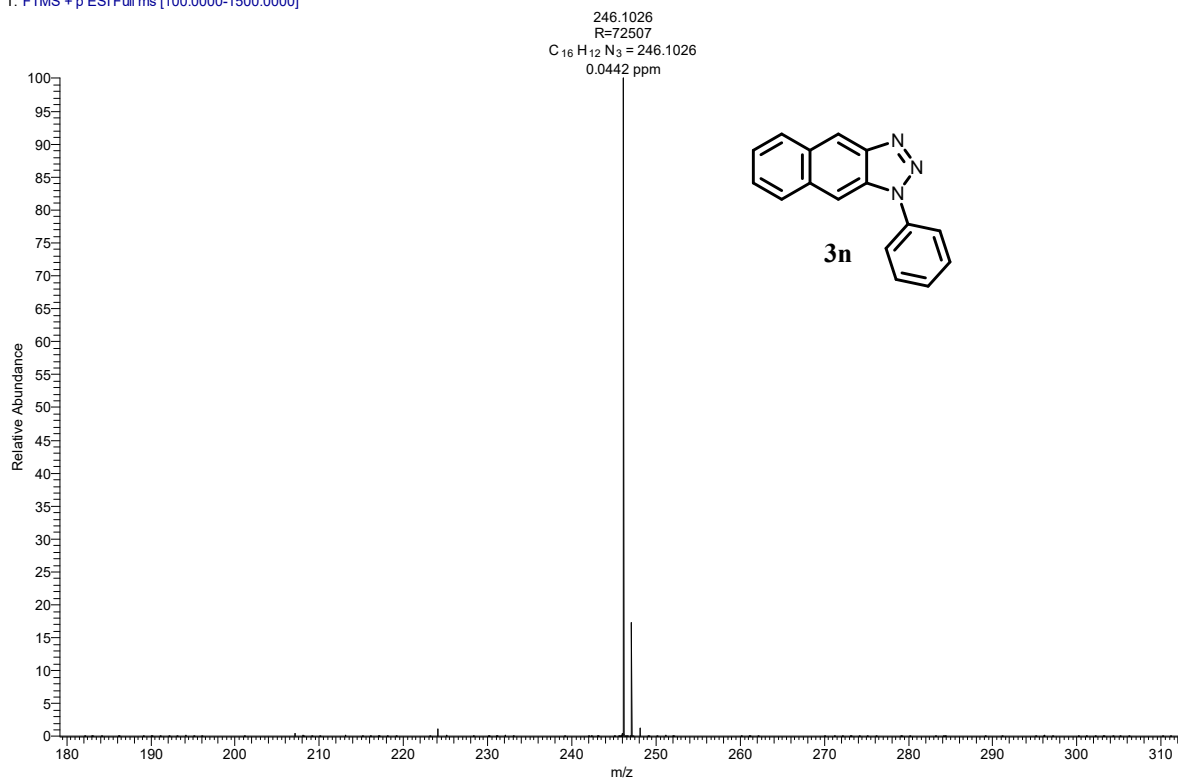
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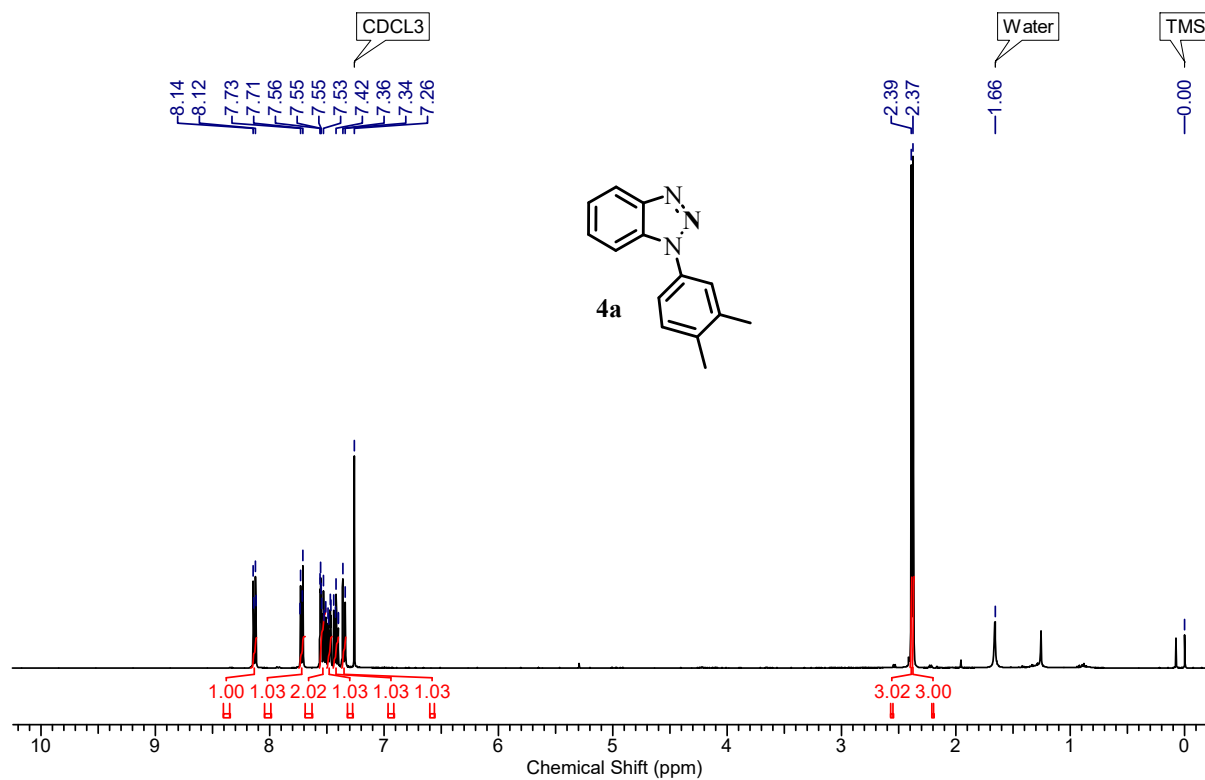
HRMS of Compound 3m



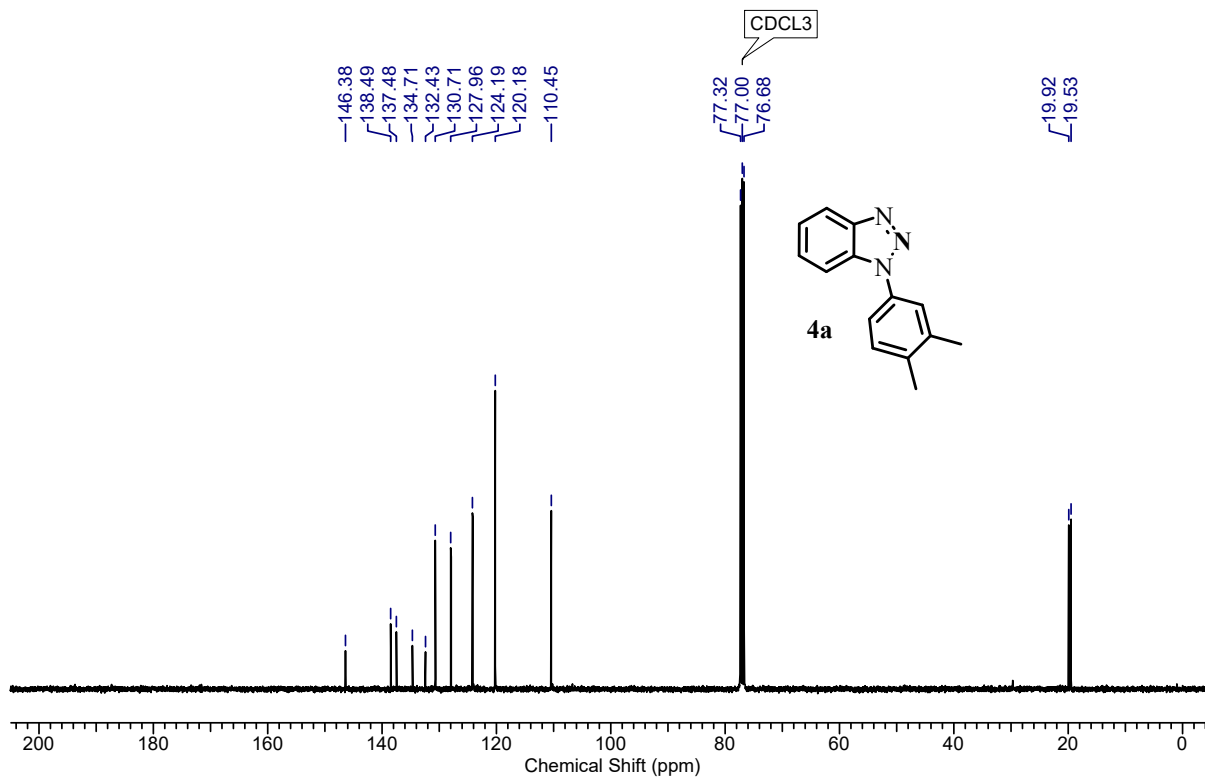
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HRMS of Compound 3n

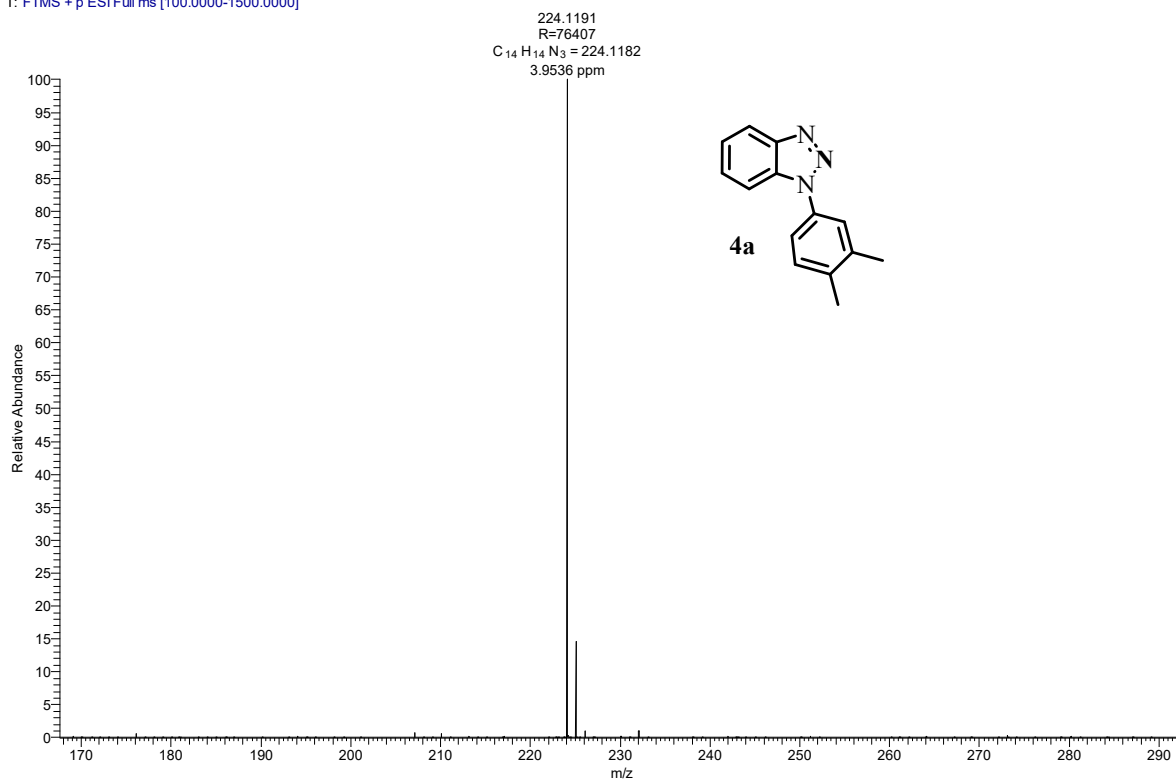


¹H NMR (CDCl₃, 400 MHz) of Compound 4a

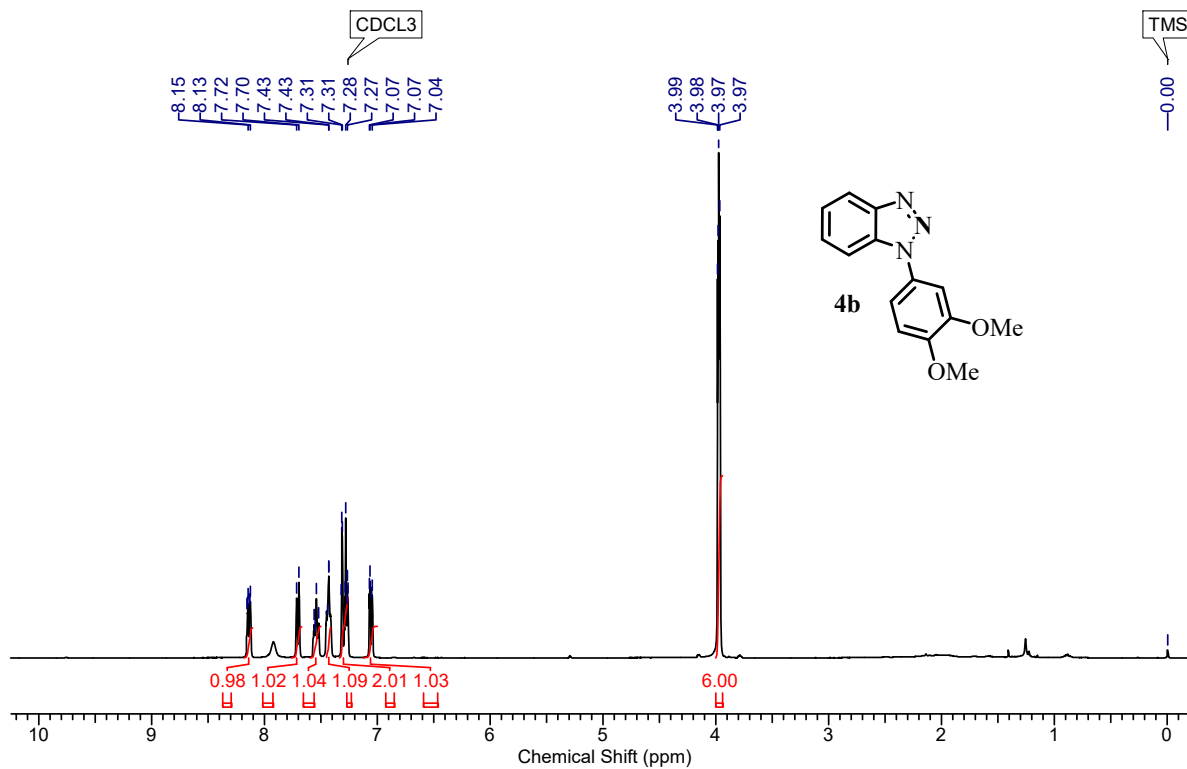


¹³C NMR (CDCl₃, 100 MHz) of Compound 4a

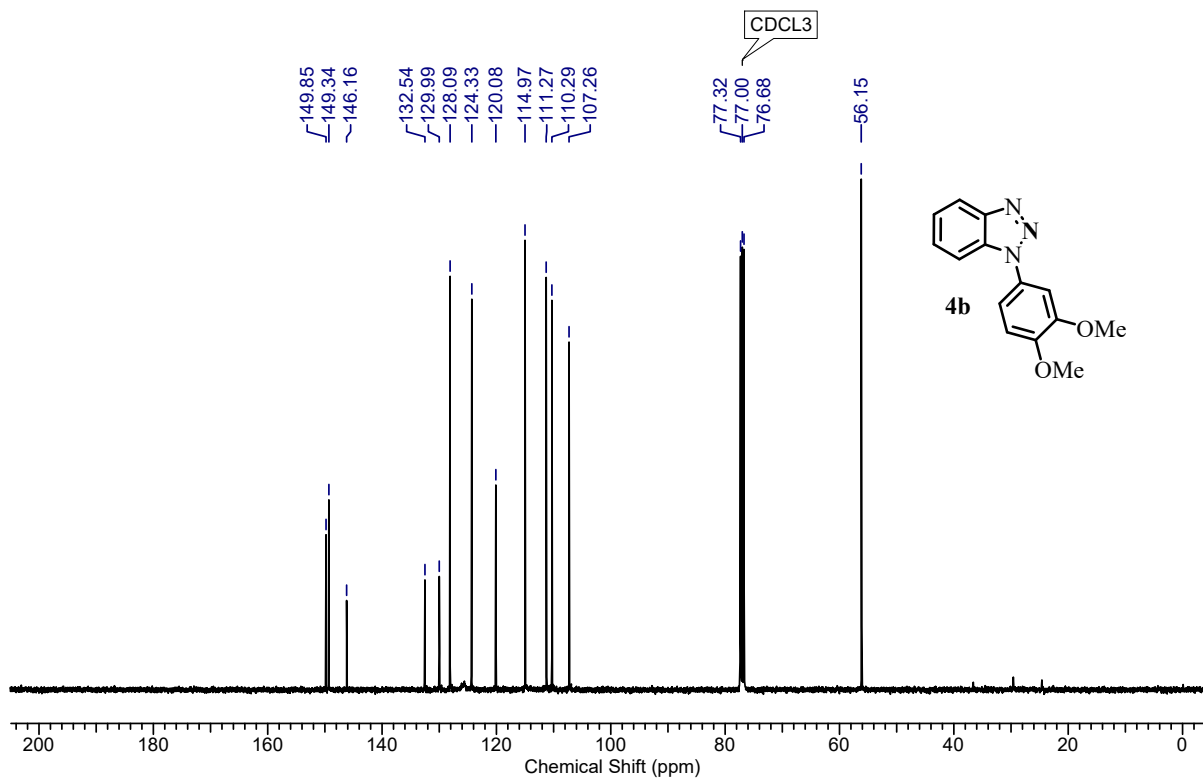
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HRMS of Compound 4a

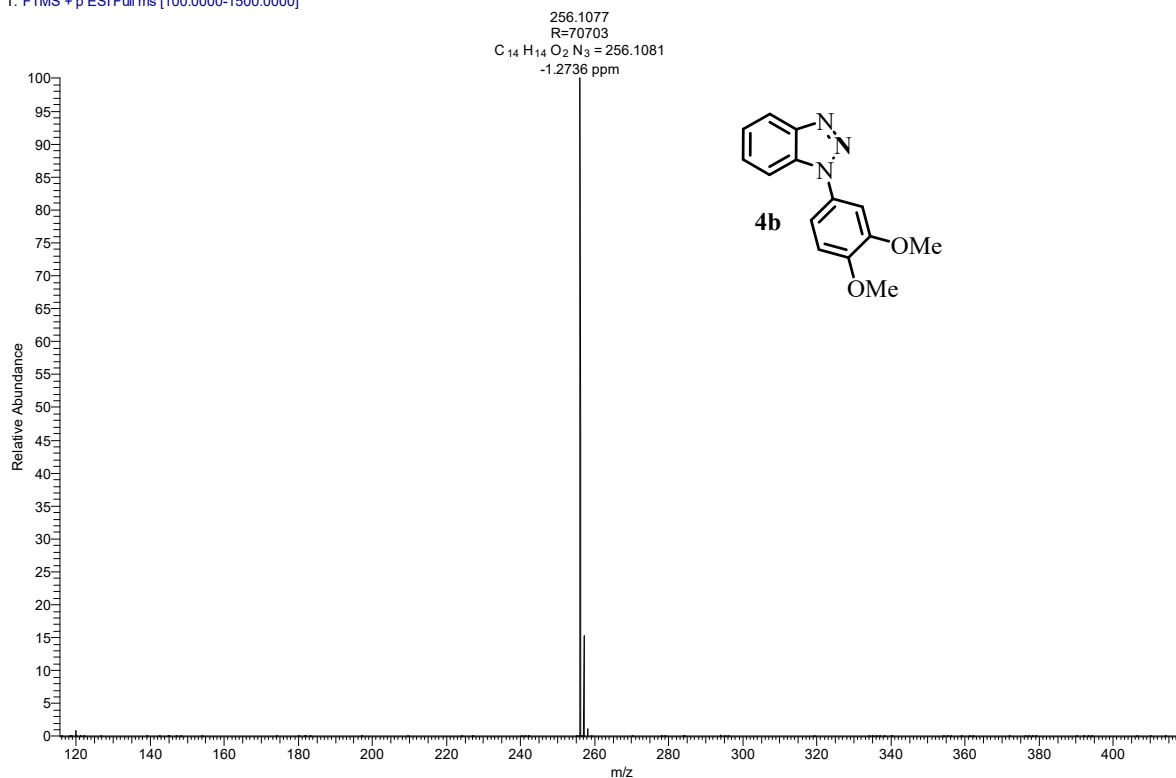


¹H NMR (CDCl₃, 400 MHz) of Compound 4b

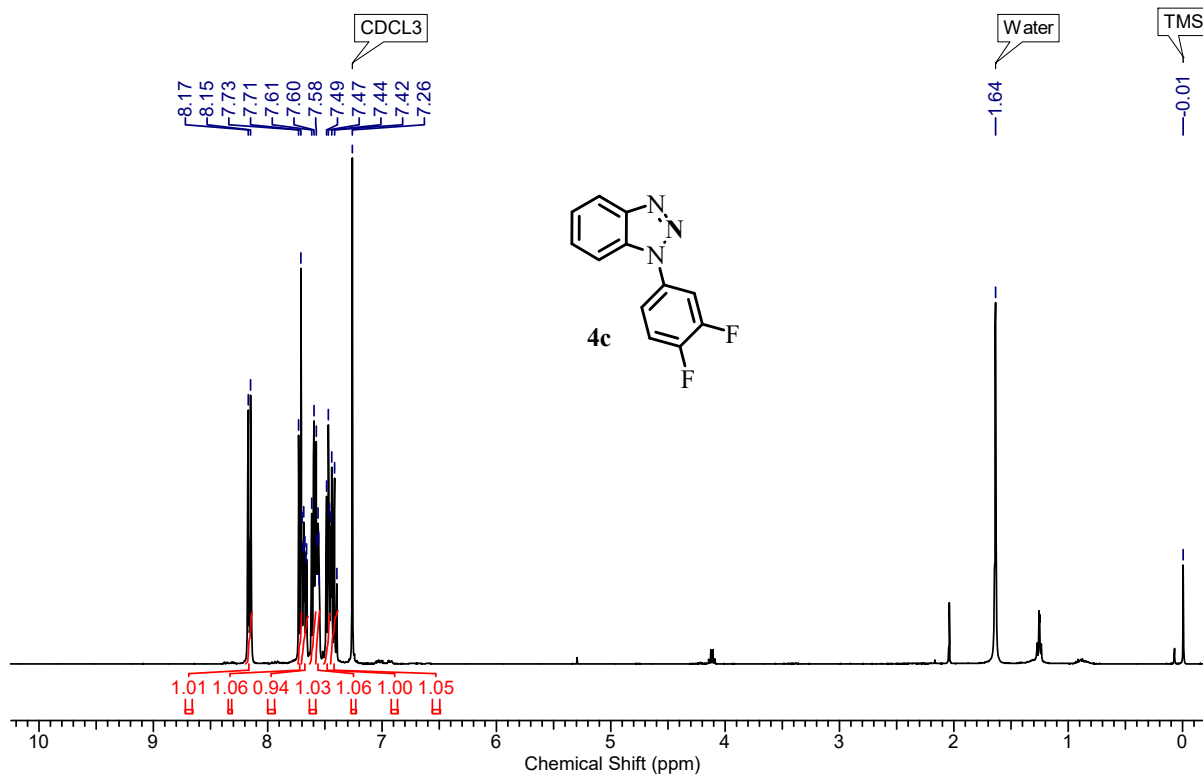


¹³C NMR (CDCl₃, 100 MHz) of Compound 4b

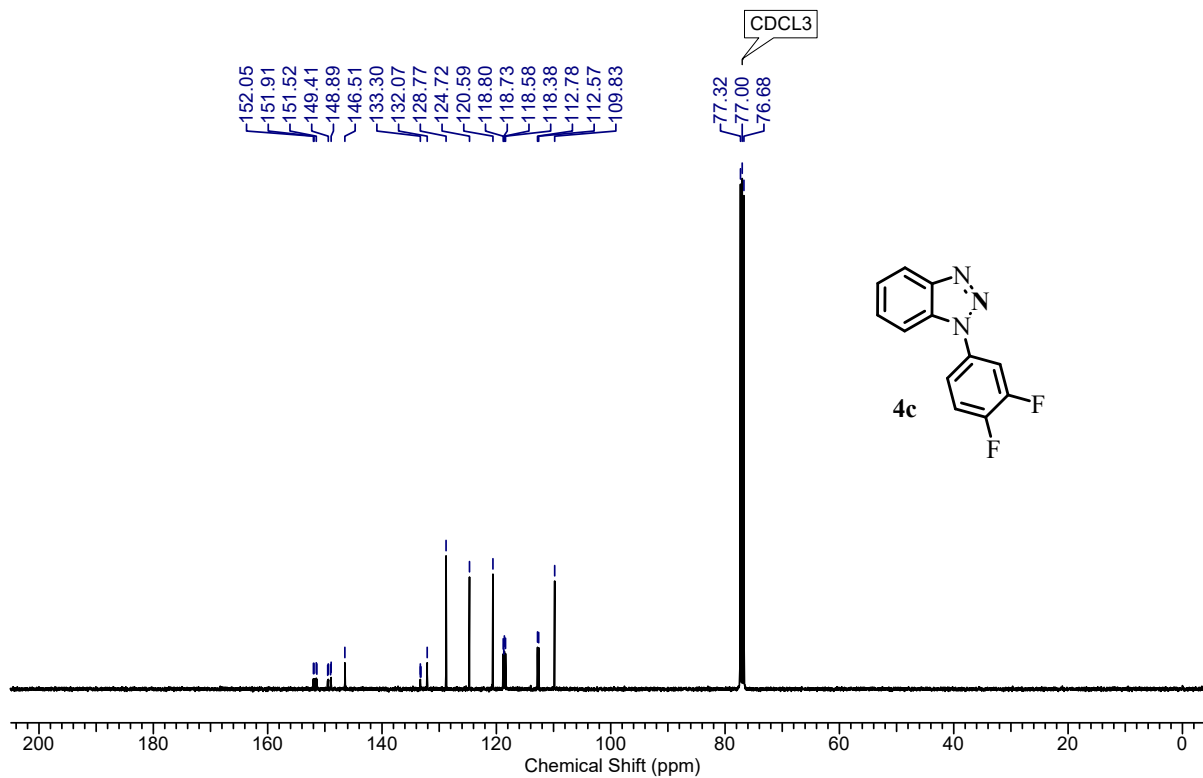
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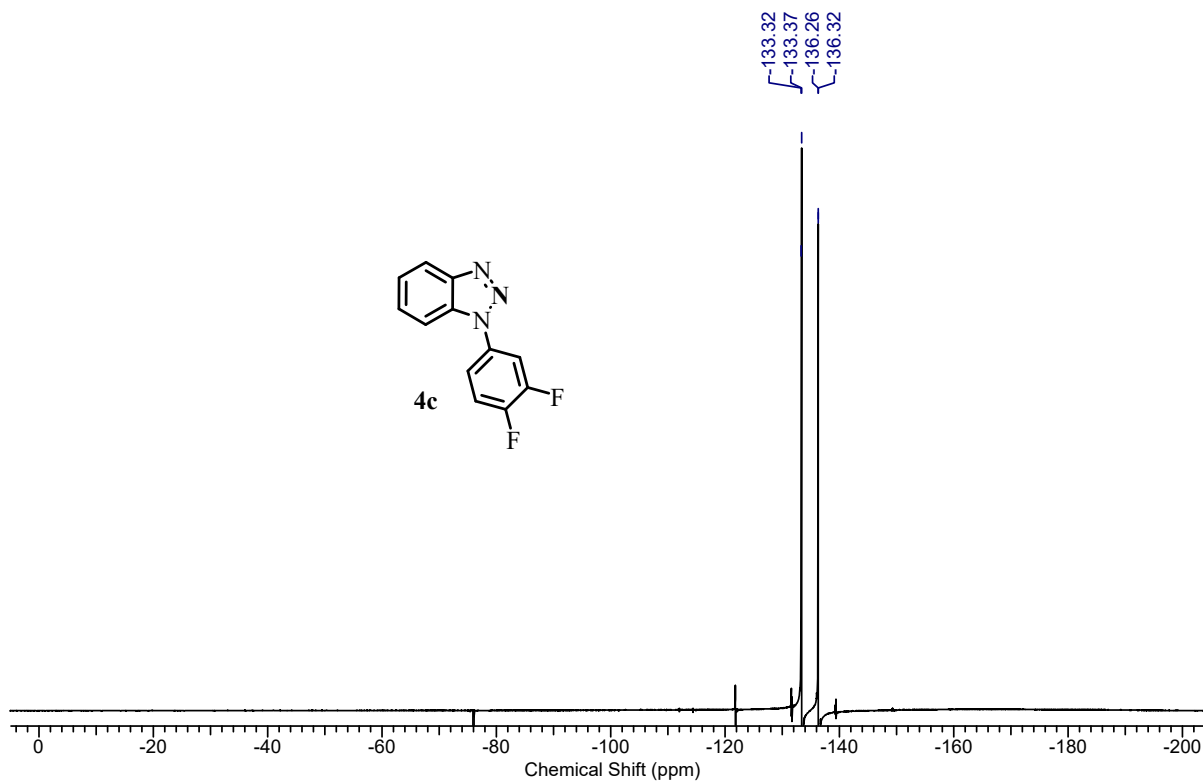
HRMS of Compound 4b



¹H NMR (CDCl₃, 400 MHz) of Compound 4c

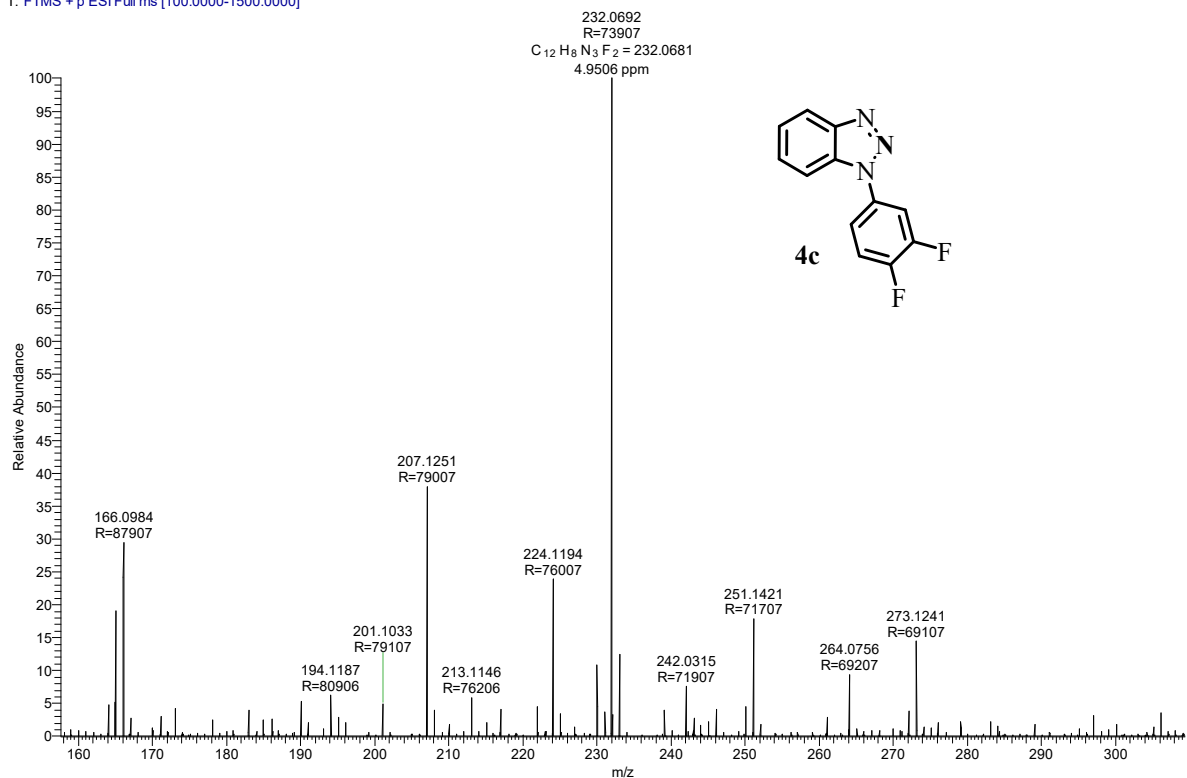


¹³C NMR (CDCl₃, 100 MHz) of Compound 4c

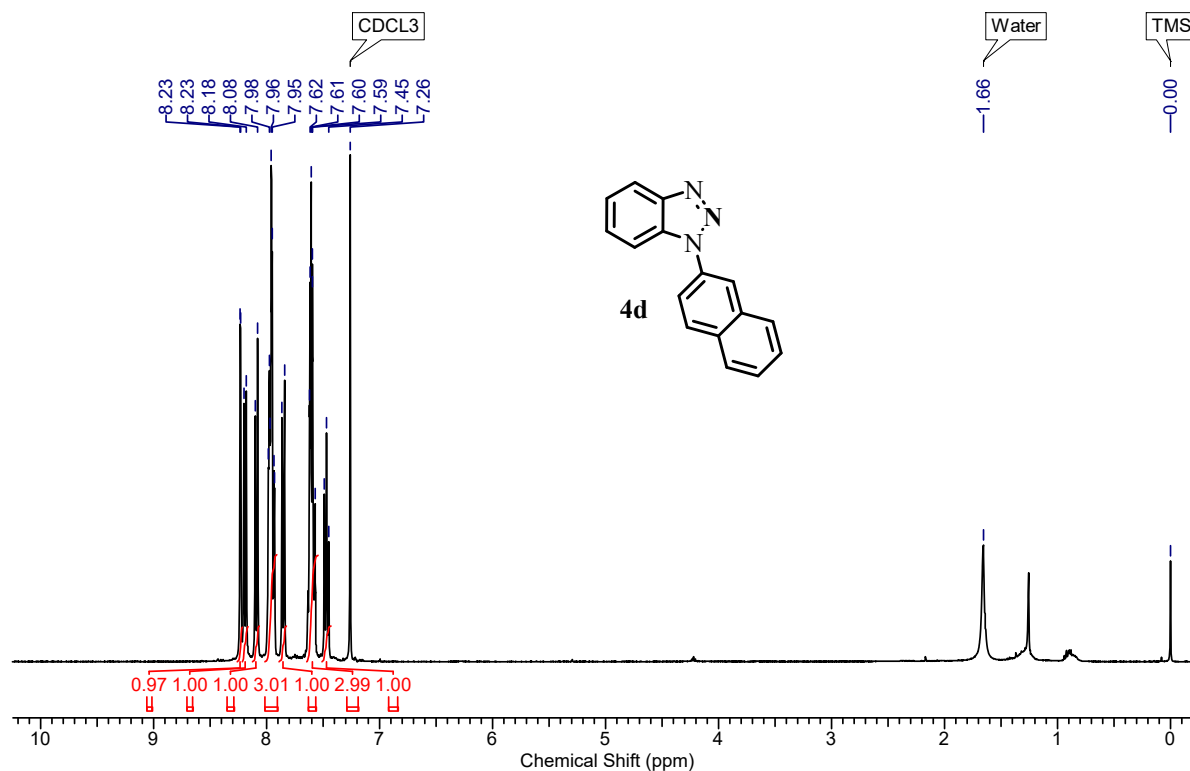


¹⁹F NMR (CDCl₃, 376 MHz) of Compound 4c

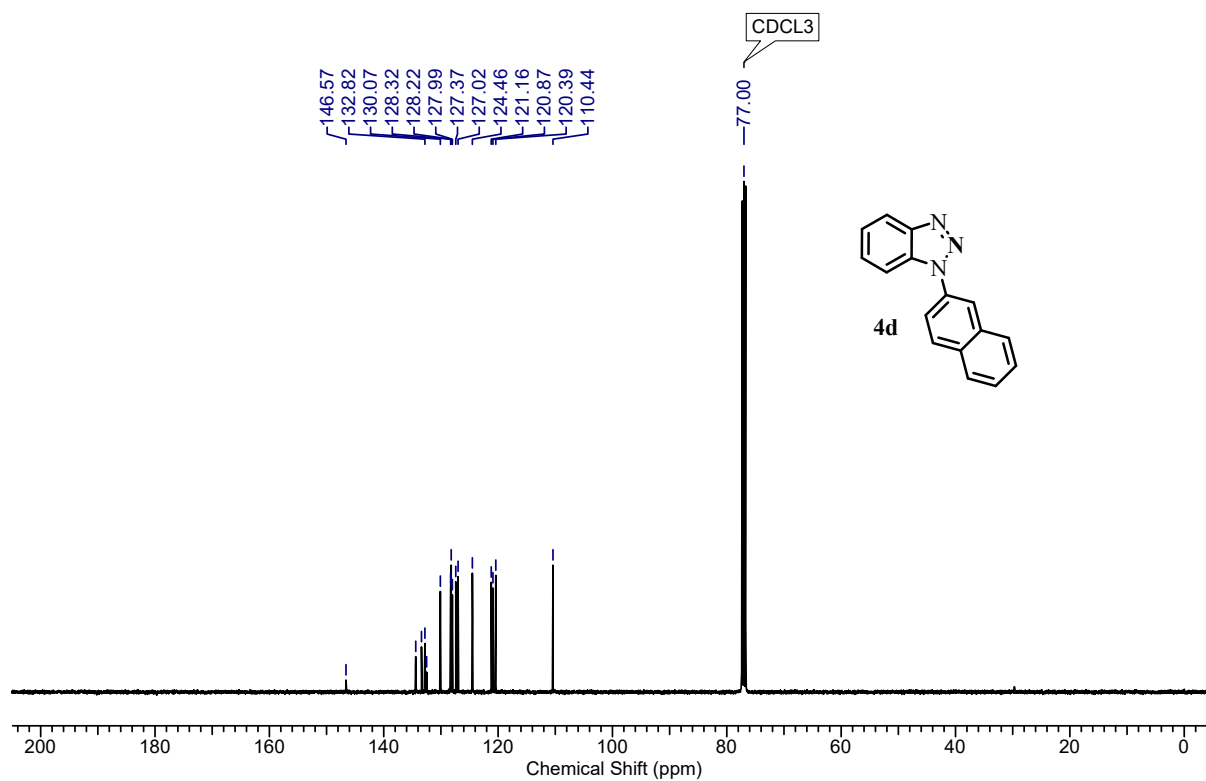
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HRMS of Compound 4c

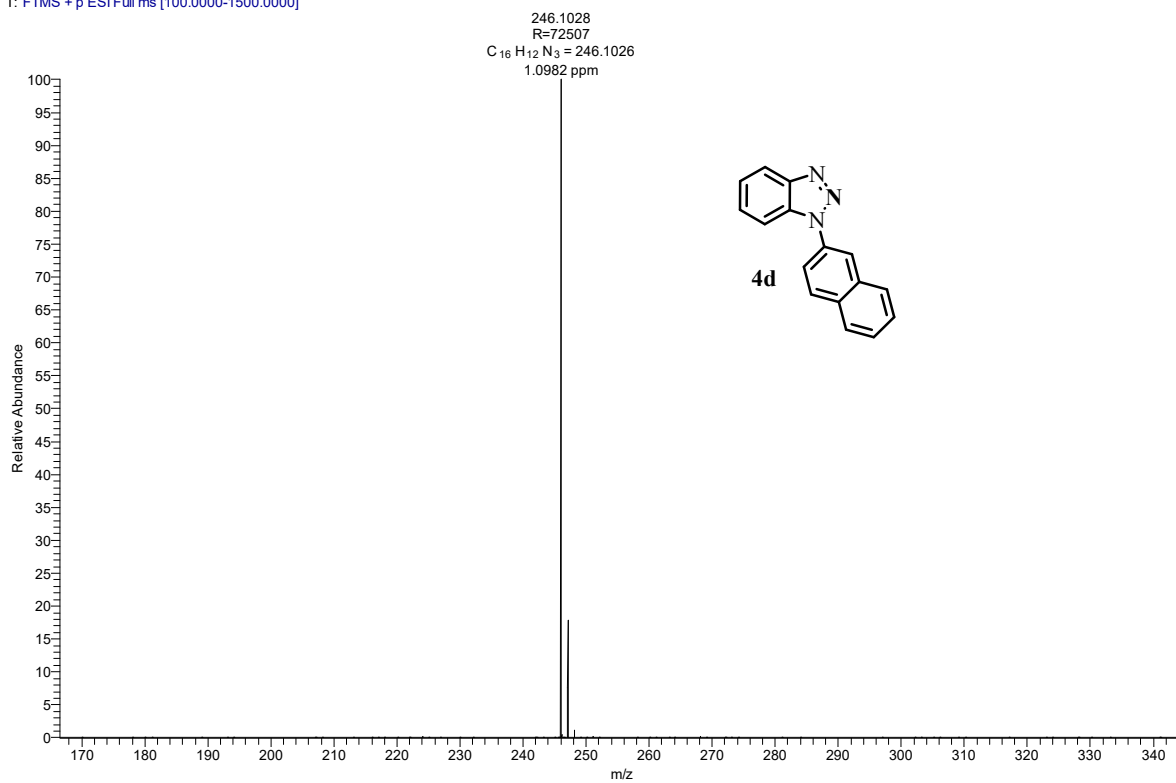


¹H NMR (CDCl₃, 400 MHz) of Compound 4d

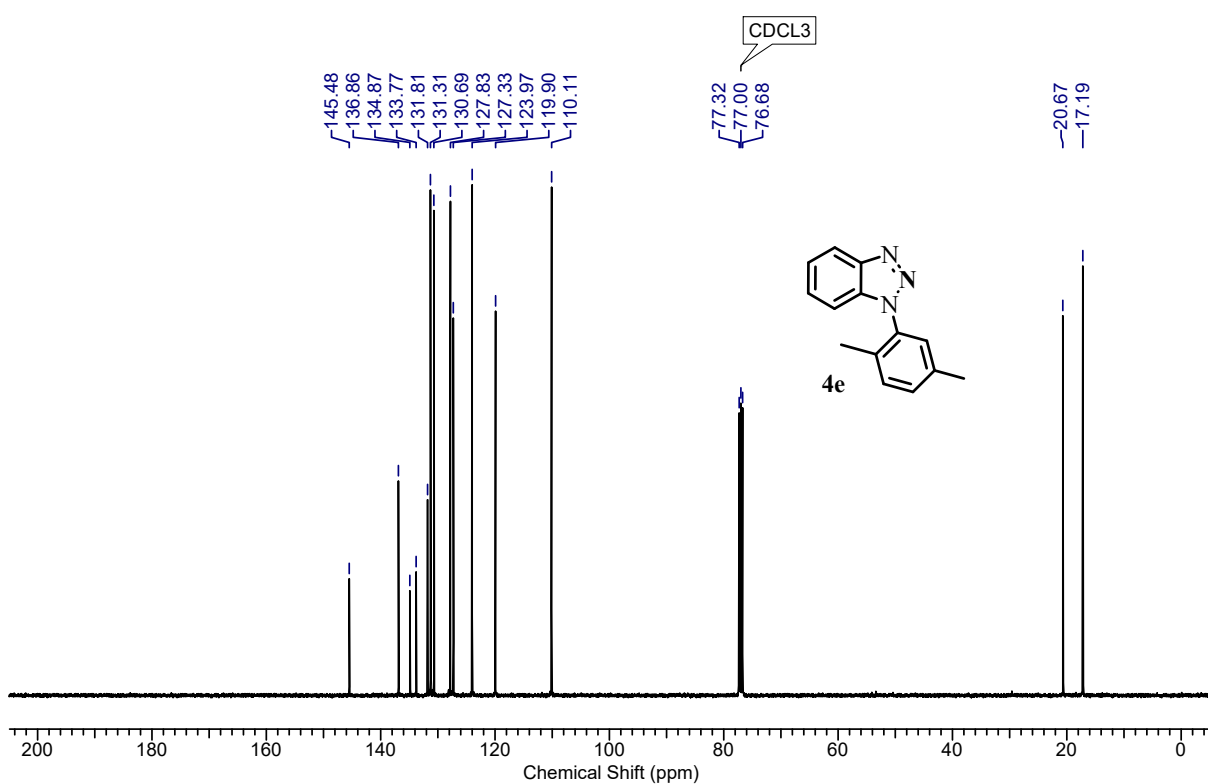
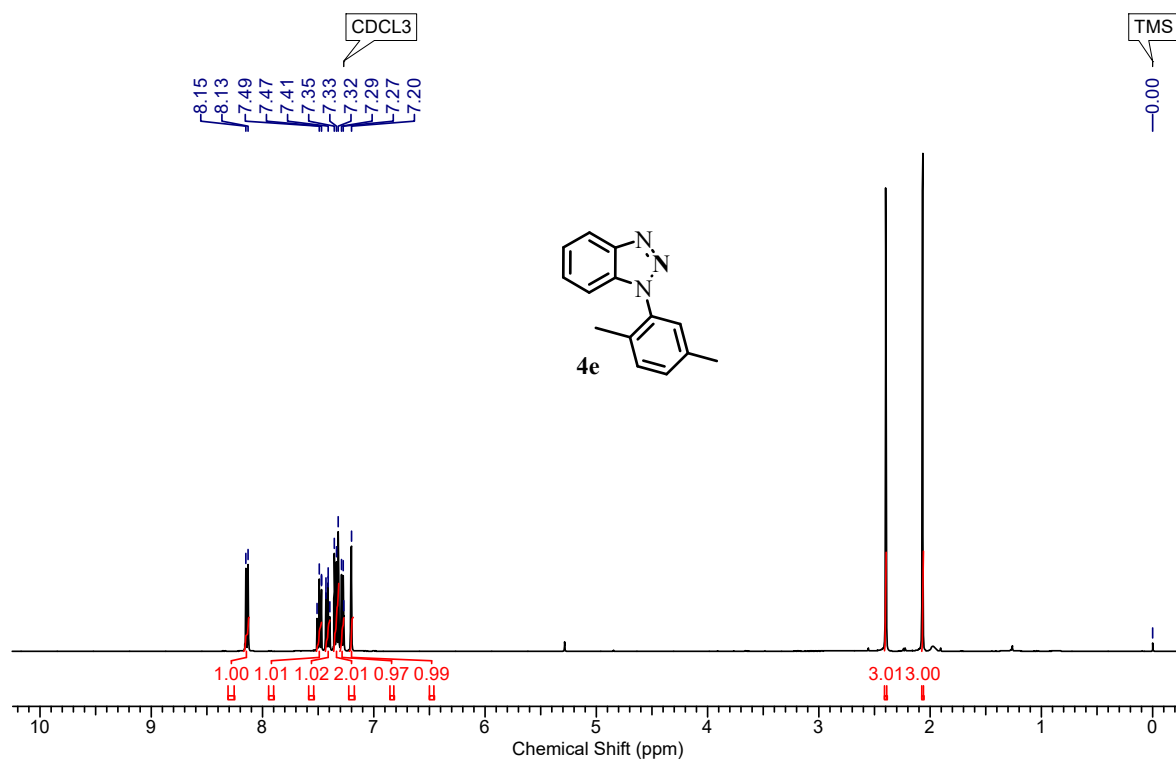


¹³C NMR (CDCl₃, 100 MHz) of Compound 4d

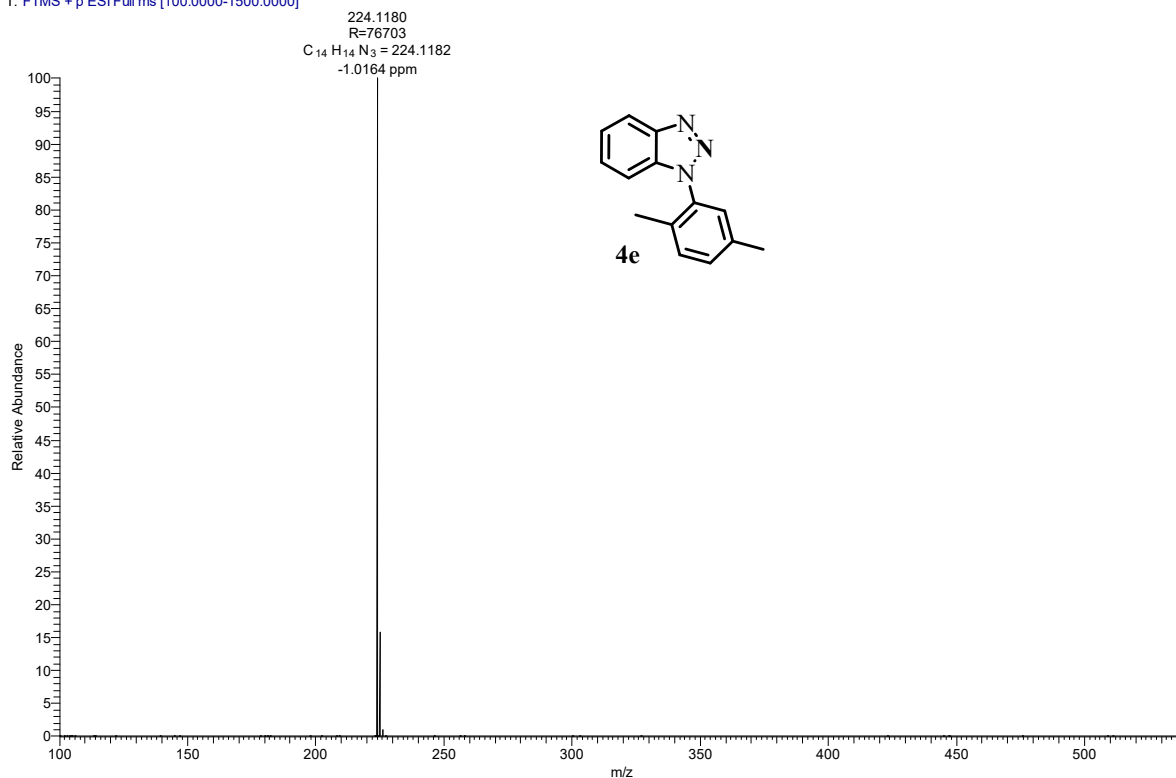
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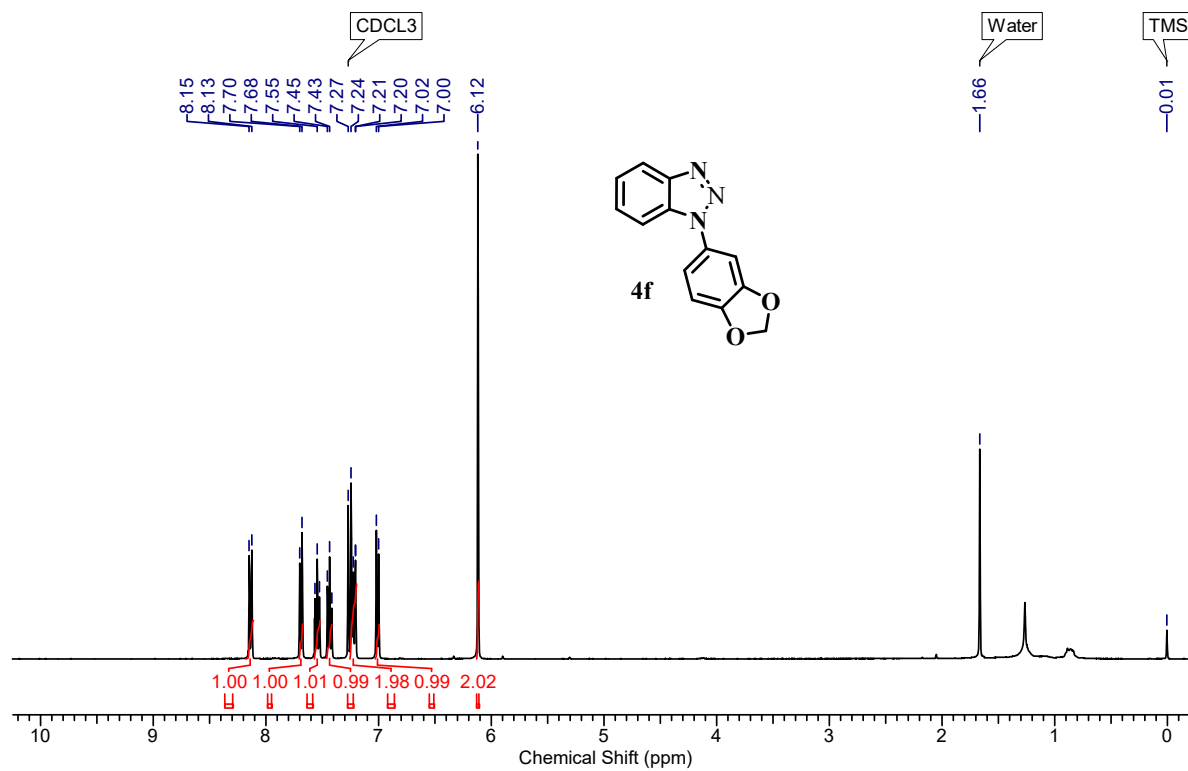
HRMS of Compound 4d



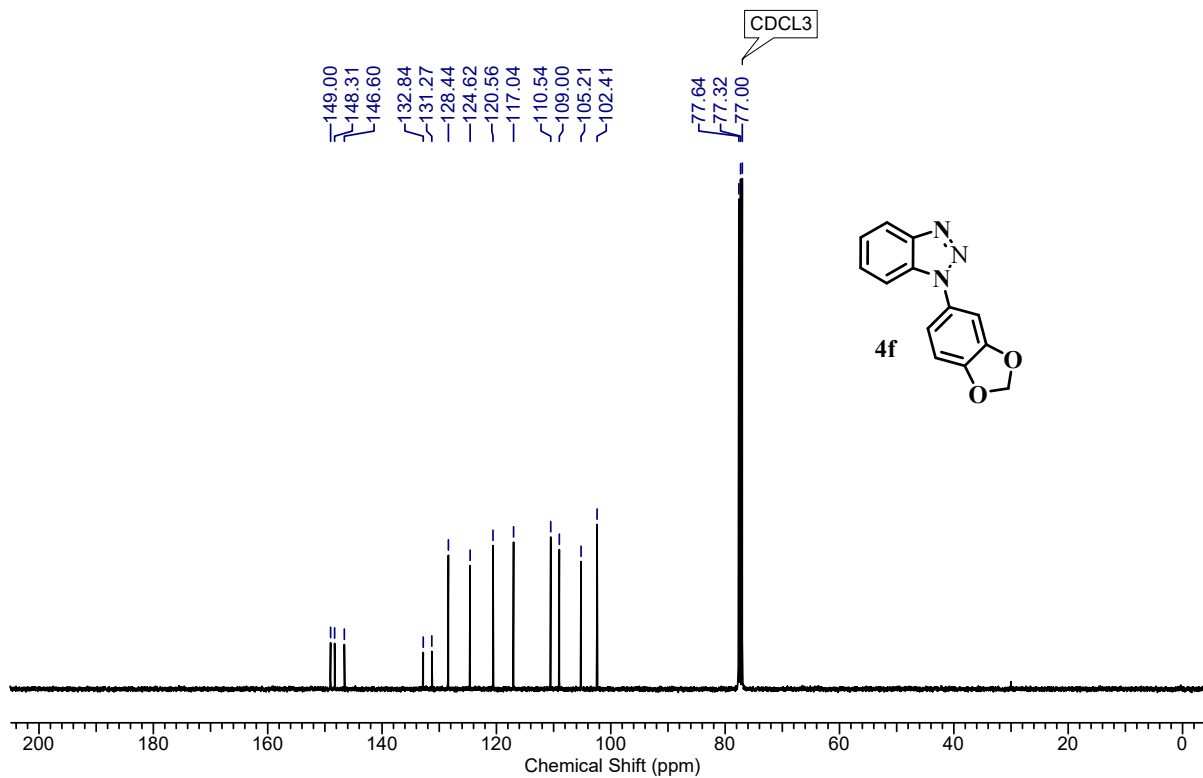
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HRMS of Compound 4e

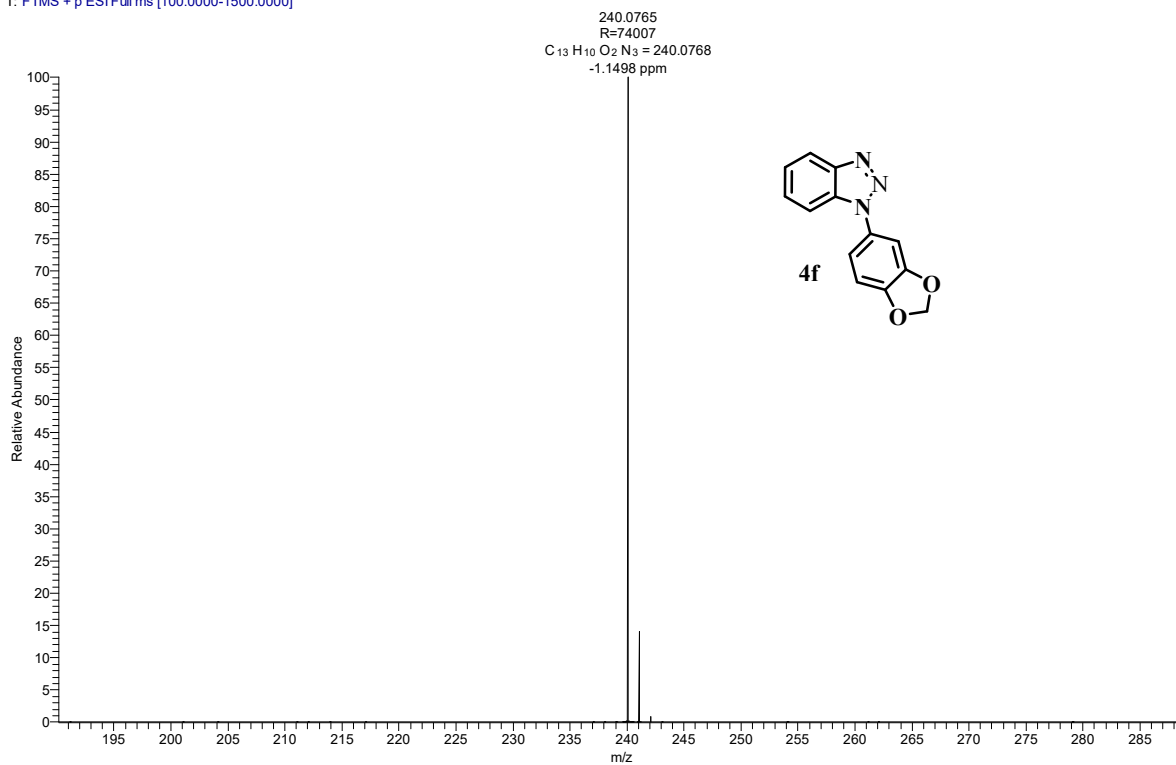


¹H NMR (CDCl₃, 400 MHz) of Compound 4f

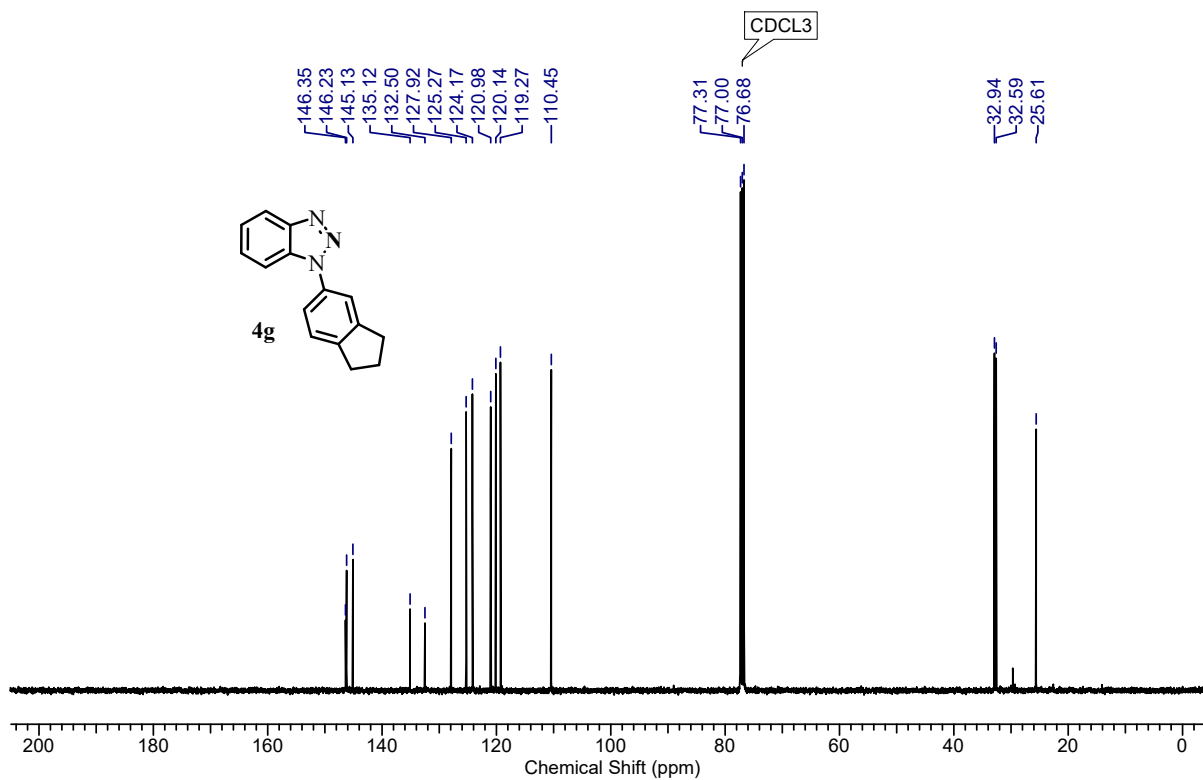
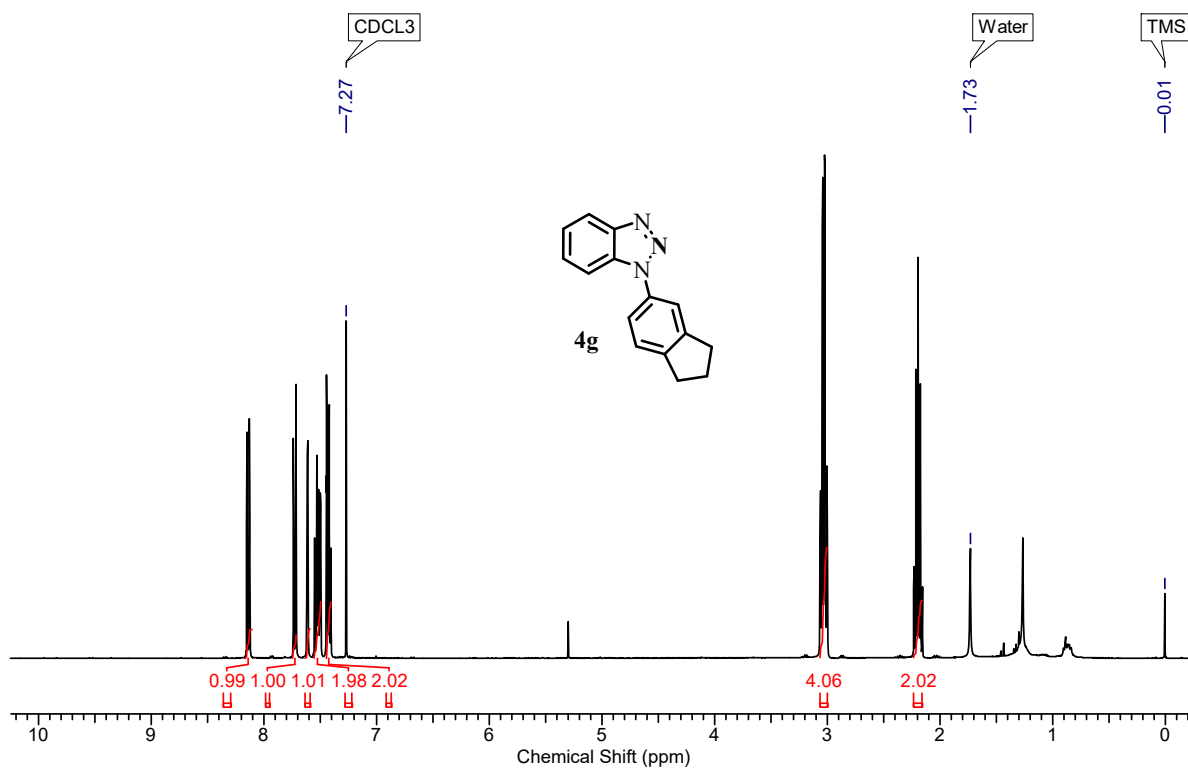


¹³C NMR (CDCl₃, 100 MHz) of Compound 4f

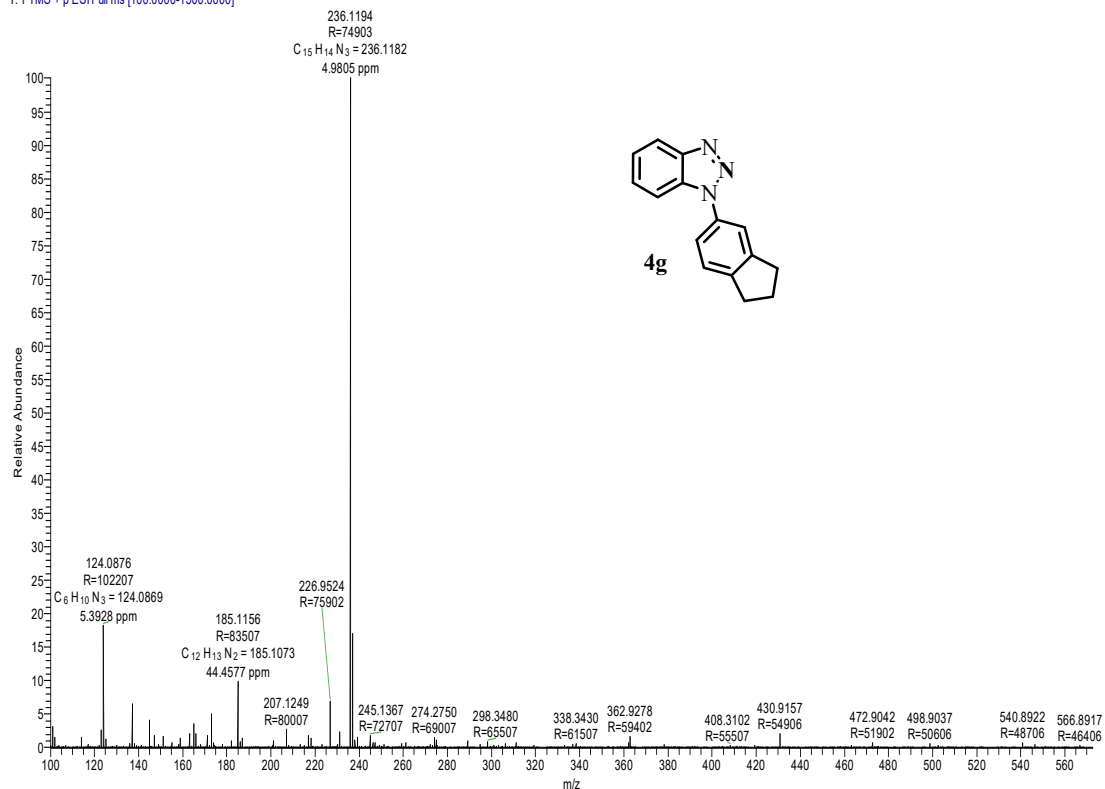
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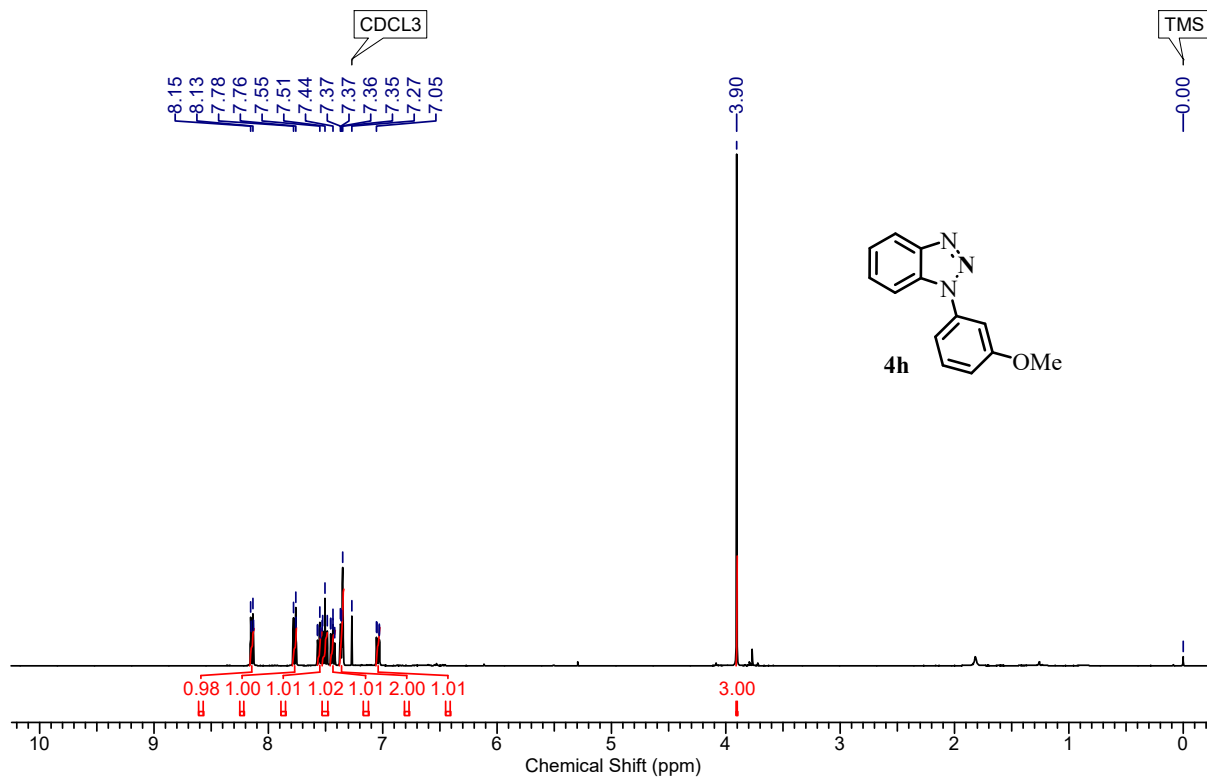
HRMS of Compound 4f



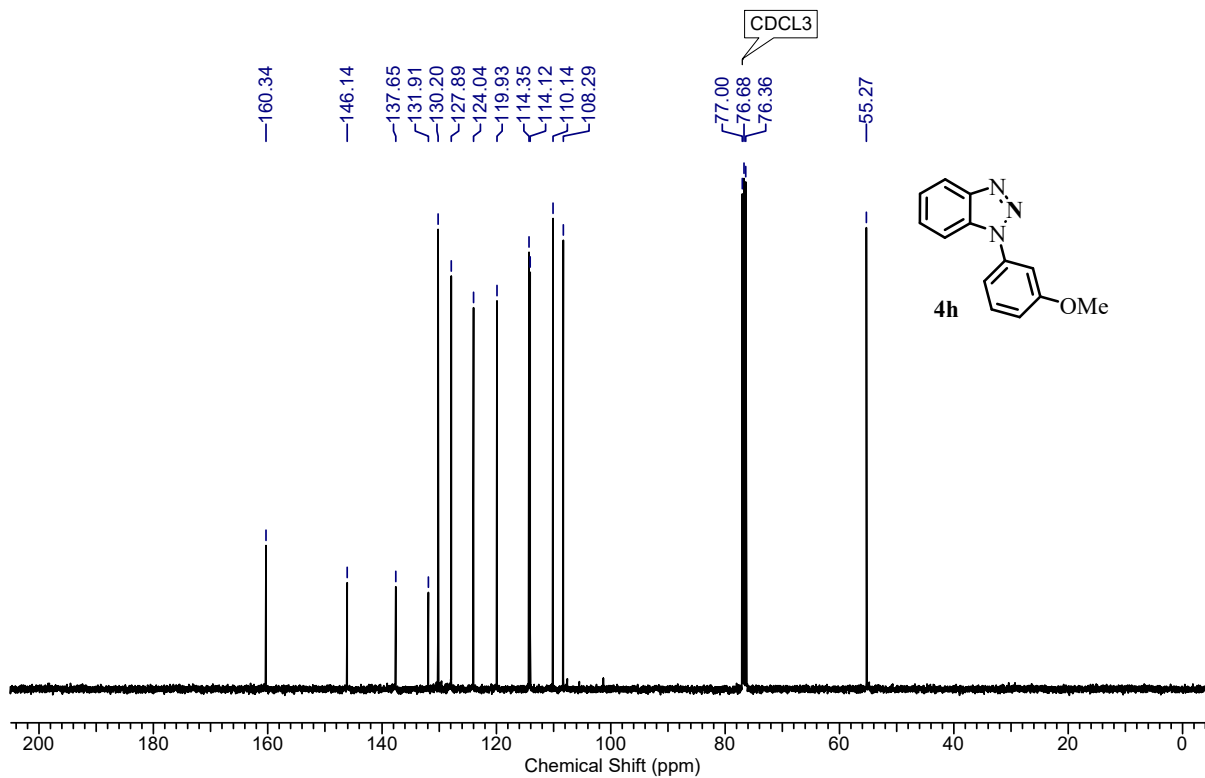
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HRMS of Compound 4g

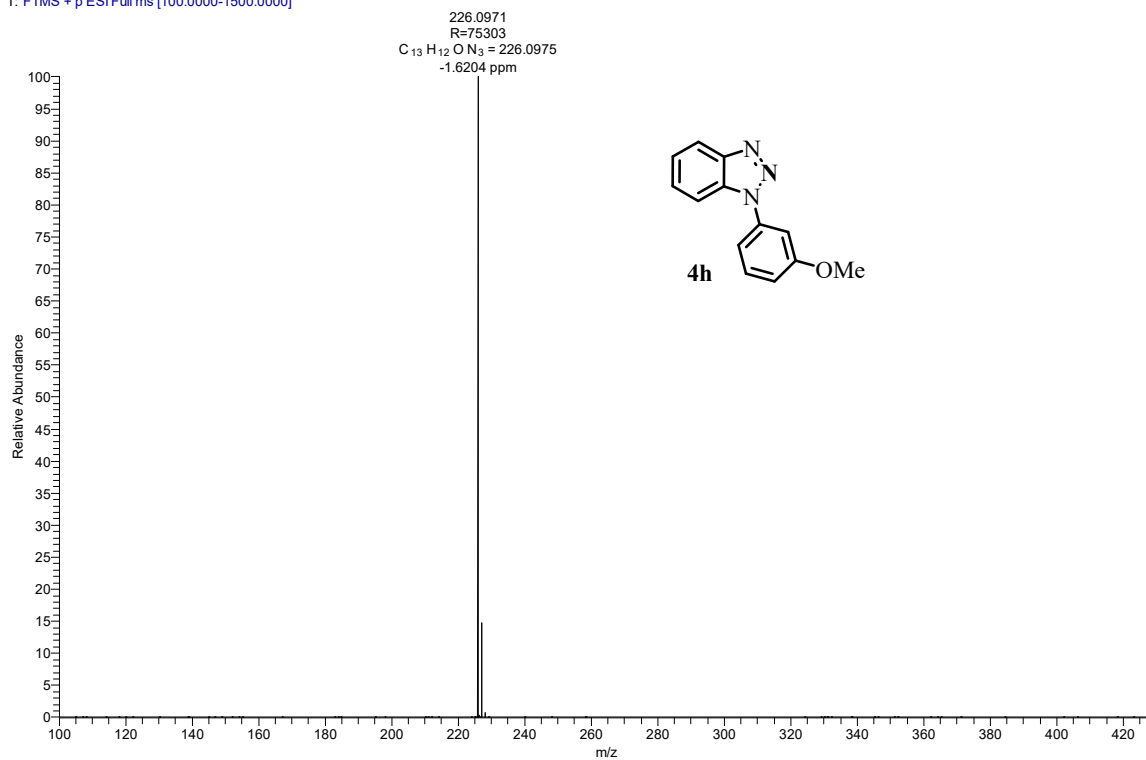


¹H NMR (CDCl₃, 400 MHz) of Compound 4h

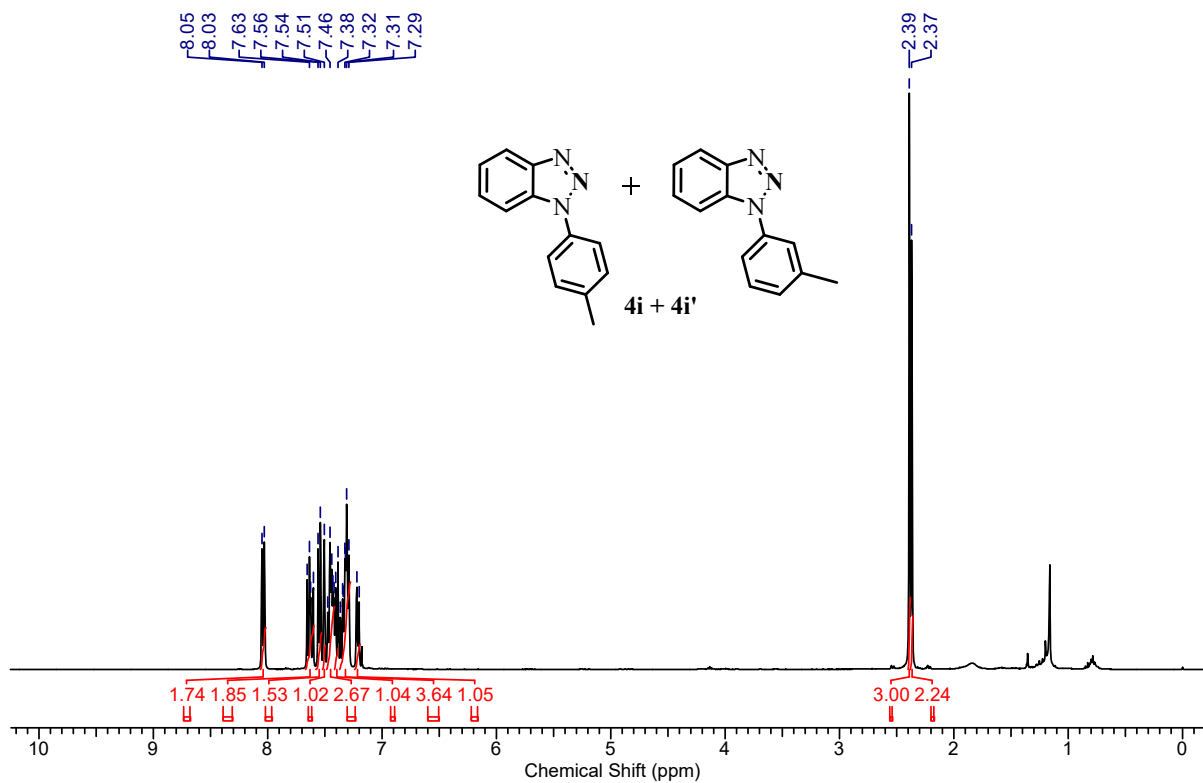


¹³C NMR (CDCl₃, 100 MHz) of Compound 4h

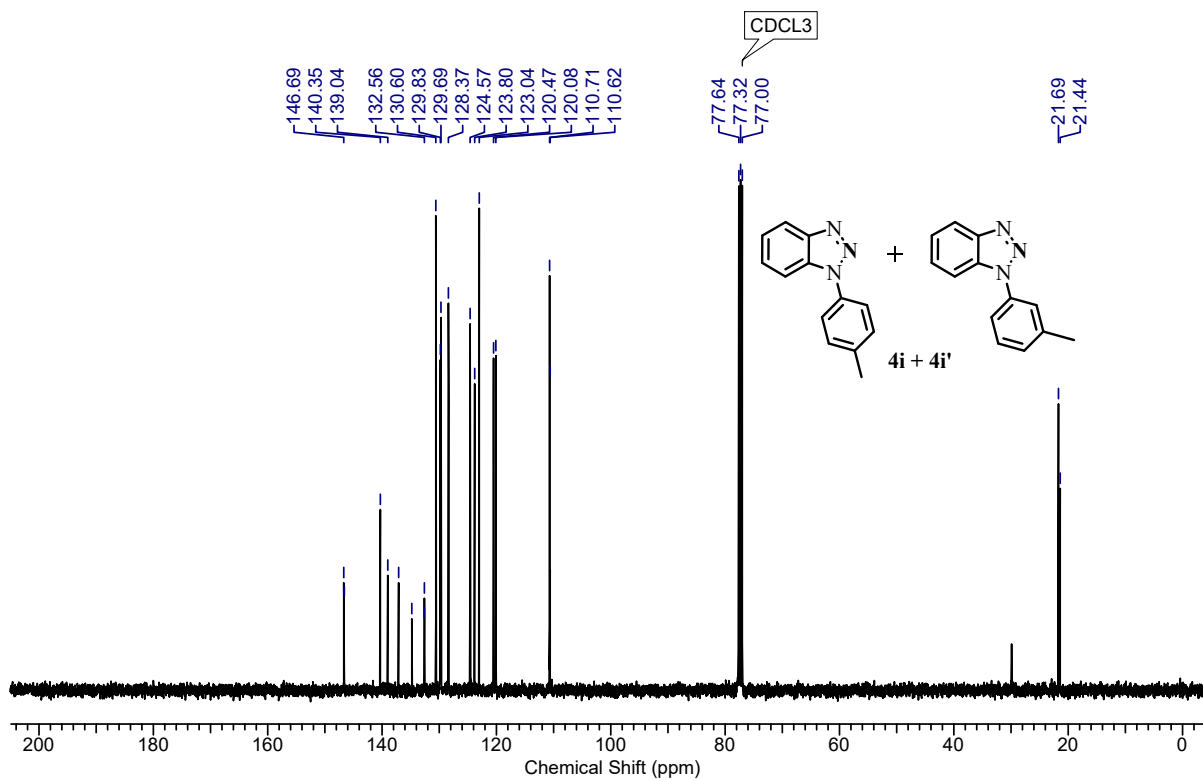
BTA-25 #348 RT: 1.98 AV: 1 NL: 1.05E10
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 4h

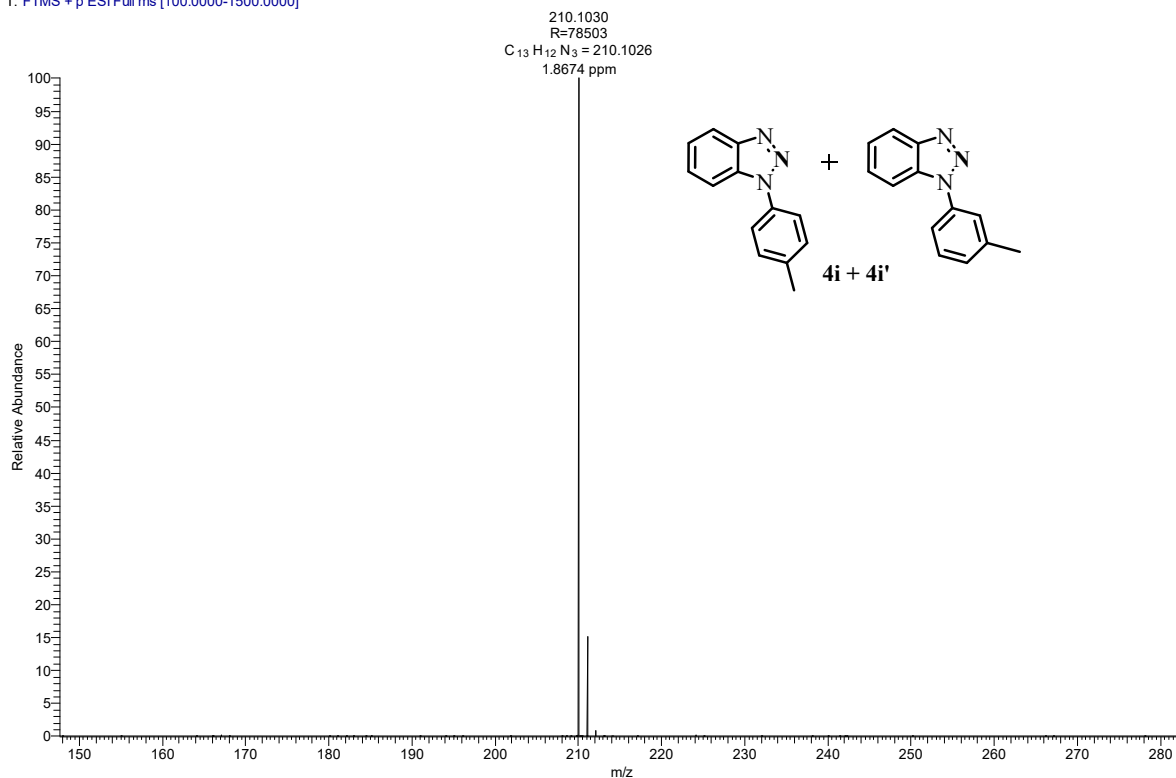


¹H NMR (CDCl₃, 400 MHz) of Compound 4i + 4i'

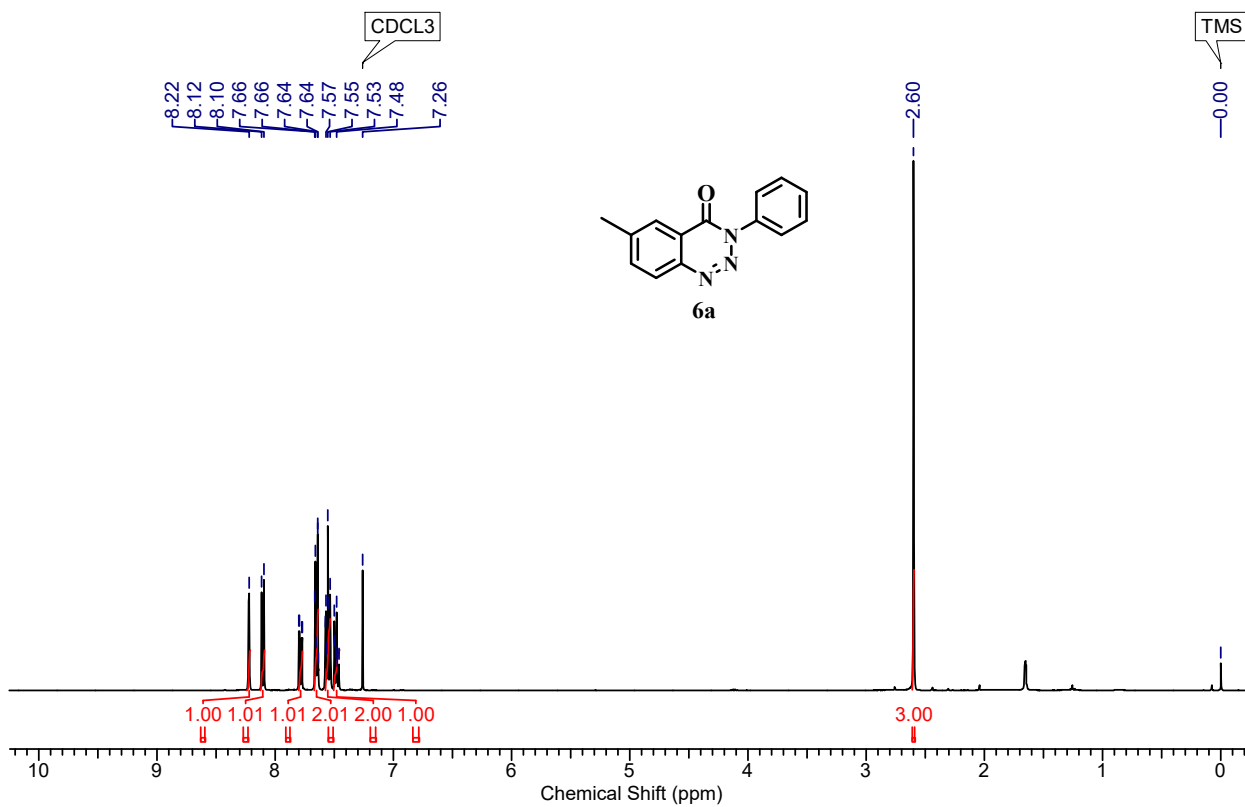


¹³C NMR (CDCl₃, 100 MHz) of Compound 4i + 4i'

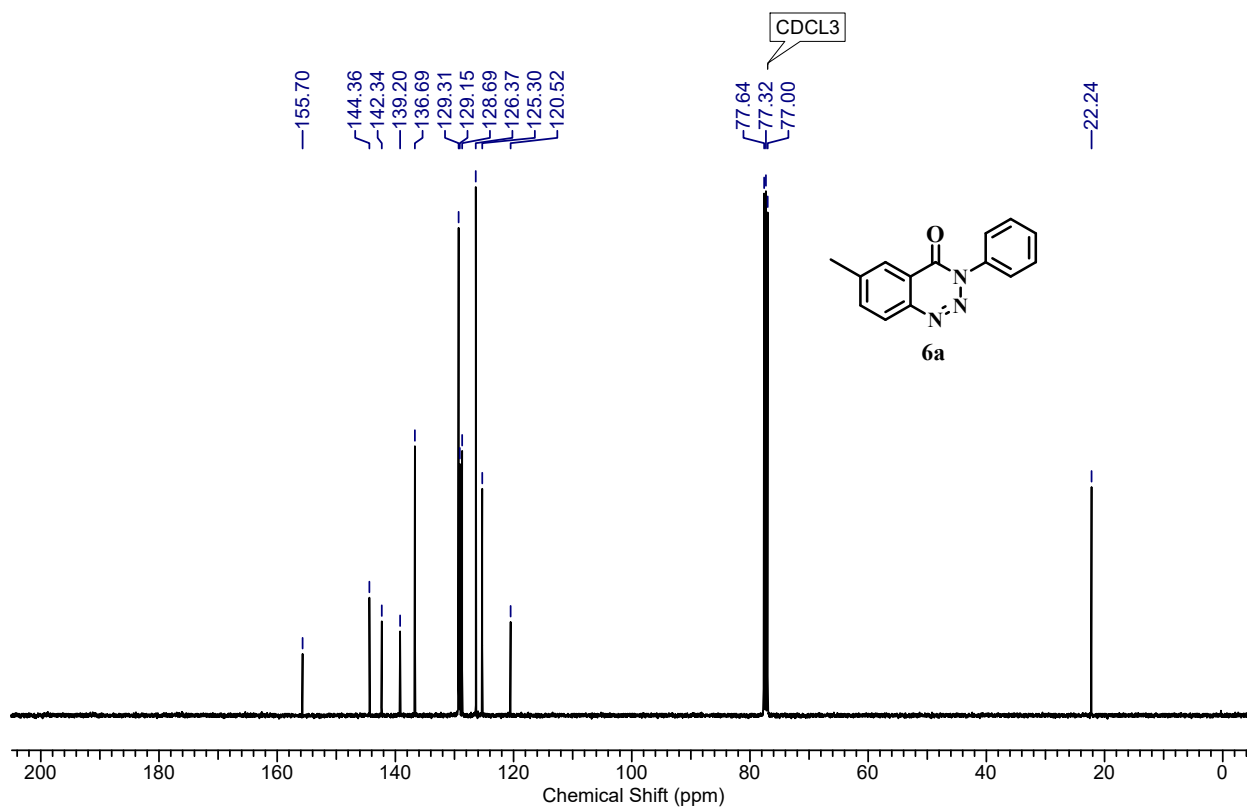
BAT-23 #379 RT: 2.04 AV: 1 NL: 3.99E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 4i + 4i'

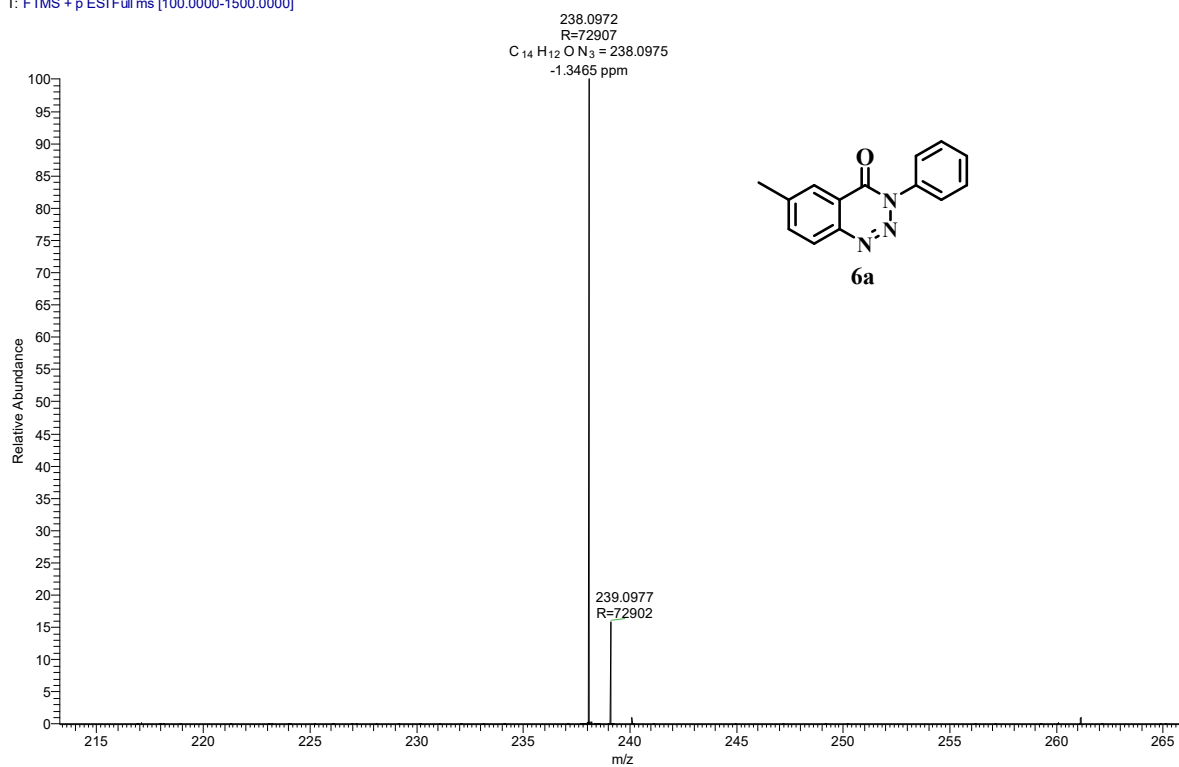


¹H NMR (CDCl₃, 400 MHz) of Compound 6a

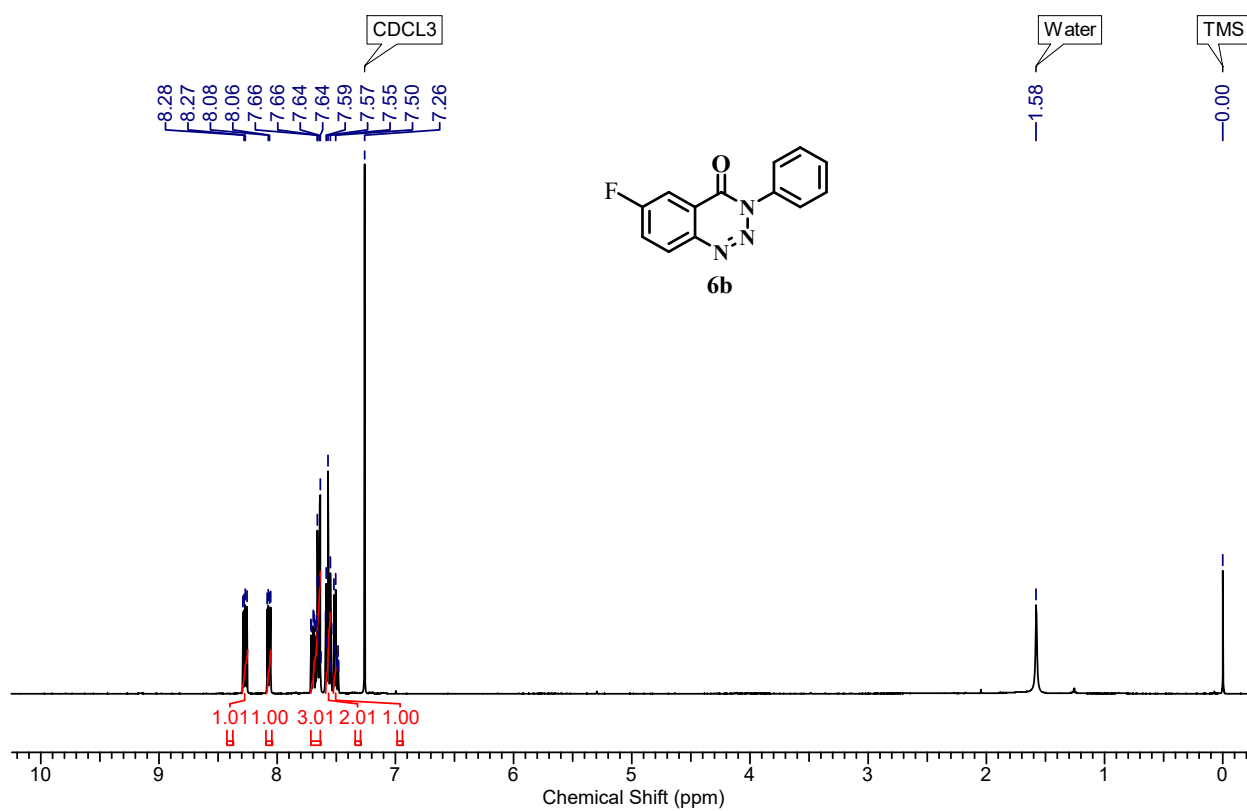


^{13}C NMR (CDCl_3 , 100 MHz) of Compound **6a**

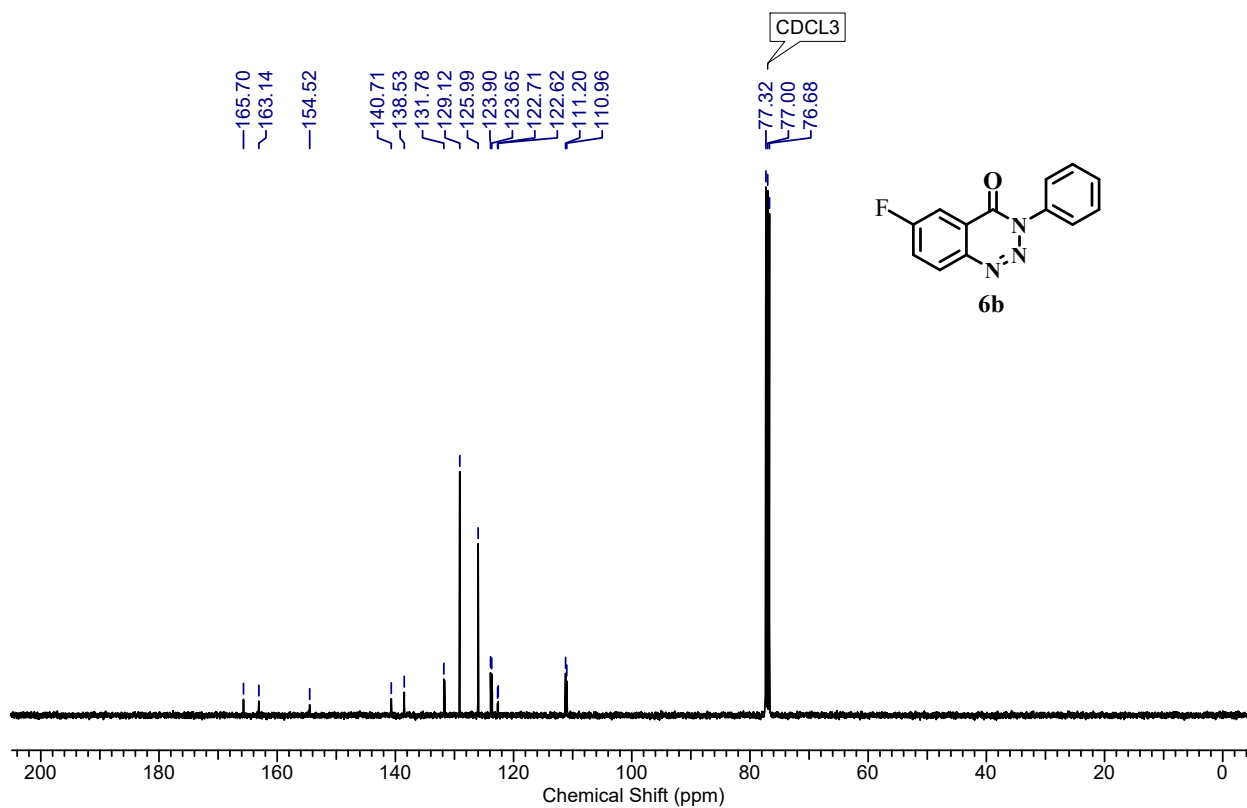
BAA-1 #303 RT: 1.84 AV: 1 NL: 6.34E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



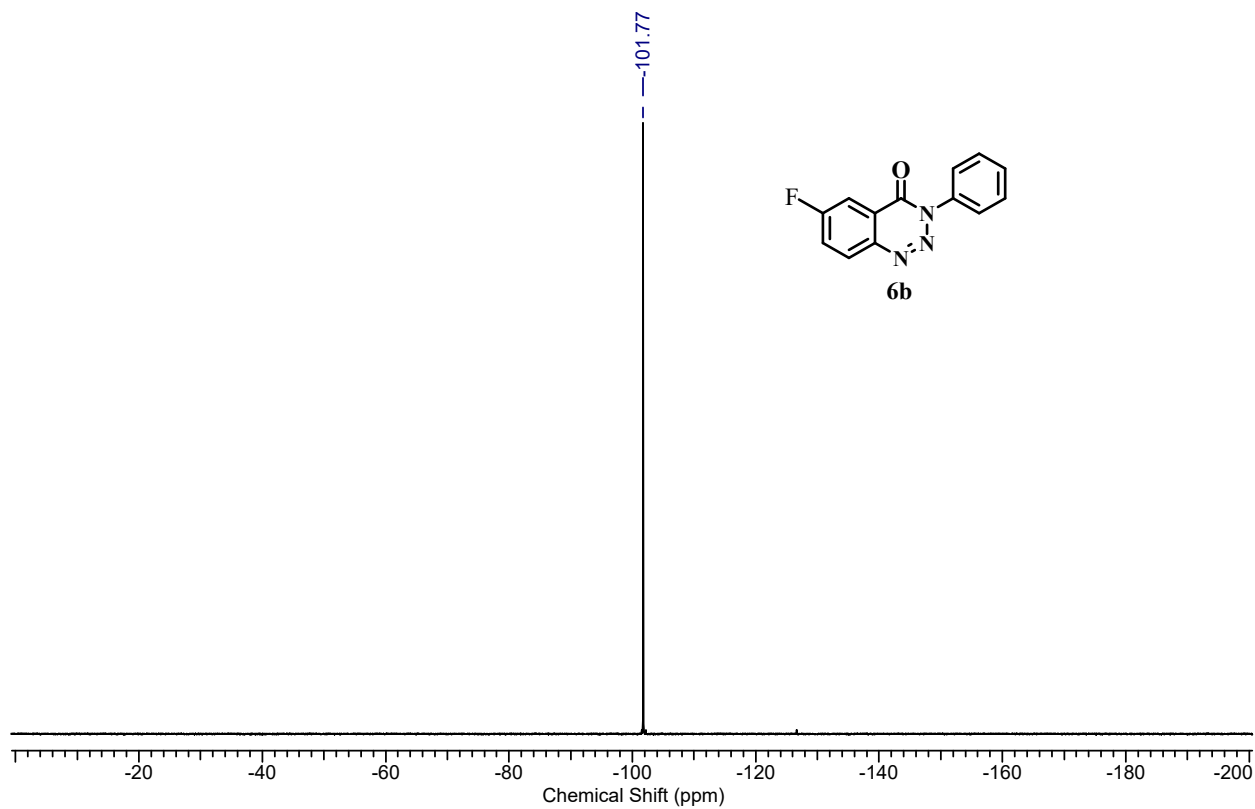
HRMS of Compound 6a



¹H NMR (CDCl₃, 400 MHz) of Compound 6b

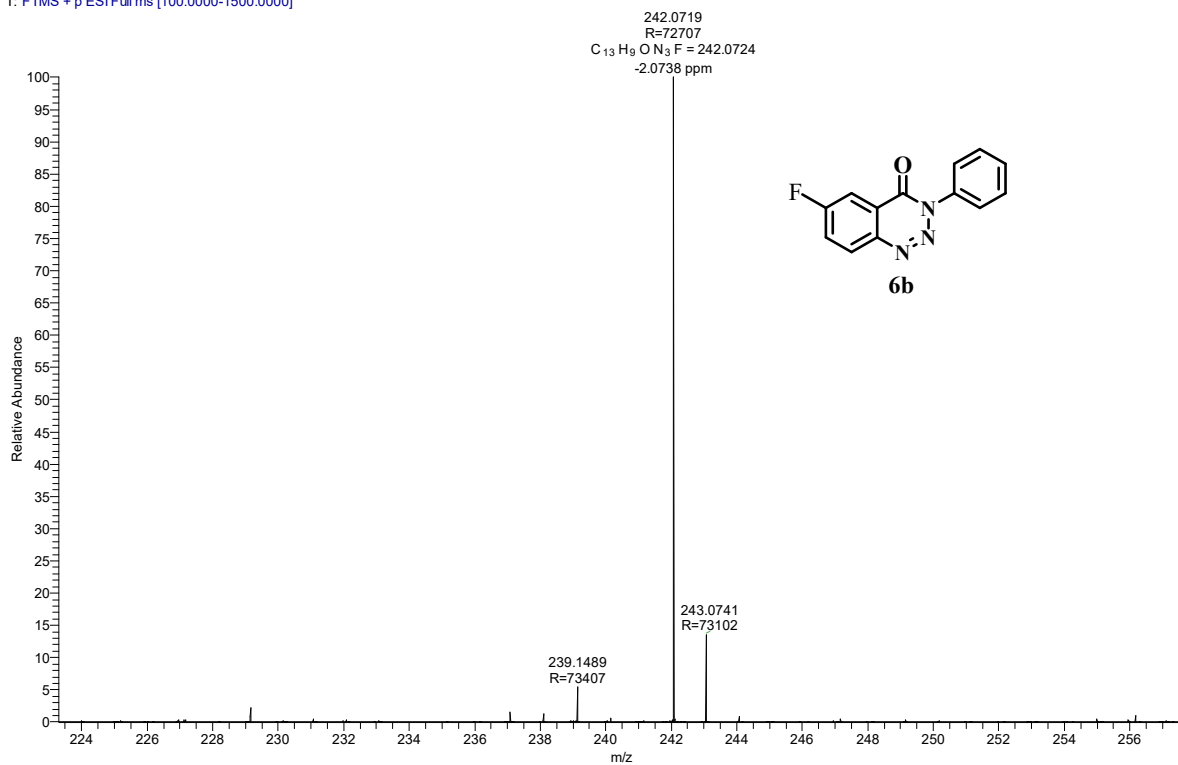


¹³C NMR (CDCl₃, 100 MHz) of Compound 6b

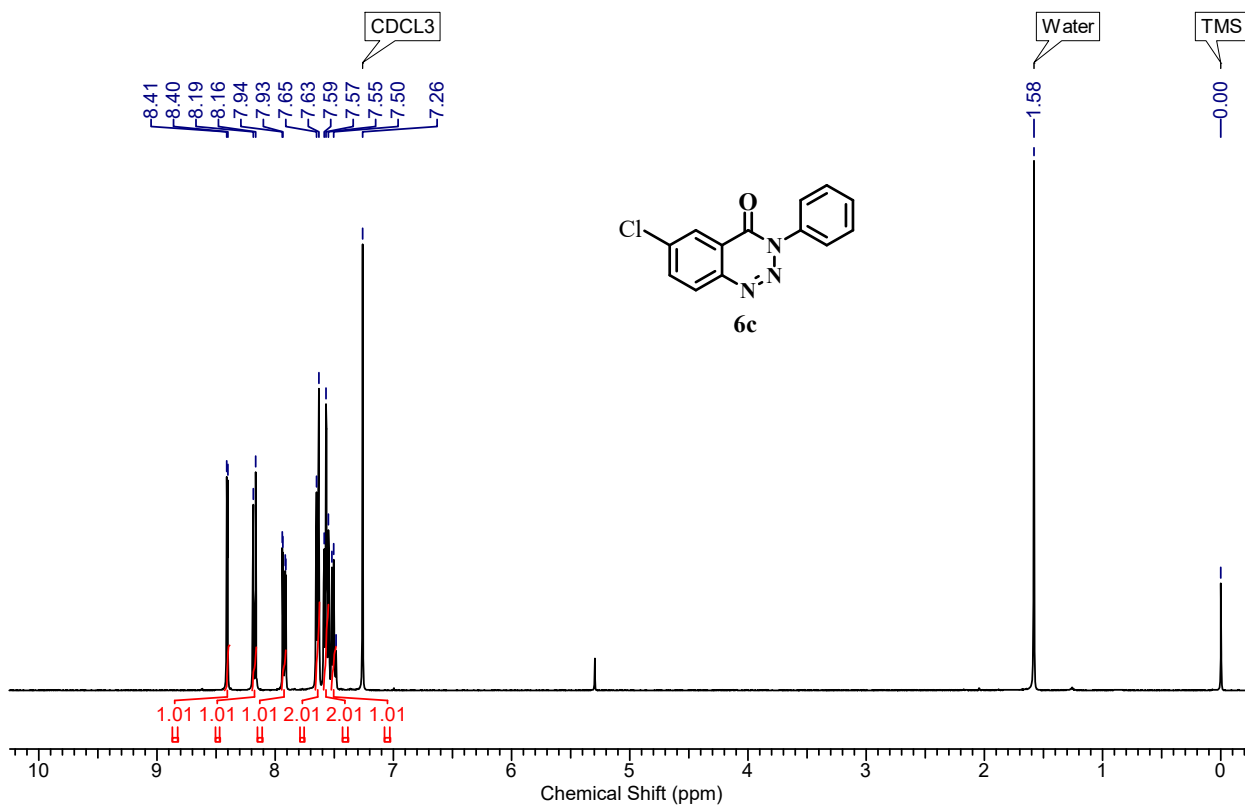


¹⁹F NMR (CDCl₃, 376 MHz) of Compound 6b

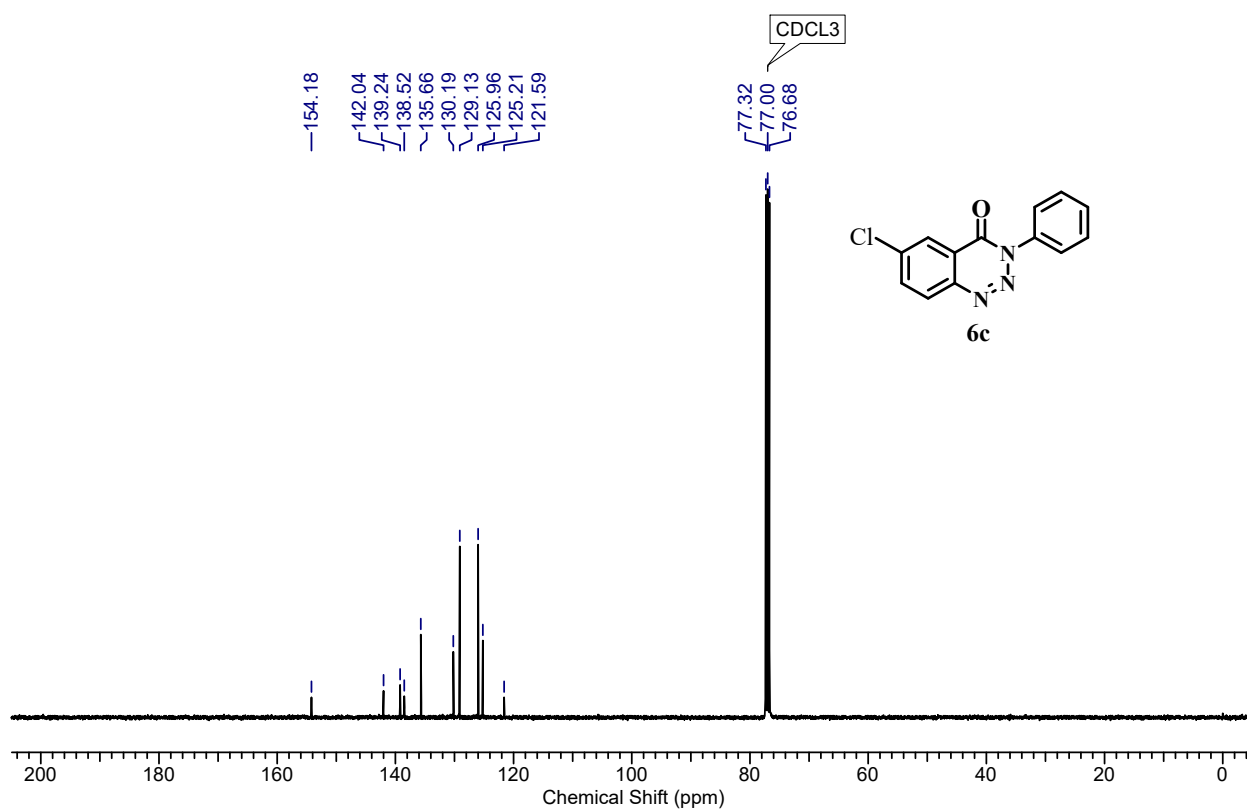
BAA-2 #297 RT: 1.78 AV: 1 NL: 5.22E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 6b

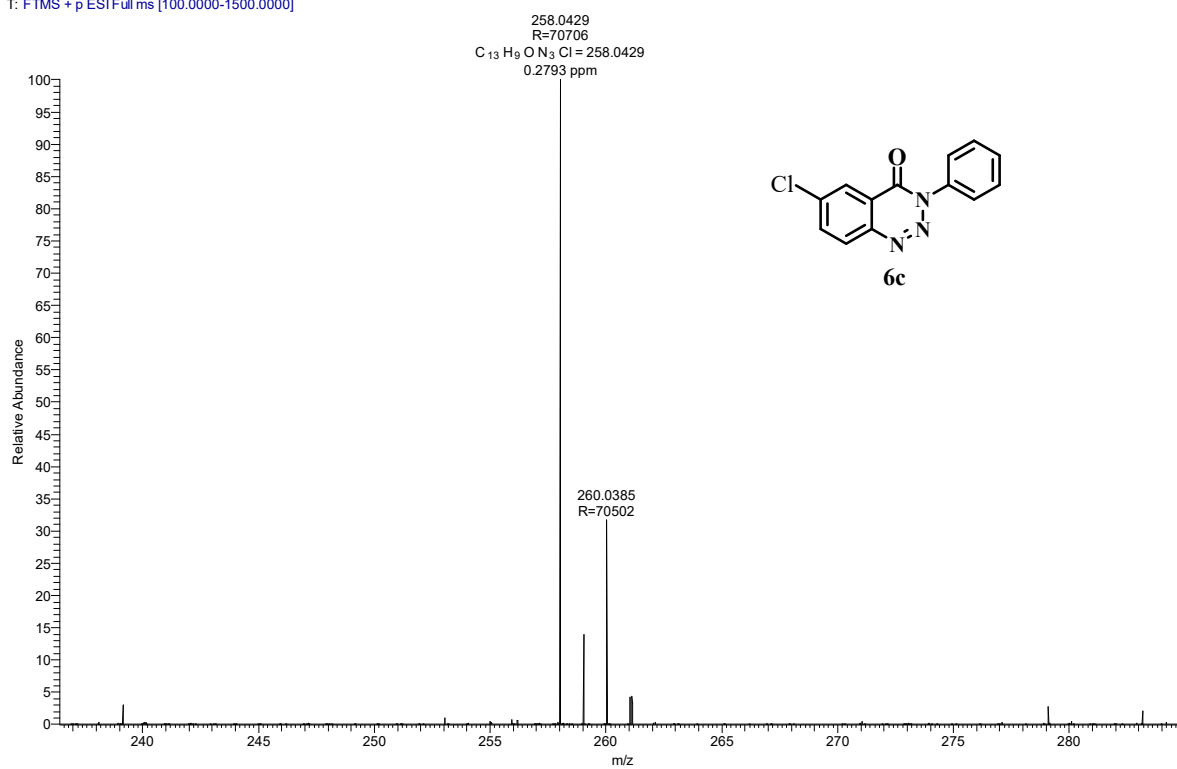


¹H NMR (CDCl₃, 400 MHz) of Compound 6c

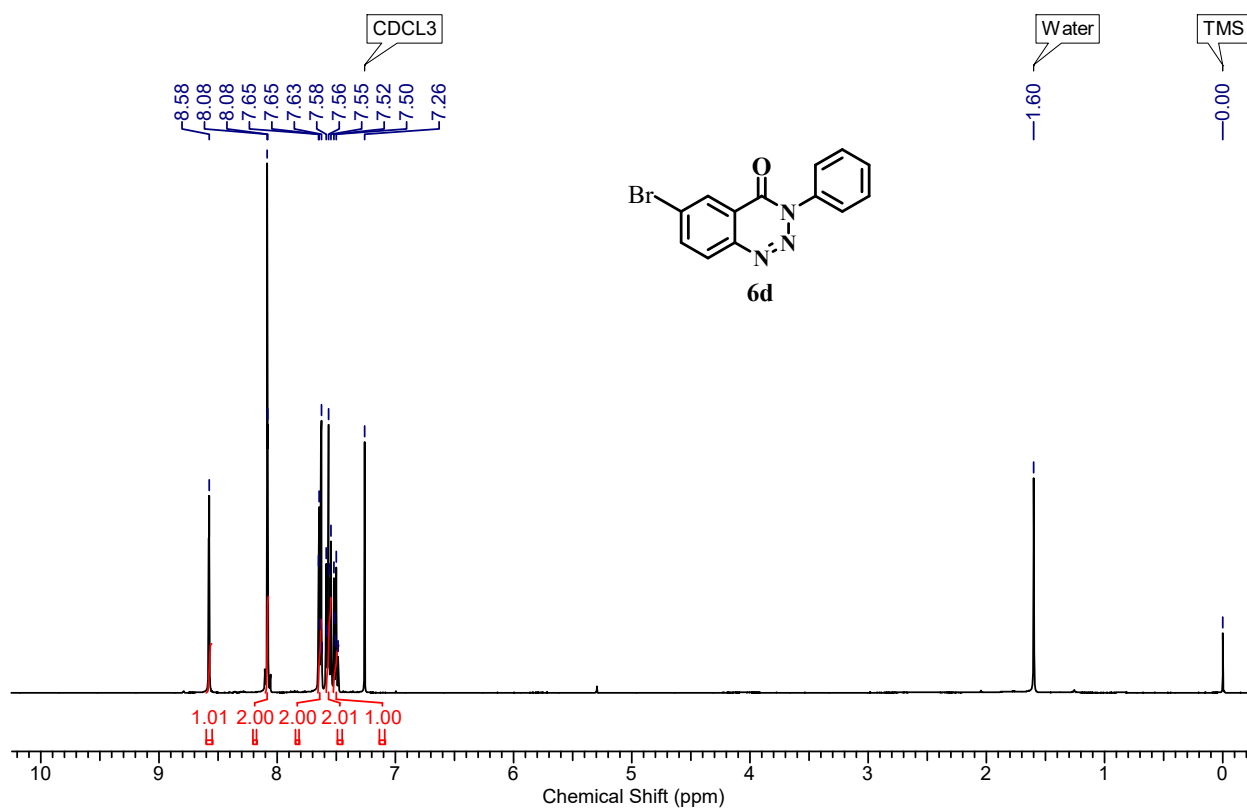


¹³C NMR (CDCl₃, 100 MHz) of Compound 6c

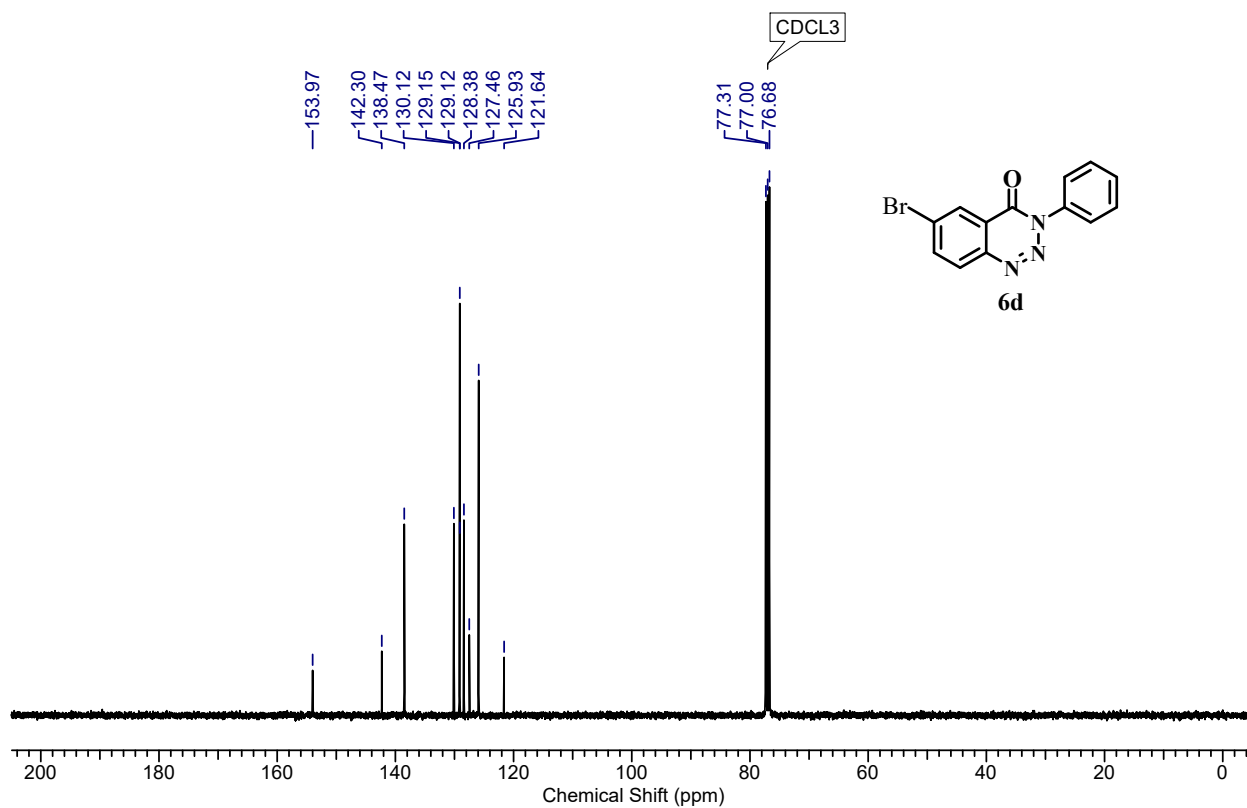
BAA-3 #315 RT: 1.88 AV: 1 NL: 7.49E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 6c

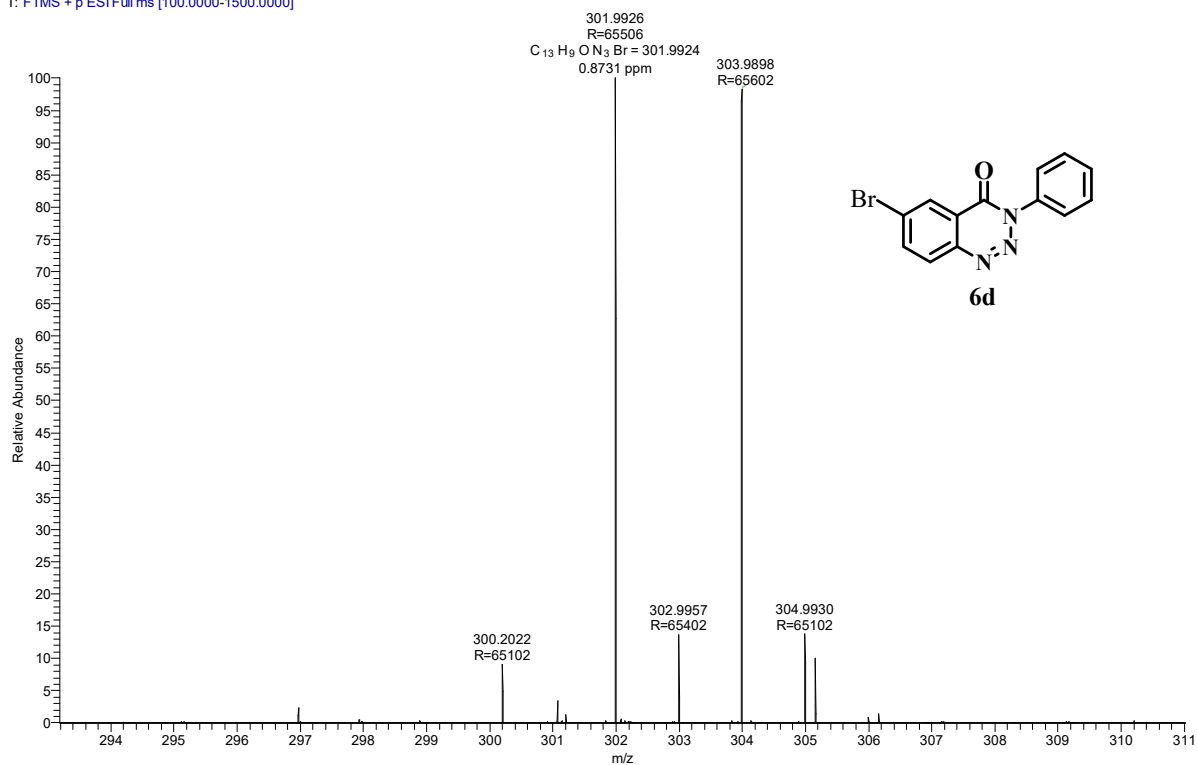


¹H NMR (CDCl₃, 400 MHz) of Compound 6d

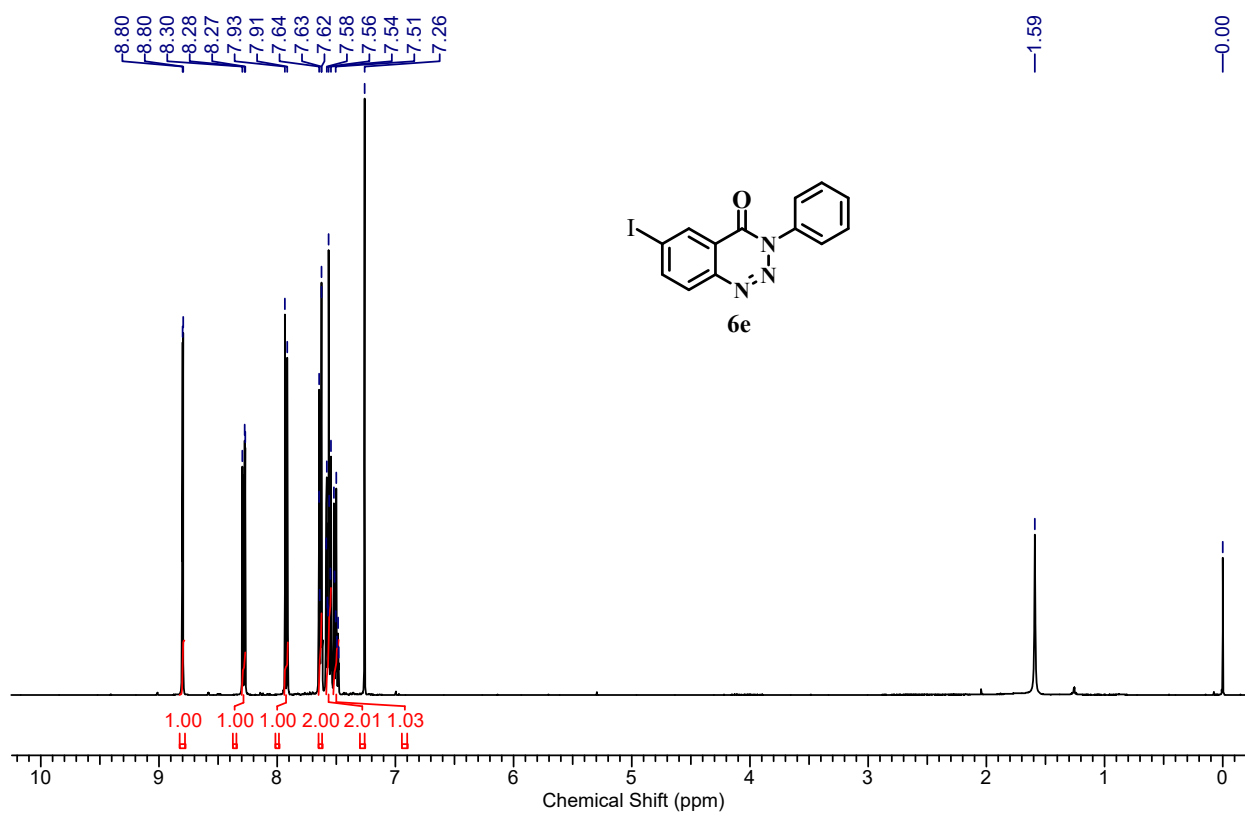


^{13}C NMR (CDCl_3 , 100 MHz) of Compound **6d**

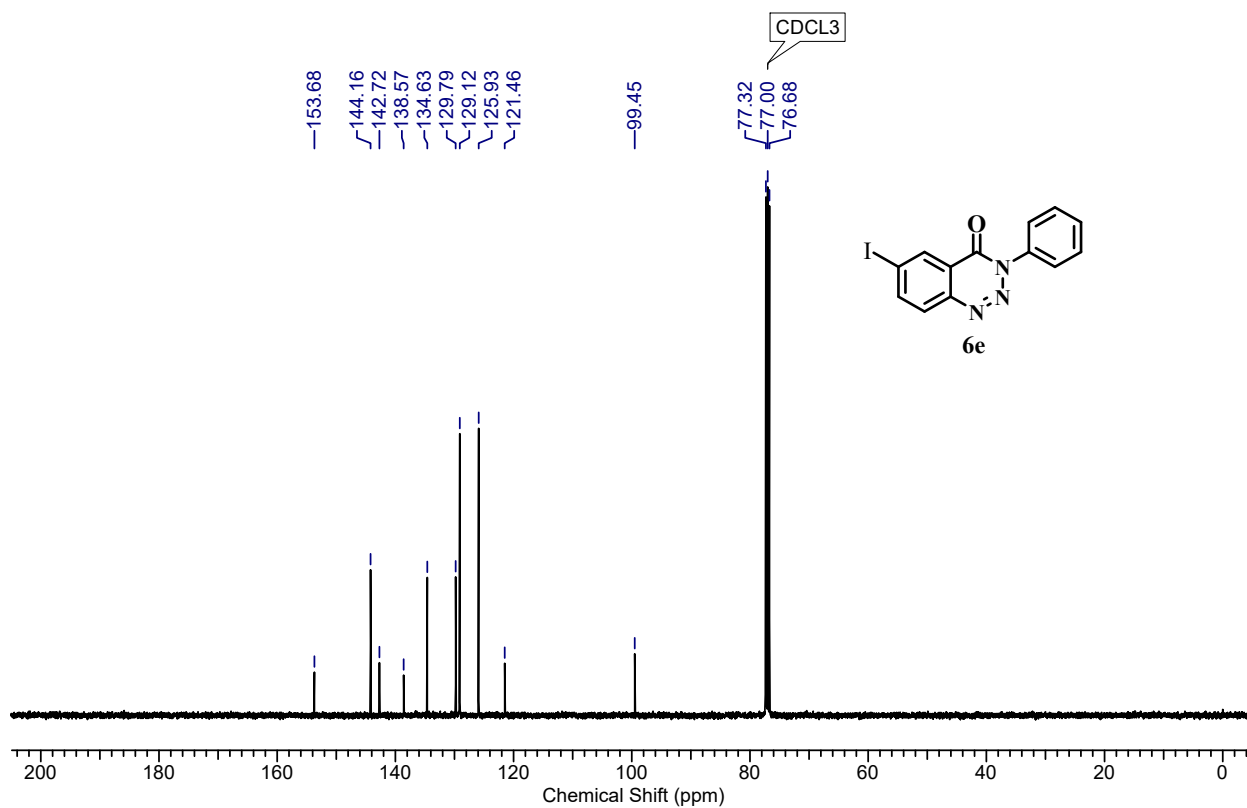
BAA-4 #319 RT: 1.90 AV: 1 NL: 2.18E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 6d

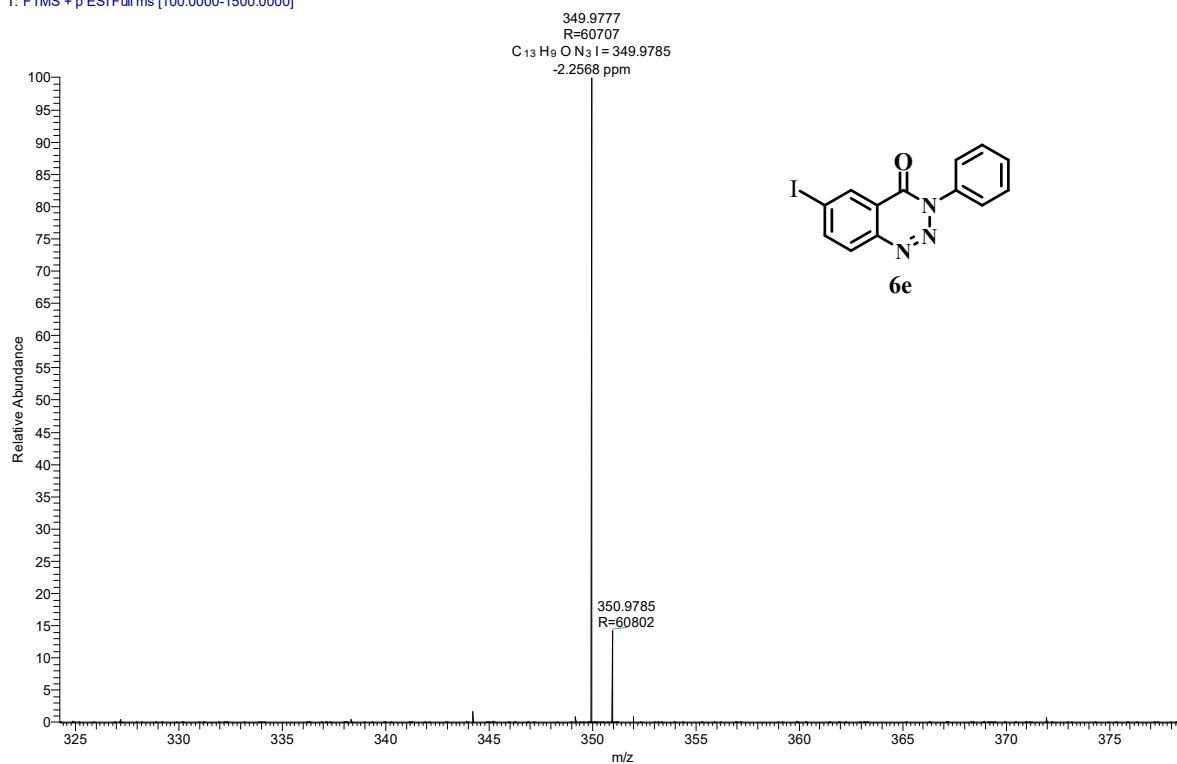


¹H NMR (CDCl₃, 400 MHz) of Compound 6e

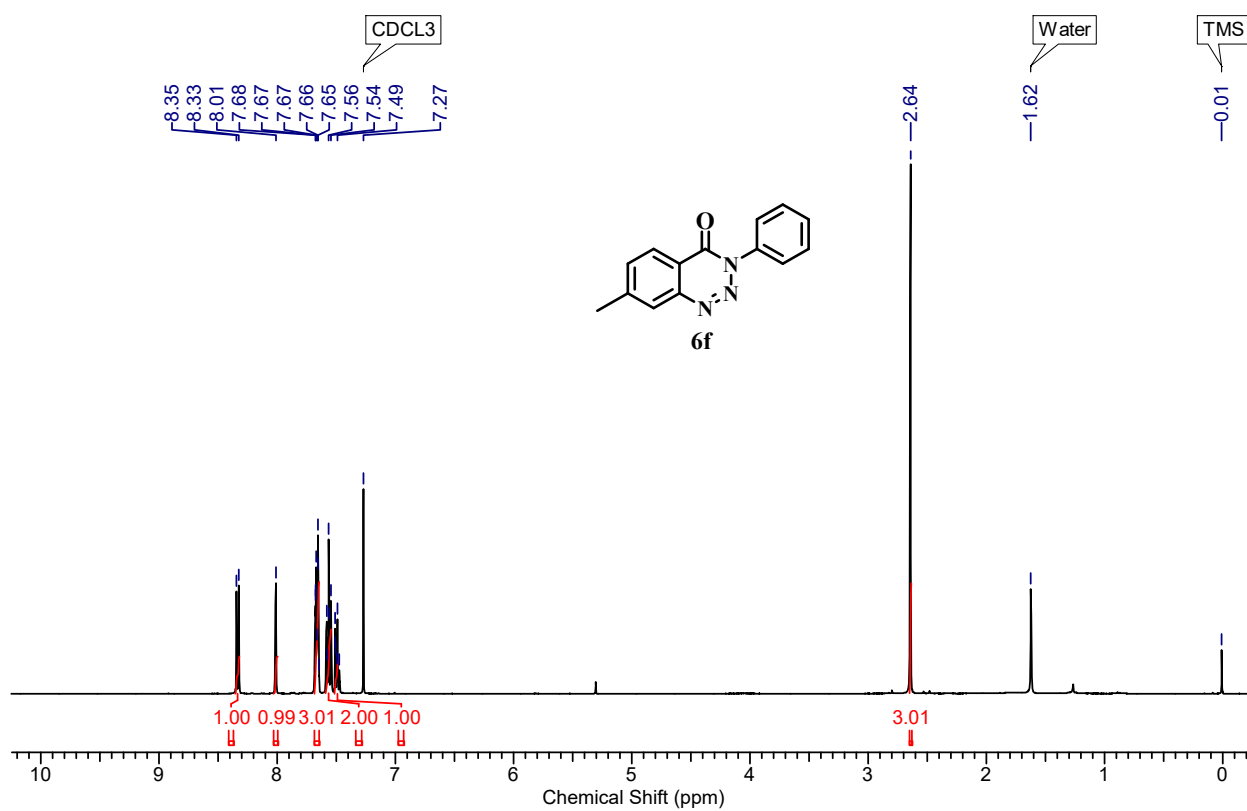


¹³C NMR (CDCl₃, 100 MHz) of Compound 6e

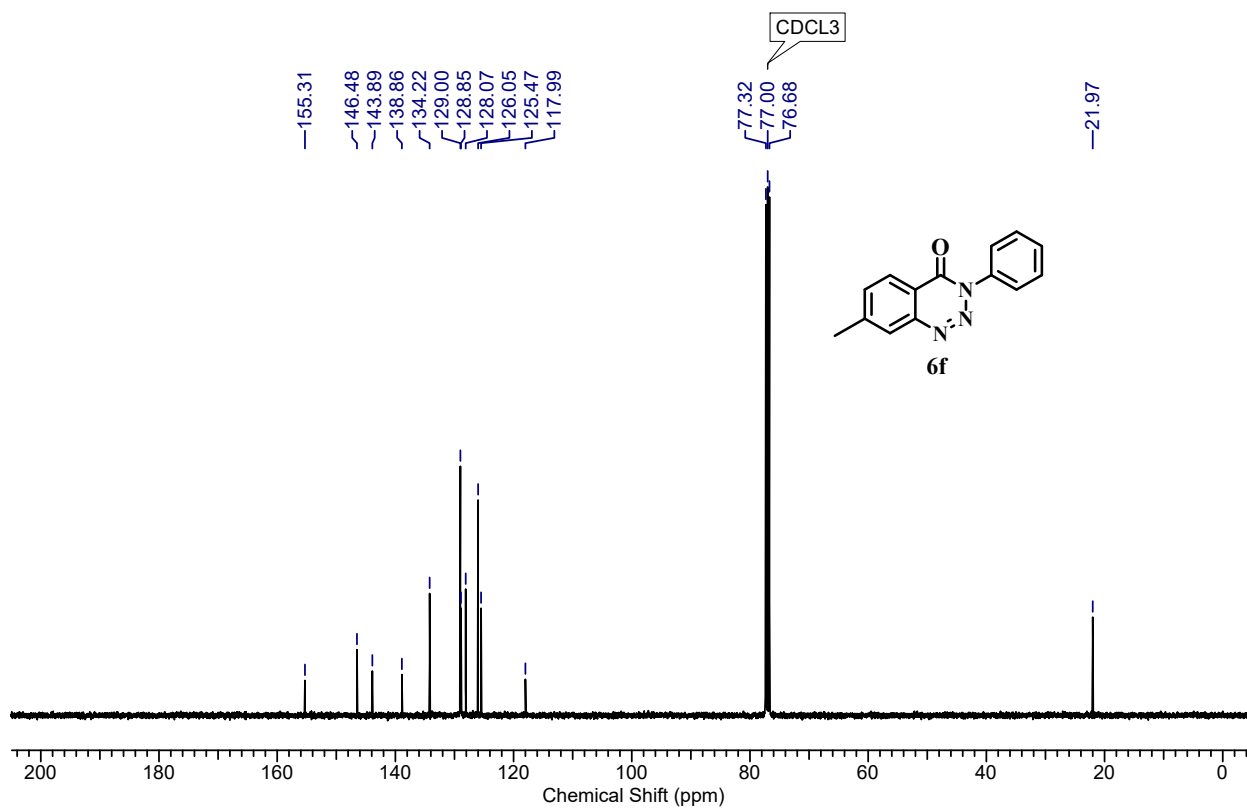
BAA-5 #323 RT: 1.92 AV: 1 NL: 9.03E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 6e

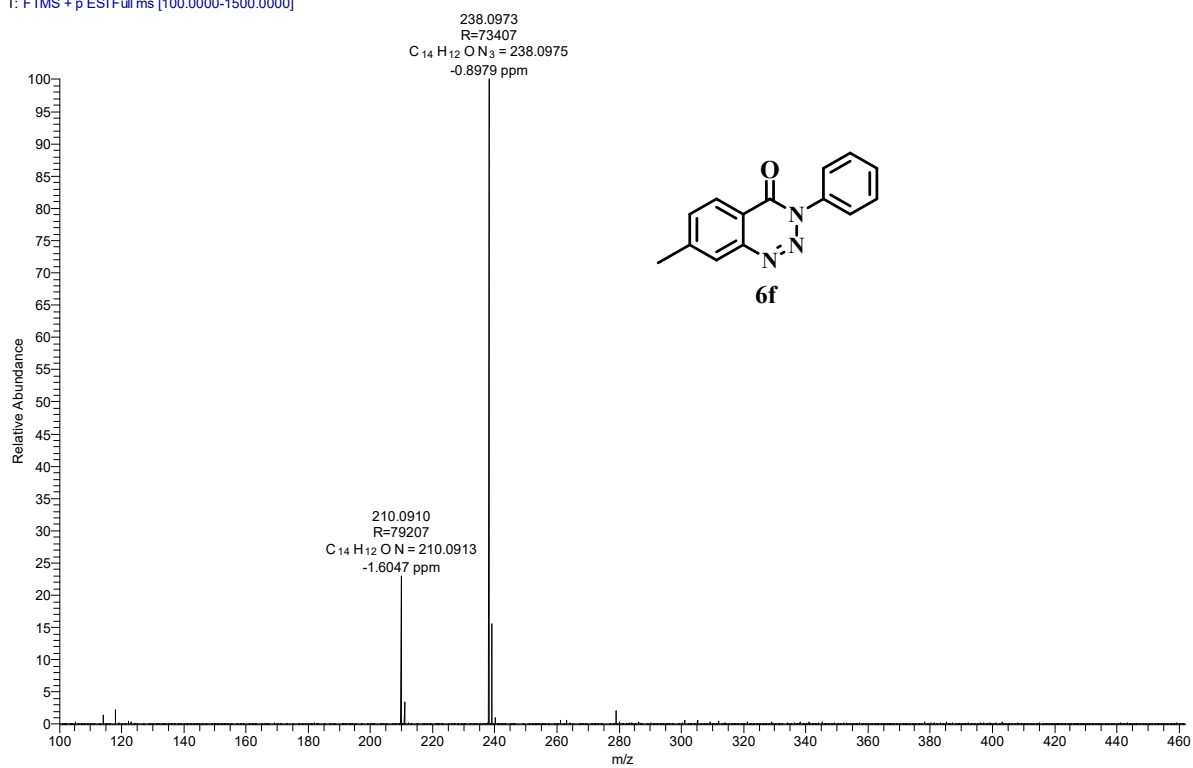


¹H NMR (CDCl₃, 400 MHz) of Compound 6f

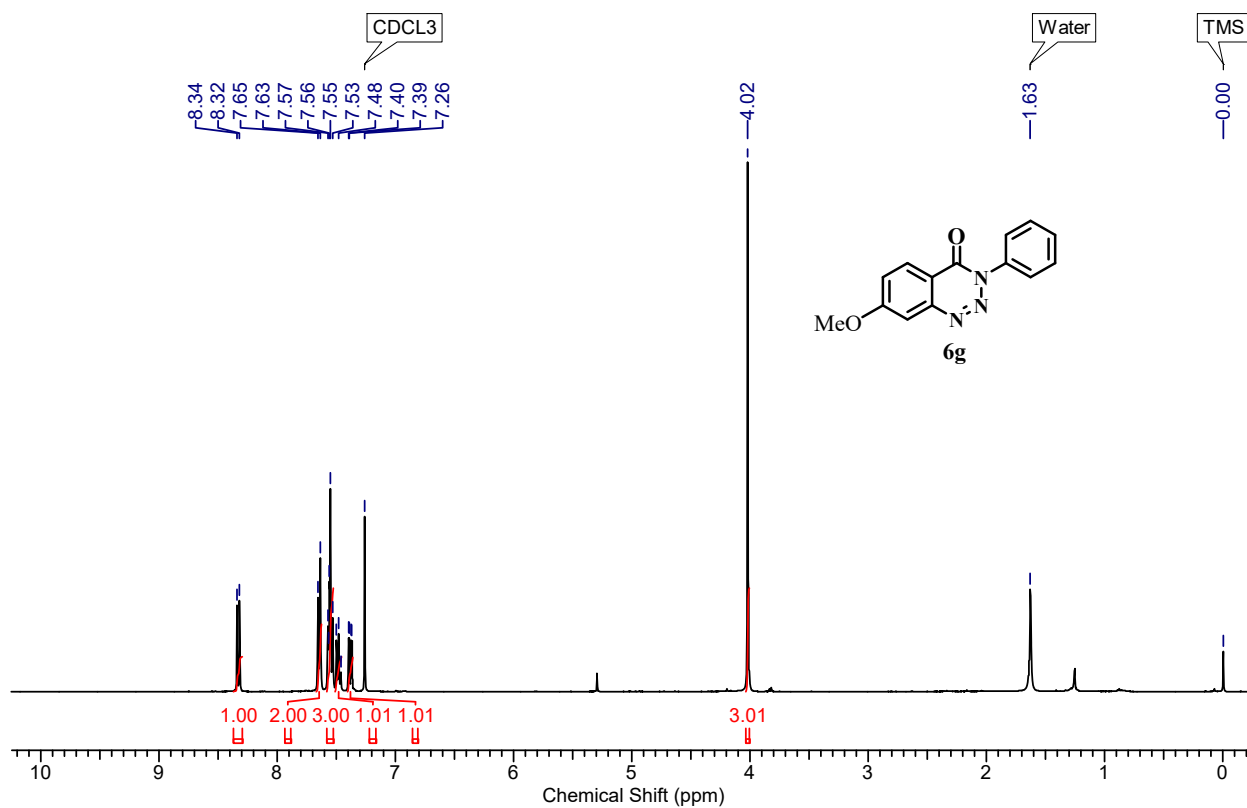


^{13}C NMR (CDCl_3 , 100 MHz) of Compound 6f

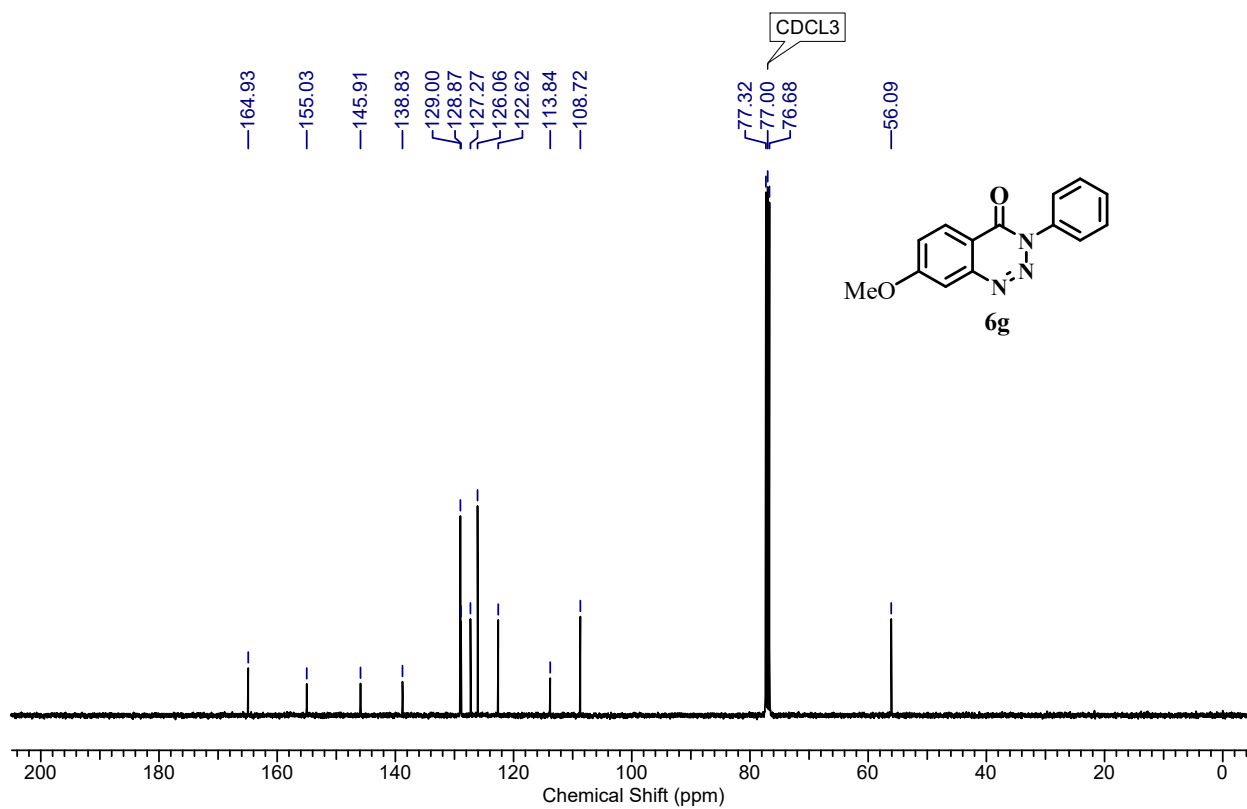
BAA-6 #331 RT: 1.85 AV: 1 NL: 5.52E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 6f

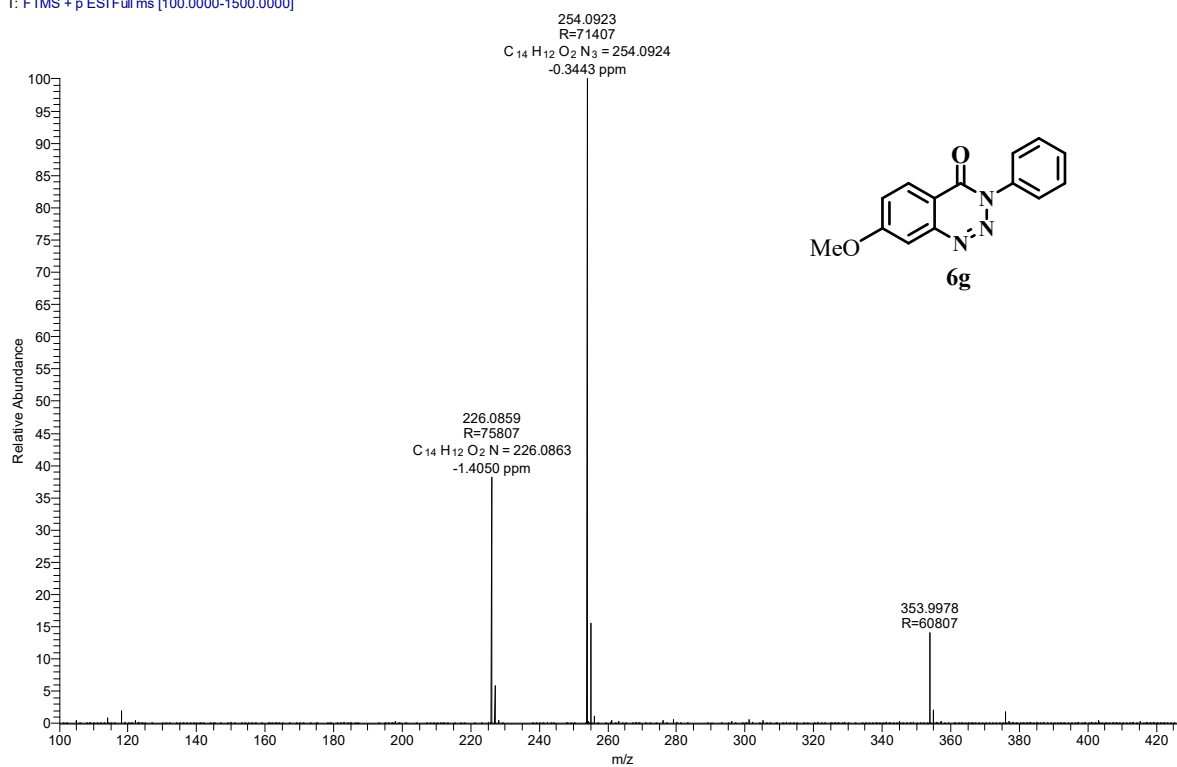


¹H NMR (CDCl₃, 400 MHz) of Compound 6g

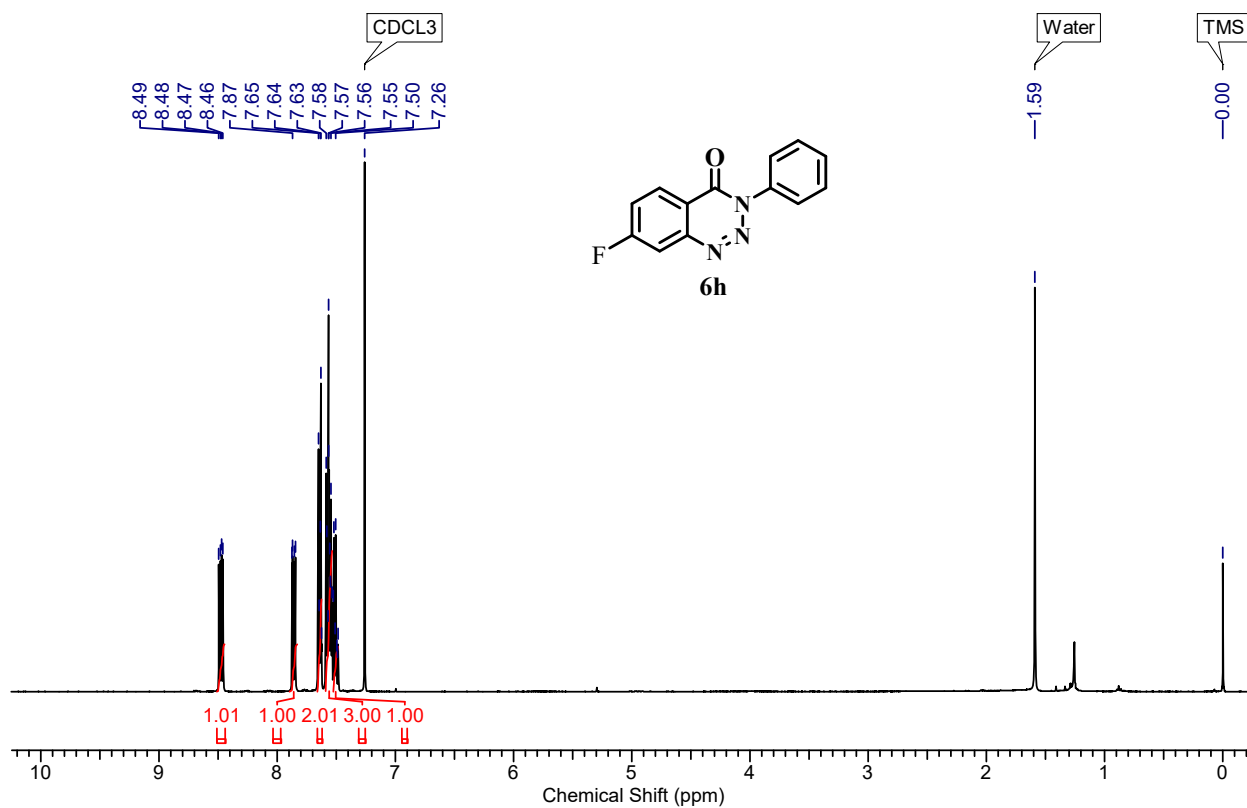


^{13}C NMR (CDCl_3 , 100 MHz) of Compound 6g

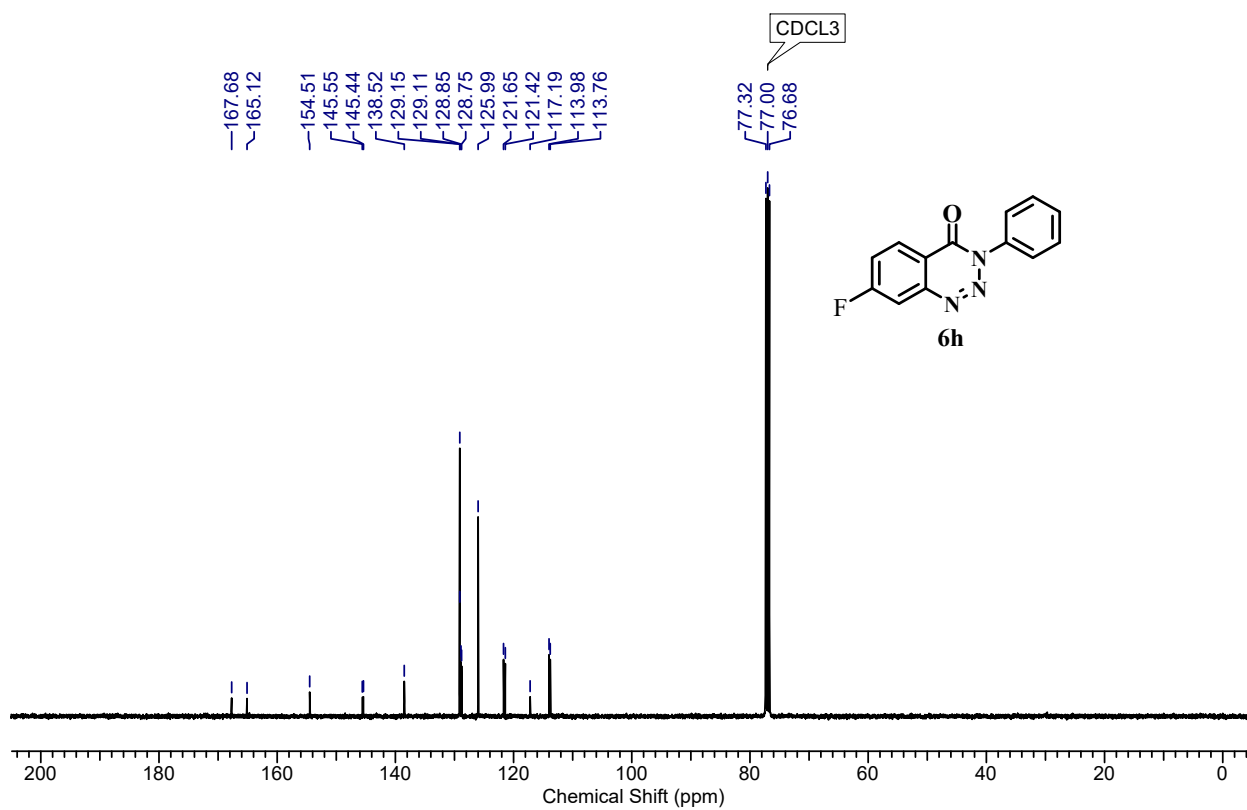
BAA-7 #331 RT: 1.82 AV: 1 NL: 6.58E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



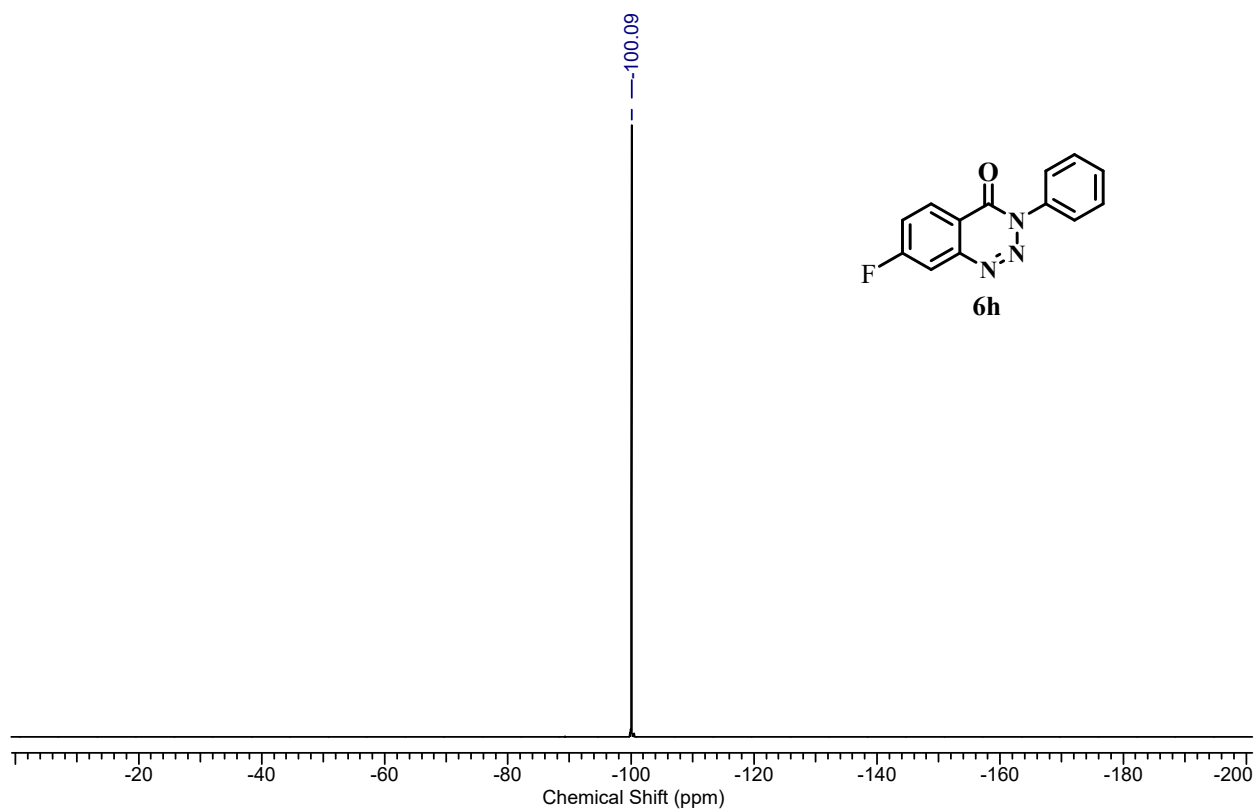
HRMS of Compound 6g



¹H NMR (CDCl₃, 400 MHz) of Compound 6h

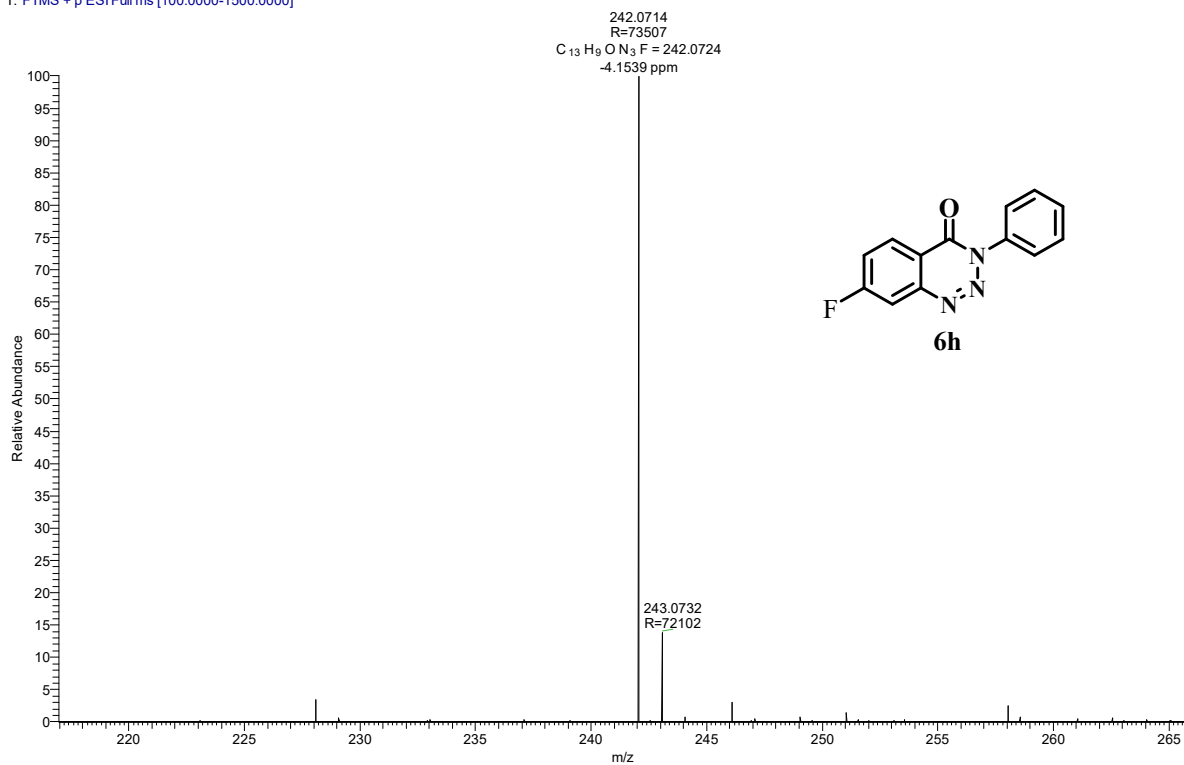


¹³C NMR (CDCl₃, 100 MHz) of Compound 6h

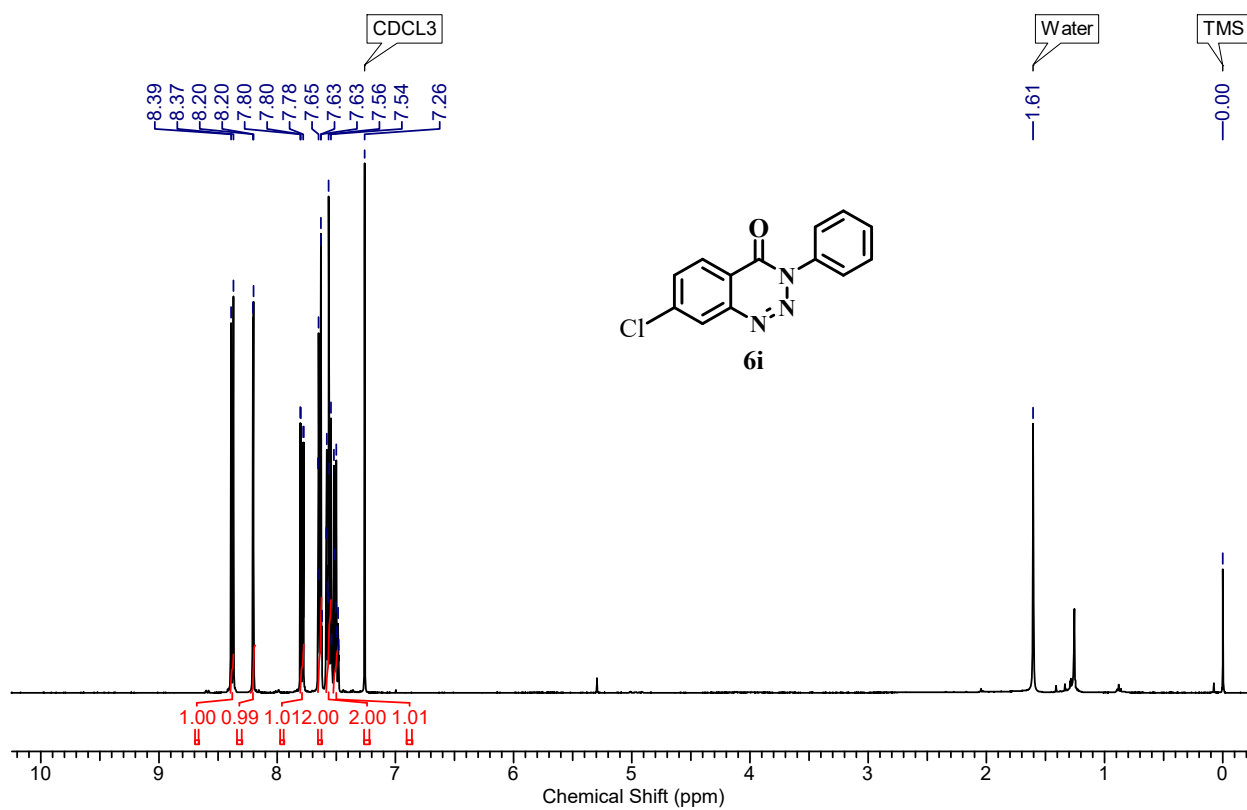


¹⁹F NMR (CDCl₃, 376 MHz) of Compound 6h

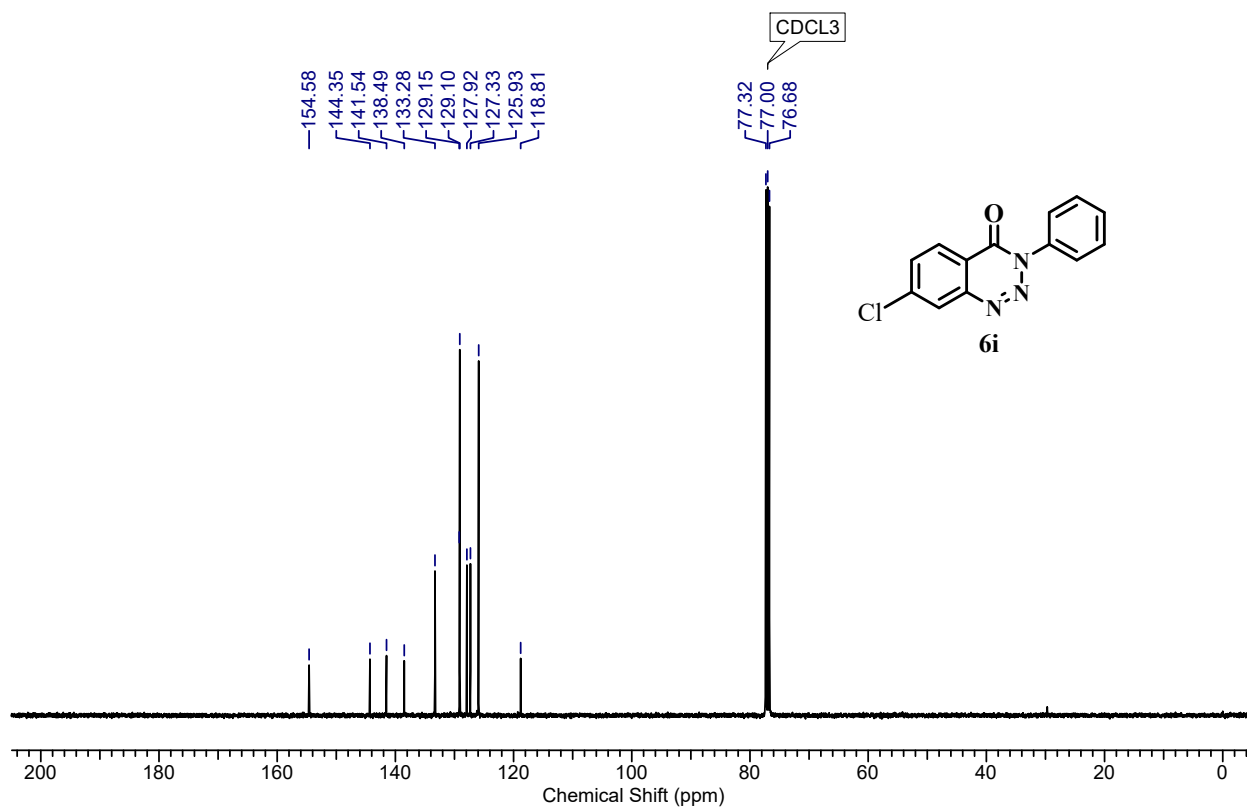
BAA-8 #452 RT: 2.43 AV: 1 NL: 1.21E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 6h

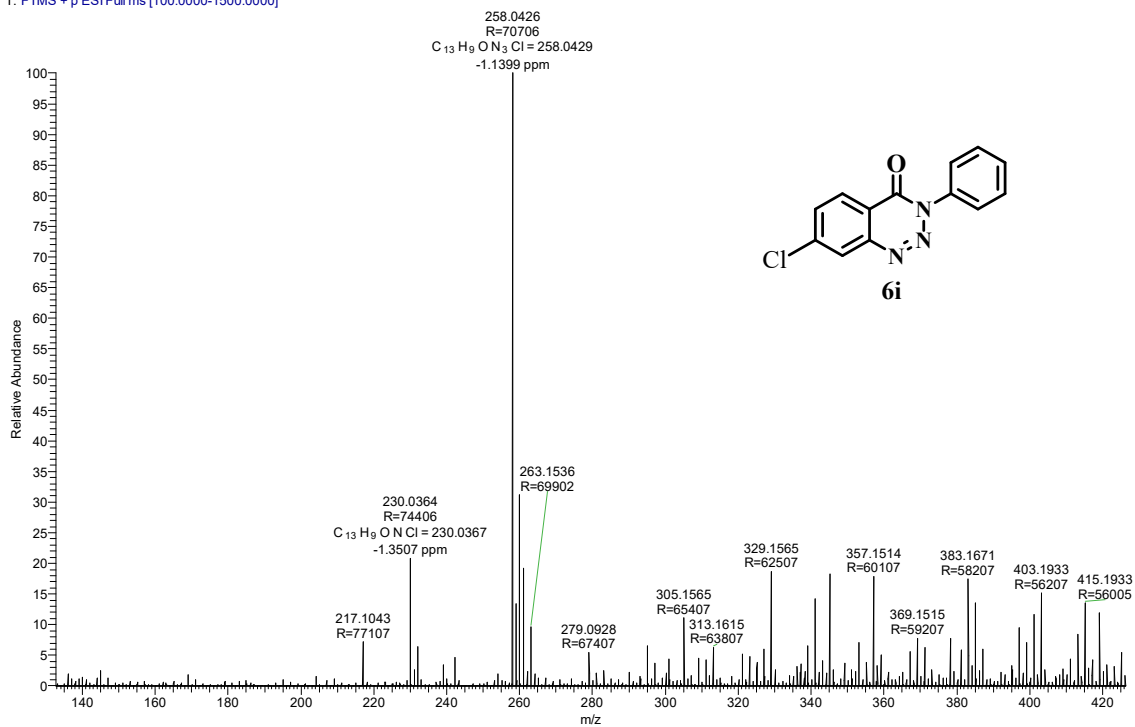


¹H NMR (CDCl₃, 400 MHz) of Compound 6i

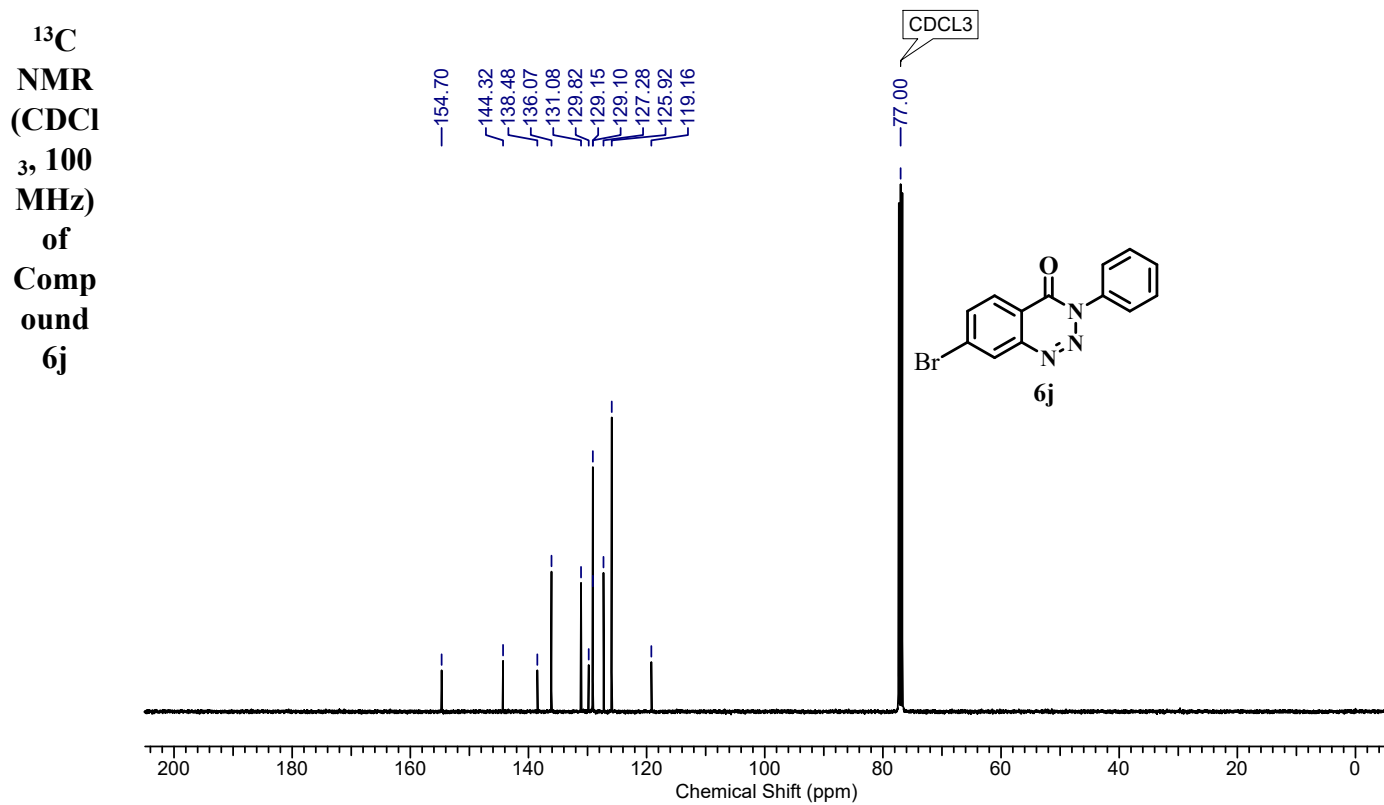
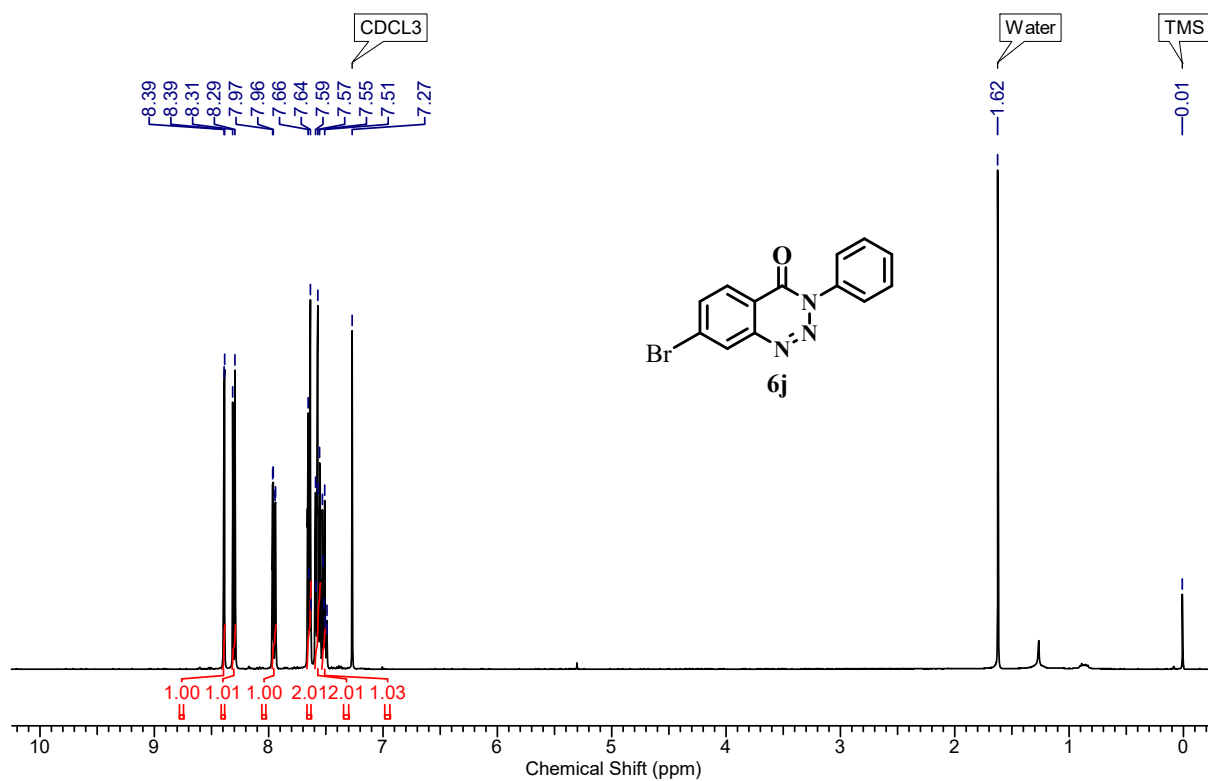


¹³C NMR (CDCl₃, 100 MHz) of Compound 6i

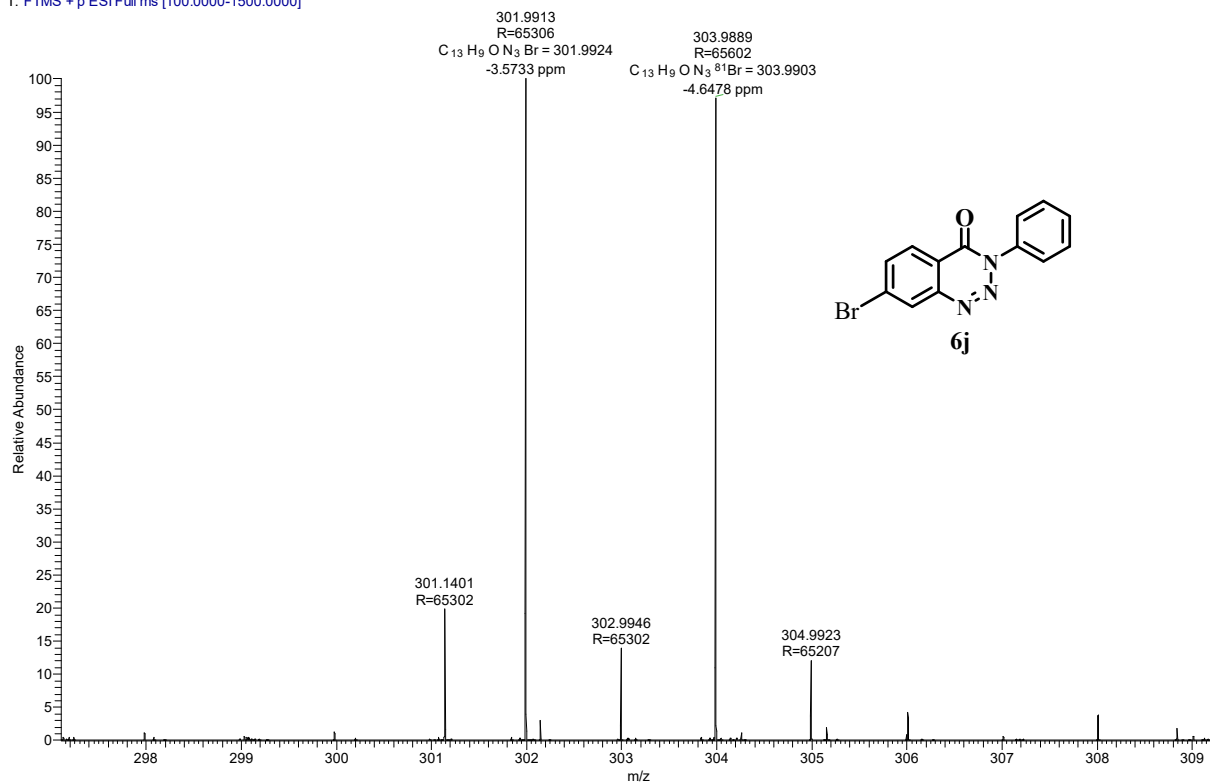
BAA-9 #344 RT: 1.88 AV: 1 NL: 3.76E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



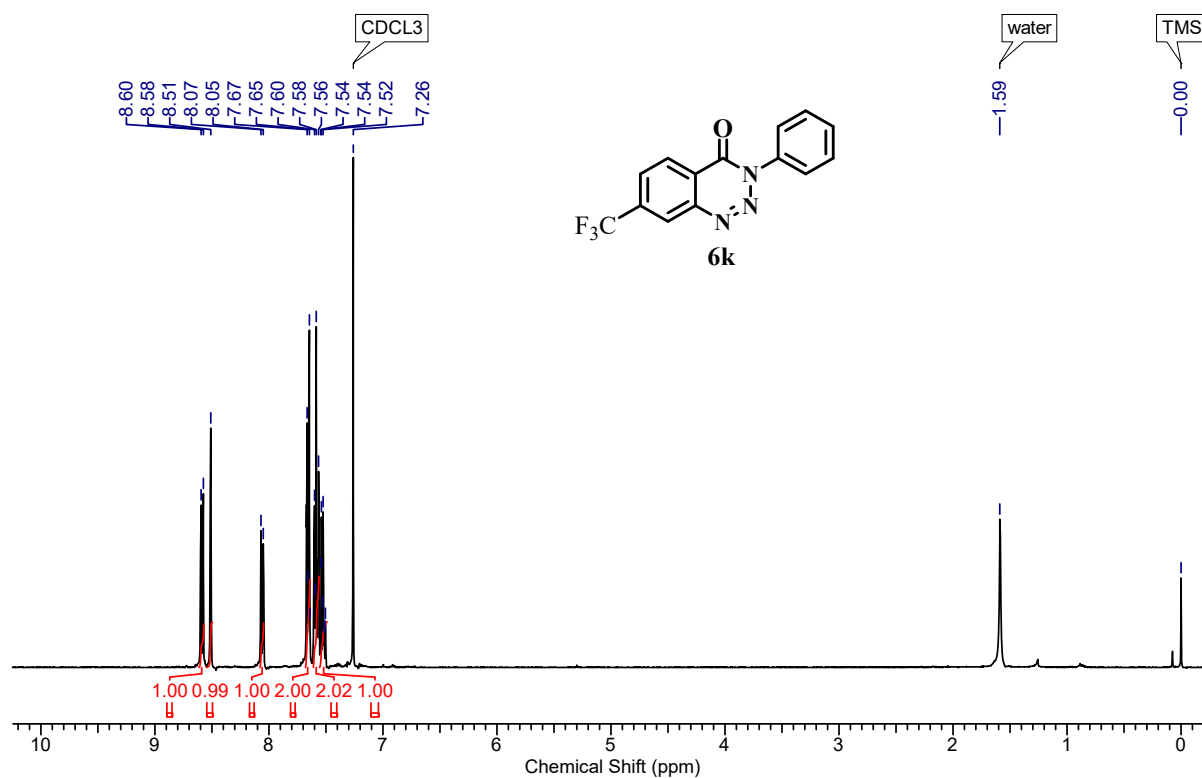
HRMS of Compound 6i



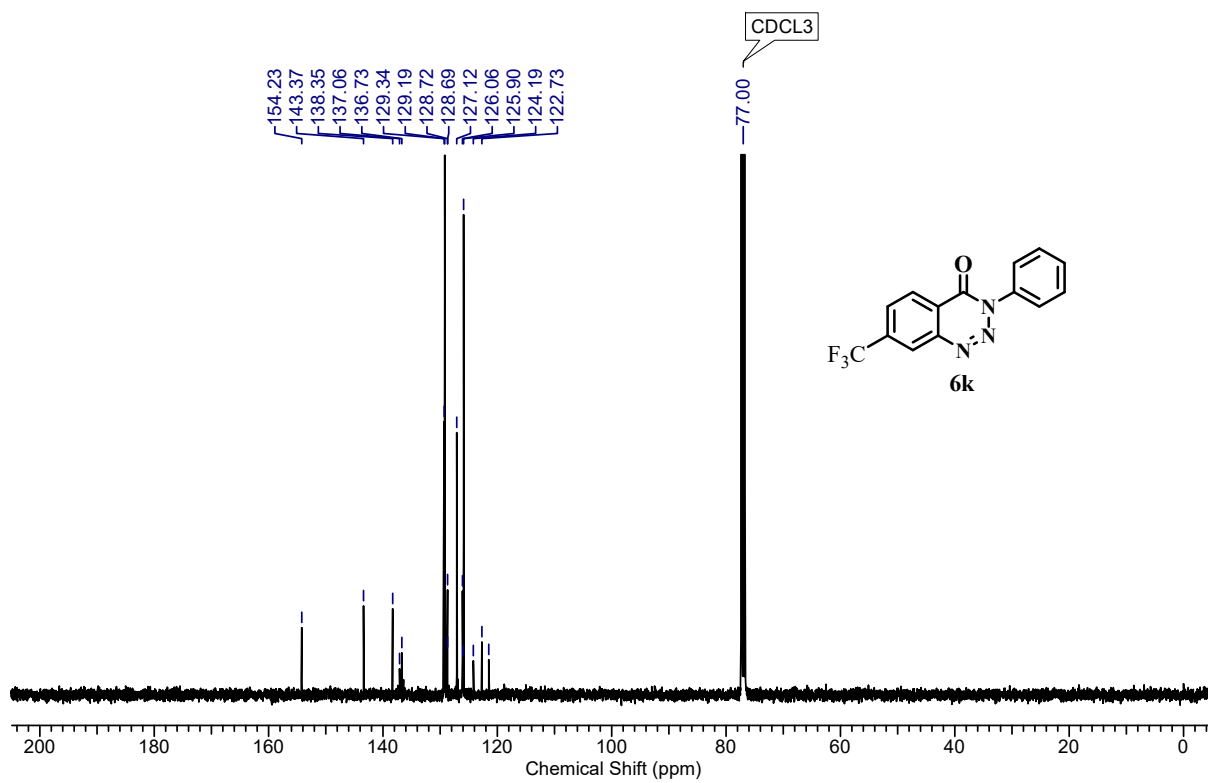
BAA-10 #393 RT: 2.24 AV: 1 NL: 2.03E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



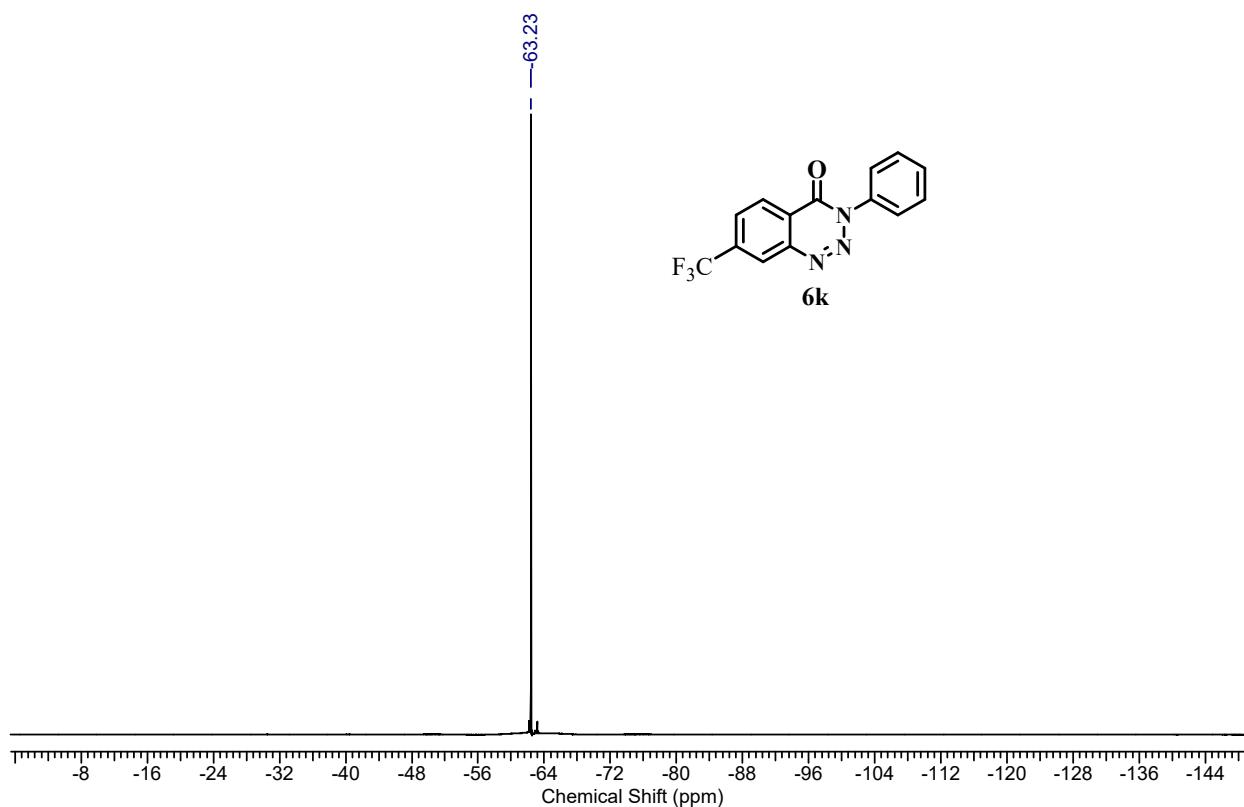
HRMS of Compound 6j



¹H NMR (CDCl₃, 400 MHz) of Compound 6k

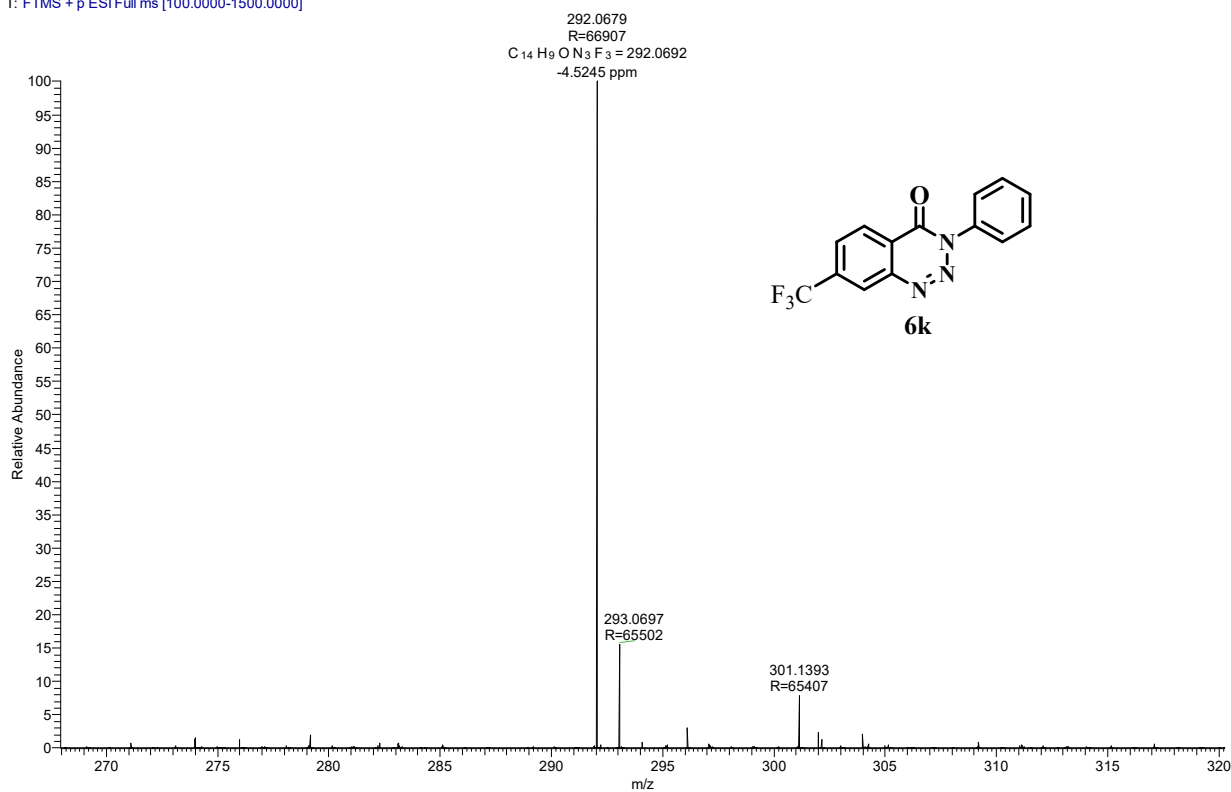


¹³C NMR (CDCl₃, 100 MHz) of Compound 6k

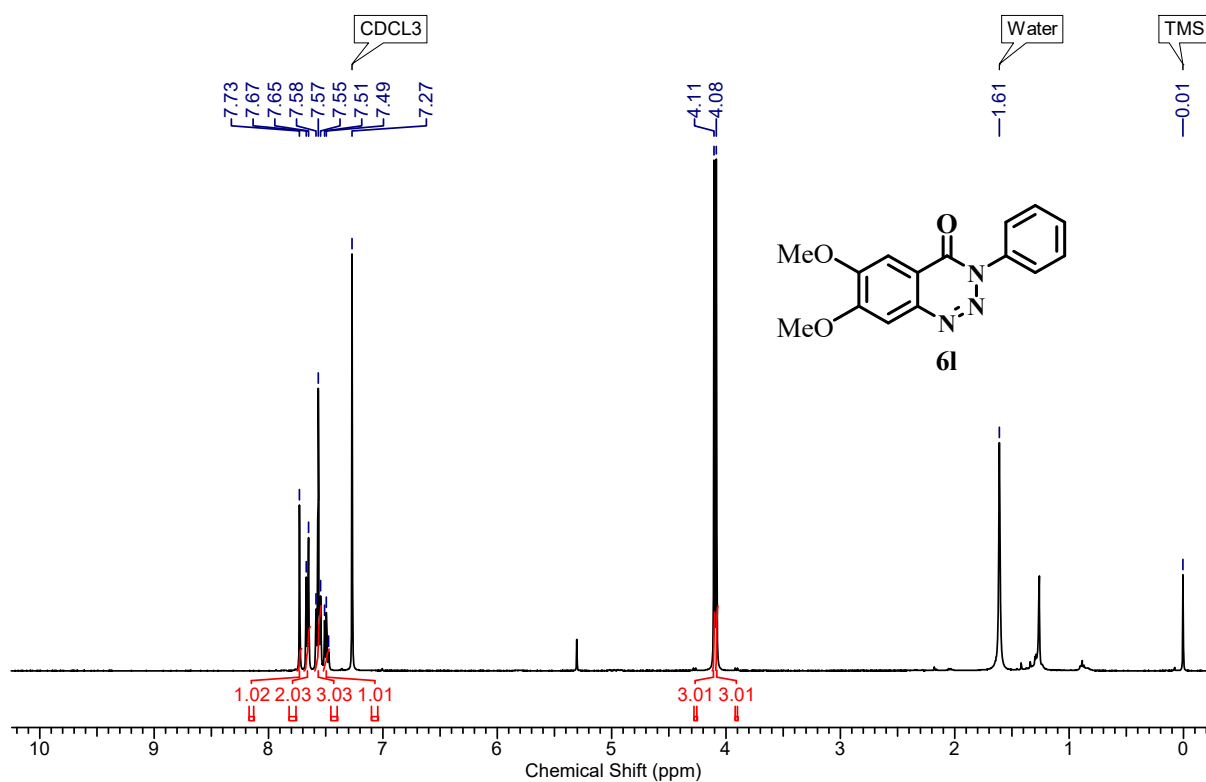


¹⁹F NMR (CDCl₃, 376 MHz) of Compound 6k

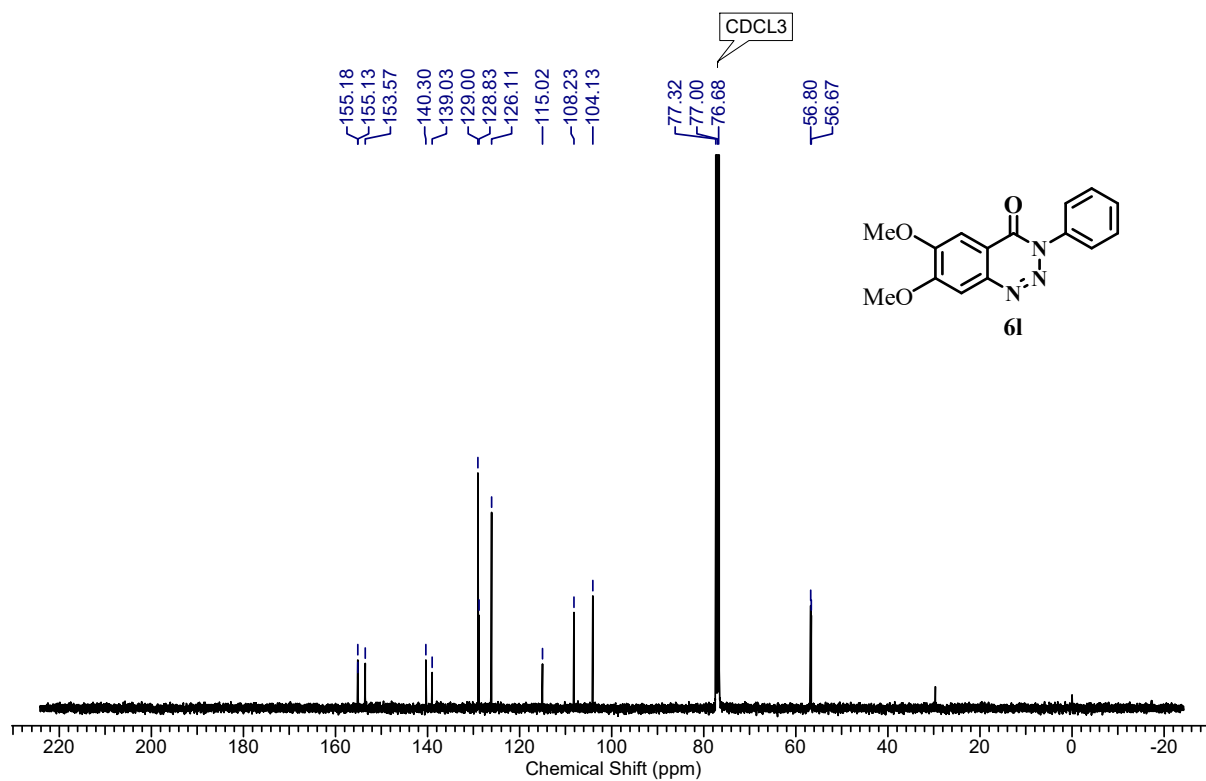
BAA-11 #386 RT: 2.20 AV: 1 NL: 7.32E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 6k

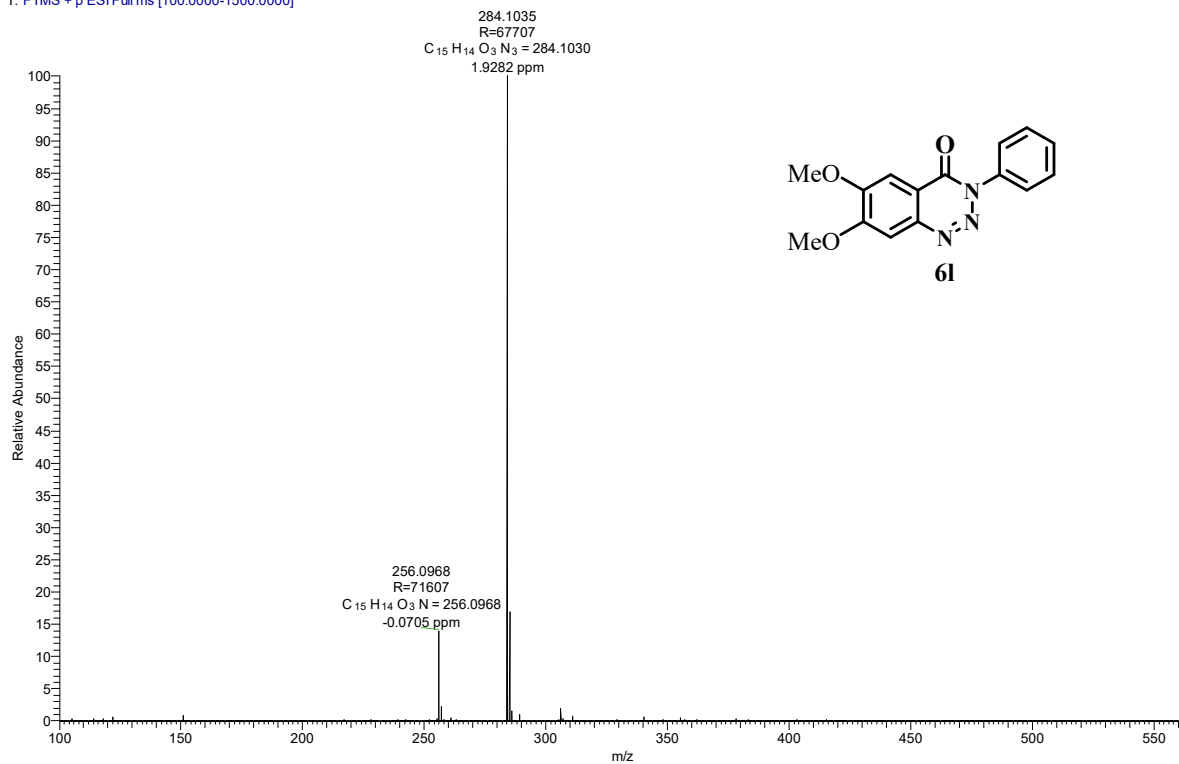


¹H NMR (CDCl₃, 400 MHz) of Compound 6l

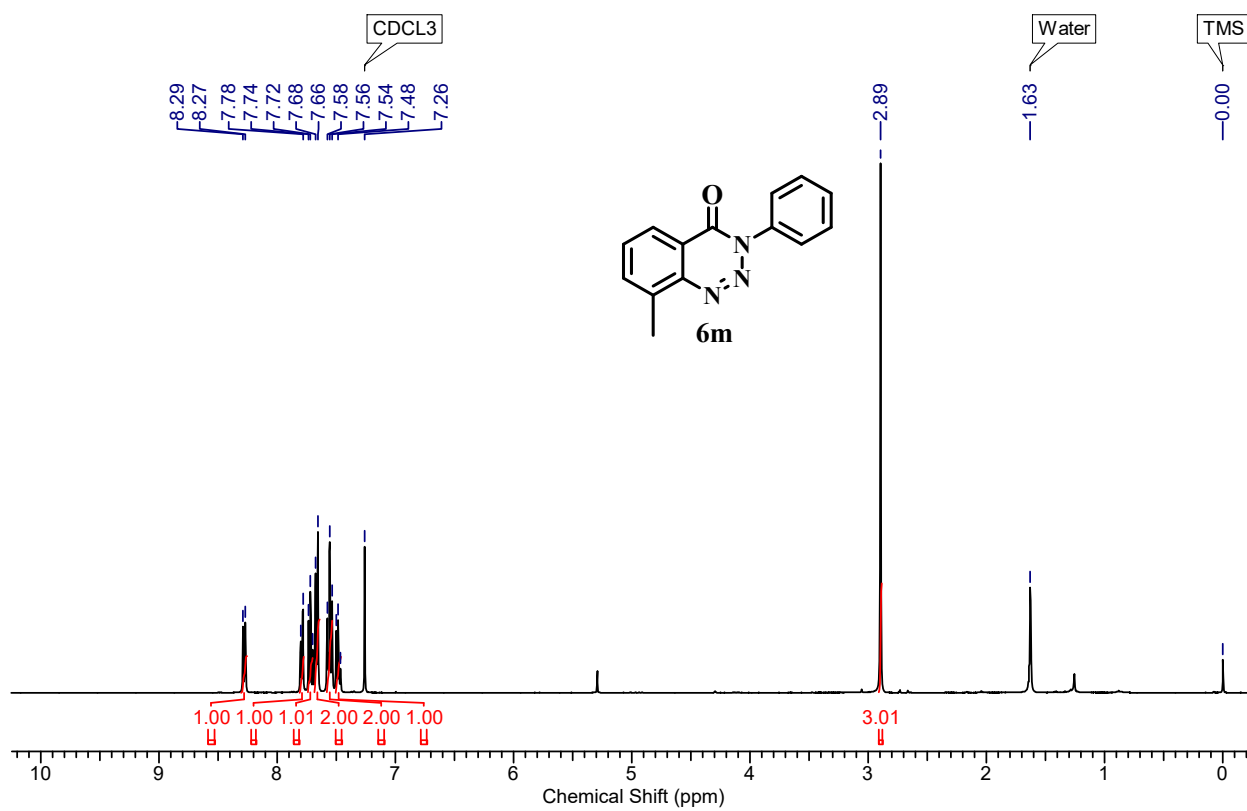


¹³C NMR (CDCl₃, 100 MHz) of Compound 6l

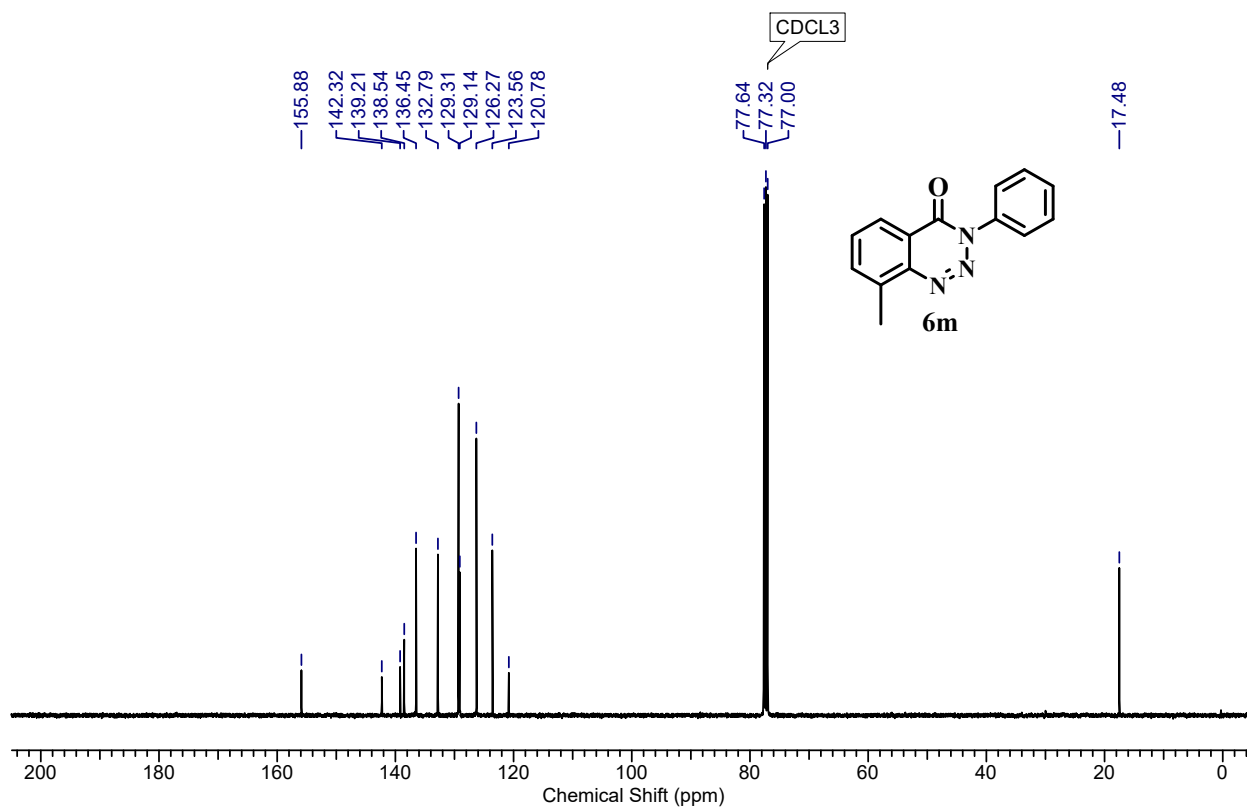
BAA-13 #319 RT: 1.74 AV: 1 NL: 1.23E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 61

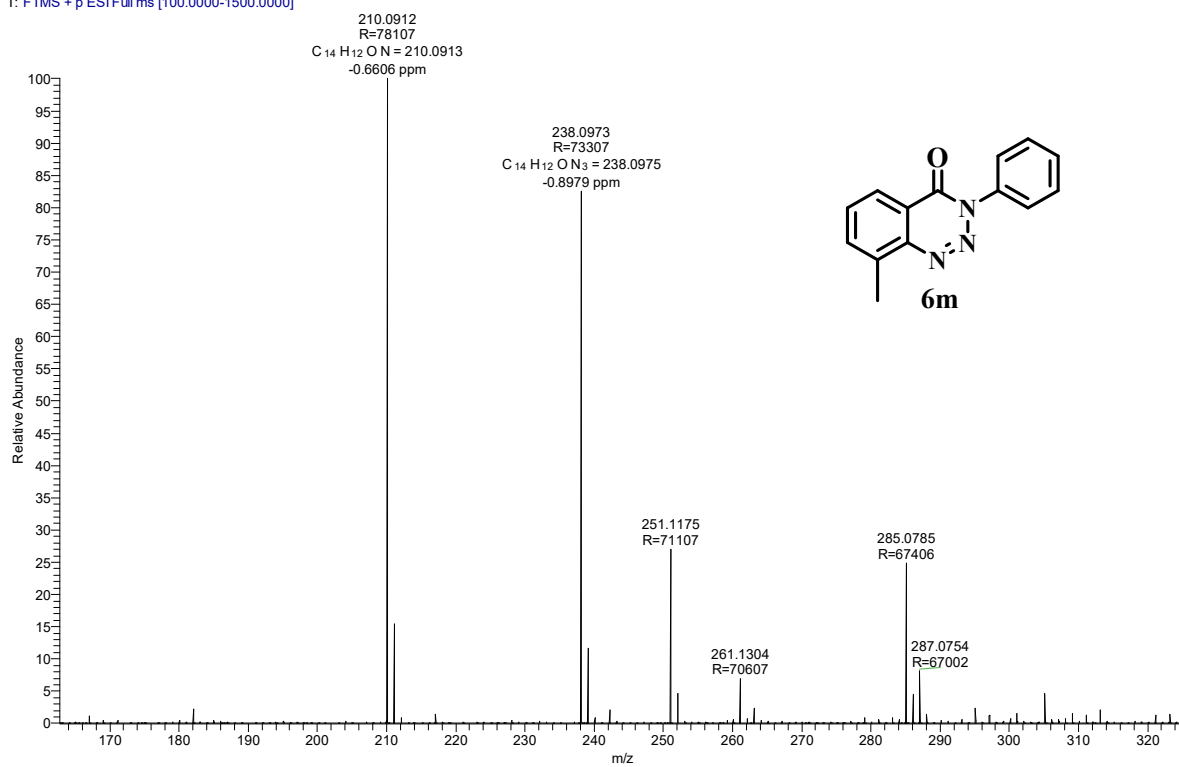


¹H NMR (CDCl₃, 400 MHz) of Compound 6m

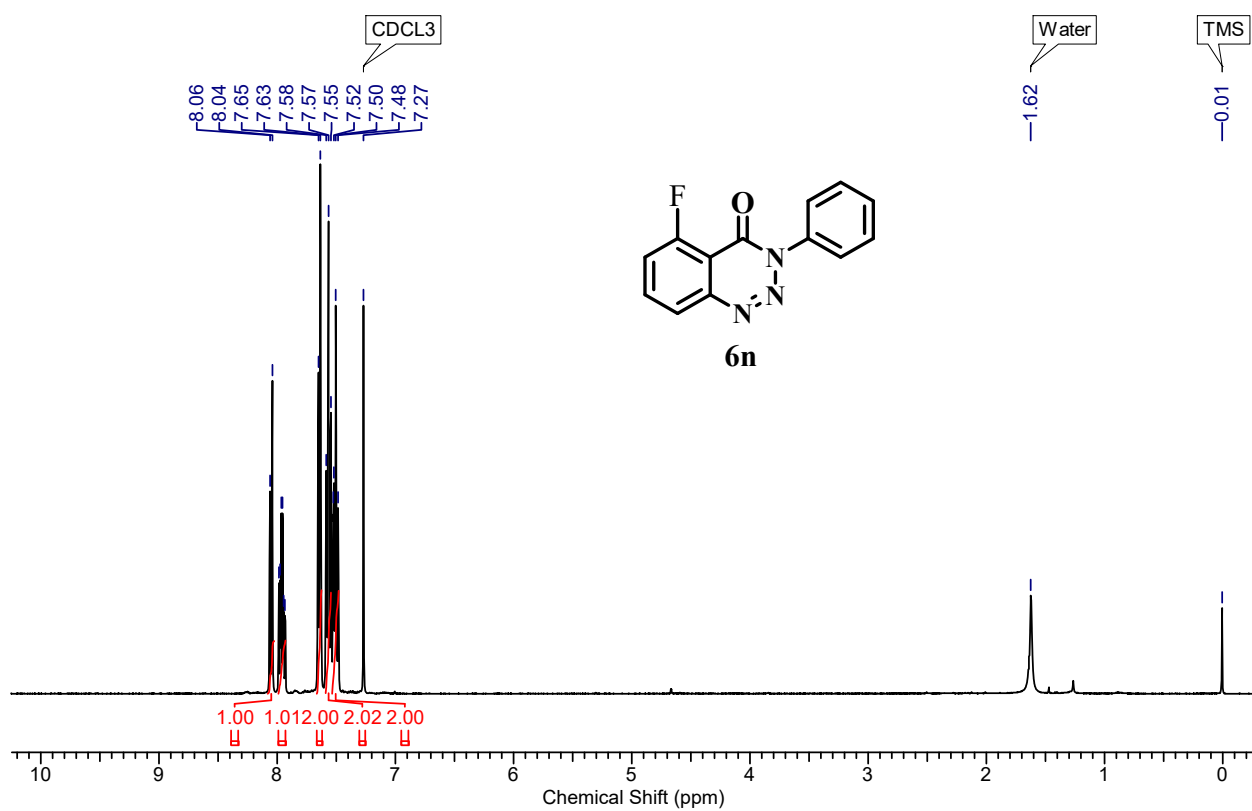


¹³C NMR (CDCl₃, 100 MHz) of Compound 6m

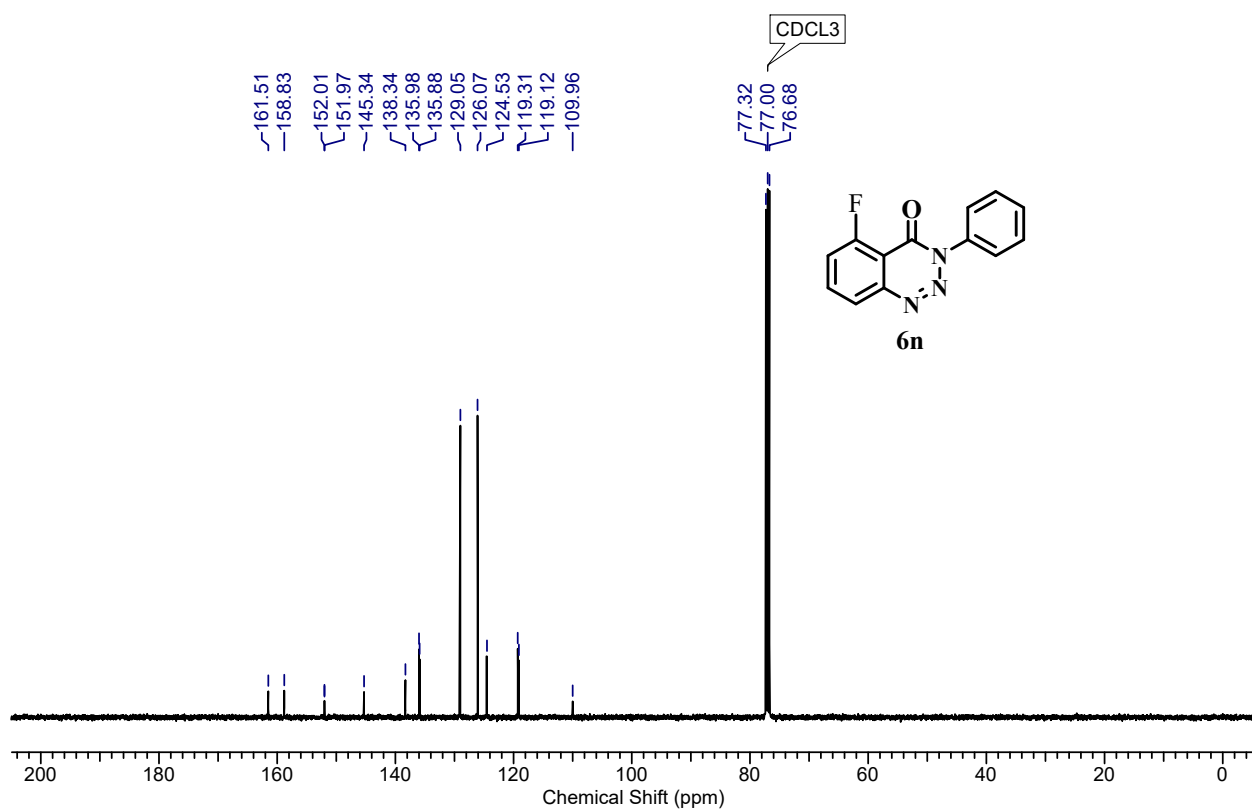
BAA-14 #347 RT: 1.90 AV: 1 NL: 1.13E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



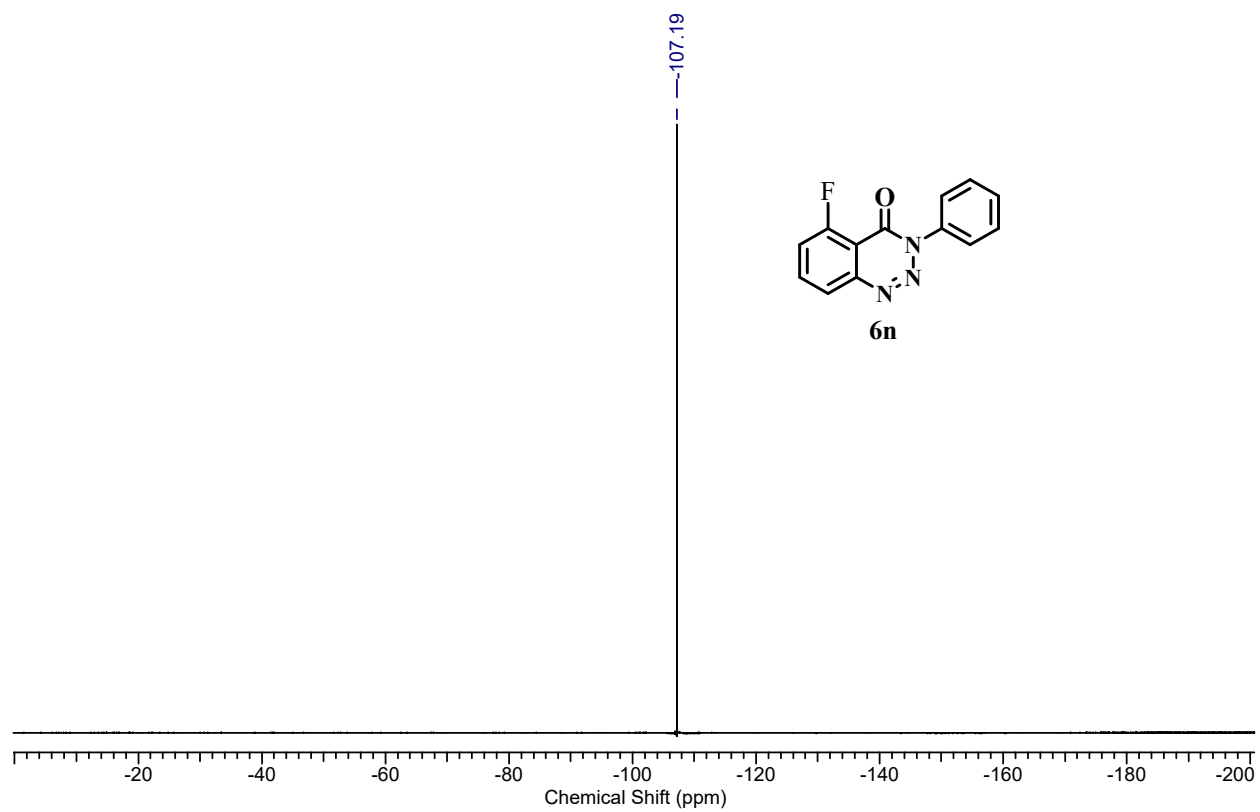
HRMS of Compound 6m



¹H NMR (CDCl₃, 400 MHz) of Compound 6n

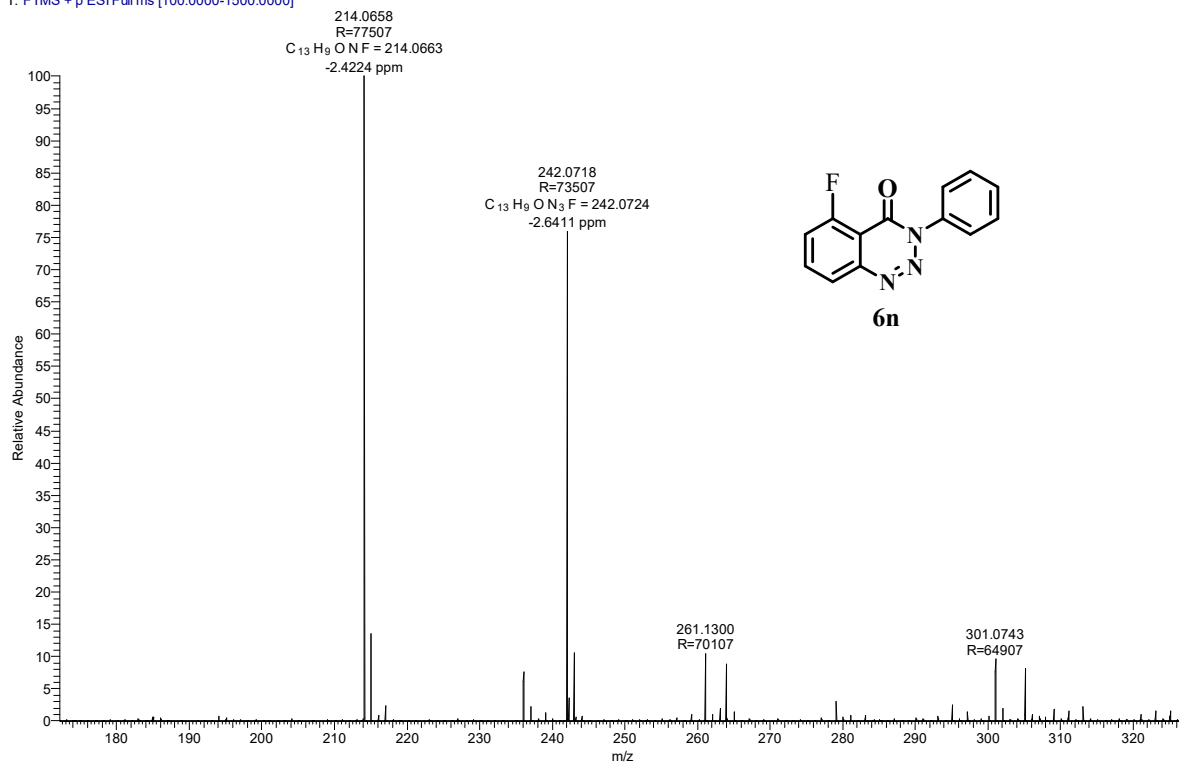


^{13}C NMR (CDCl_3 , 100 MHz) of Compound 6n

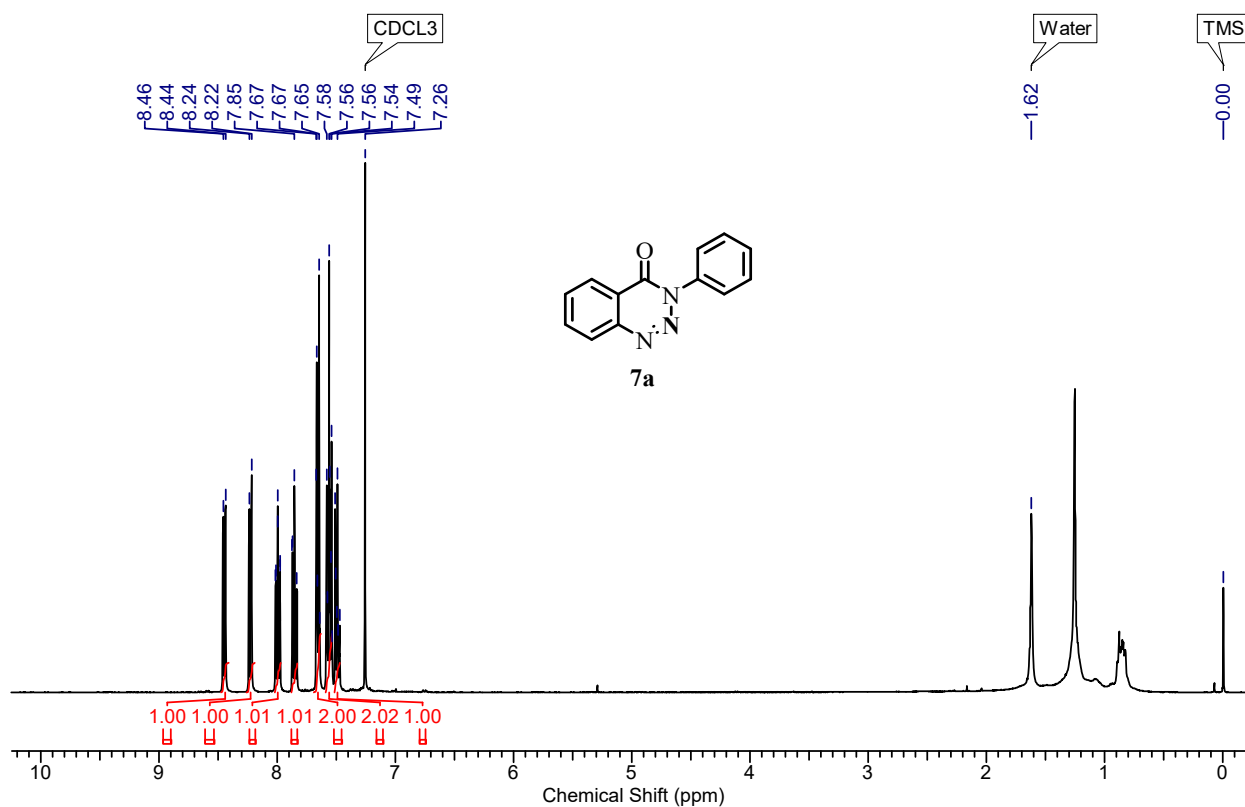


^{19}F NMR (CDCl_3 , 376 MHz) of Compound 6n

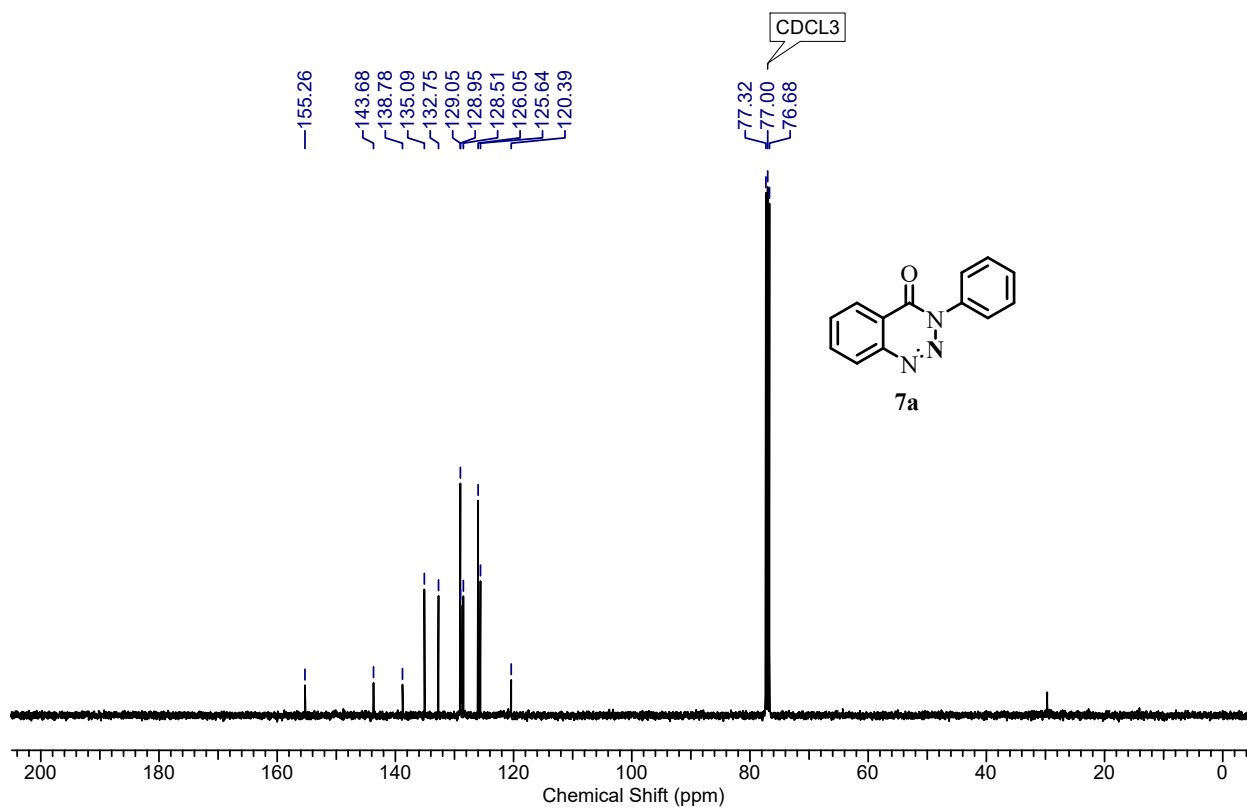
BAA-15 #318 RT: 1.77 AV: 1 NL: 6.39E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 6n

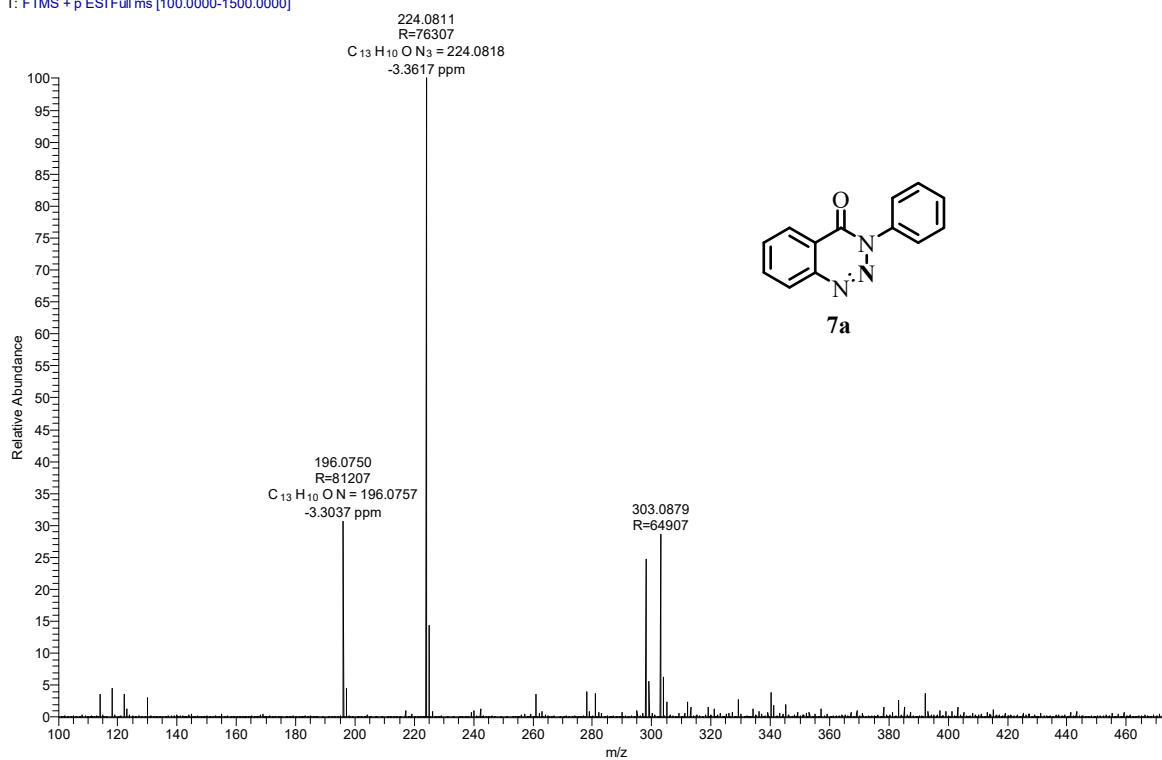


¹H NMR (CDCl₃, 400 MHz) of Compound 7a

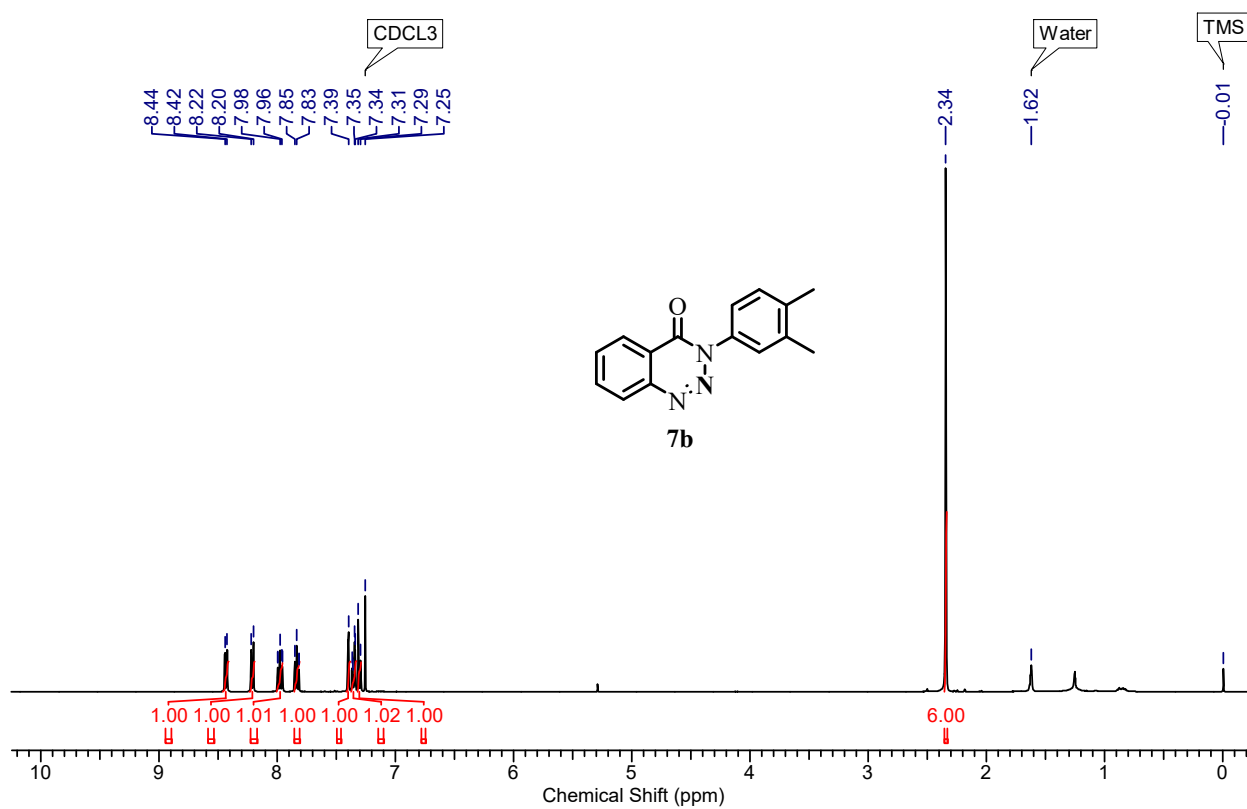


¹³C NMR (CDCl₃, 100 MHz) of Compound 7a

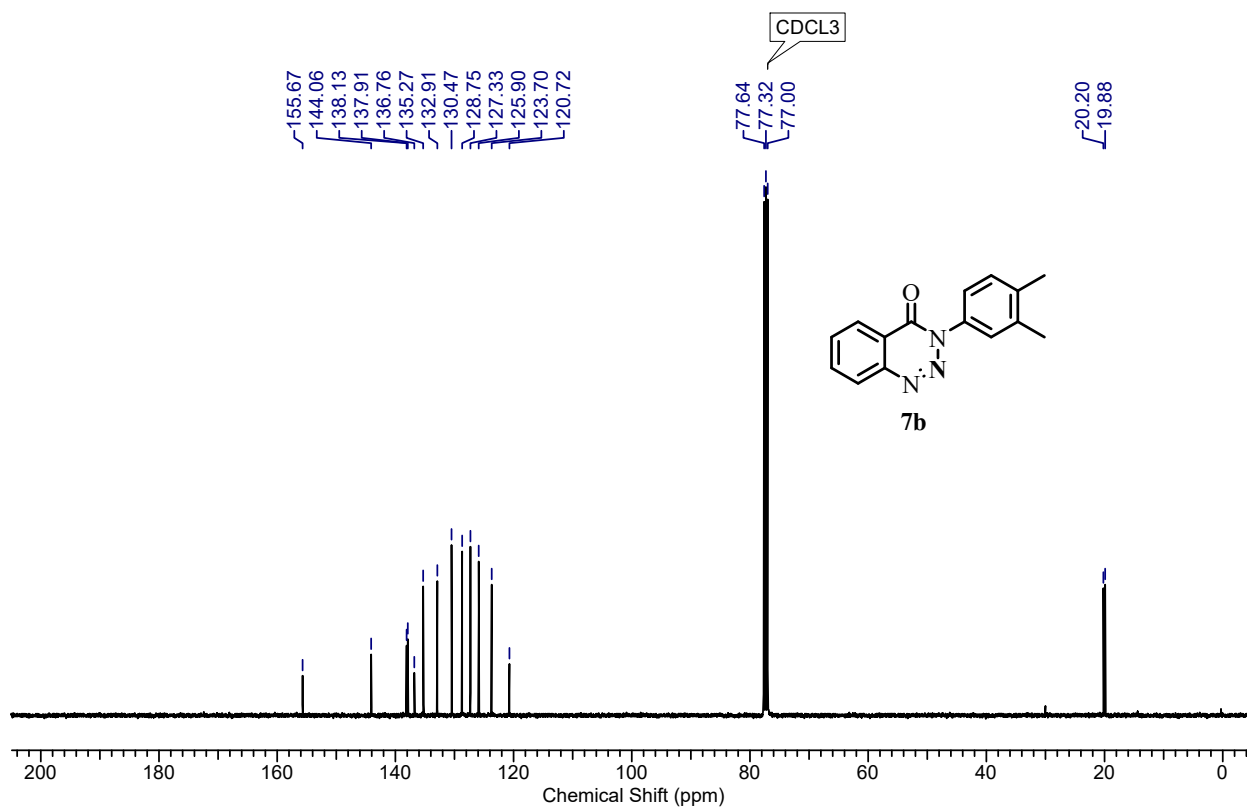
BAA-16 #310 RT: 1.76 AV: 1 NL: 2.20E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 7a

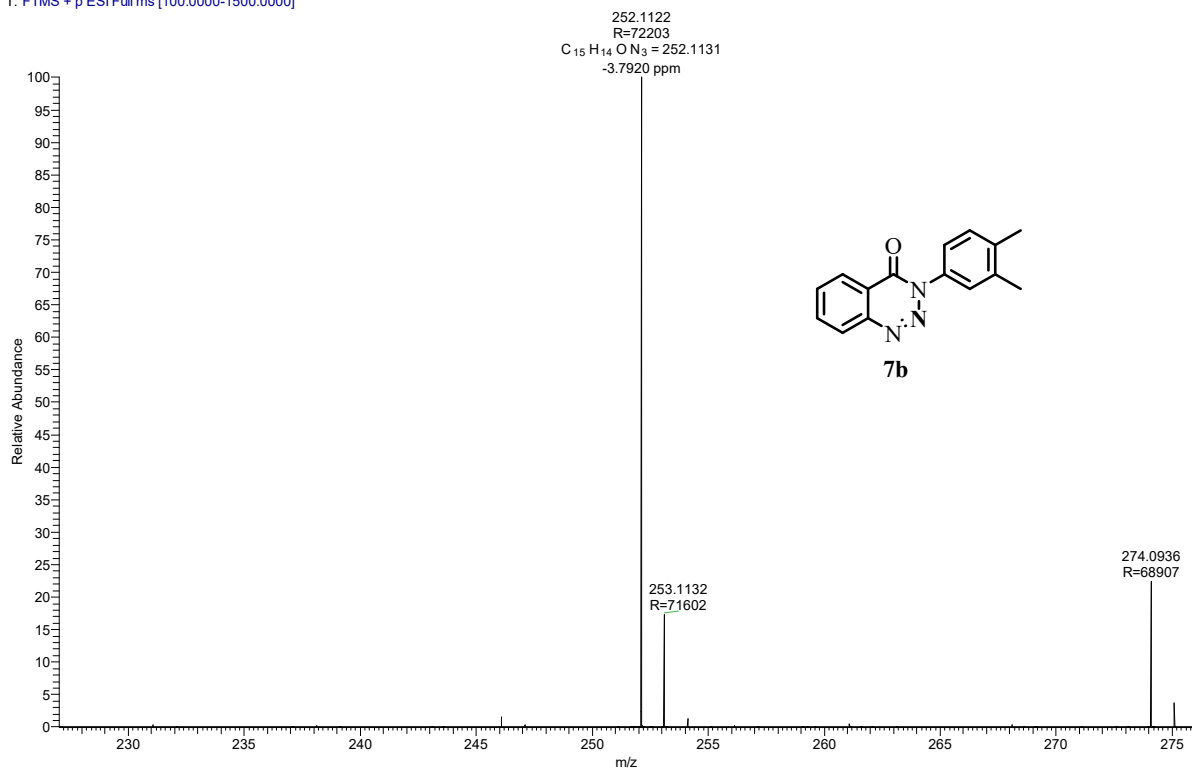


¹H NMR (CDCl₃, 400 MHz) of Compound 7b

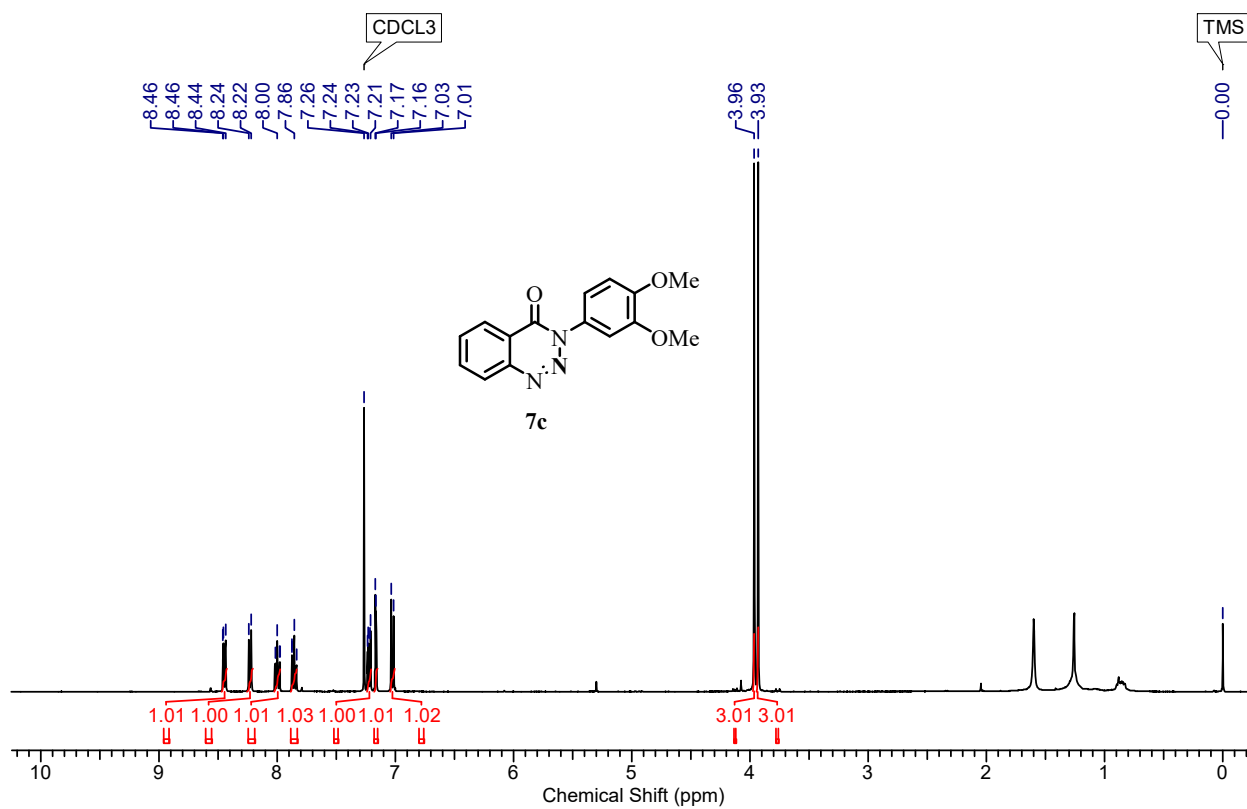


¹³C NMR (CDCl₃, 100 MHz) of Compound 7b

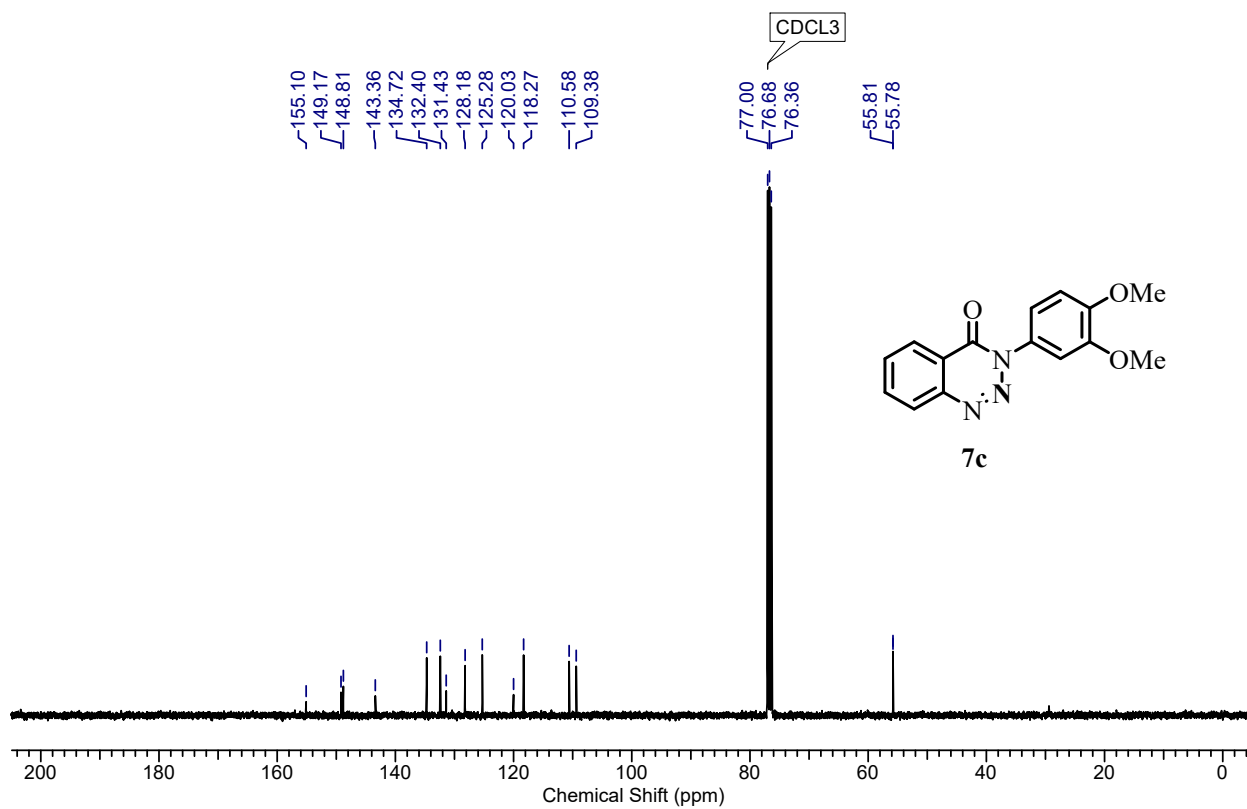
BAA-17 #477 RT: 2.55 AV: 1 NL: 4.71E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 7b

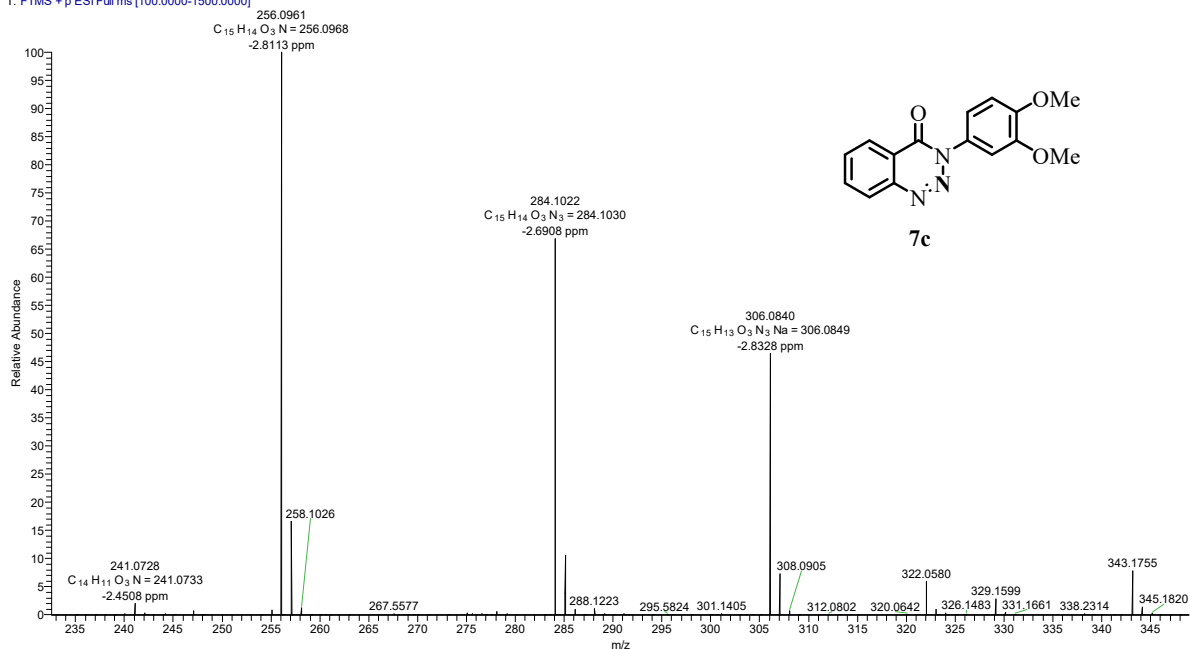


¹H NMR (CDCl₃, 400 MHz) of Compound 7c

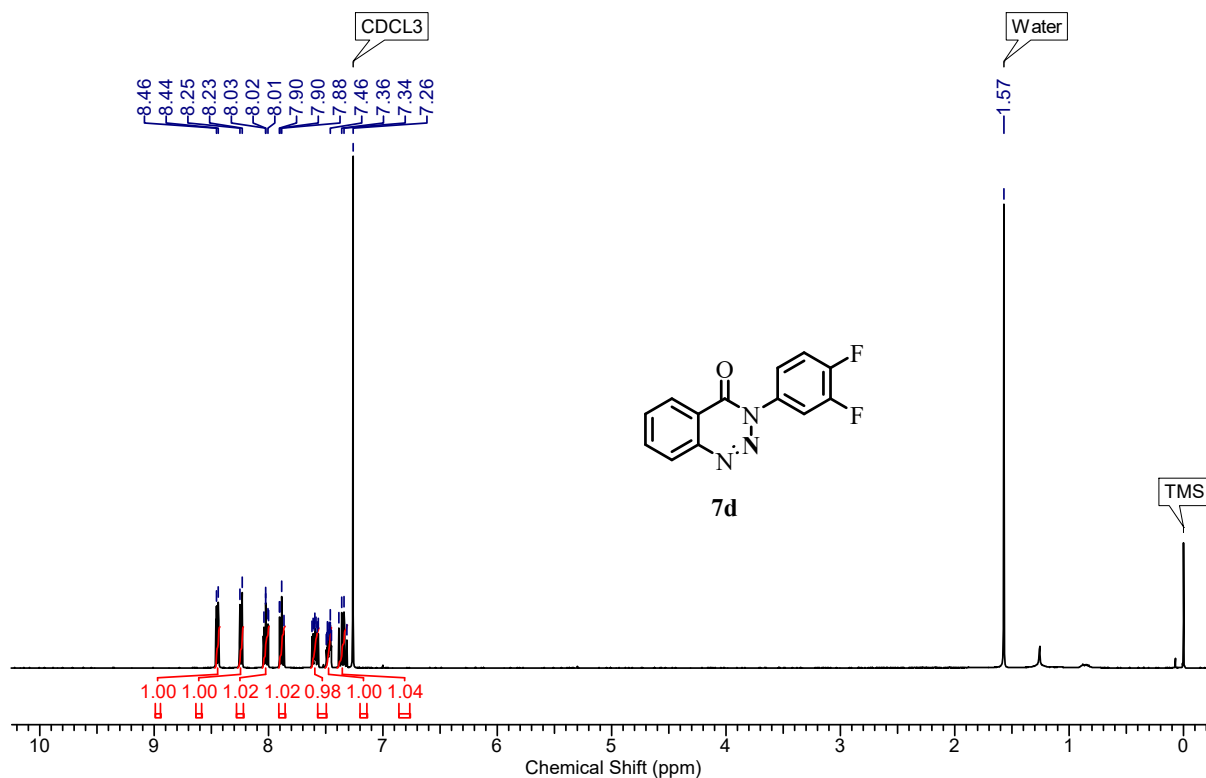


^{13}C NMR (CDCl_3 , 100 MHz) of Compound 7c

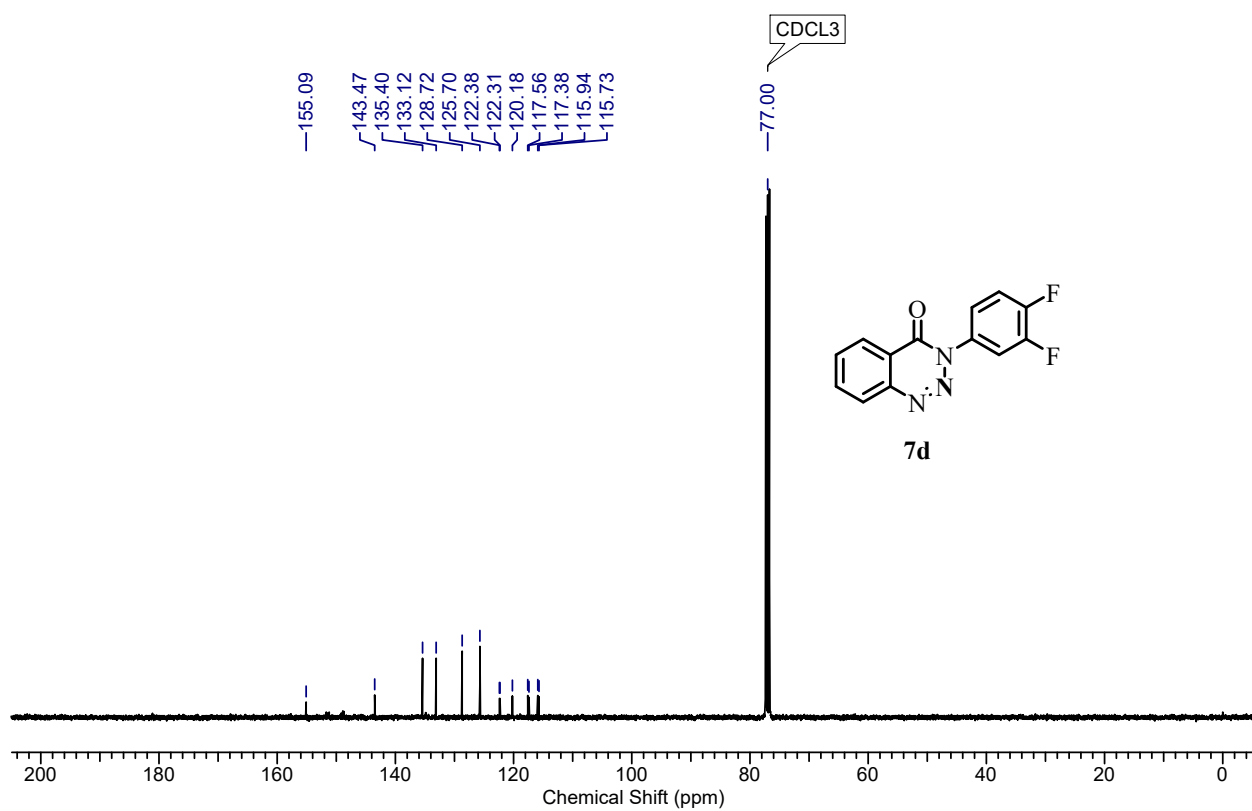
BAA-18 #313 RT: 1.82 AV: 1 NL: 3.93E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



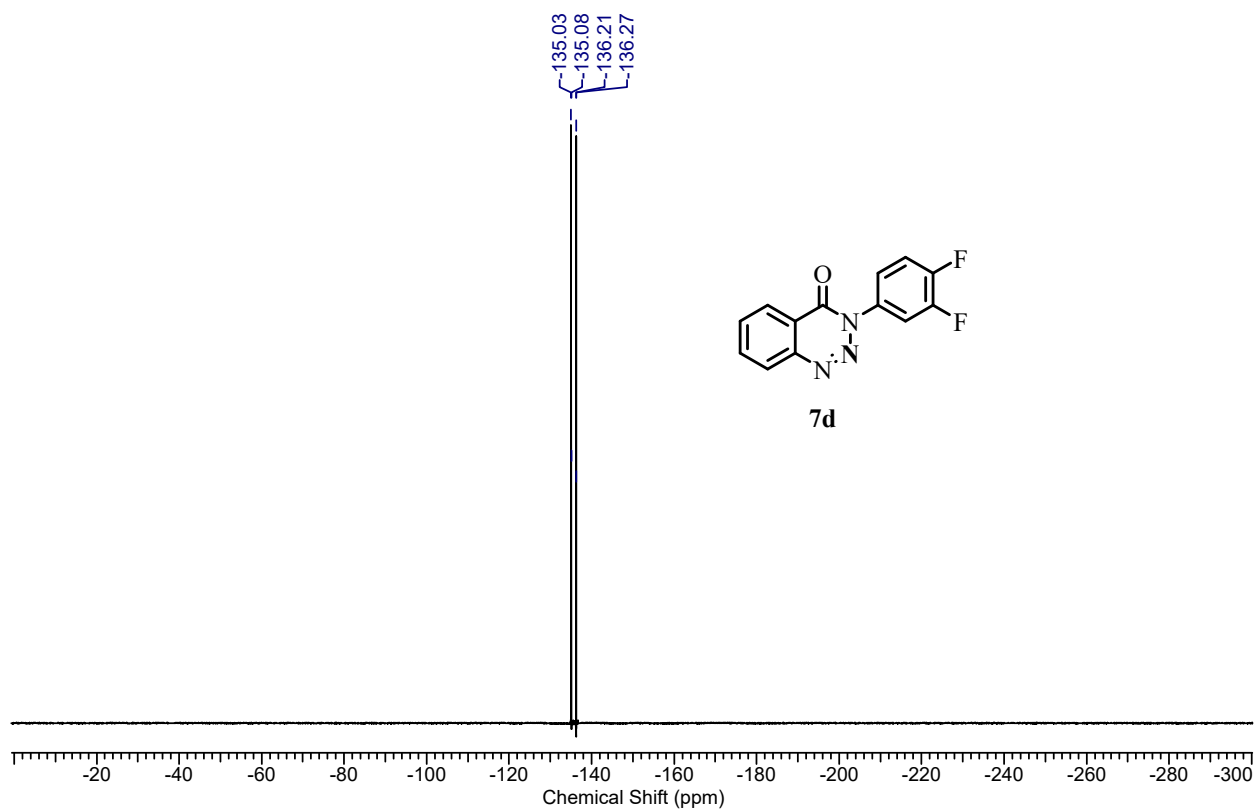
HRMS of Compound 7c



^1H NMR (CDCl_3 , 400 MHz) of Compound 7d

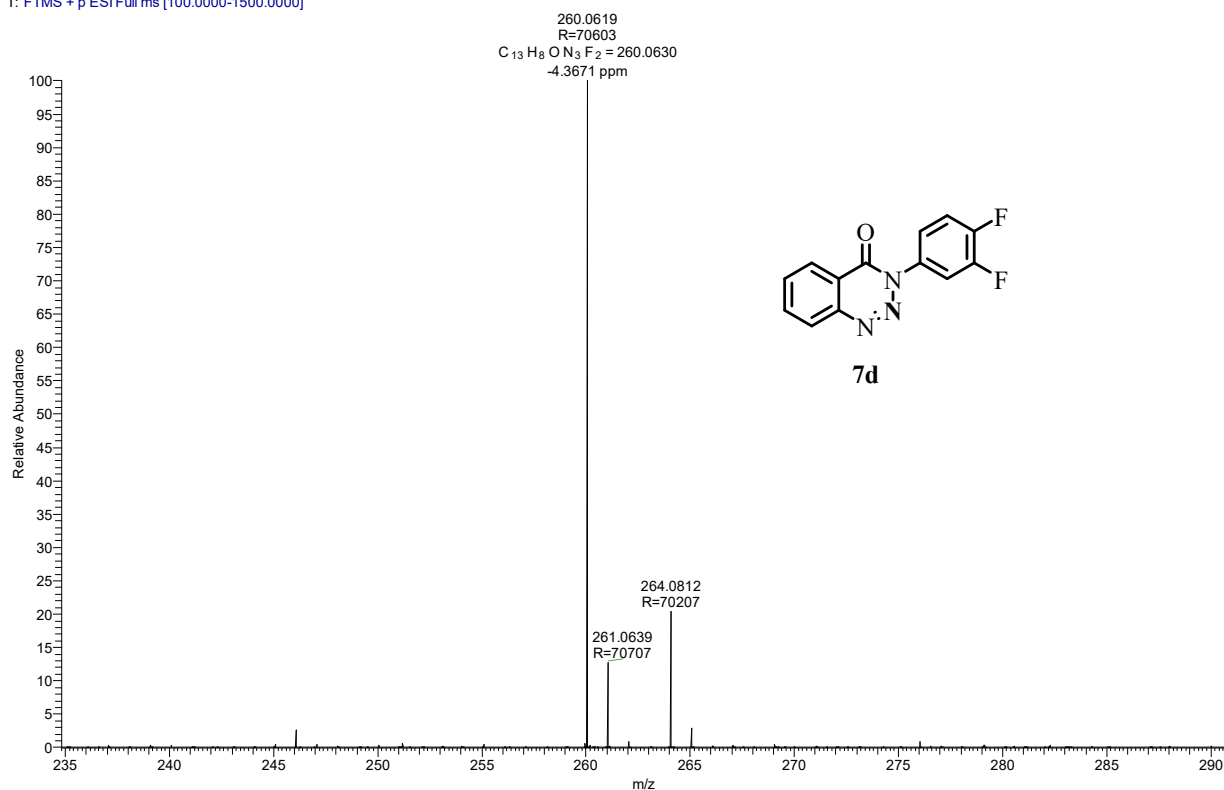


¹³C NMR (CDCl₃, 100 MHz) of Compound 7d

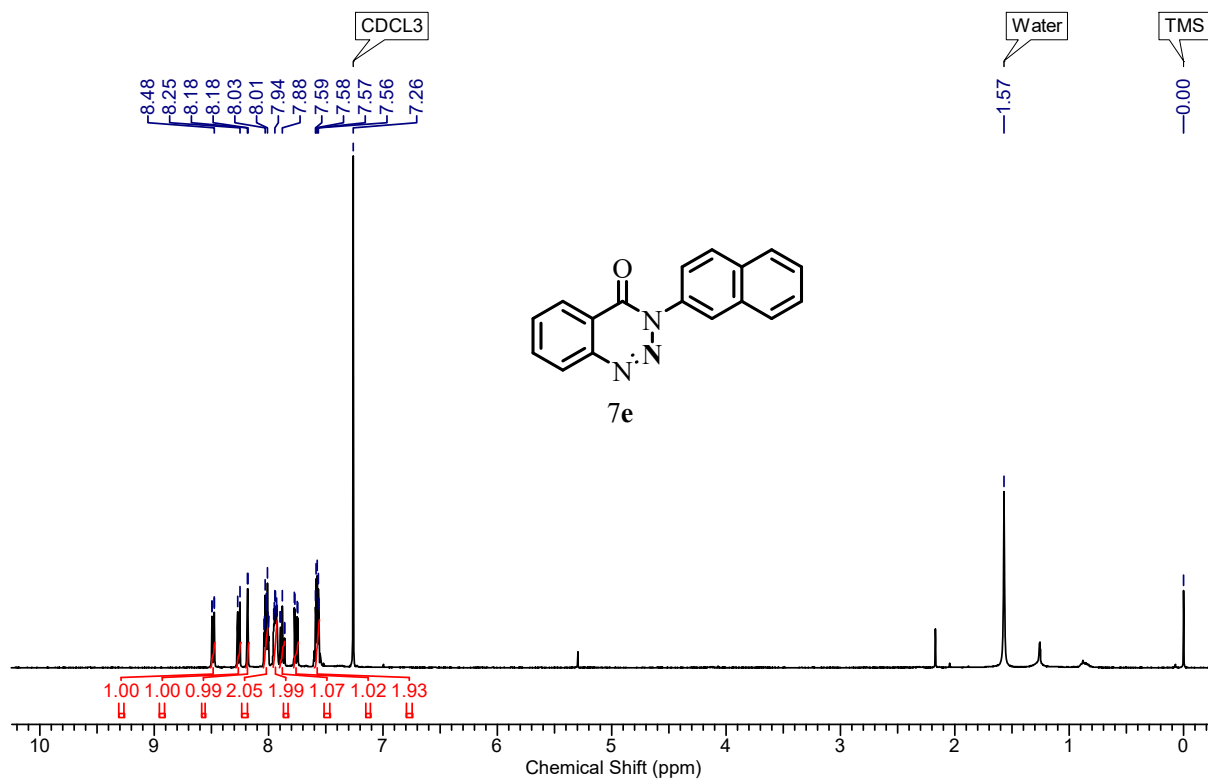


¹⁹F NMR (CDCl₃, 376 MHz) of Compound 7d

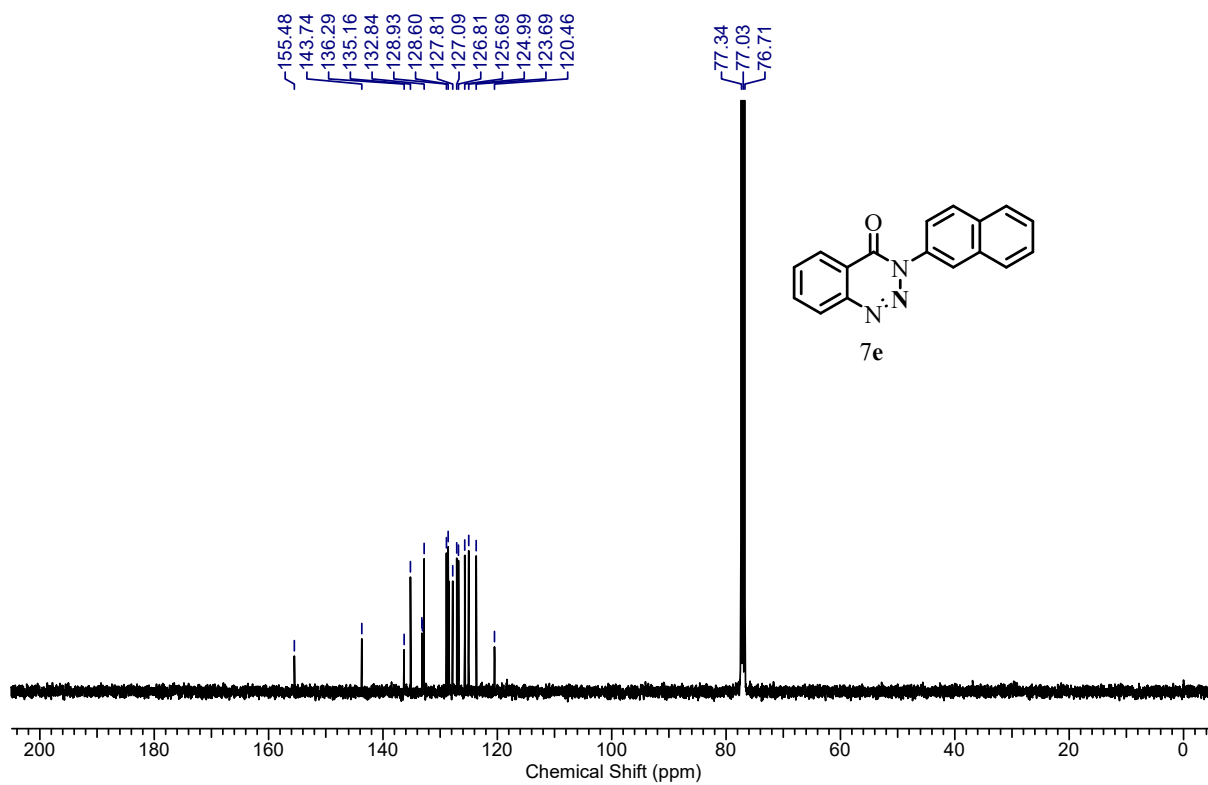
BAA-19_20250918032633 #358 RT: 2.04 AV: 1 NL: 3.47E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 7d

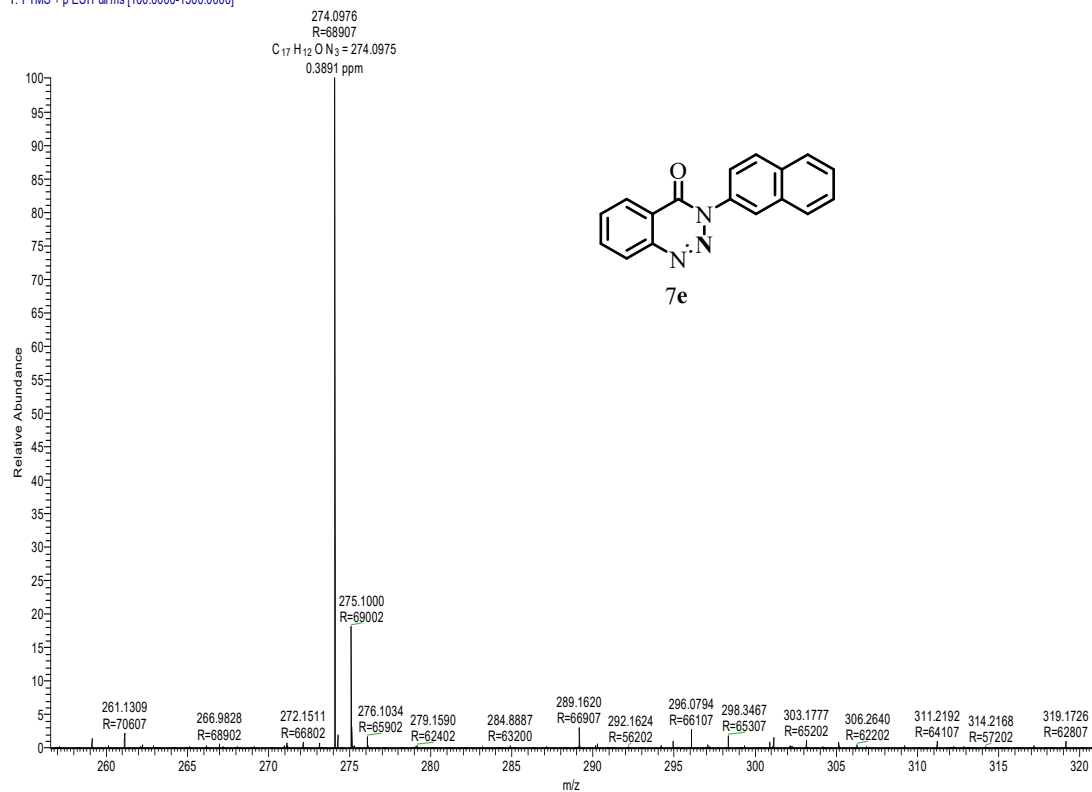


^1H NMR (CDCl_3 , 400 MHz) of Compound 7e

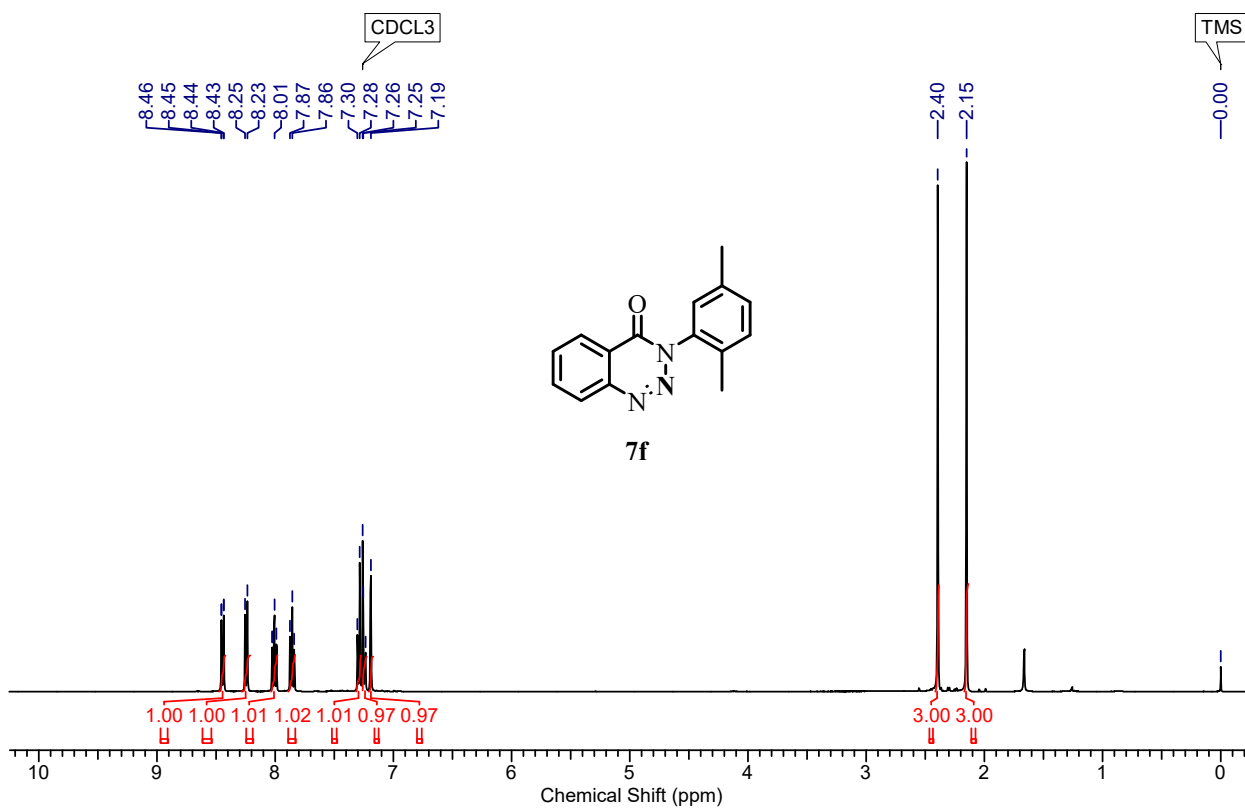


^{13}C NMR (CDCl_3 , 100 MHz) of Compound 7e

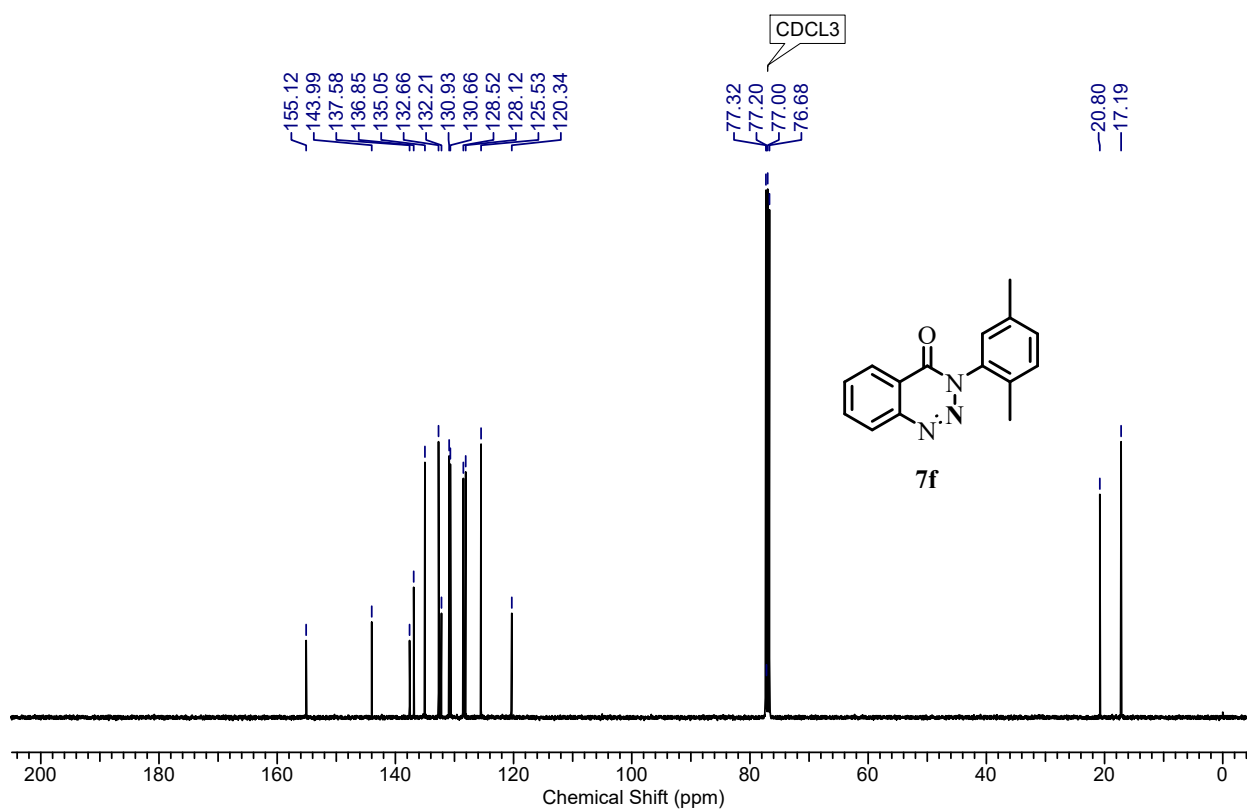
BAA-20_20260227142433 #299 RT: 1.82 AV: 1 NL: 2.36E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 7e

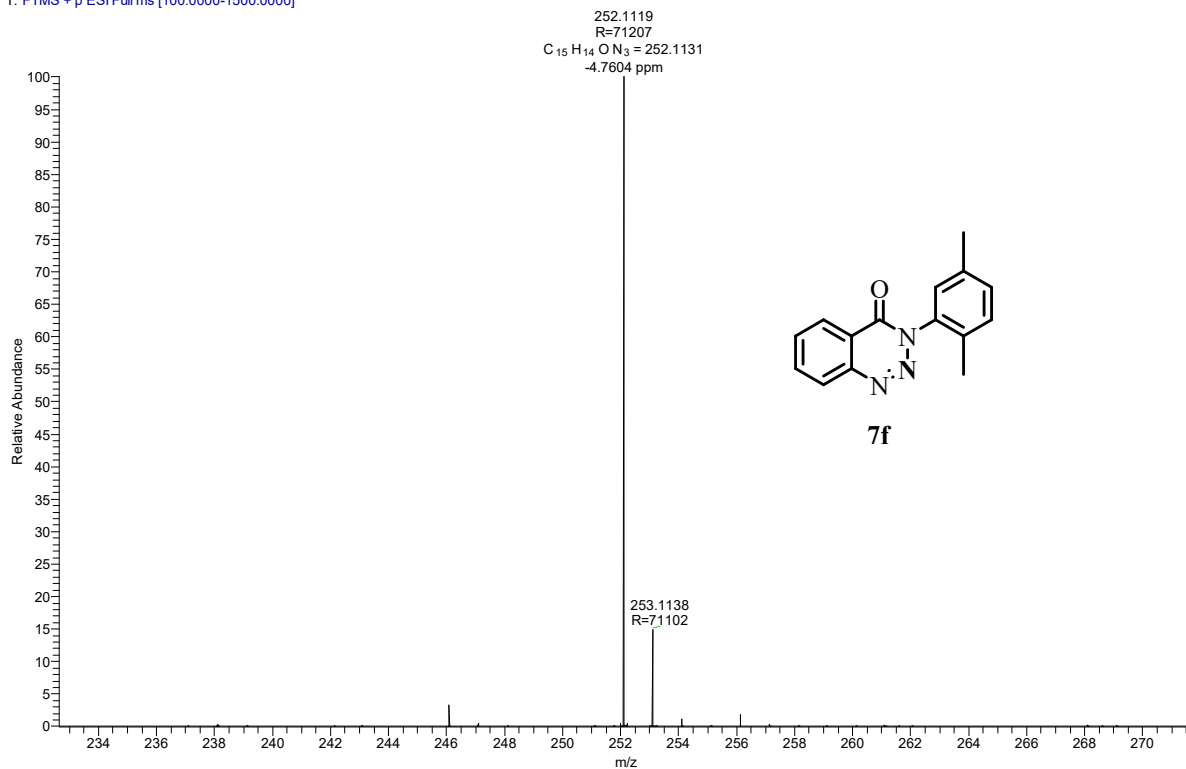


^1H NMR (CDCl_3 , 400 MHz) of Compound 7f

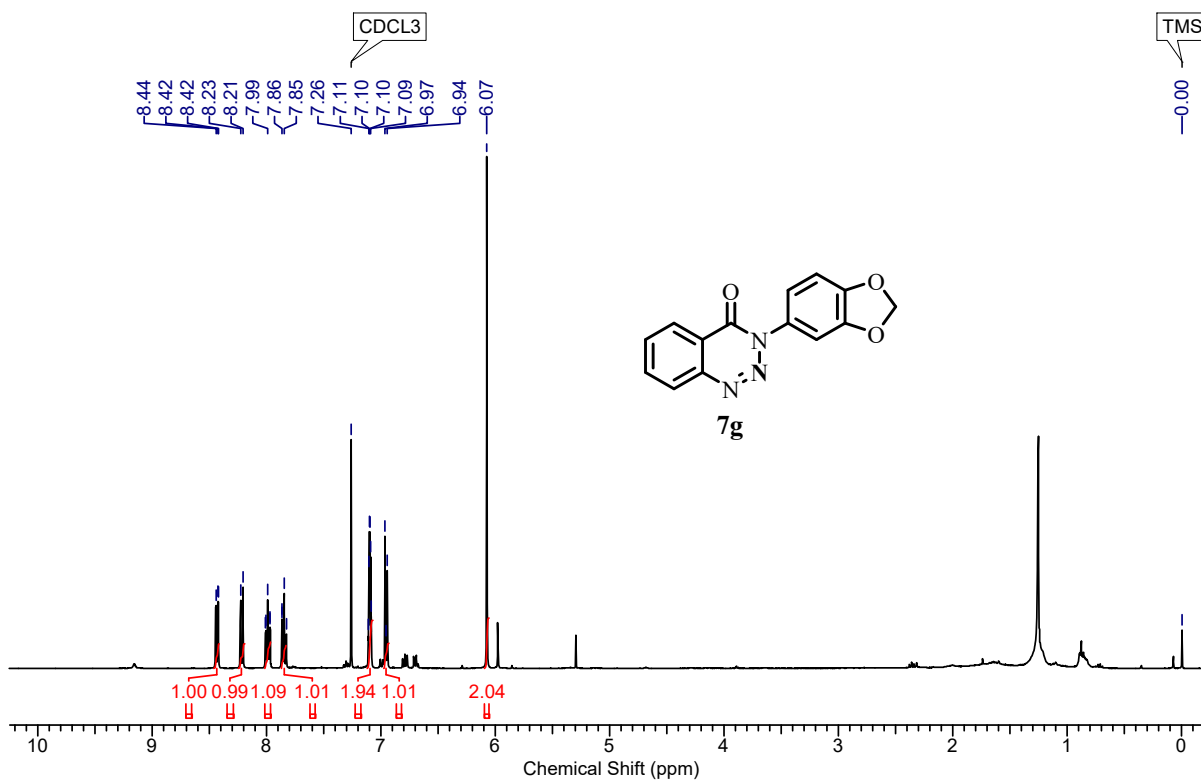


^{13}C NMR (CDCl_3 , 100 MHz) of Compound 7f

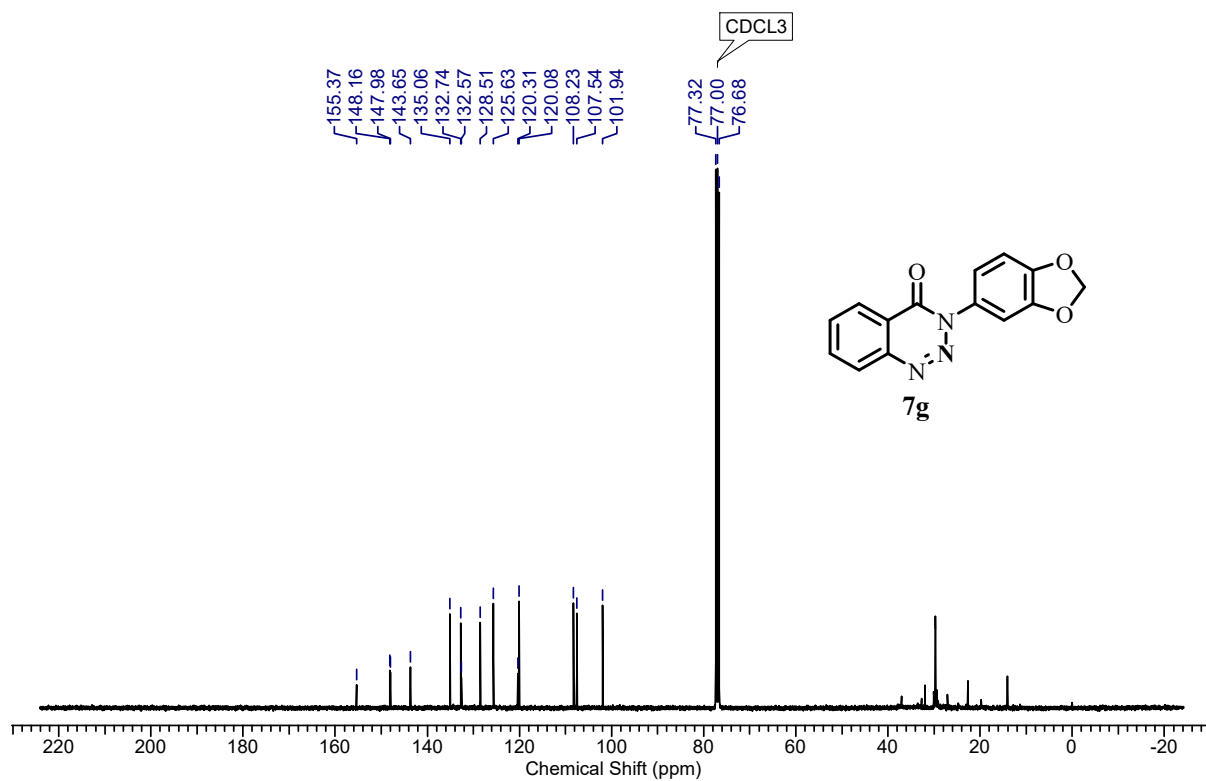
BAA-21 20250918033228 #386 RT: 2.19 AV: 1 NL: 2.35E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 7f

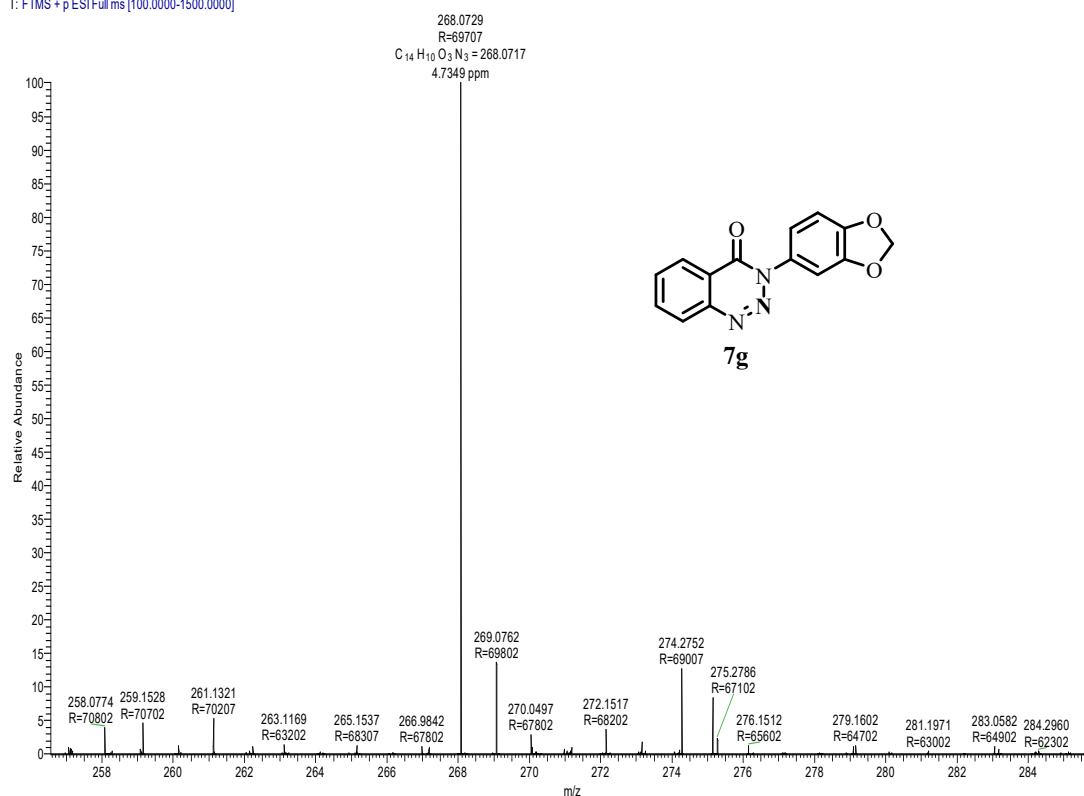


¹H NMR (CDCl₃, 400 MHz) of Compound 7g

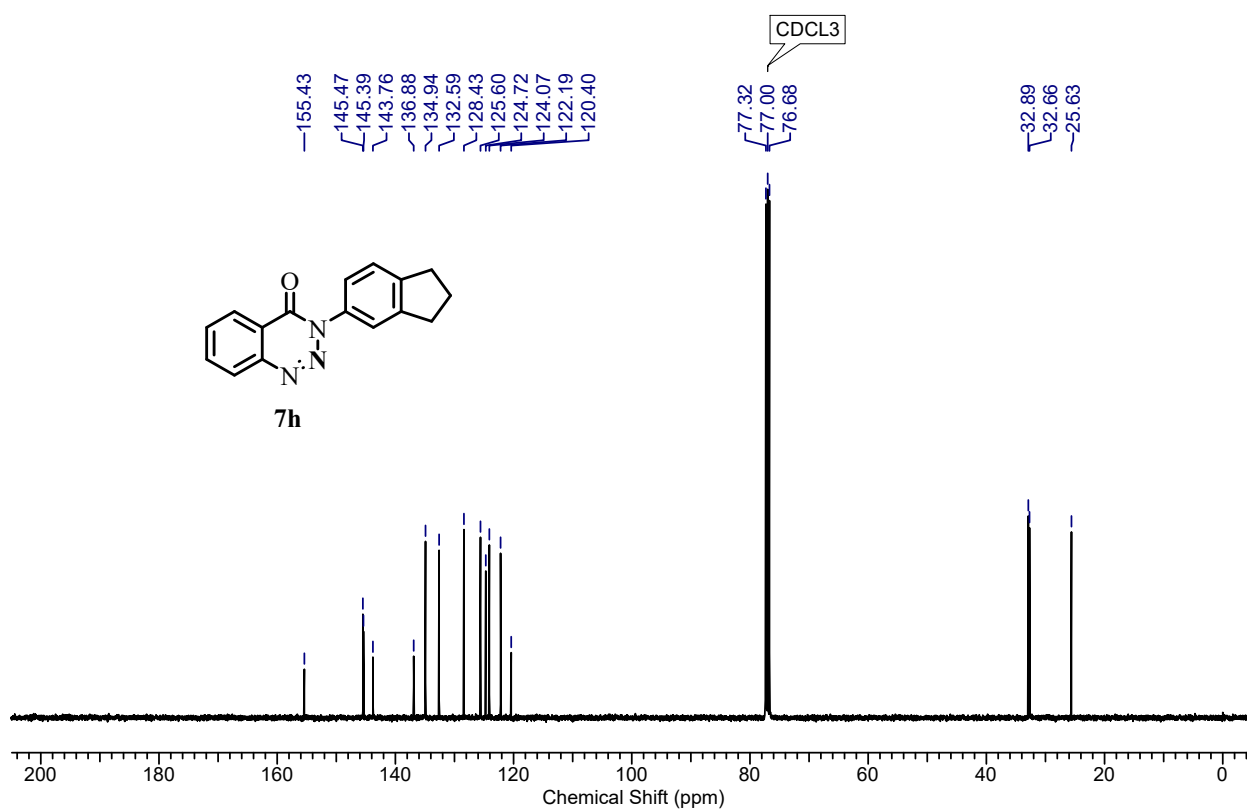
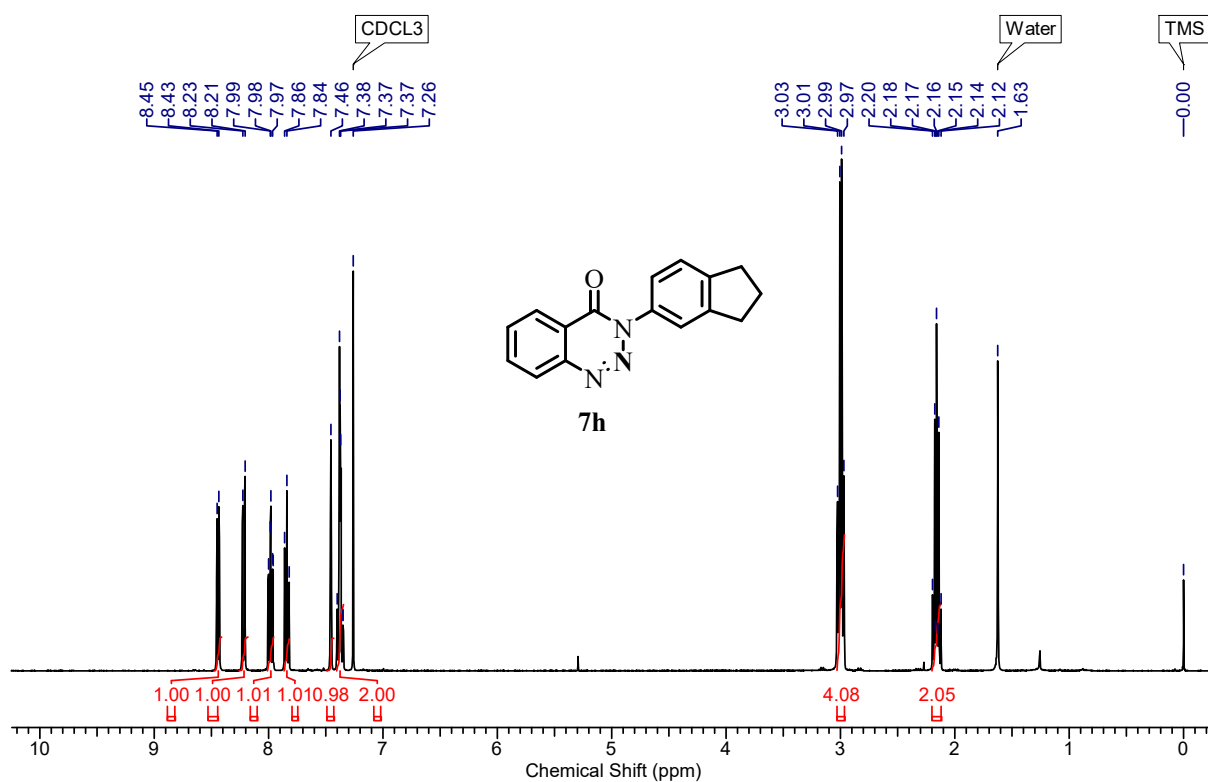


¹³C NMR (CDCl₃, 100 MHz) of Compound 7g

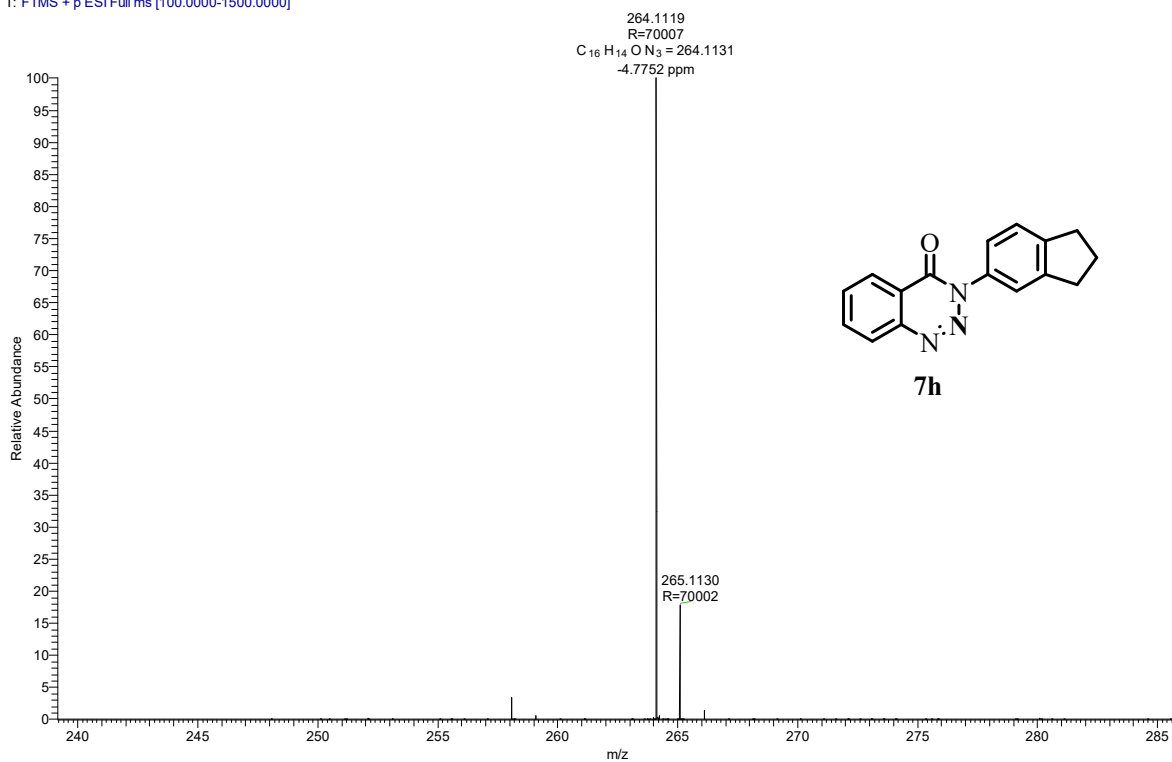
BAA-22 #328 RT: 1.95 AV: 1 NL: 9.95E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]



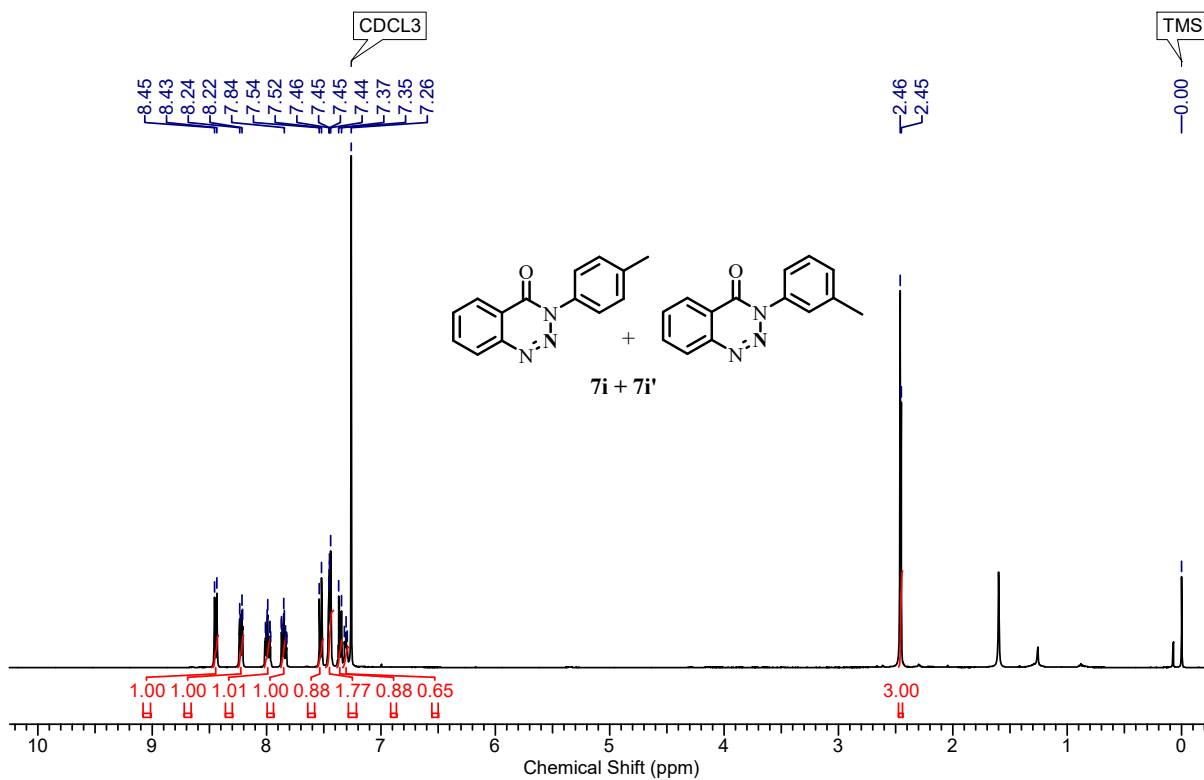
HRMS of Compound 7g



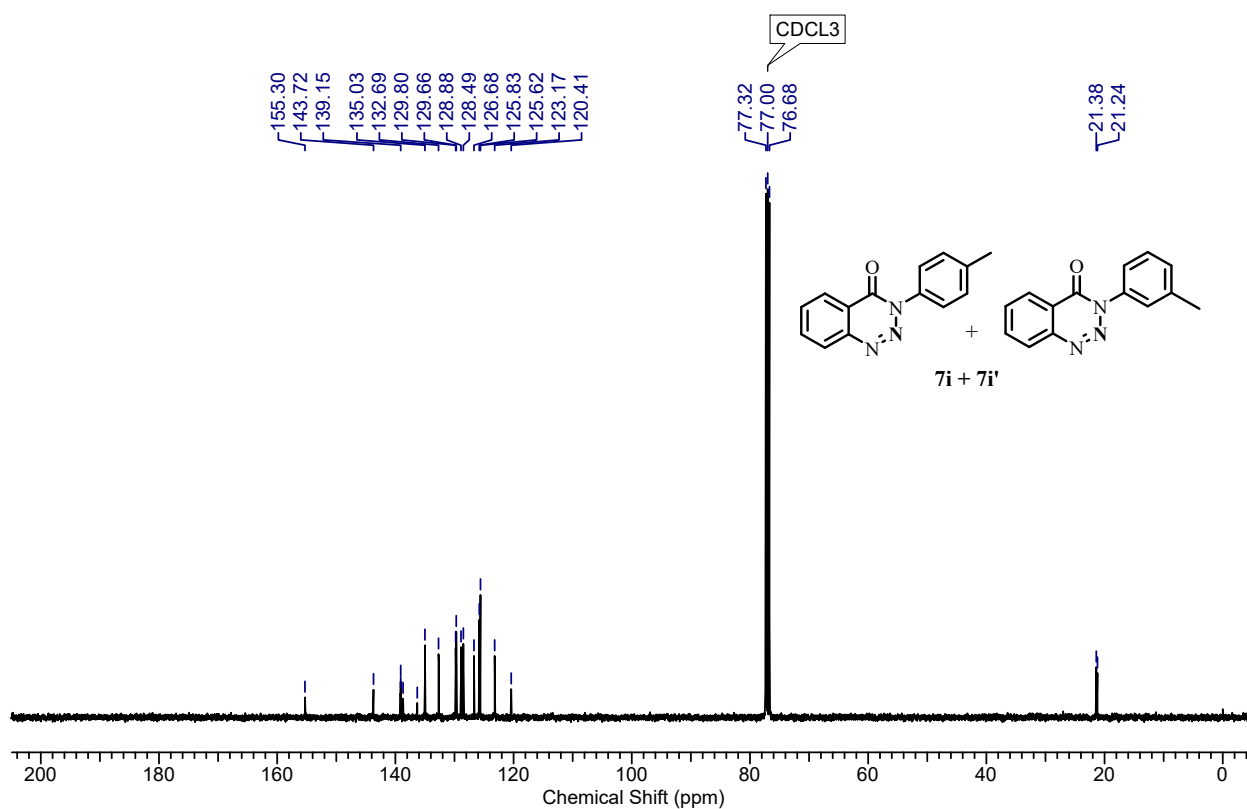
BAA-23_20250918033822 #420 RT: 2.37 AV: 1 NL: 1.72E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 7h

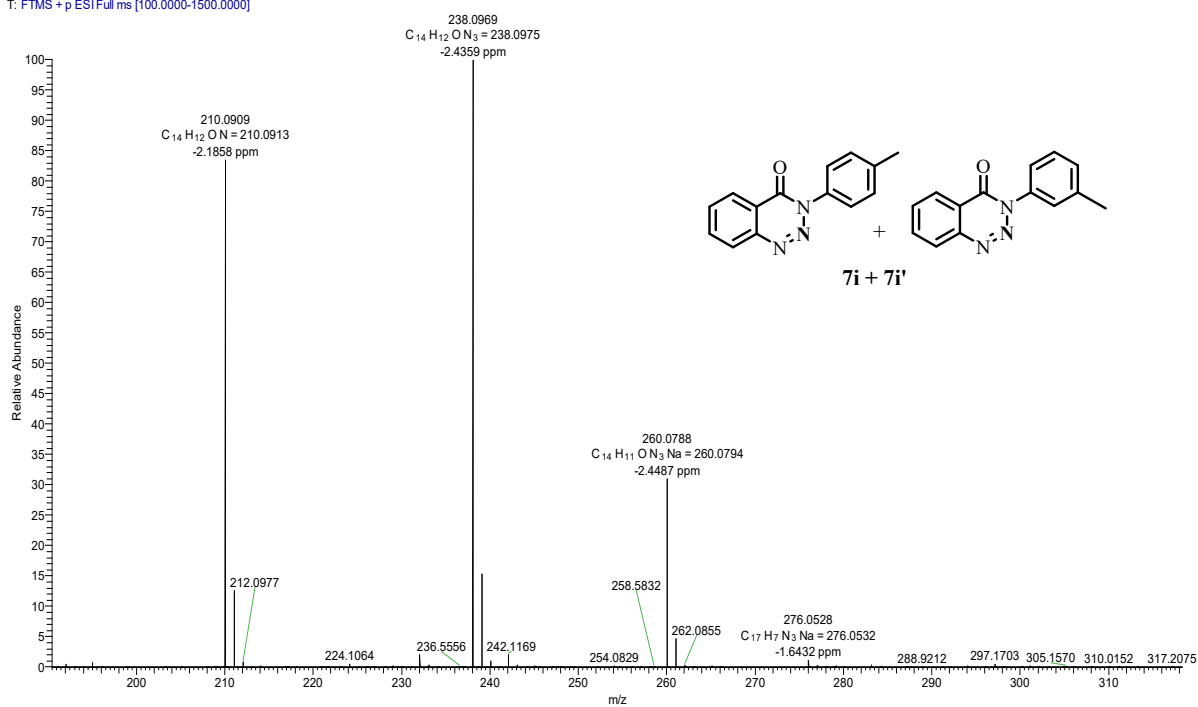


¹H NMR (CDCl₃, 400 MHz) of Compound 7i + 7i'

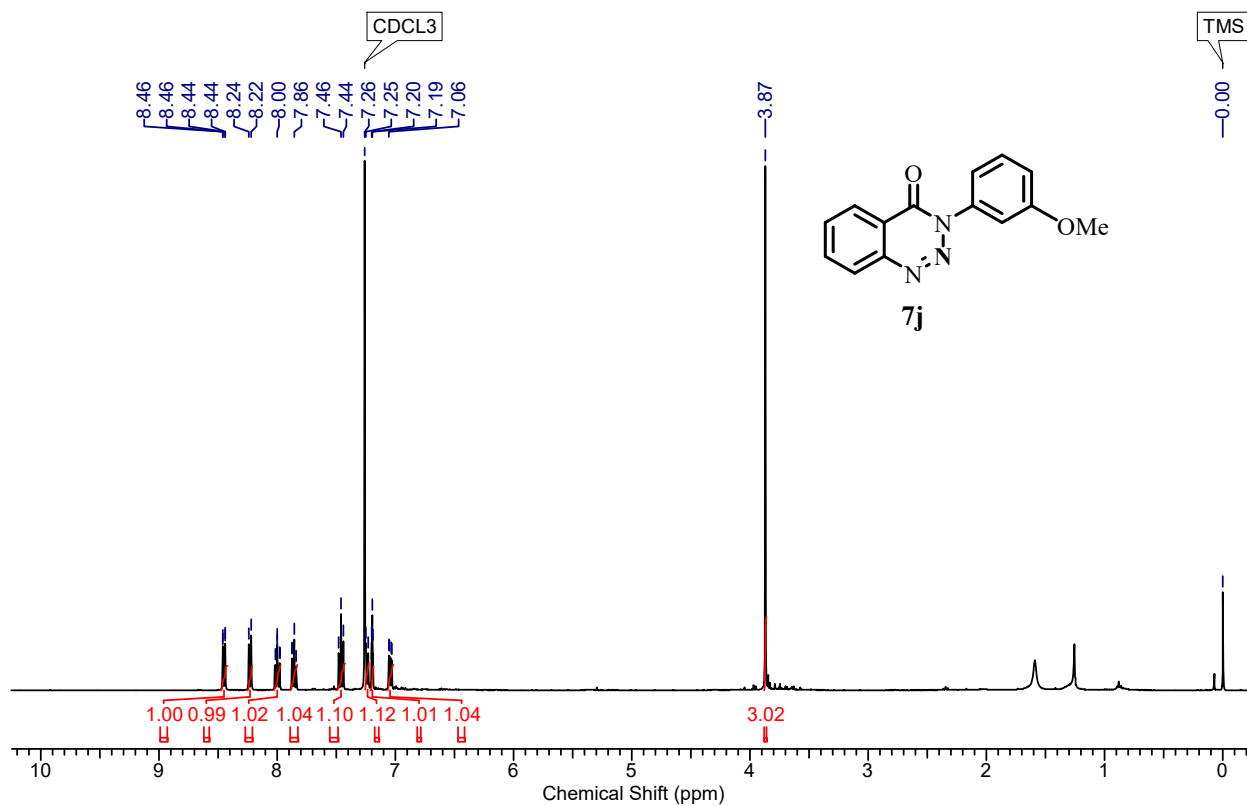


¹³C NMR (CDCl₃, 100 MHz) of Compound 7i + 7i'

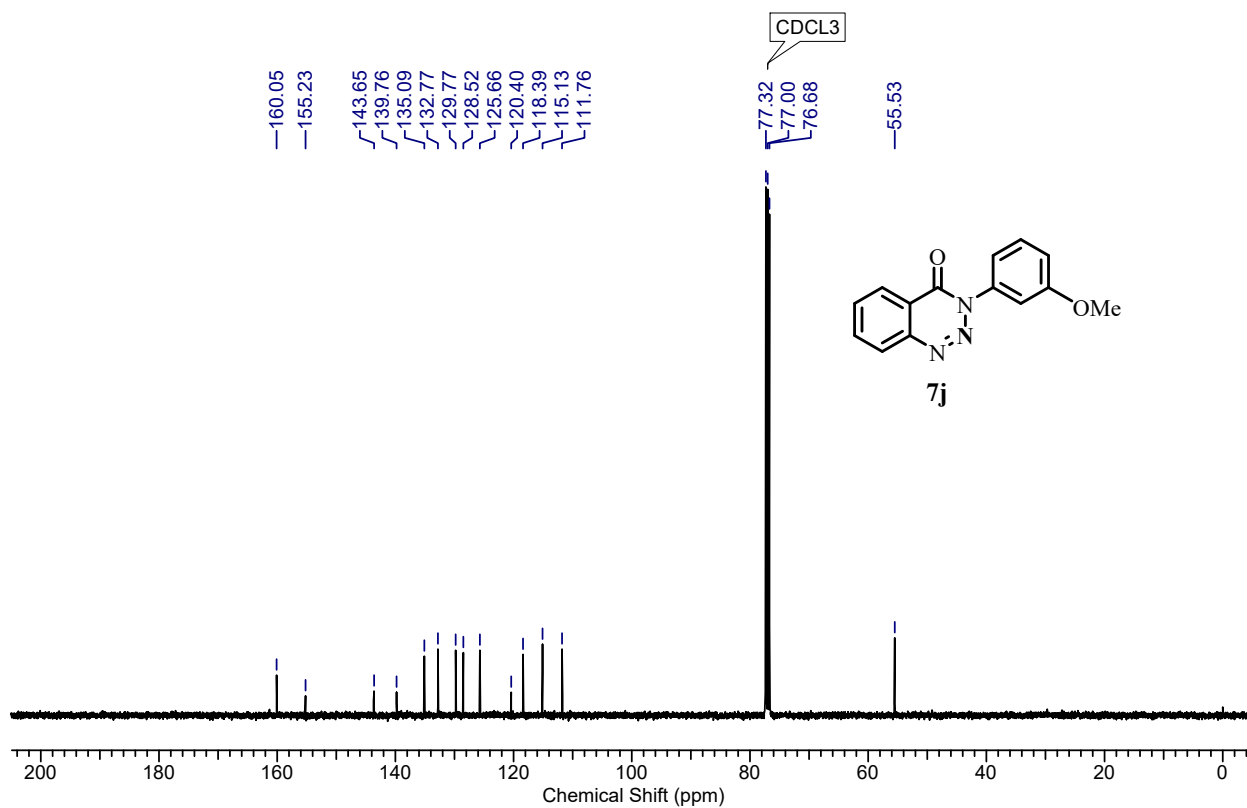
BAA-24 #343 RT: 1.99 AV: 1 NL: 7.44E8
T: FTMS + p ESIFull.ms [100.0000-1500.0000]



HRMS of Compound 7i + 7i'

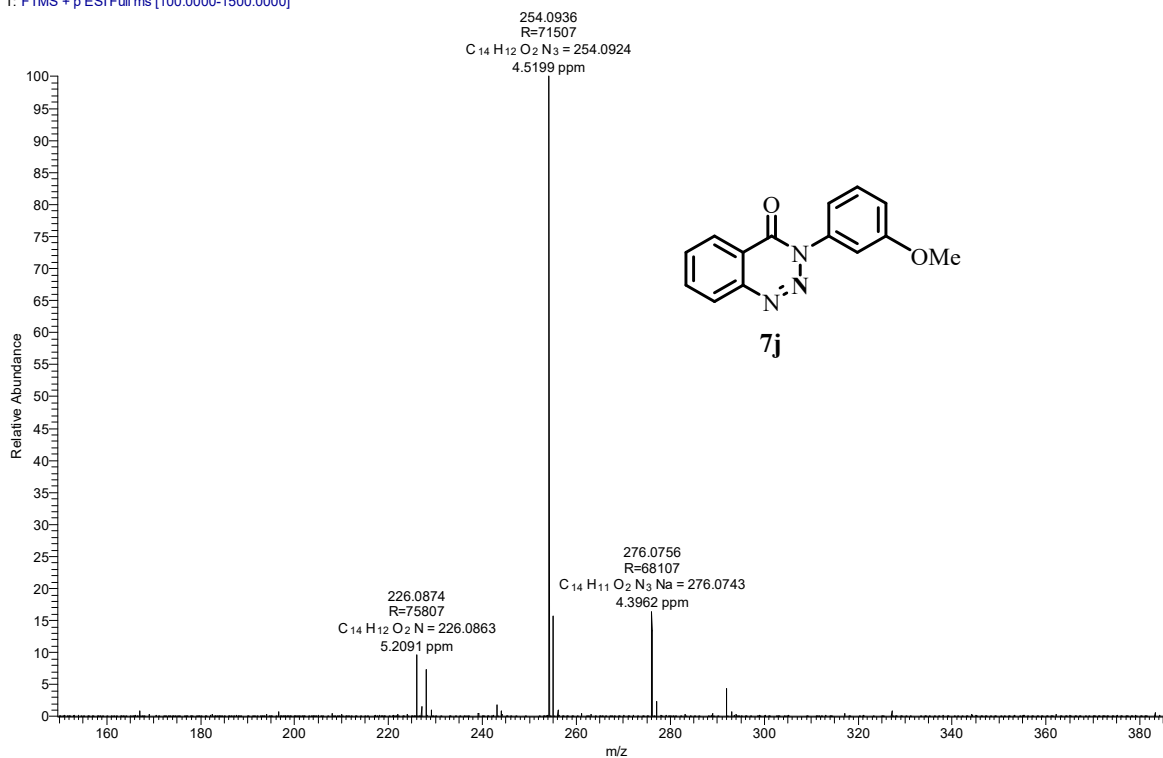


¹H NMR (CDCl₃, 400 MHz) of Compound 7j

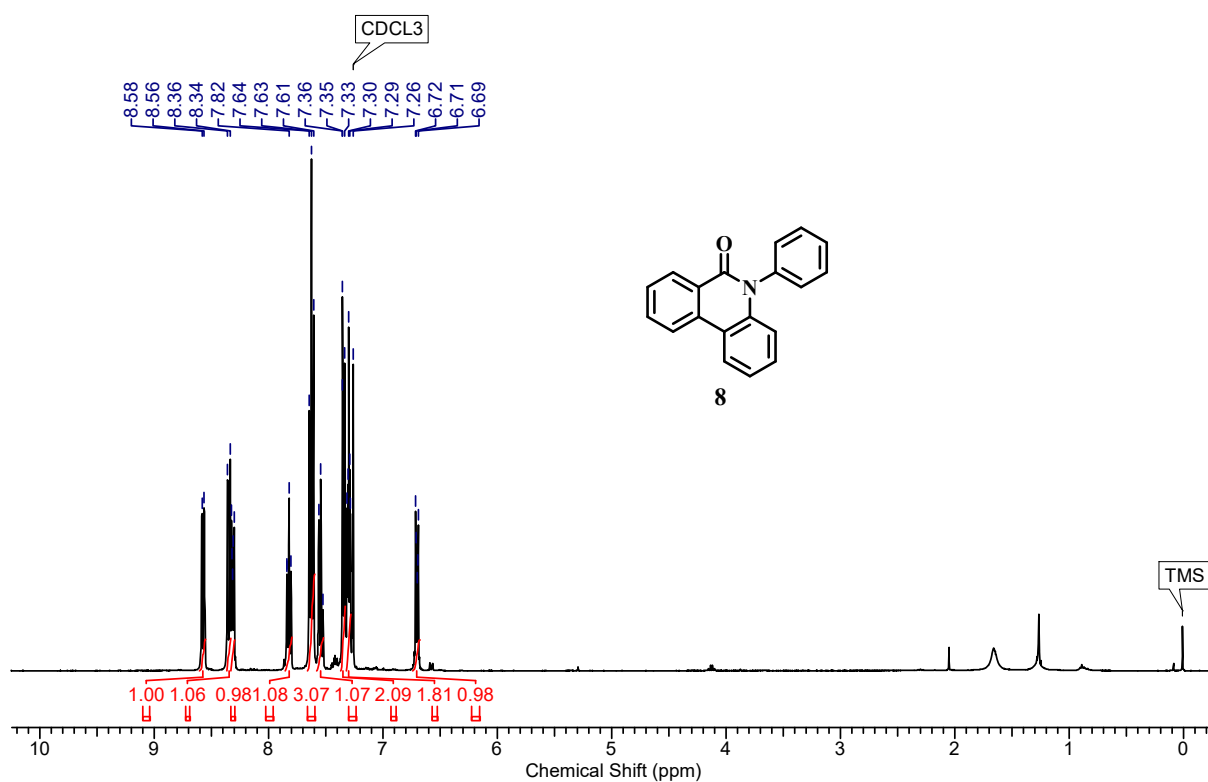


¹³C NMR (CDCl₃, 100 MHz) of Compound 7j

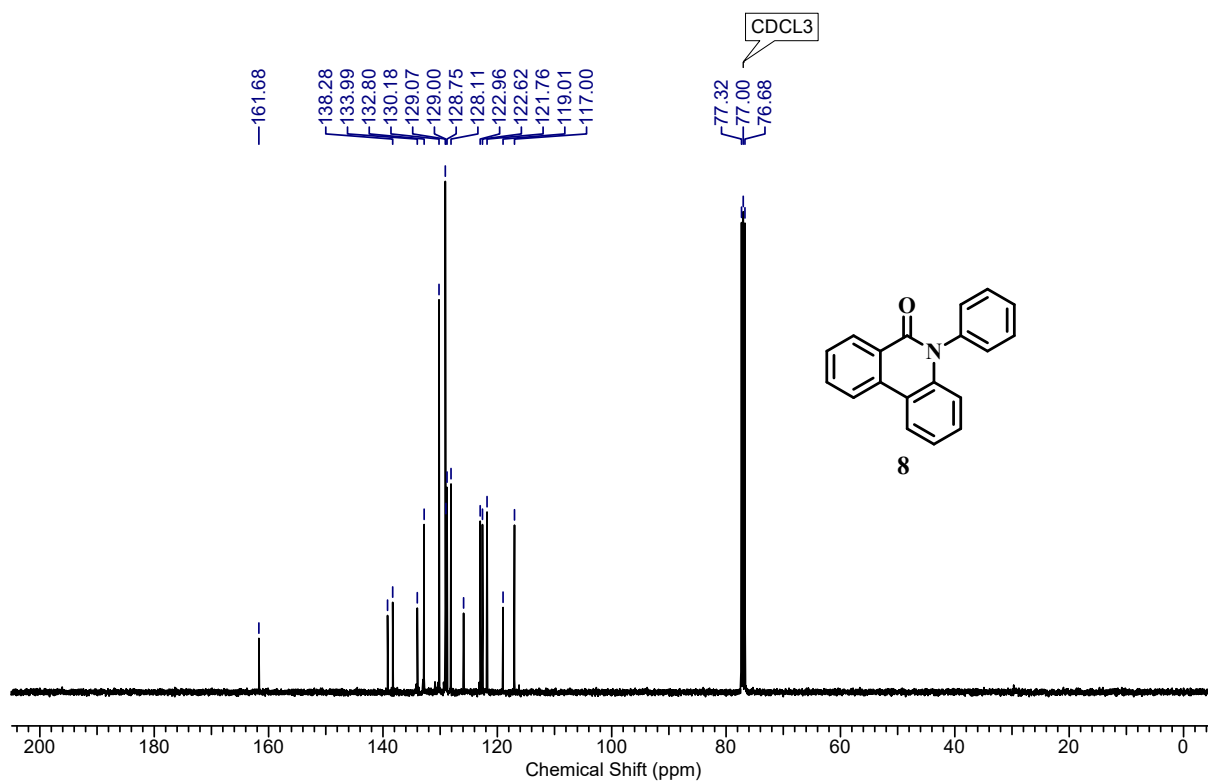
BAA-25 #404 RT: 2.13 AV: 1 NL: 8.72E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



HRMS of Compound 7j

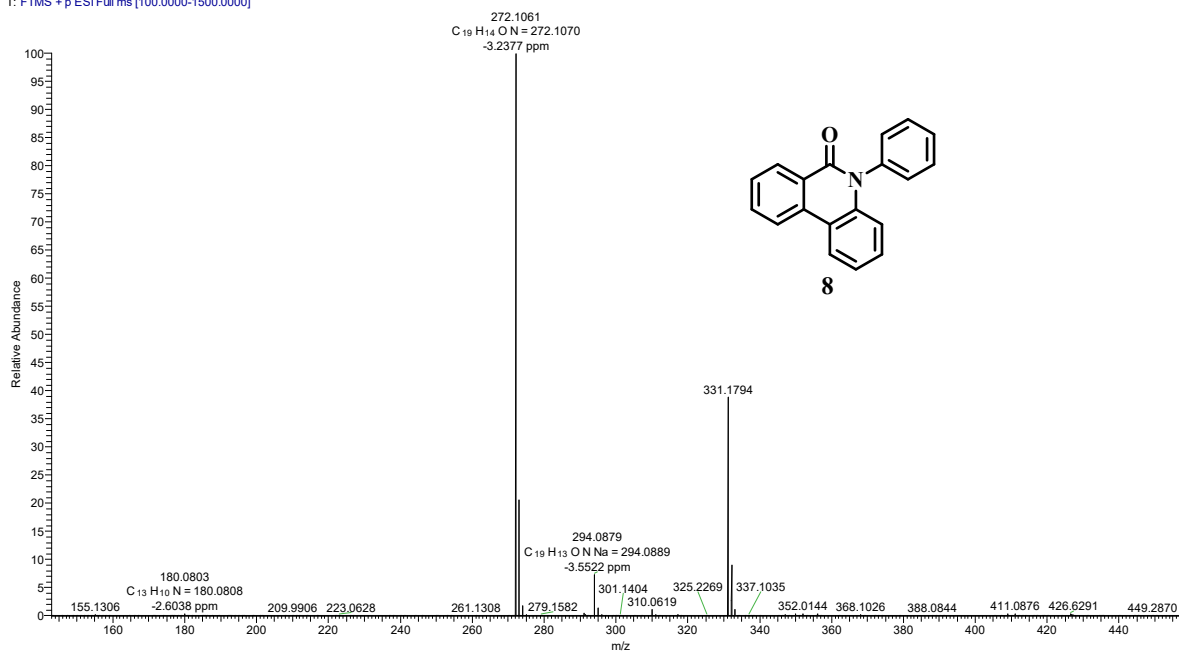


¹H NMR (CDCl₃, 400 MHz) of Compound 8

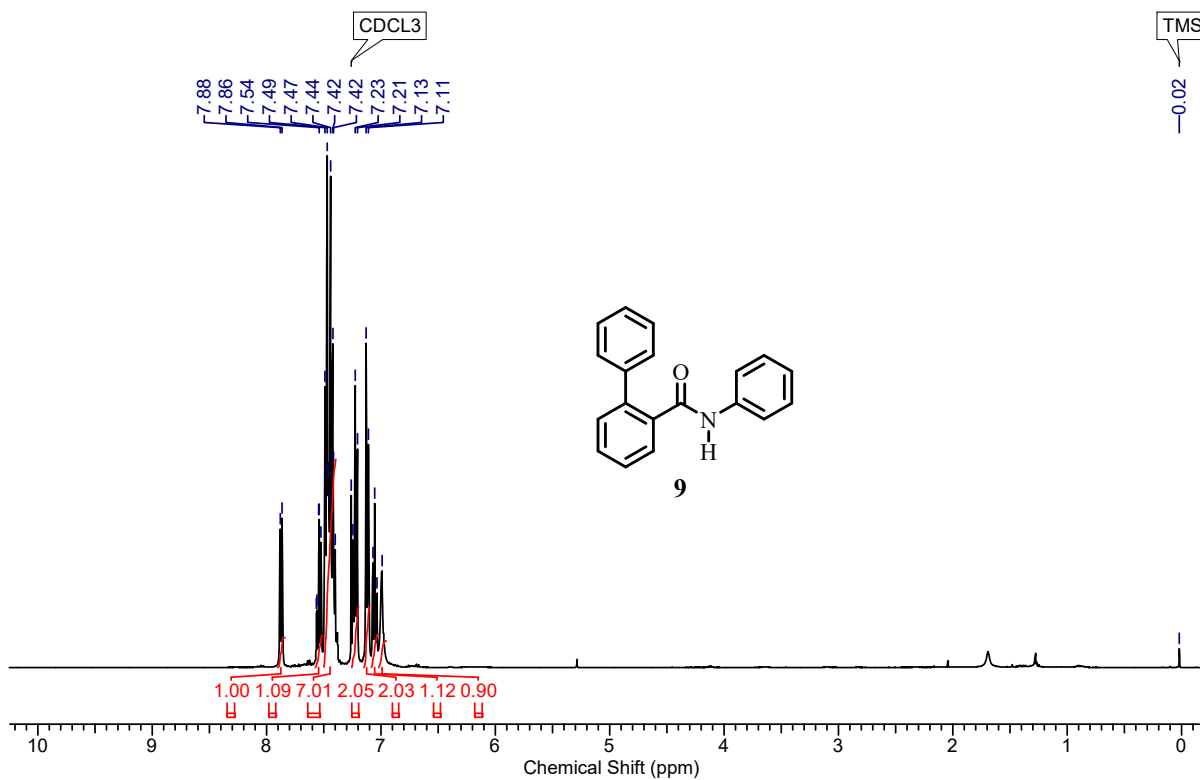


¹³C NMR (CDCl₃, 100 MHz) of Compound 8

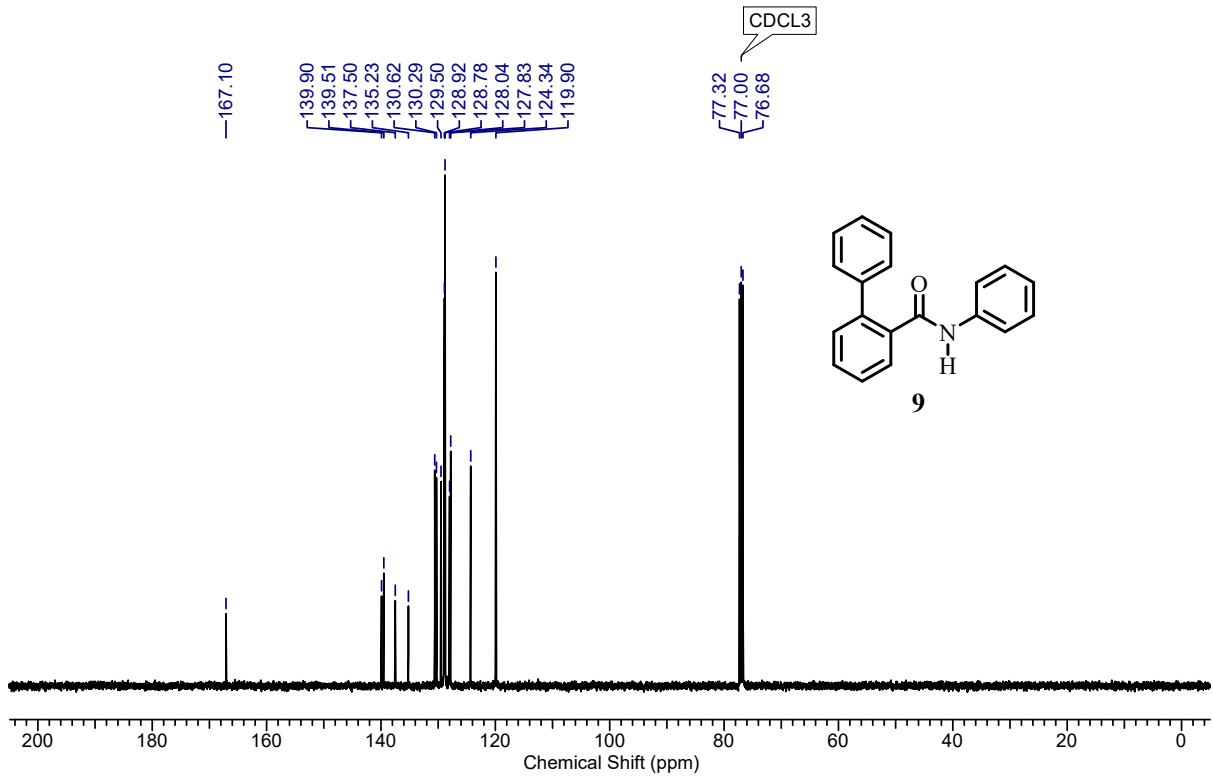
BAA-8A #375 RT: 2.23 AV: 1 NL: 1.73E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



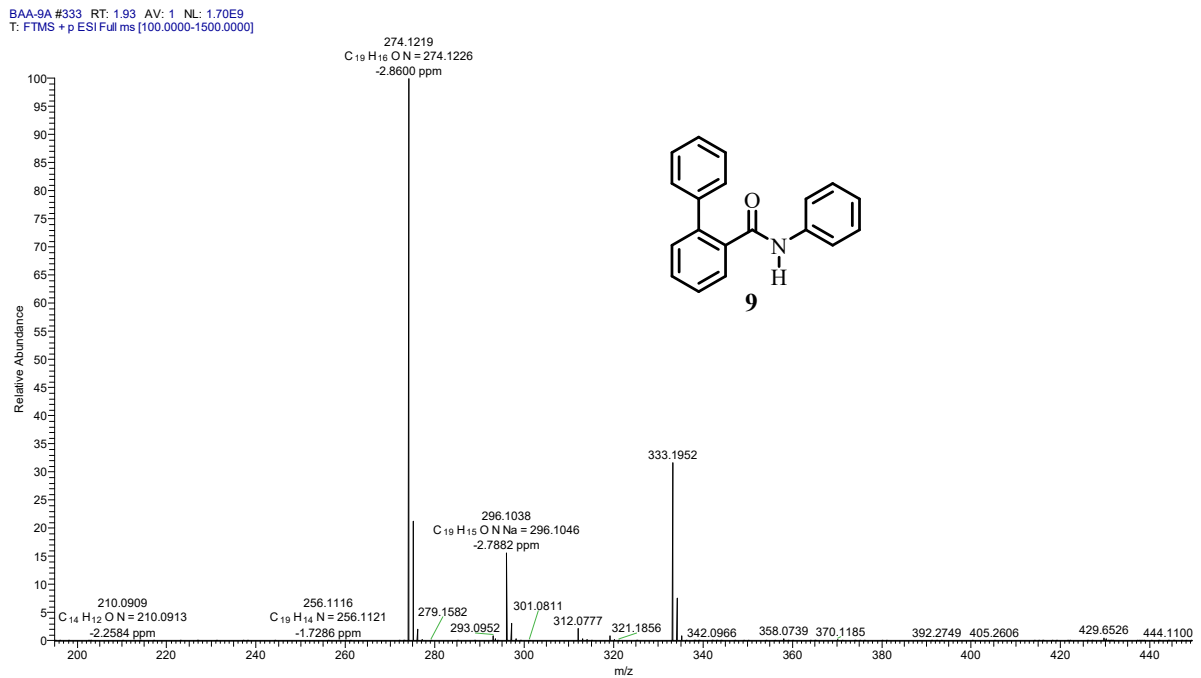
HRMS of Compound 8



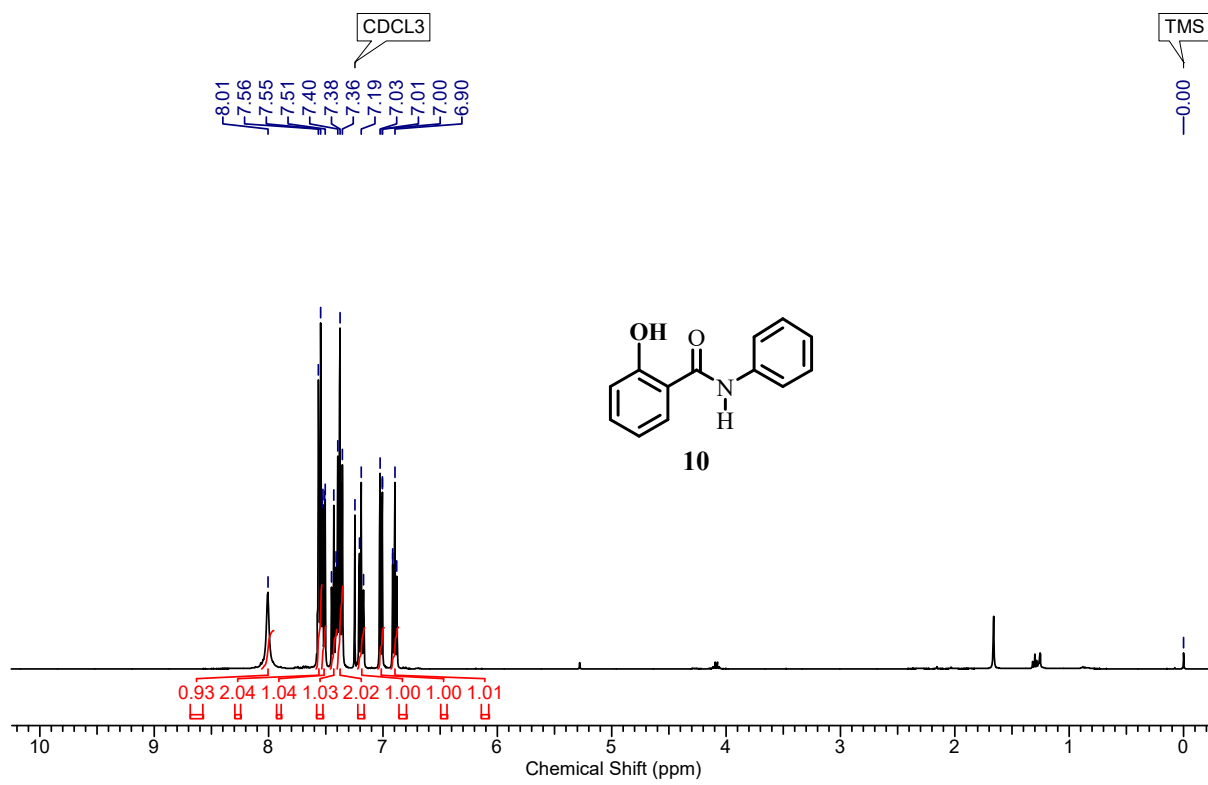
¹H NMR (CDCl₃, 400 MHz) of Compound 9



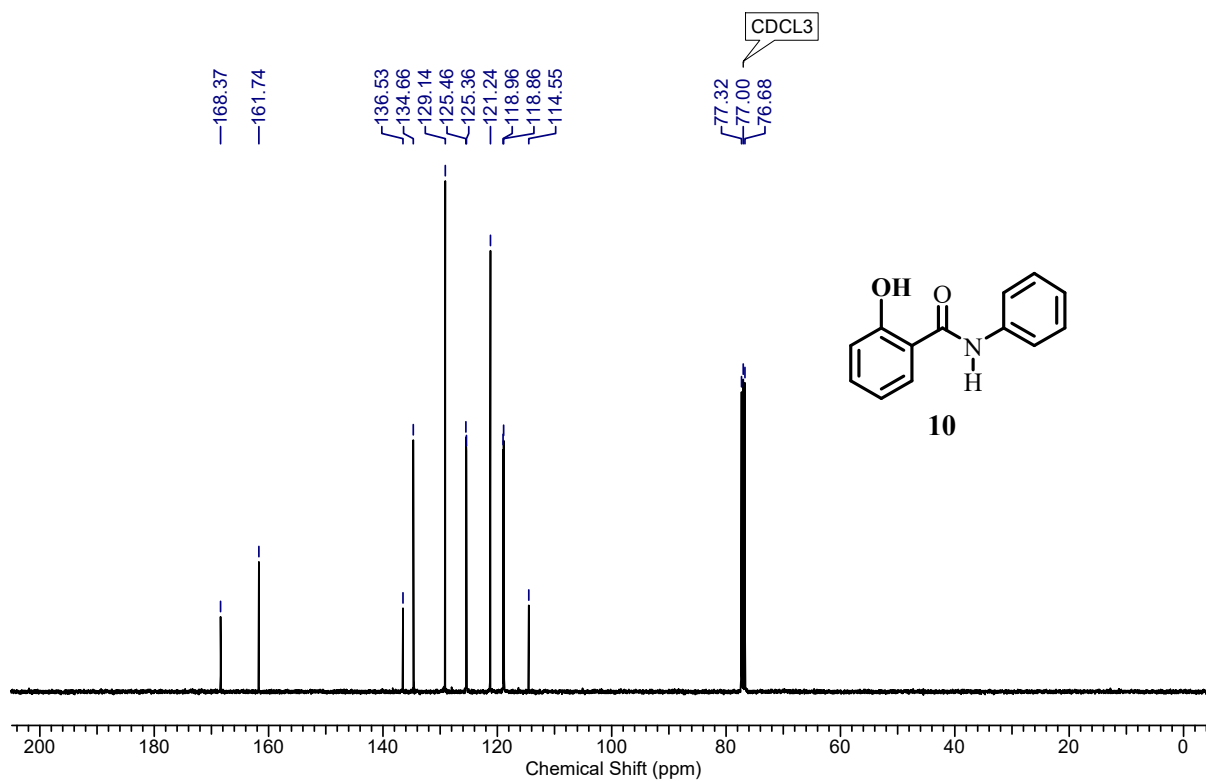
¹³C NMR (CDCl₃, 100 MHz) of Compound 9



HRMS of Compound 9

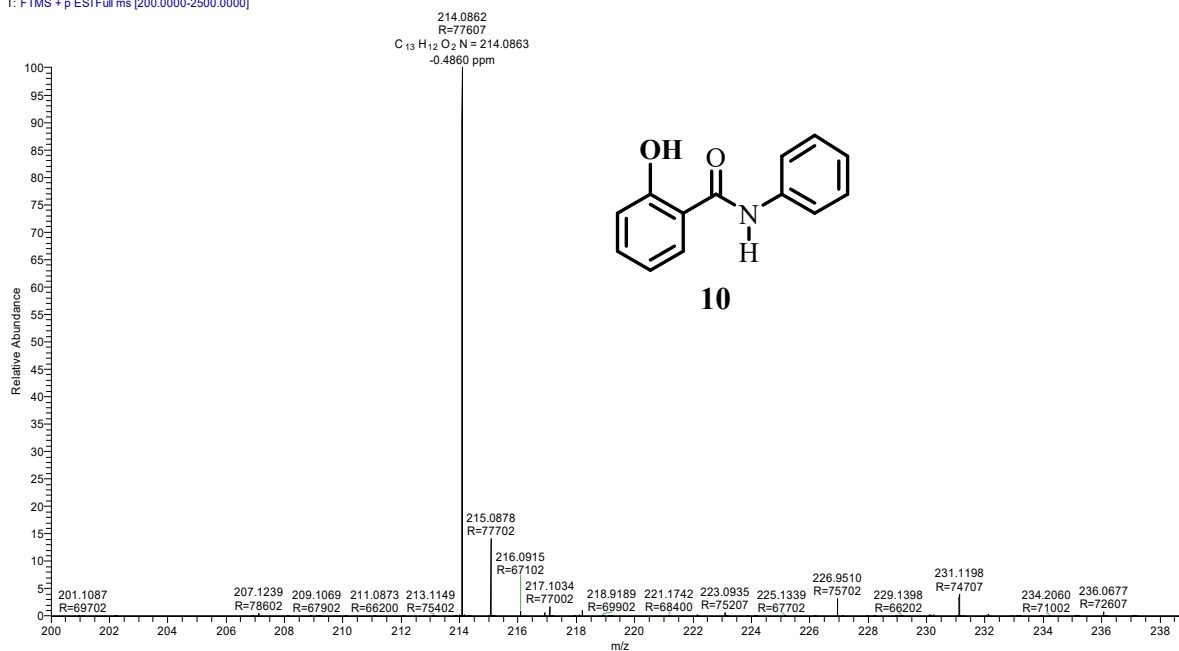


¹H NMR (CDCl₃, 400 MHz) of Compound 10



¹³C NMR (CDCl₃, 100 MHz) of Compound 10

BAA-10A #213 RT: 1.76 AV: 1 NL: 1.55E7
T: FTMS + p ESI Full ms [200.0000-2500.0000]



HRMS of Compound 10