

N-Aryl Benzimidazole and Benzotriazole Derivatives and Their Hybrids as Cytotoxic Agents: Design, Synthesis and Structure-Activity Relationship Studies

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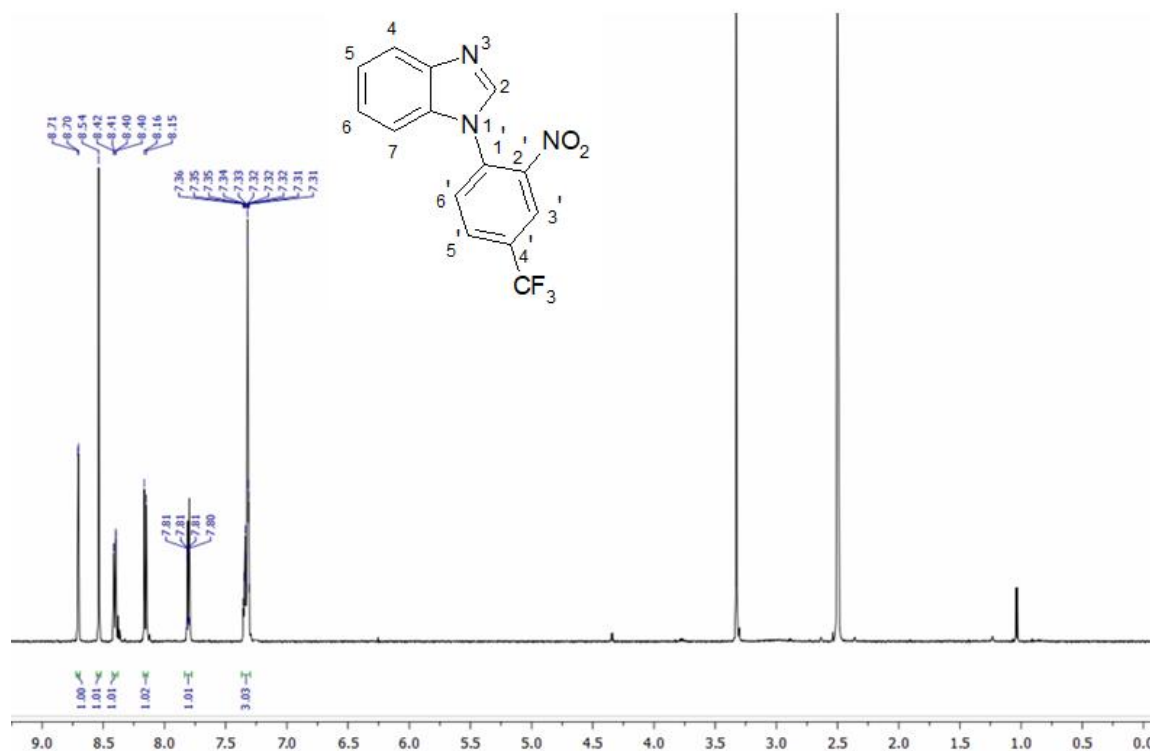
⁴ N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, 47 Leninsky Prosp., 119991 Moscow, Russia

⁵ Institute of Pharmacy, Yaroslavl State Medical University of the Ministry of Health of the Russian Federation, 5 Revolutsionnaya st., 150000 Yaroslavl, Russia

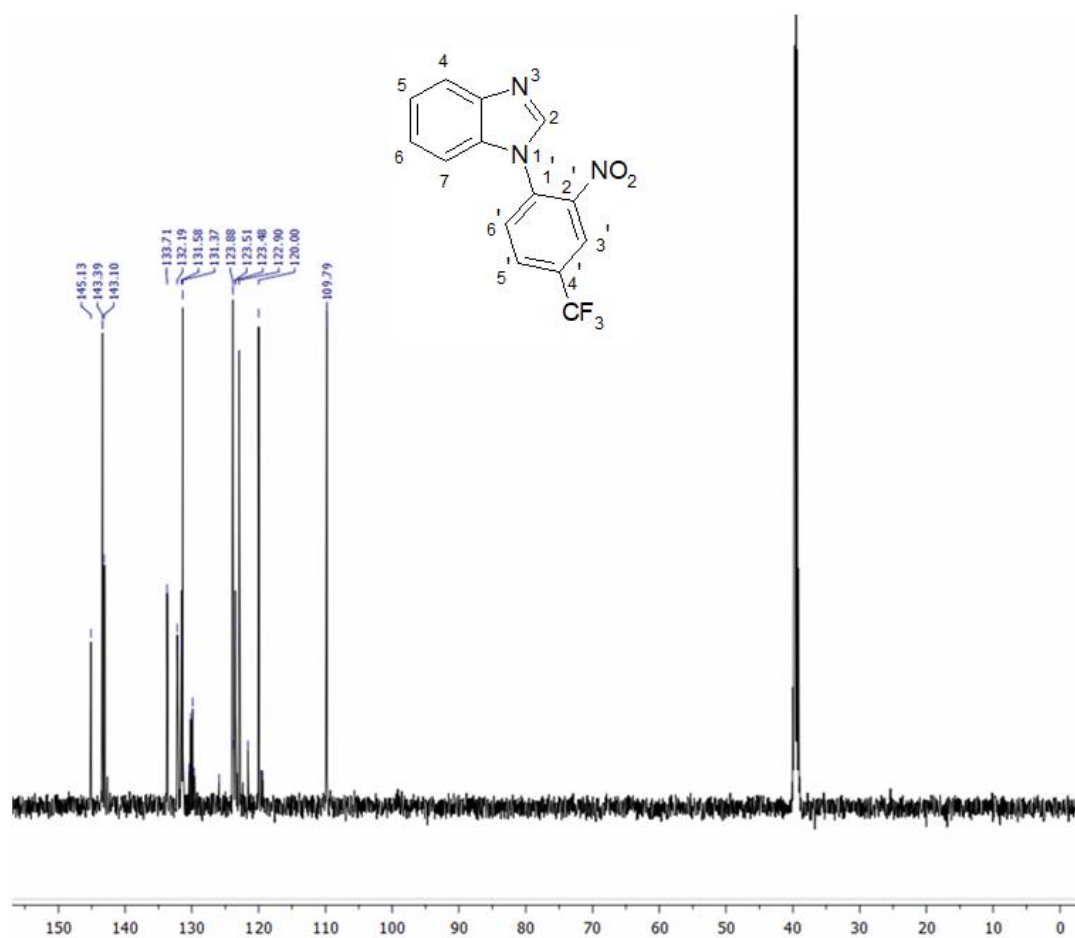
* Correspondence: begunov@uniyar.ac.ru (RB); neganovam@ineos.ac.ru (MN)

Table of Contents:

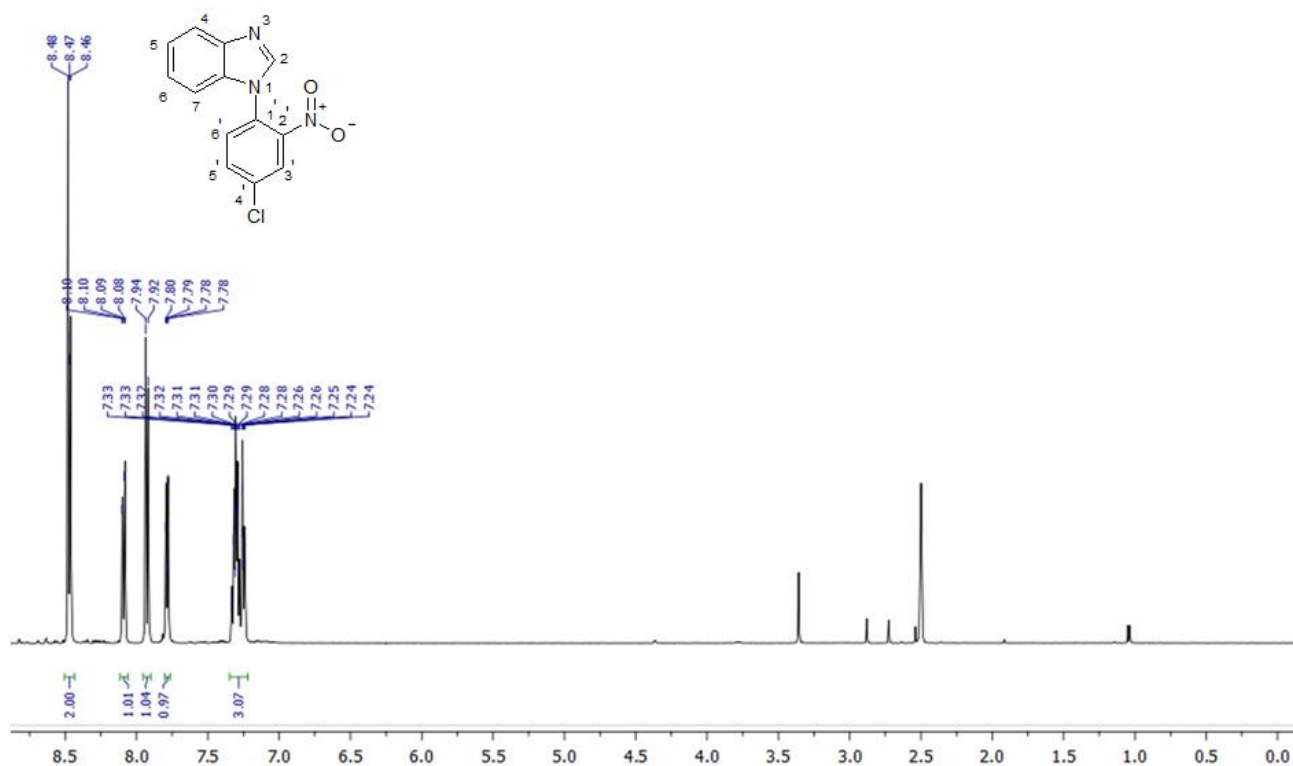
| | |
|--|---------|
| 1. ¹ H and ¹³ C NMR spectra of compounds 3a-3e | S2-S6 |
| 2. ¹ H and ¹³ C NMR spectra of compounds 4a-4e | S7-S11 |
| 3. ¹ H and ¹³ C NMR spectra of compounds 5a-5d | S12-S15 |
| 4. ¹ H and ¹³ C NMR spectra of compounds 6a-6d | S16-S19 |
| 5. ¹ H and ¹³ C NMR spectra of compounds 7a-7c | S20-S22 |
| 6. ¹ H and ¹³ C NMR spectra of compounds 8a, 8b | S23-S24 |



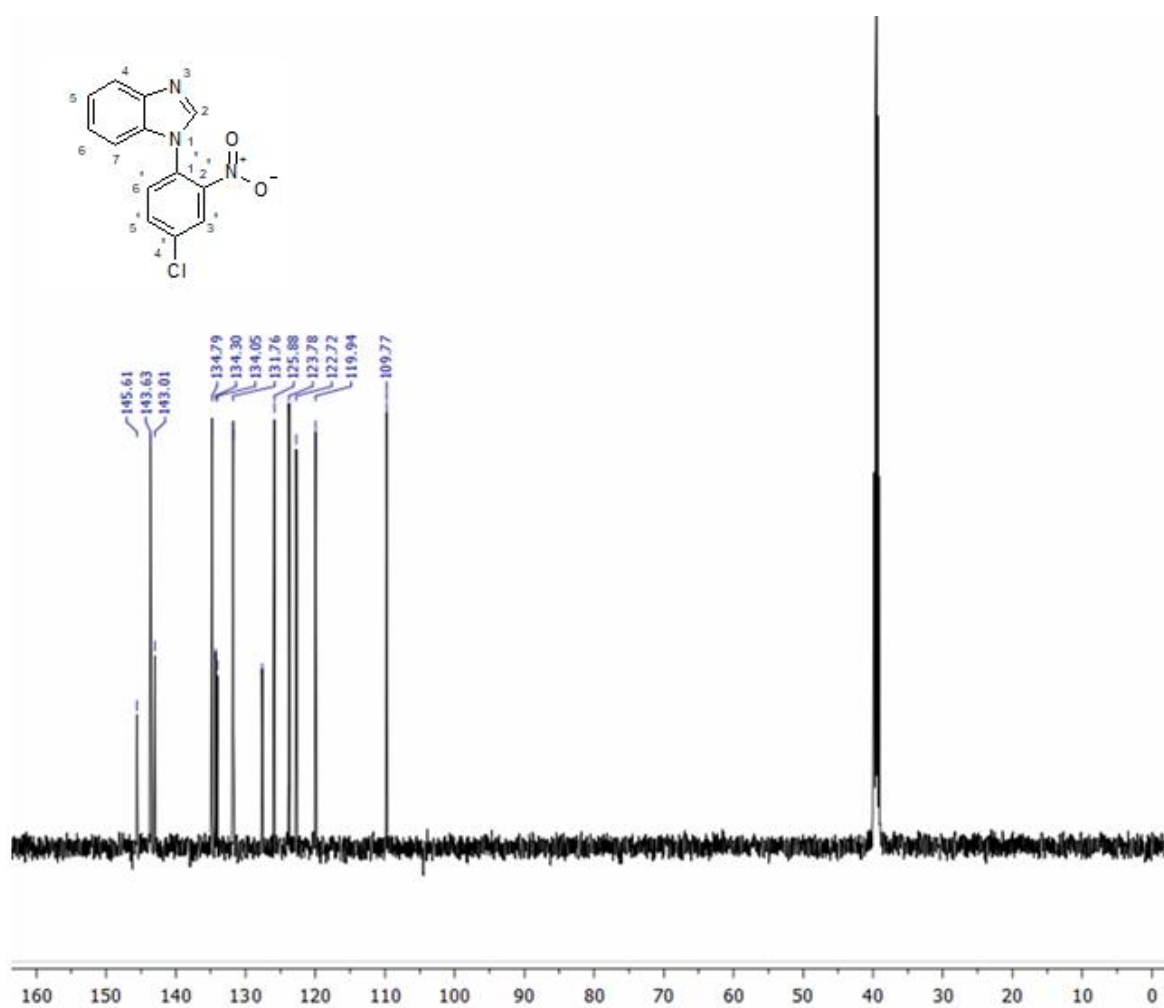
¹H NMR spectra of 1-(2-nitro-4-(trifluoromethyl)phenyl)-1H-benzimidazole (**3a**) (DMSO-*d*₆)



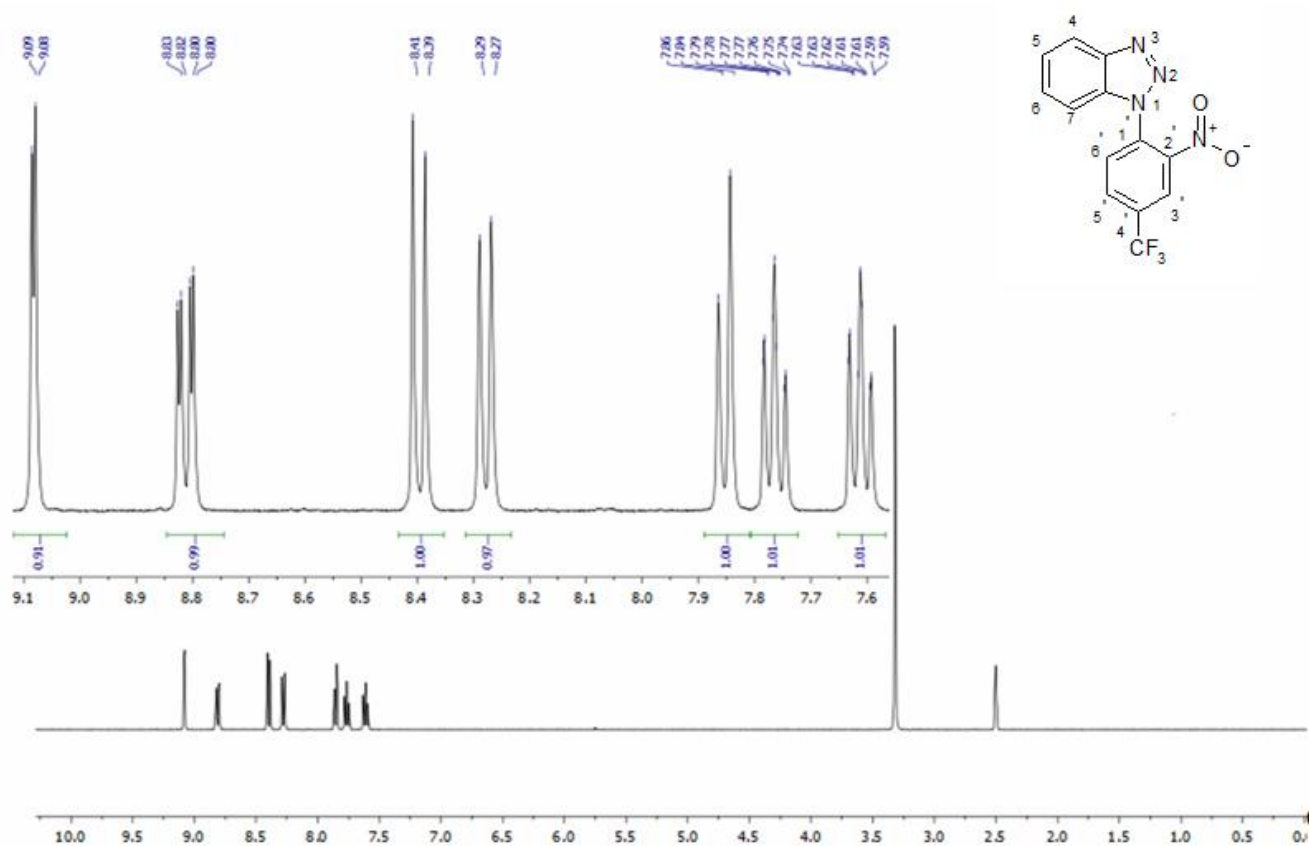
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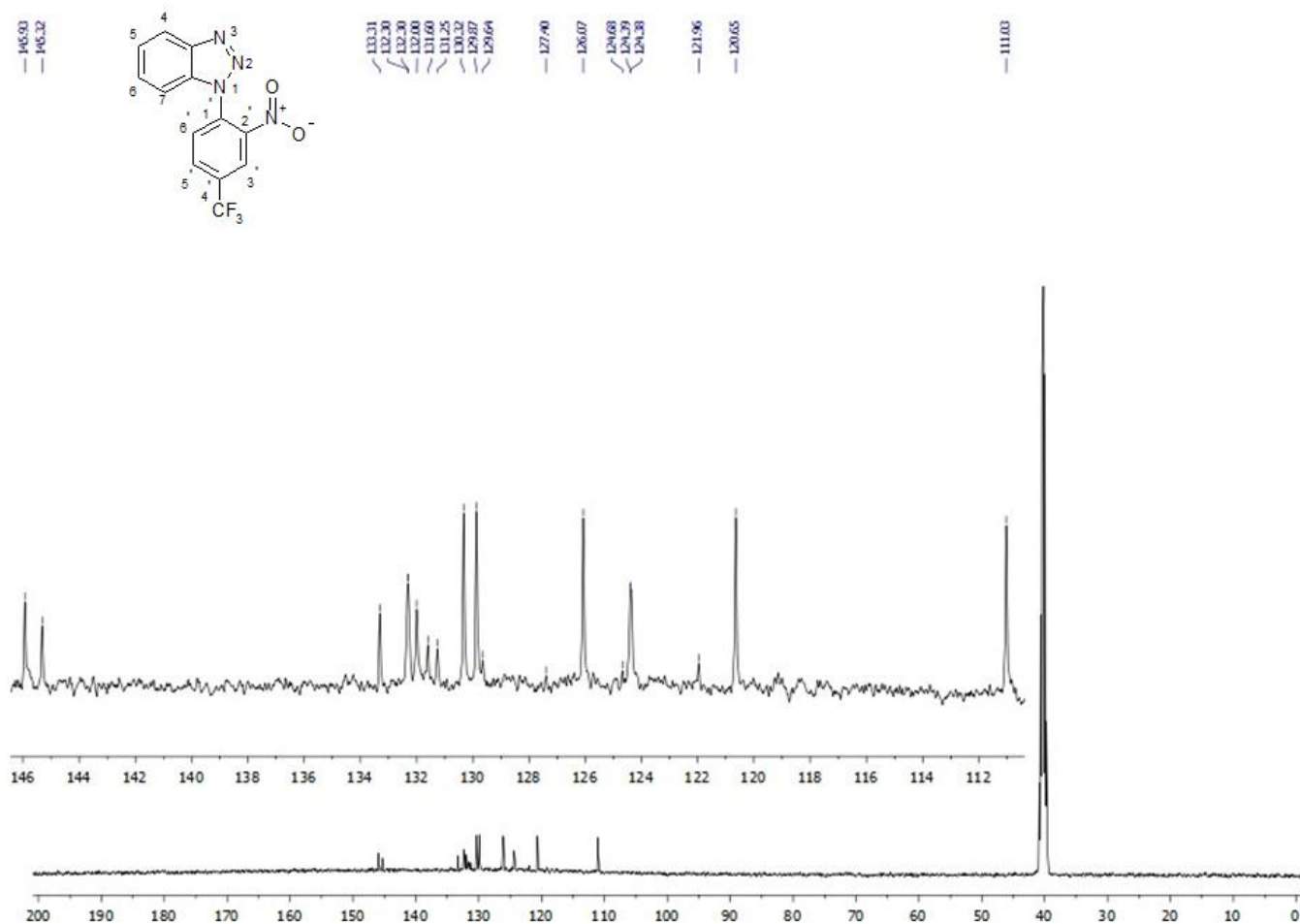
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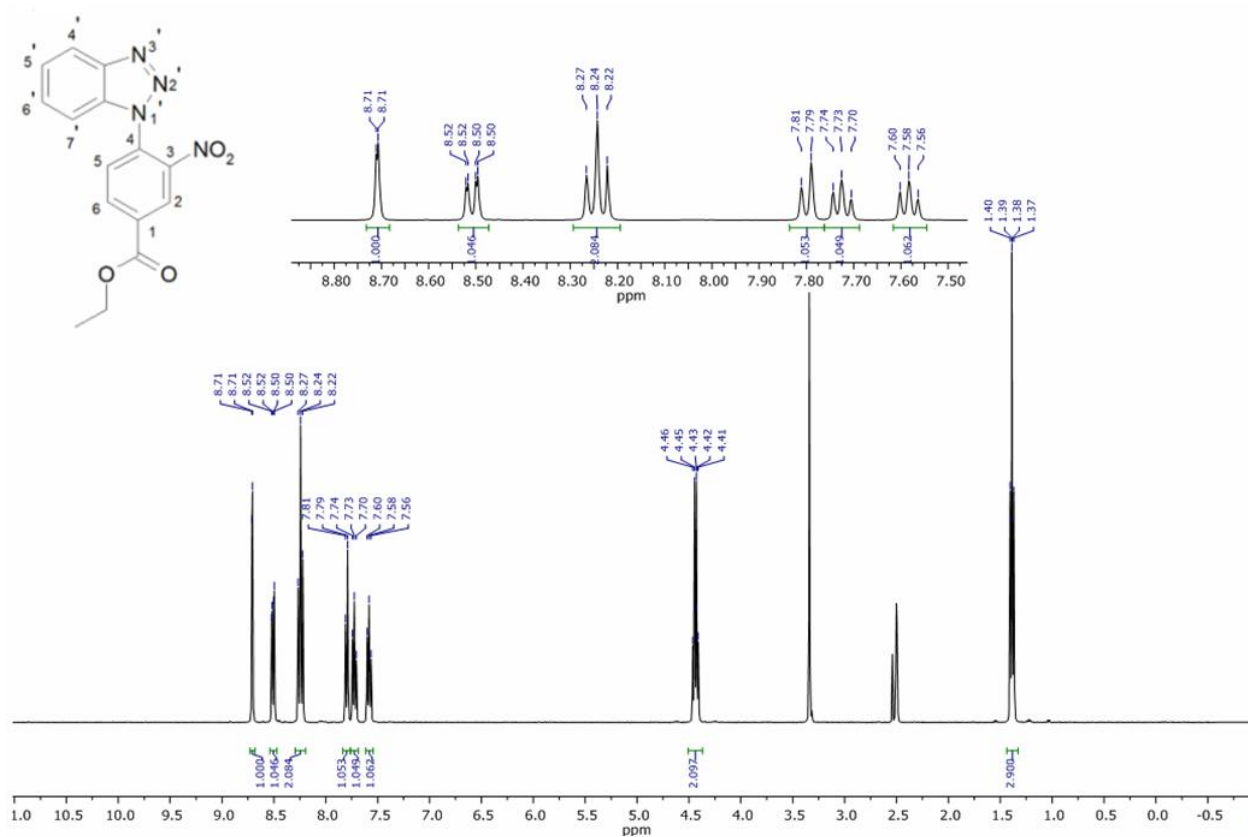
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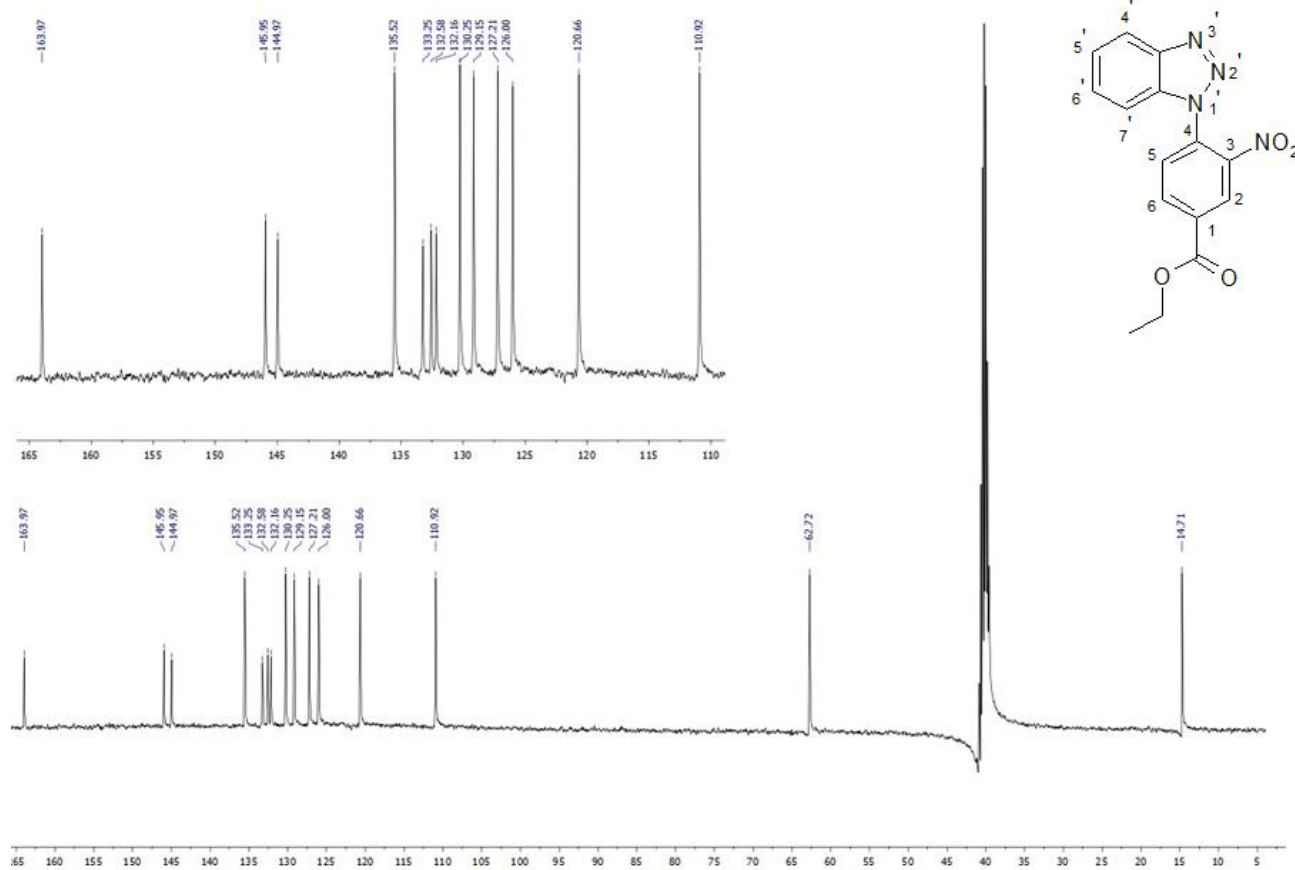
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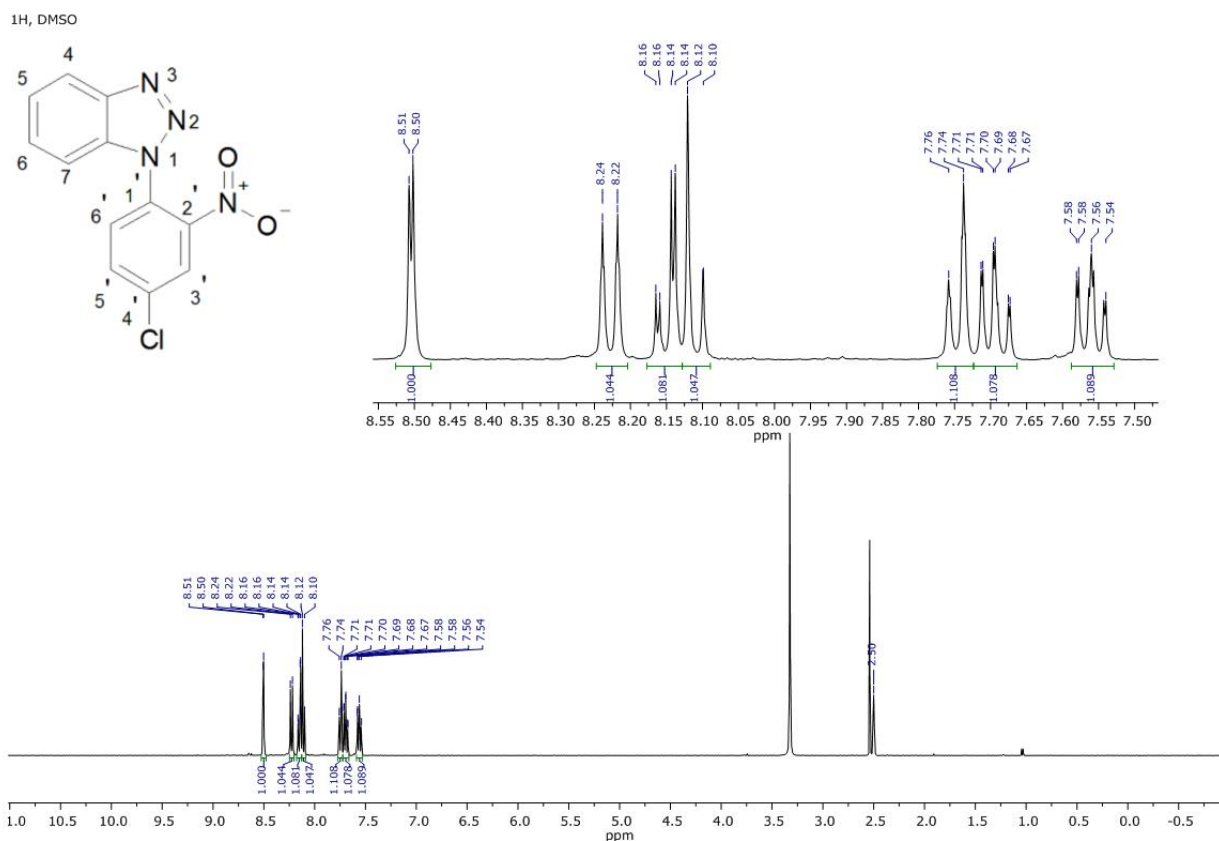
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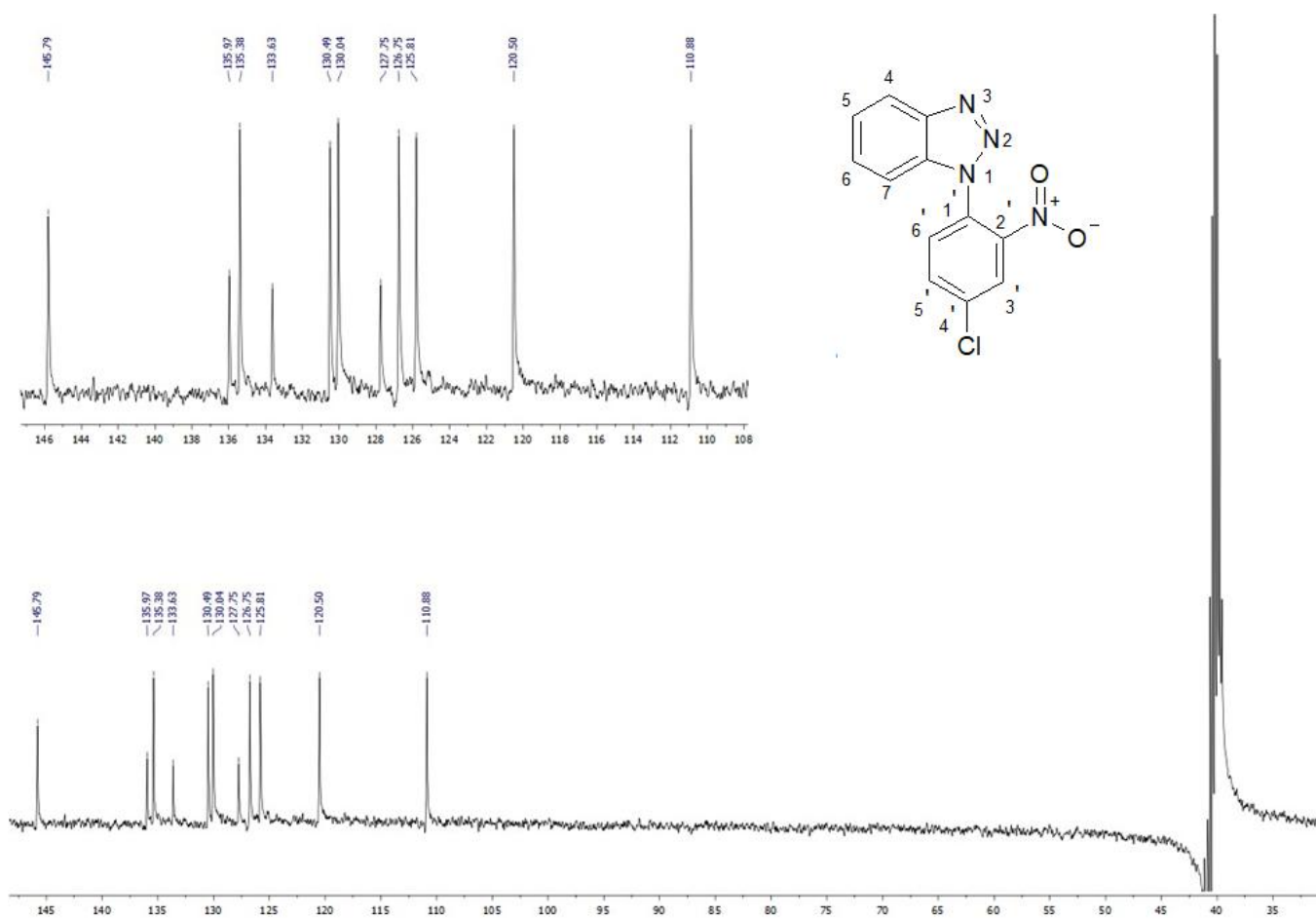
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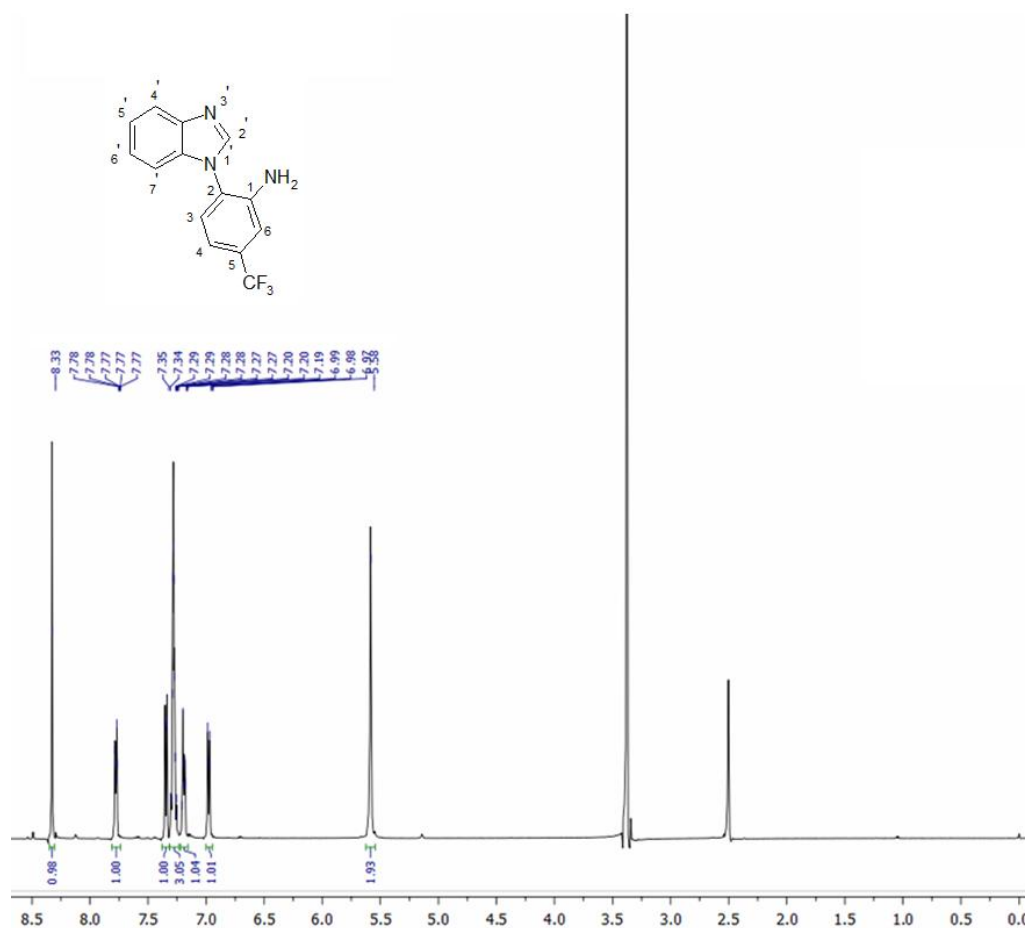
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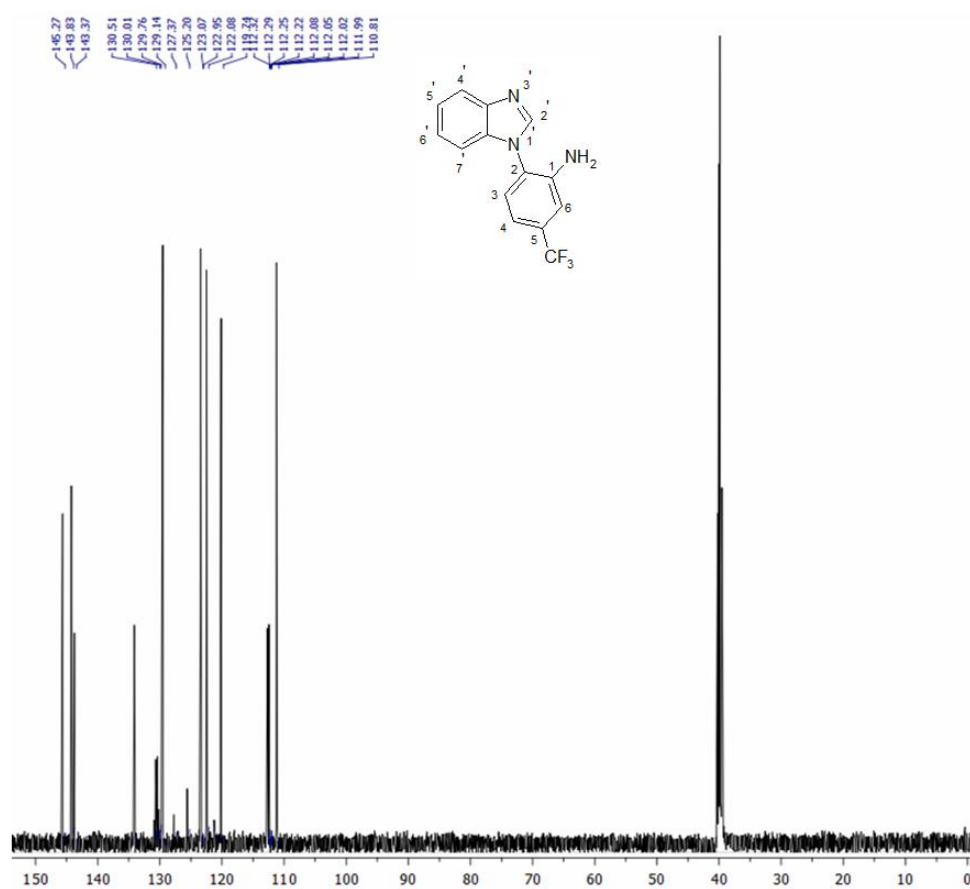
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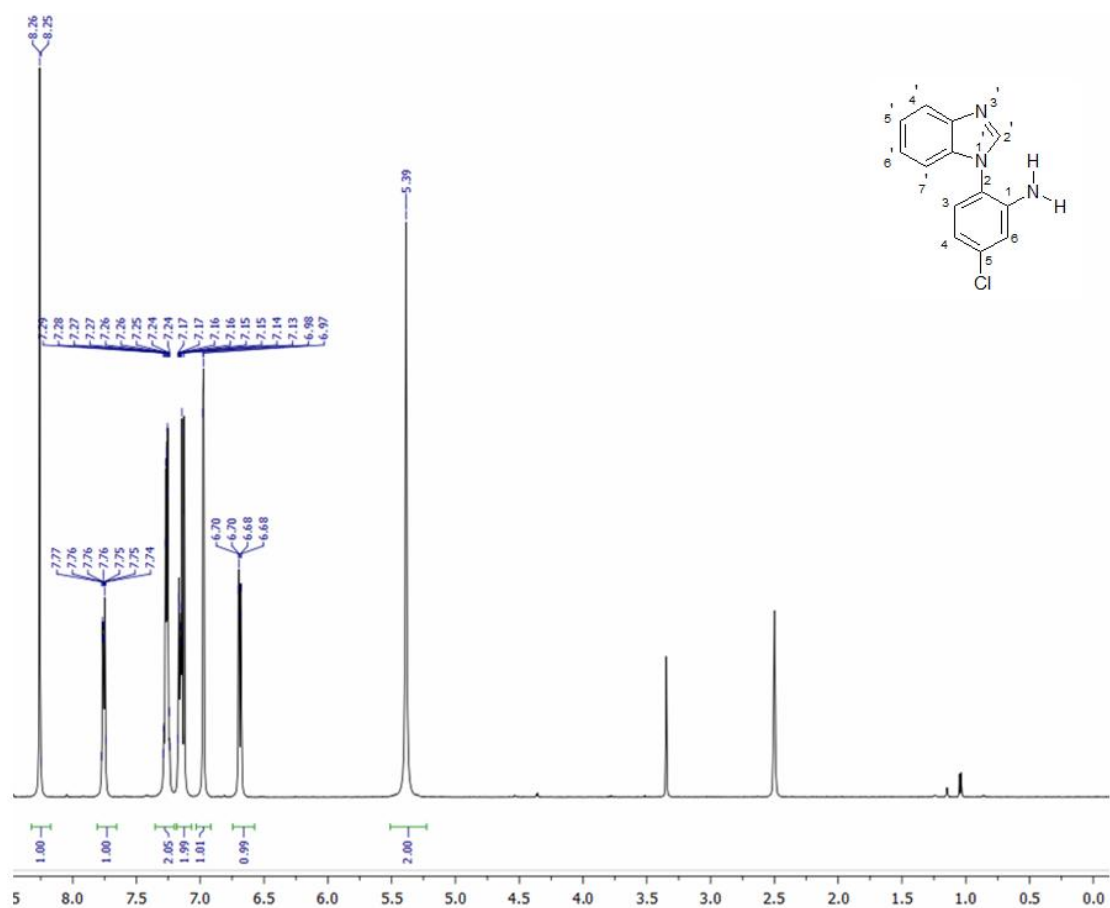
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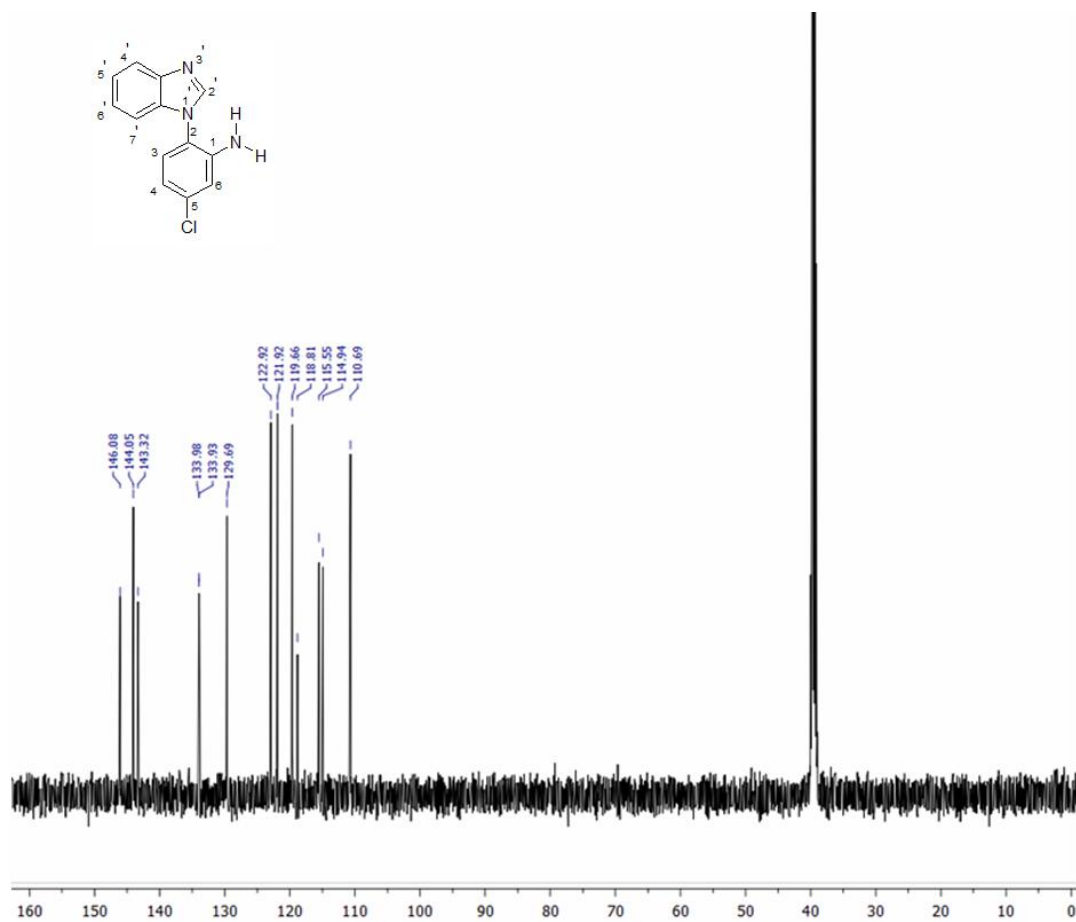
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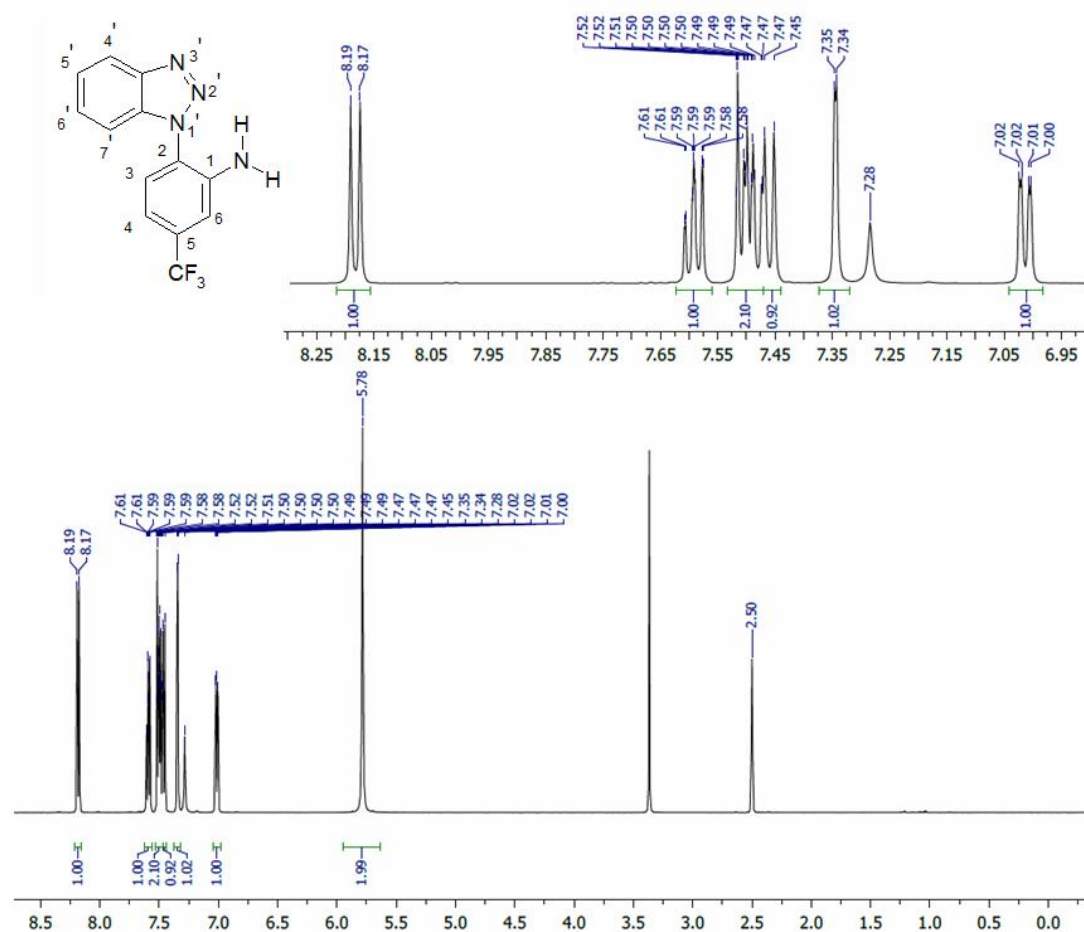
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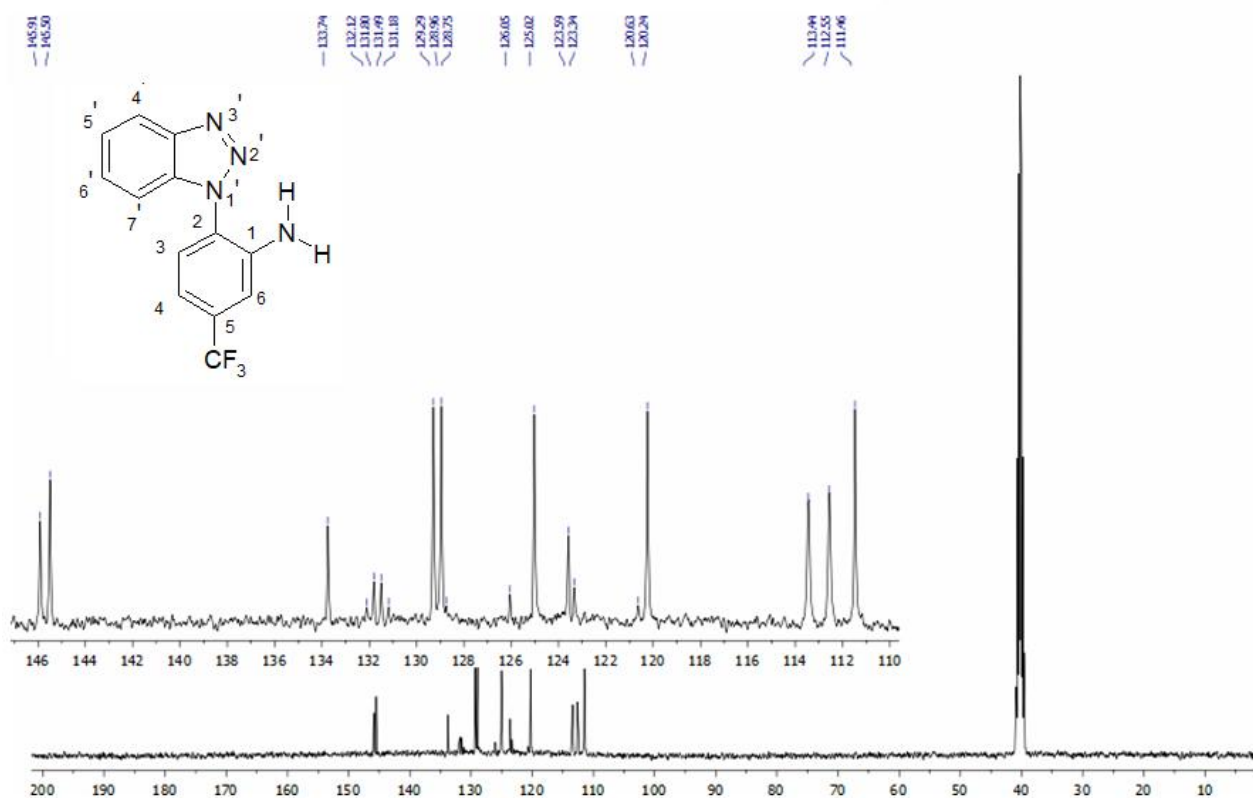
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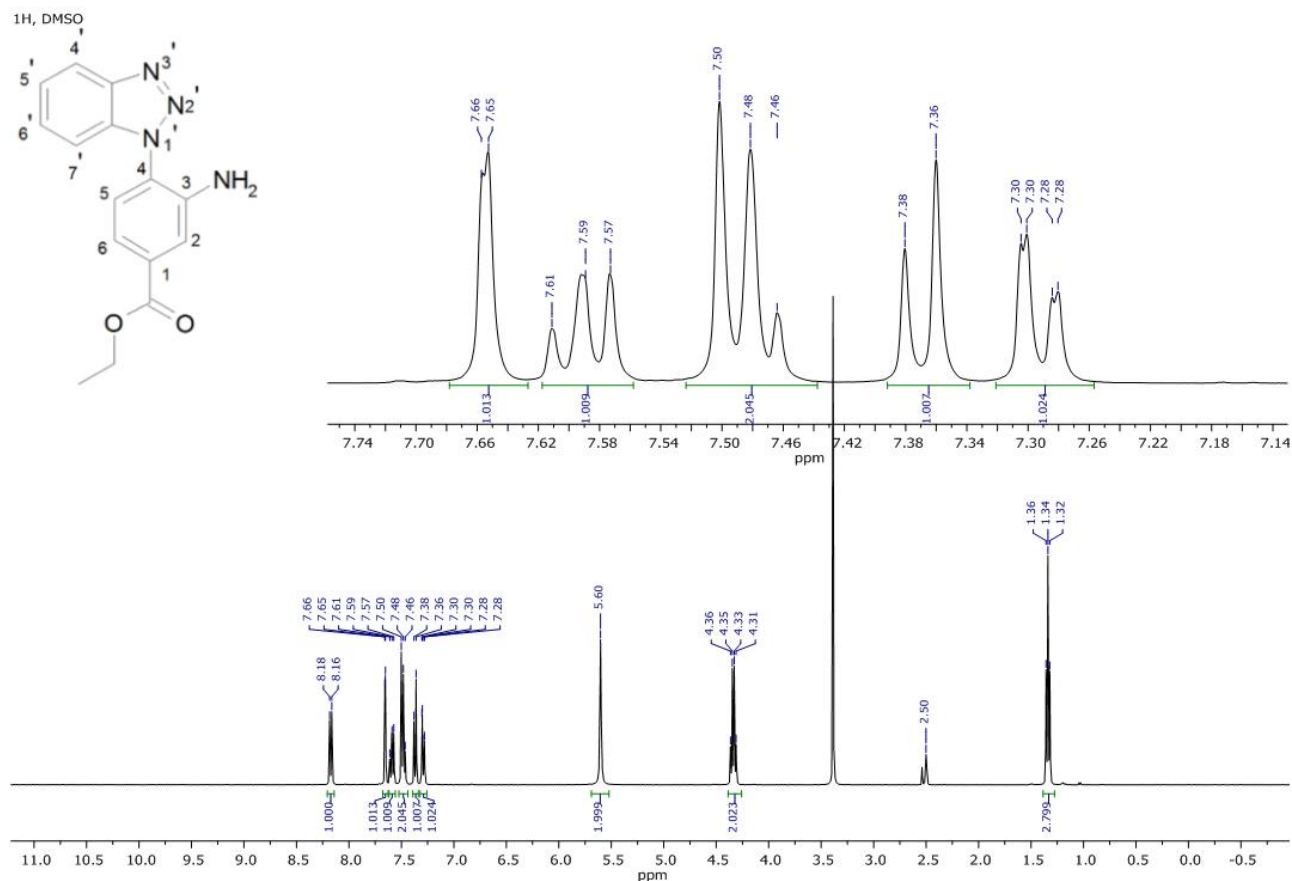
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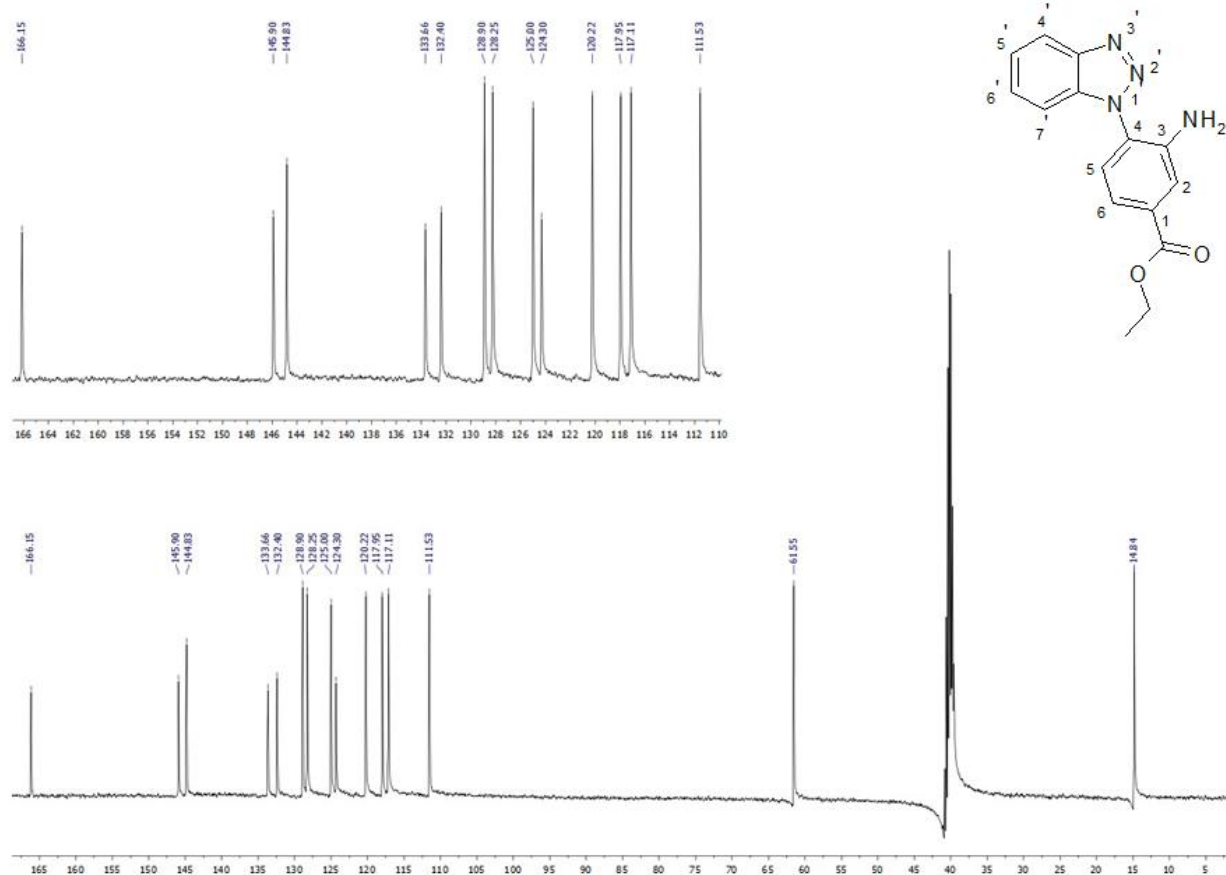
¹H NMR spectra of 2-(1*H*-benzotriazol-1-yl)-5-(trifluoromethyl)aniline (**4c**) (DMSO-*d*₆)



¹³C NMR spectra of 2-(1*H*-benzotriazol-1-yl)-5-(trifluoromethyl)aniline (**4c**) (DMSO-*d*₆)

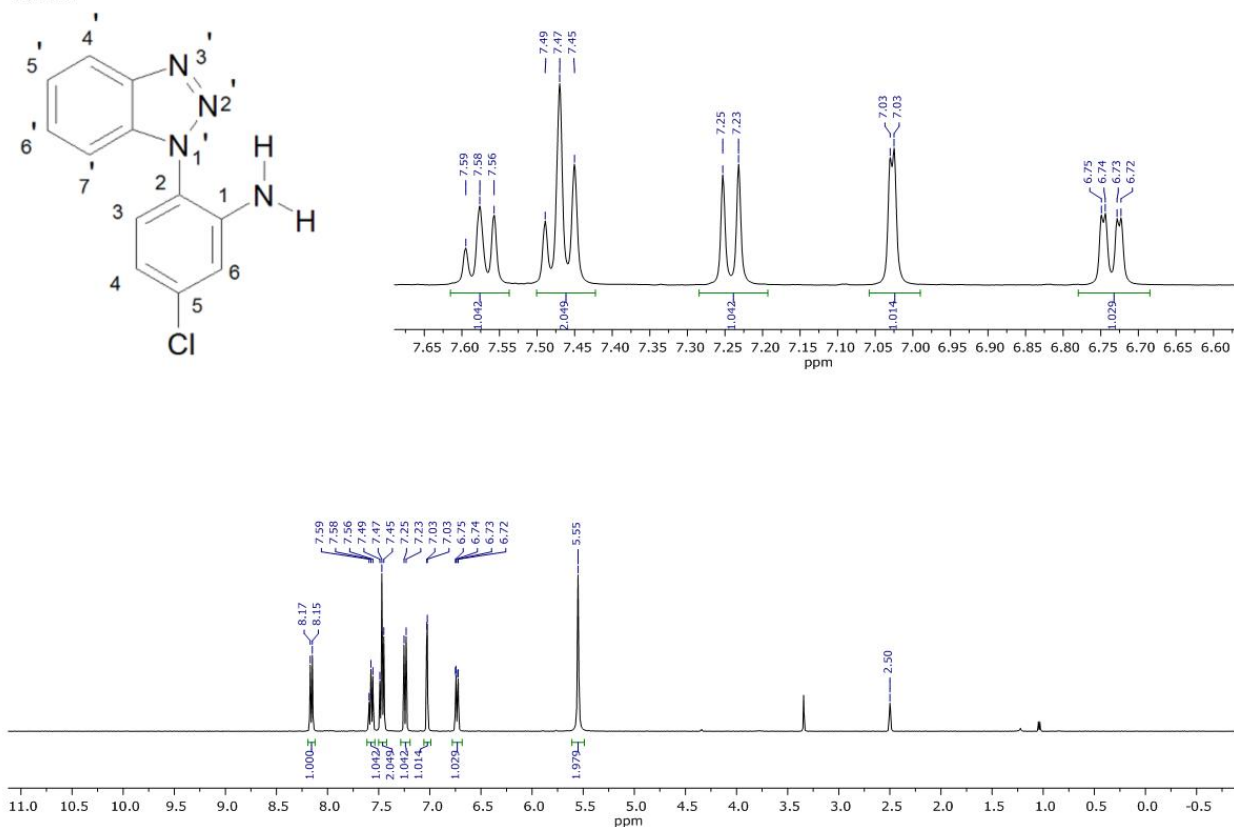


¹H NMR spectra of ethyl 3-amino-4-(1H-benzotriazol-1-yl)benzoate (**4d**) (DMSO-*d*₆)

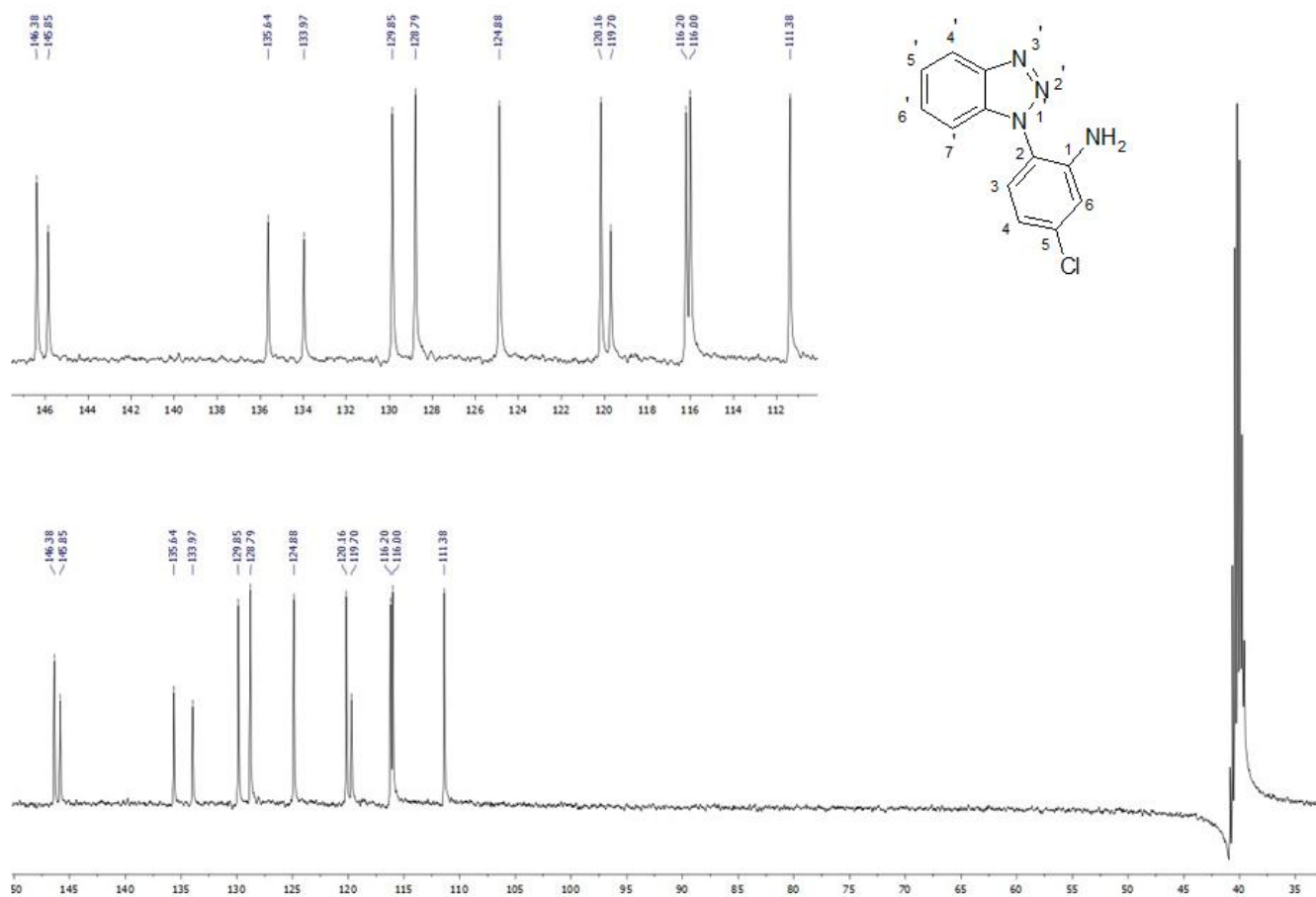


¹³C NMR spectra of ethyl 3-amino-4-(1H-benzotriazol-1-yl)benzoate (**4d**) (DMSO-*d*₆)

¹H, DMSO

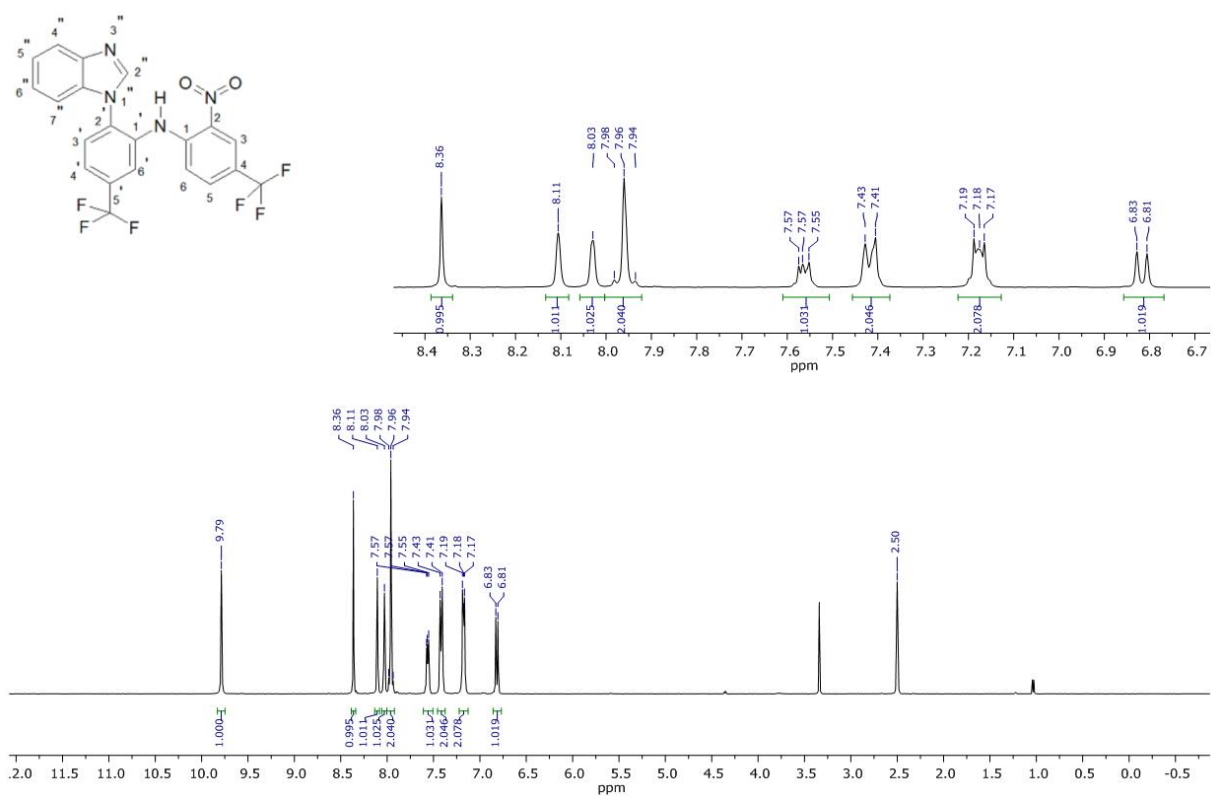


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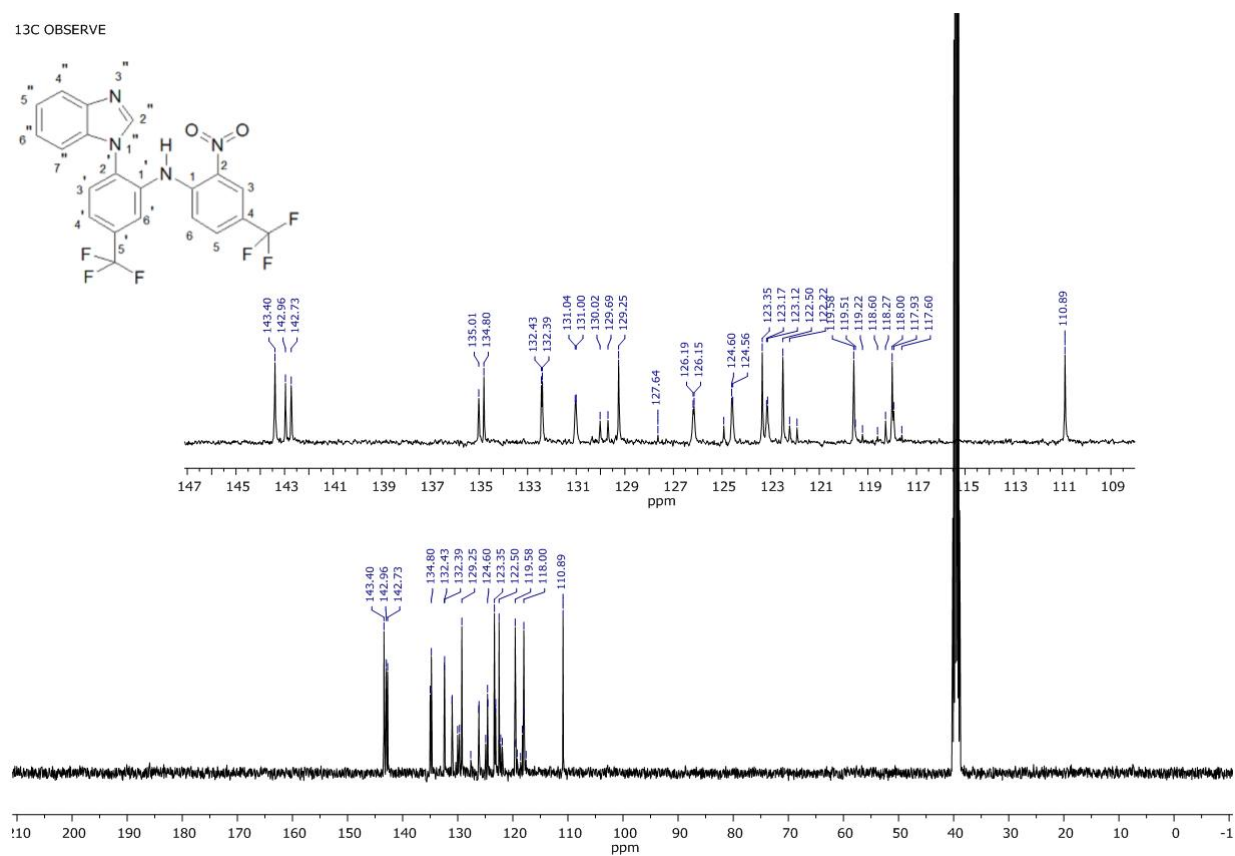
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¹H, DMSO



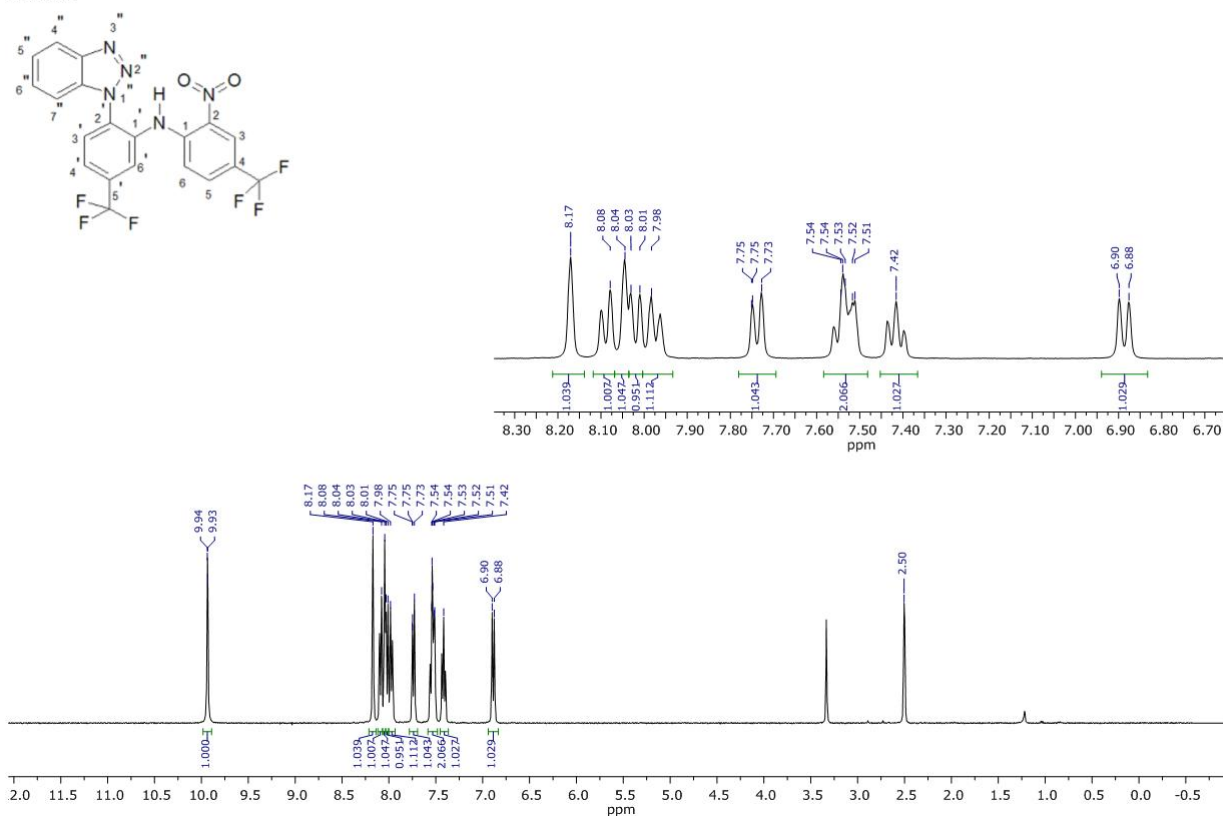
¹H NMR spectra of *N*-[2-(1*H*-benzimidazol-1-yl)-5-(trifluoromethyl)phenyl]-2-nitro-4-(trifluoromethyl)aniline (**5a**) (DMSO-*d*₆)

¹³C OBSERVE



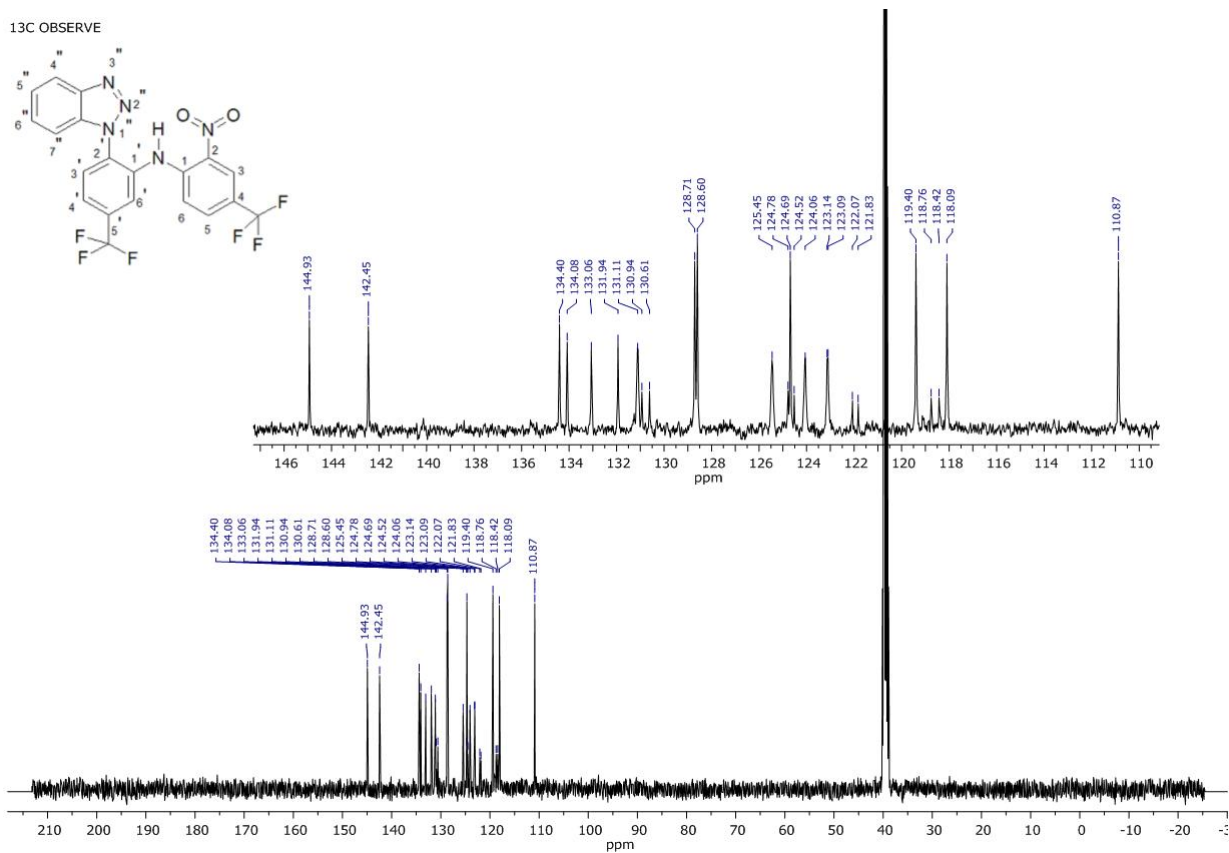
¹³C NMR spectra of *N*-[2-(1*H*-benzimidazol-1-yl)-5-(trifluoromethyl)phenyl]-2-nitro-4-(trifluoromethyl)aniline (**5a**) (DMSO-*d*₆)

¹H, DMSO

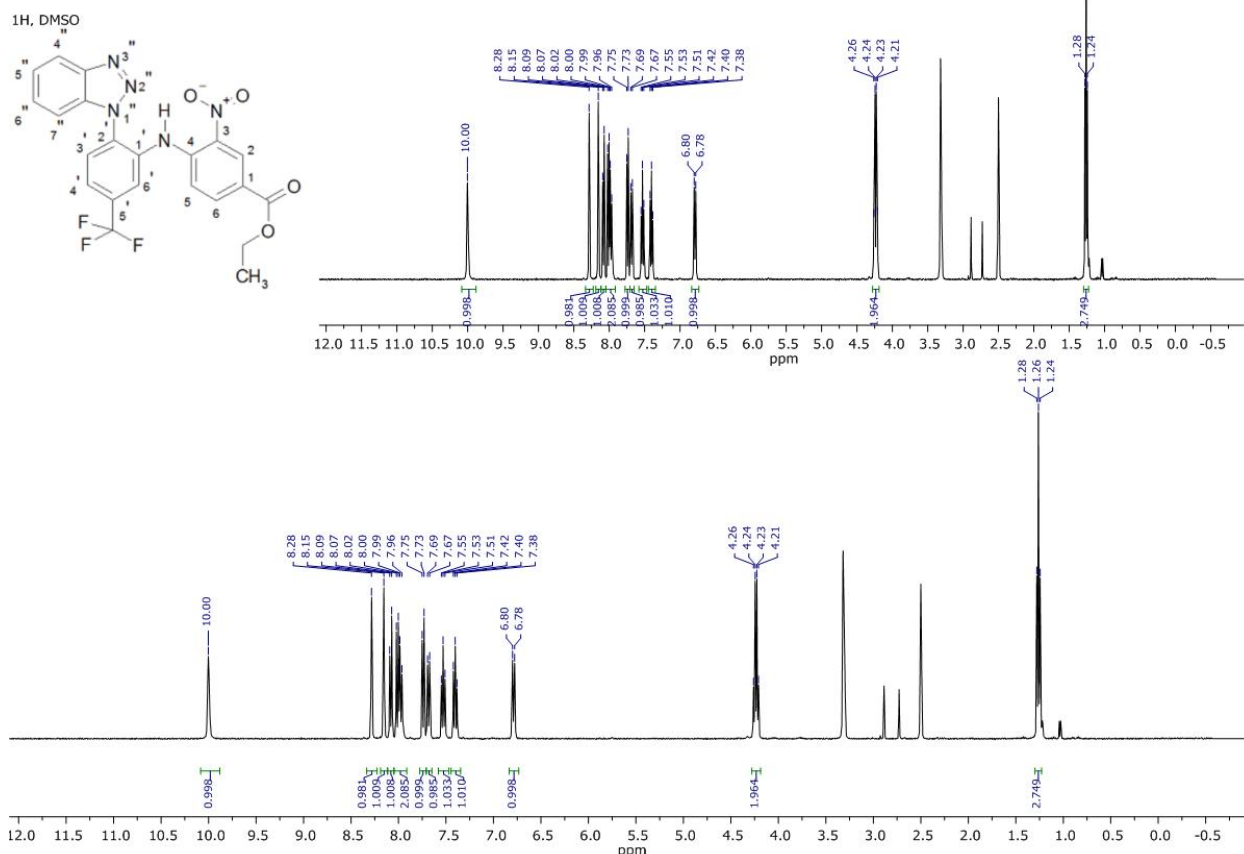


¹H NMR spectra of N-[2-(1*H*-benzotriazol-1-yl)-5-(trifluoromethyl)phenyl]-2-nitro-4-(trifluoromethyl)aniline (**5b**) (DMSO-*d*₆)

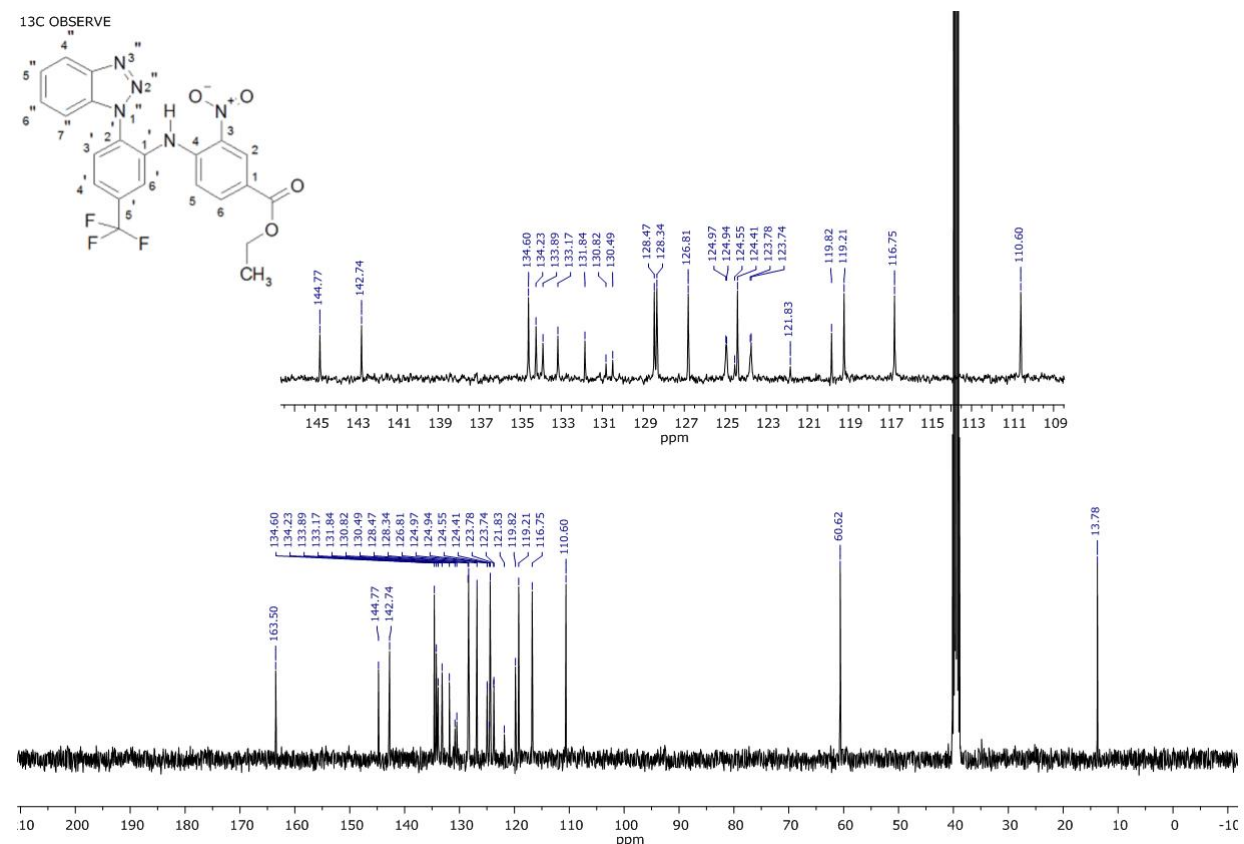
¹³C OBSERVE



¹³C NMR spectra of N-[2-(1*H*-benzotriazol-1-yl)-5-(trifluoromethyl)phenyl]-2-nitro-4-(trifluoromethyl)aniline (**5b**) (DMSO-*d*₆)

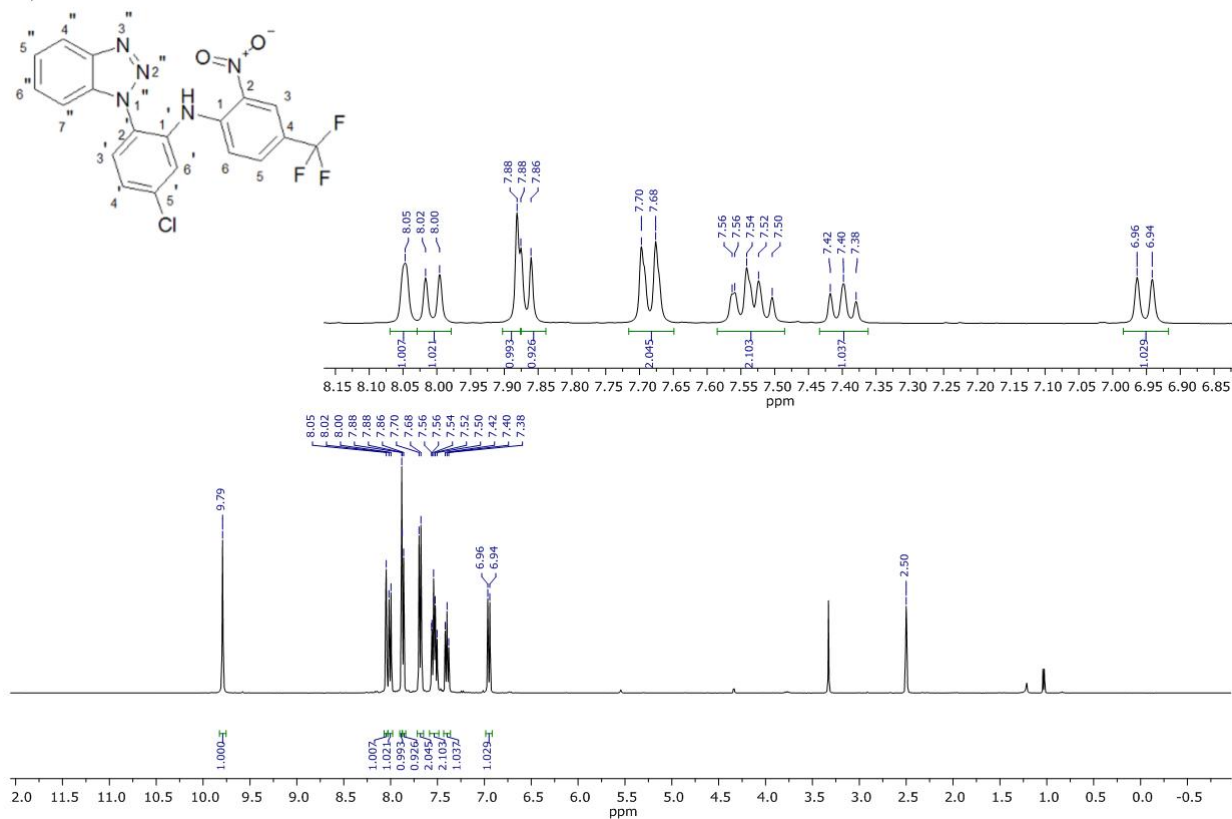


¹H NMR spectra of ethyl 4-[2-(1*H*-benzotriazol-1-yl)-5-(trifluoromethyl)anilino]-3-nitrobenzoate (**5c**) (DMSO-*d*₆)



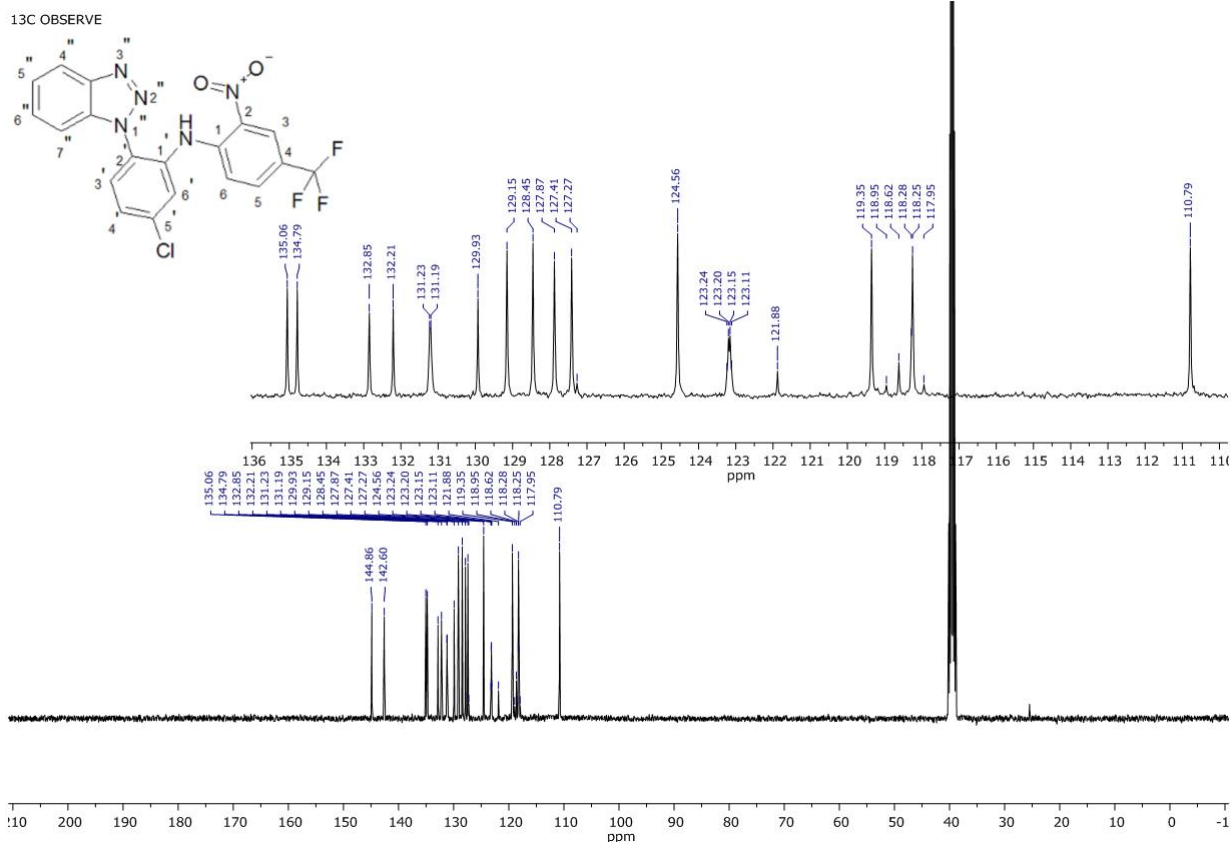
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¹H, DMSO



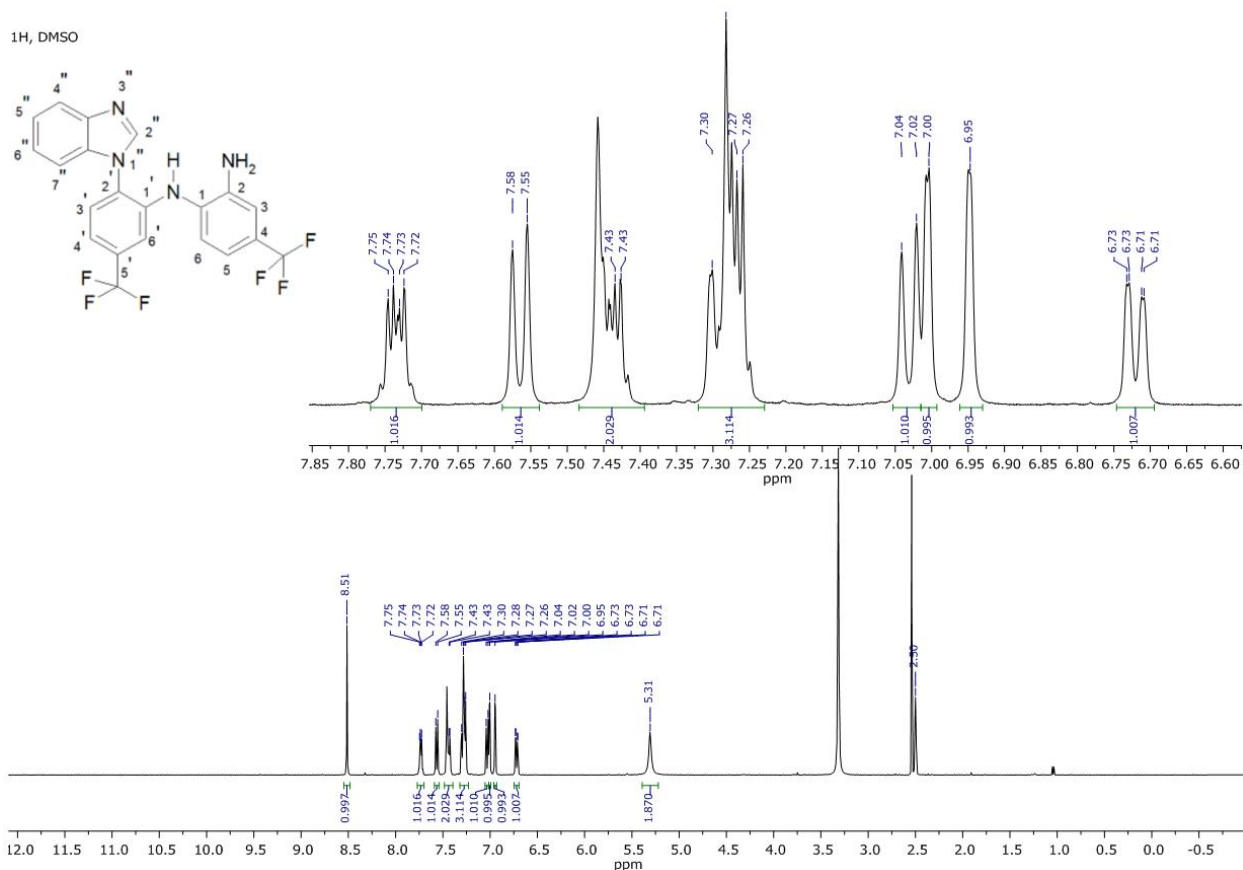
¹H NMR spectra of *N*-[2-(1*H*-benzotriazol-1-yl)-5-chlorophenyl]-2-nitro-4-(trifluoromethyl)aniline (**5d**) (DMSO-*d*₆)

¹³C OBSERVE



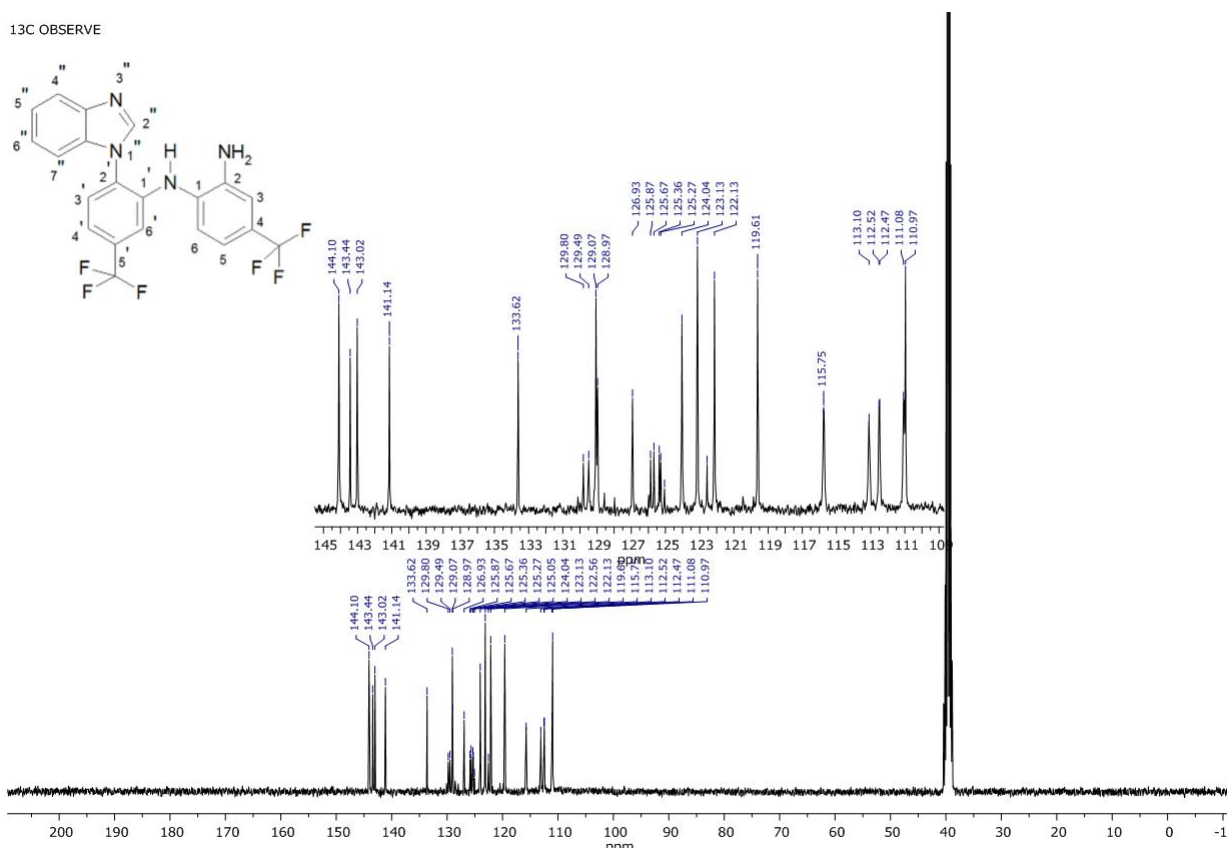
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¹H, DMSO



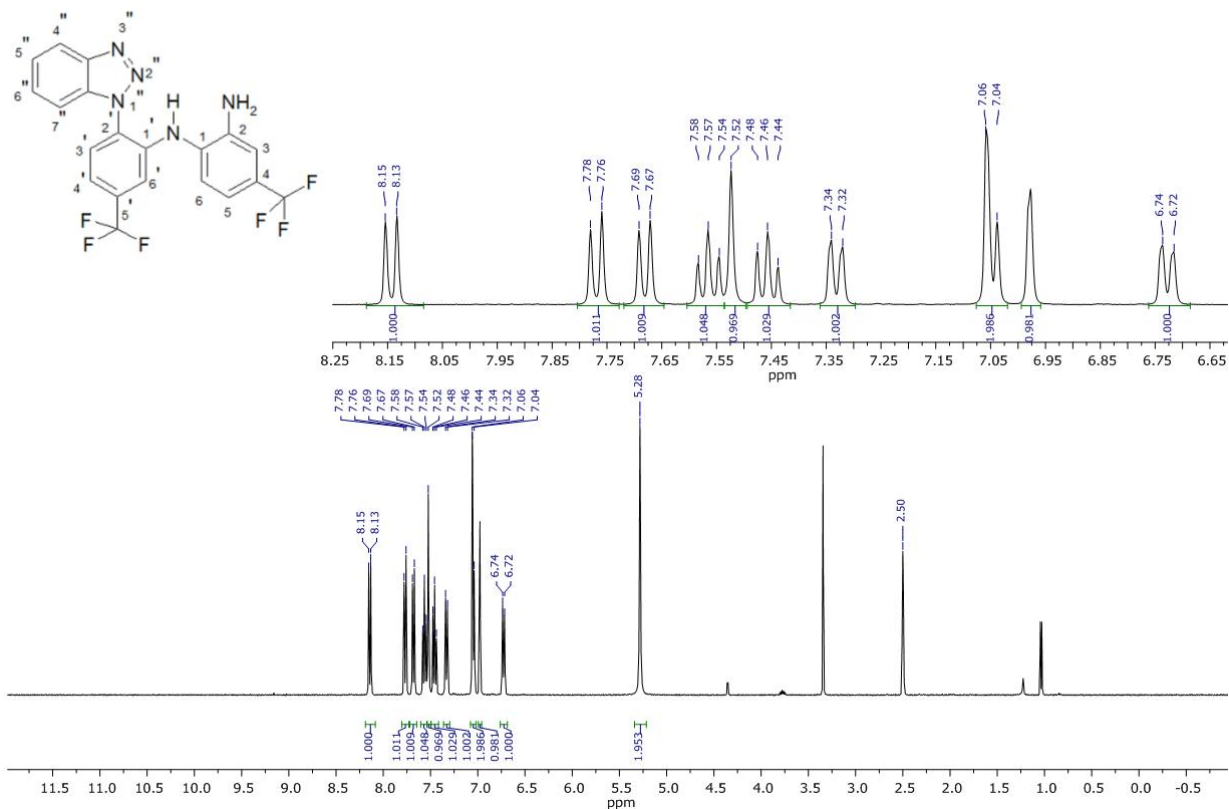
¹H NMR spectra of *N*-[2-(1*H*-benzimidazol-1-yl)-5-(trifluoromethyl)phenyl]-2-amino-4-(trifluoromethyl)aniline (**6a**) (DMSO-*d*₆)

¹³C OBSERVE



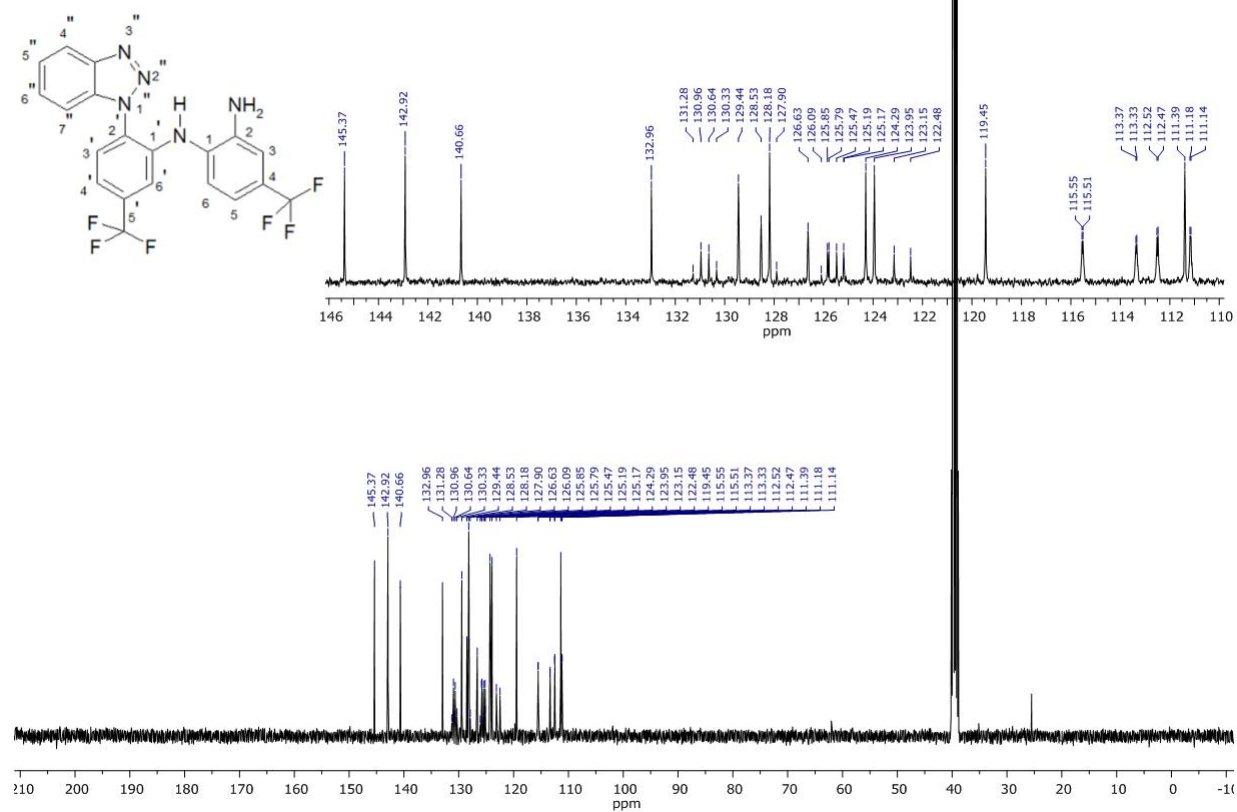
¹³C NMR spectra of *N*-[2-(1*H*-benzimidazol-1-yl)-5-(trifluoromethyl)phenyl]-2-amino-4-(trifluoromethyl)aniline (**6a**) (DMSO-*d*₆)

¹H, DMSO

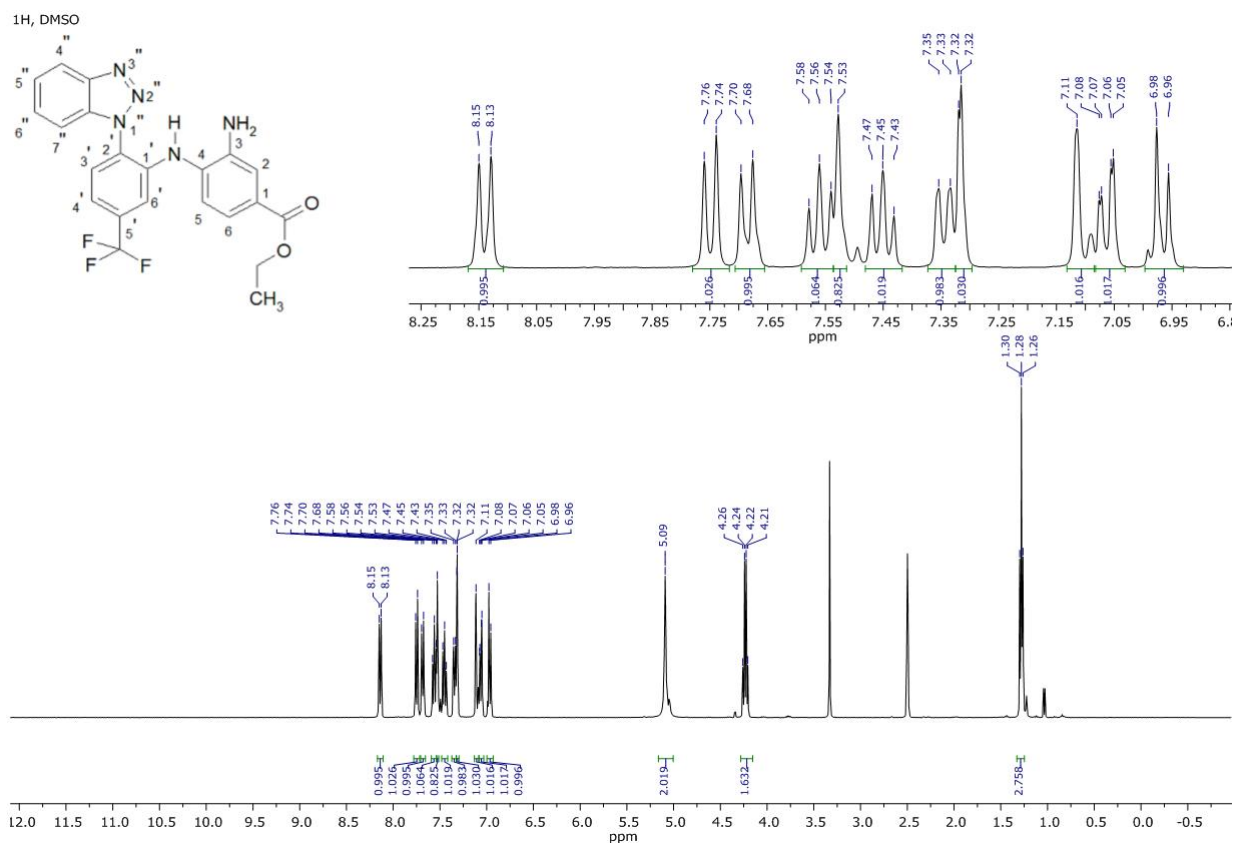


¹H NMR spectra of *N*-[2-(1*H*-benzotriazol-1-yl)-5-(trifluoromethyl)phenyl]-2-amino-4-(trifluoromethyl)aniline (**6b**) (DMSO-*d*₆)

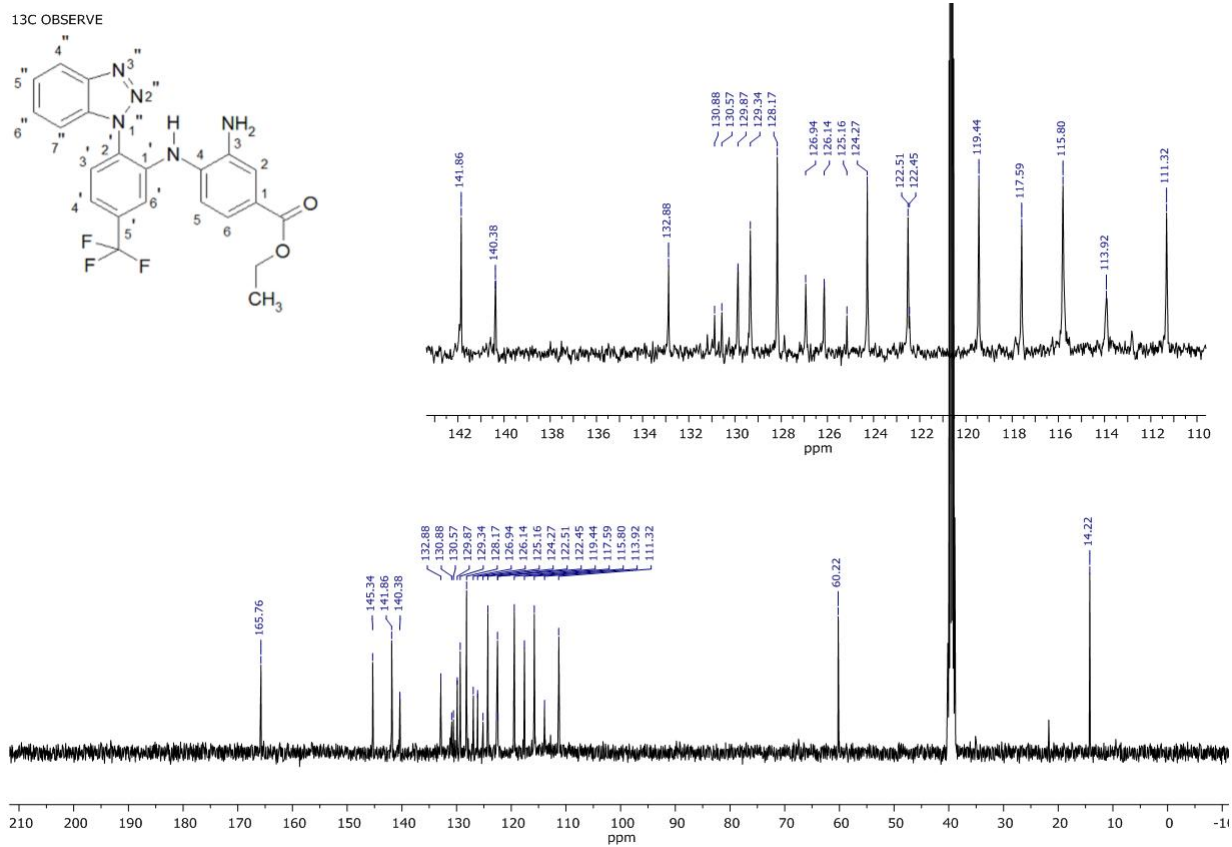
¹³C OBSERVE



¹³C NMR spectra of *N*-[2-(1*H*-benzotriazol-1-yl)-5-(trifluoromethyl)phenyl]-2-amino-4-(trifluoromethyl)aniline (**6b**) (DMSO-*d*₆)

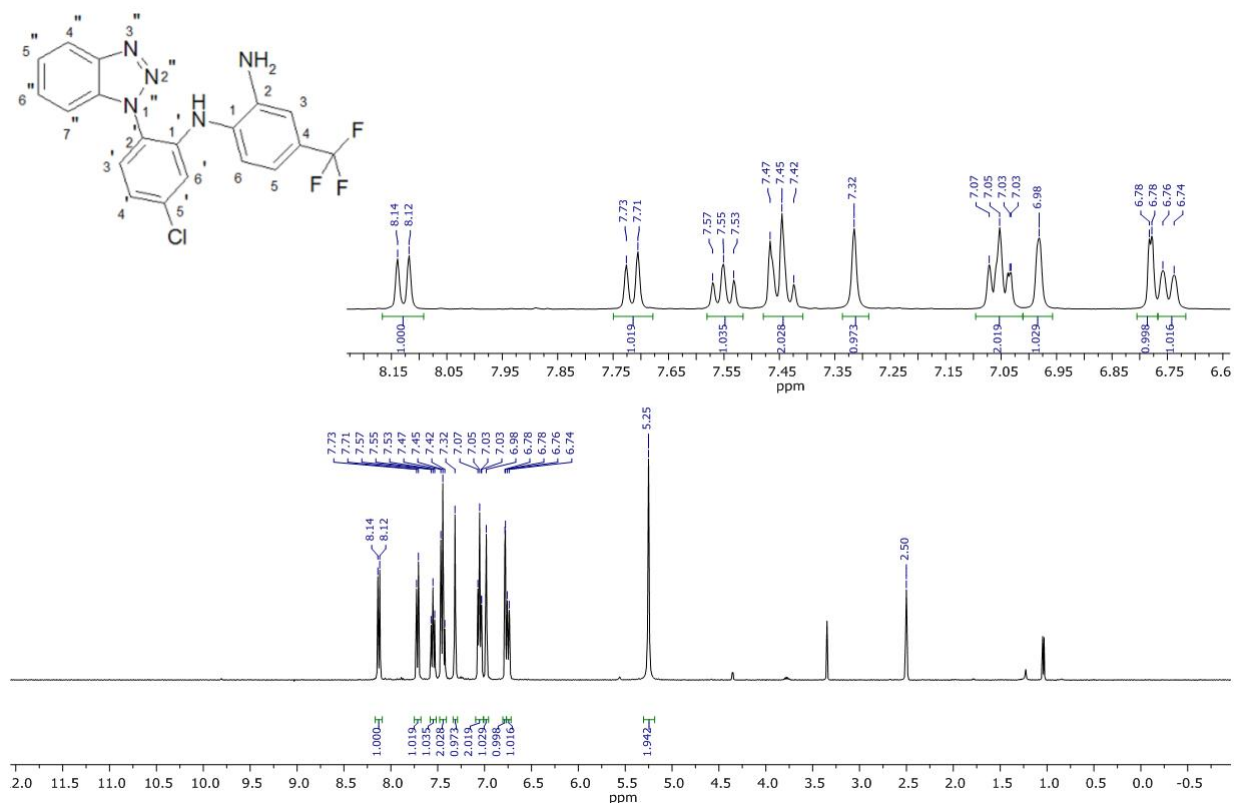


¹H NMR spectra of ethyl 3-amino-4-[2-(1H-benzotriazol-1-yl)-5-(trifluoromethyl)anilino]-benzoate (**6c**) (DMSO-*d*₆)



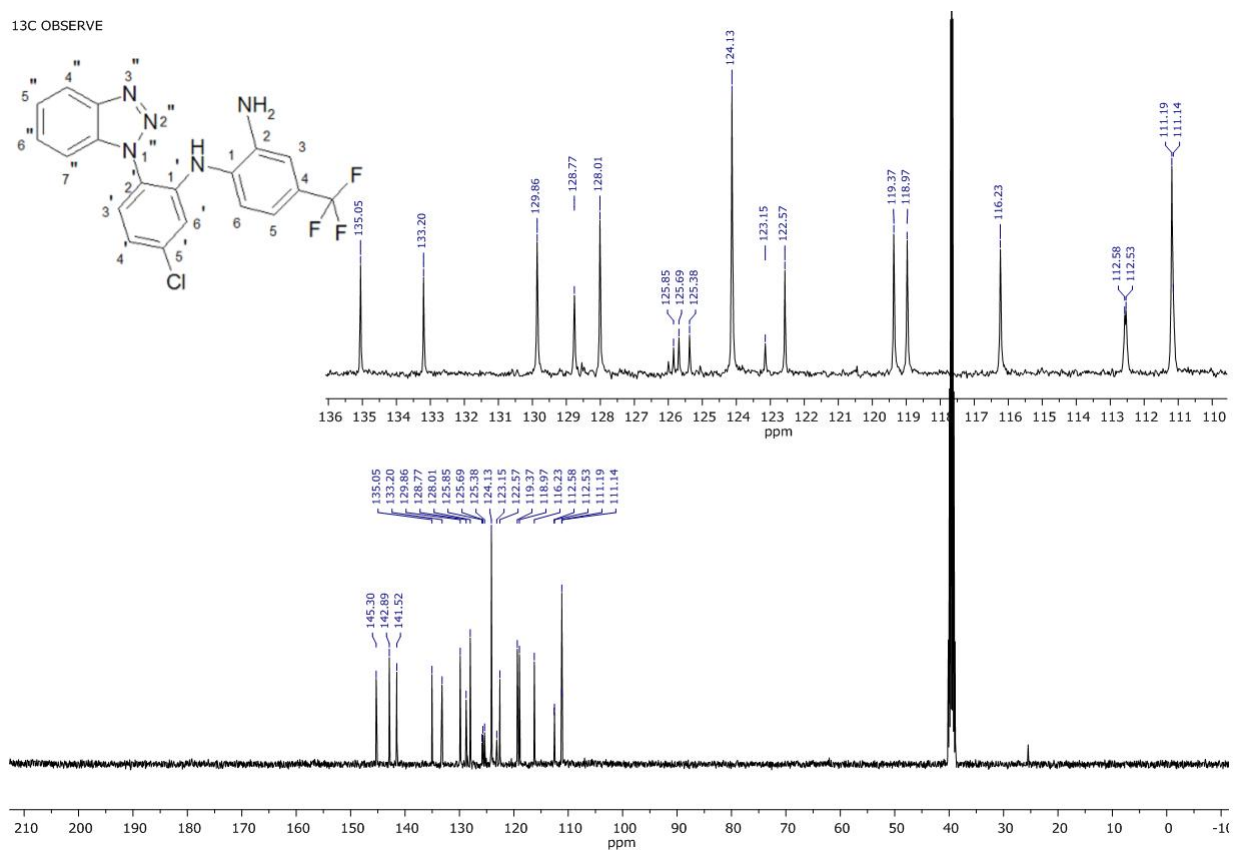
¹³C NMR spectra of ethyl 3-amino-4-[2-(1H-benzotriazol-1-yl)-5-(trifluoromethyl)anilino]-benzoate (**6c**) (DMSO-*d*₆)

¹H, DMSO



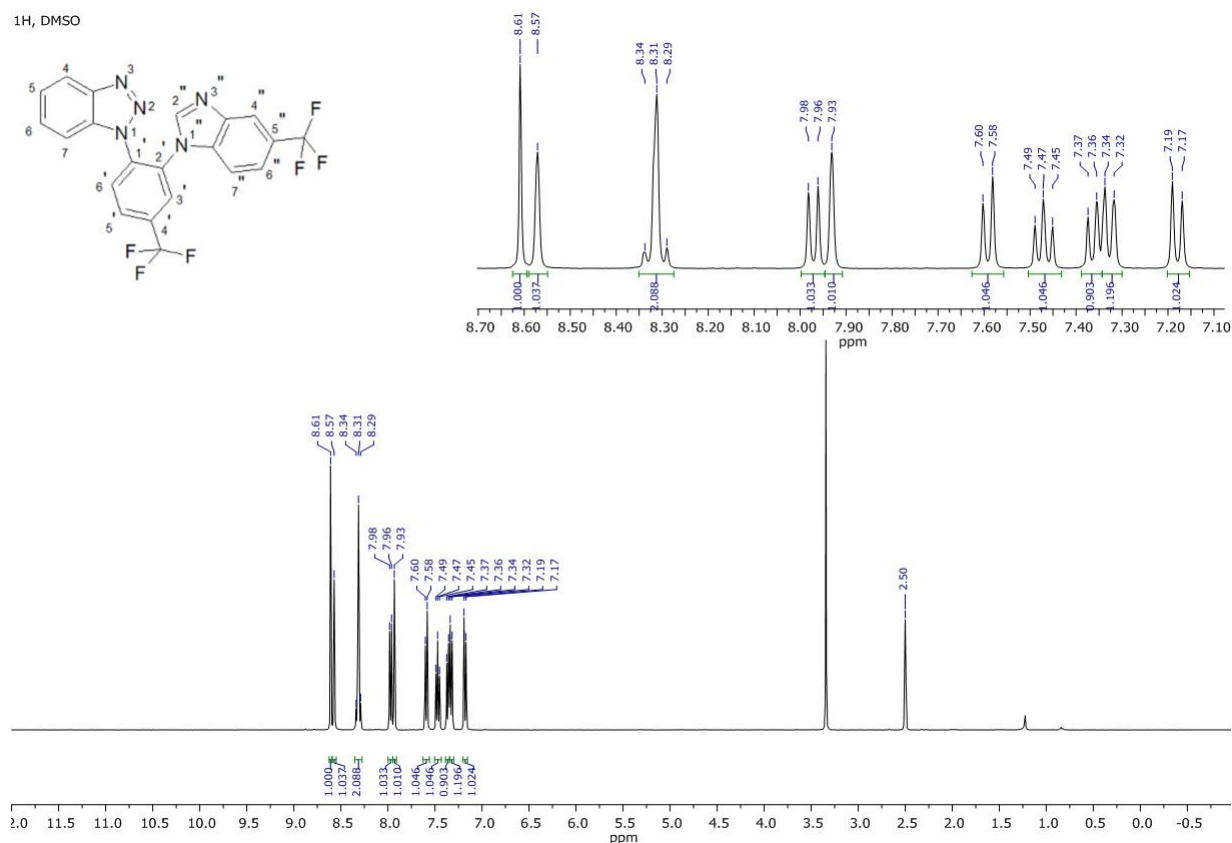
¹H NMR spectra of *N*-[2-(1*H*-benzotriazol-1-yl)-5-chlorophenyl]-2-amino-4-(trifluoromethyl)aniline (**6d**) (DMSO-*d*₆)

¹³C OBSERVE



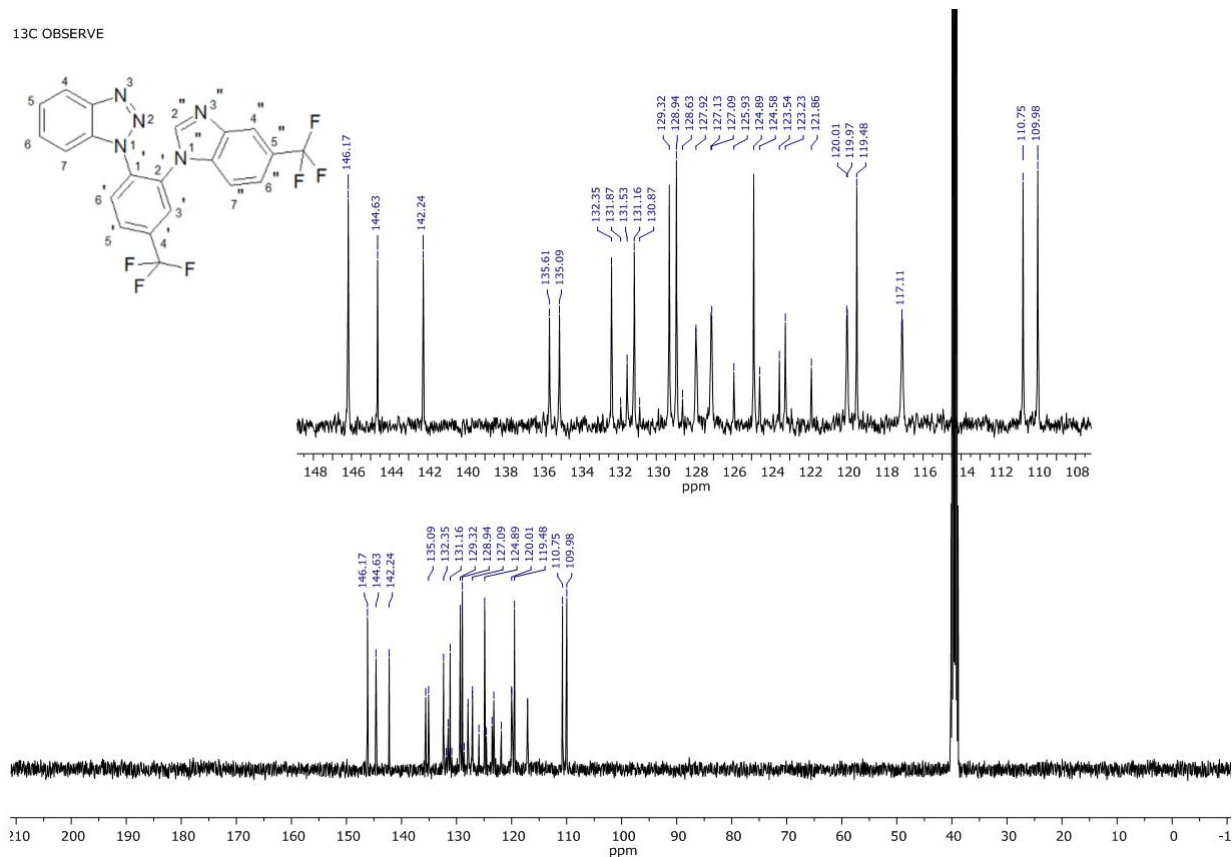
¹³C NMR spectra of *N*-[2-(1*H*-benzotriazol-1-yl)-5-chlorophenyl]-2-amino-4-(trifluoromethyl)aniline (**6d**) (DMSO-*d*₆)

¹H, DMSO



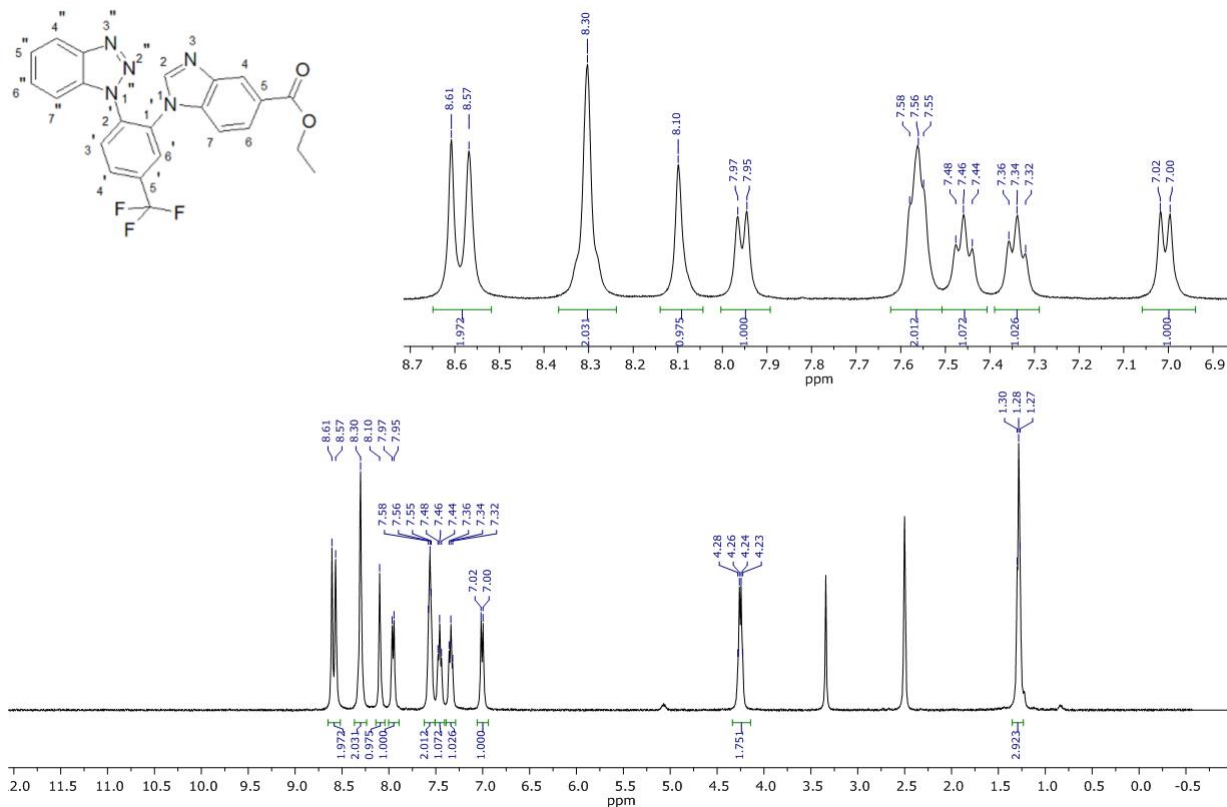
¹H NMR spectra of 1-{4-(trifluoromethyl)-2-[5-(trifluoromethyl)-1H-benzimidazol-1-yl]phenyl}-1H-benzotriazole (**7a**) (DMSO-*d*₆)

¹³C OBSERVE



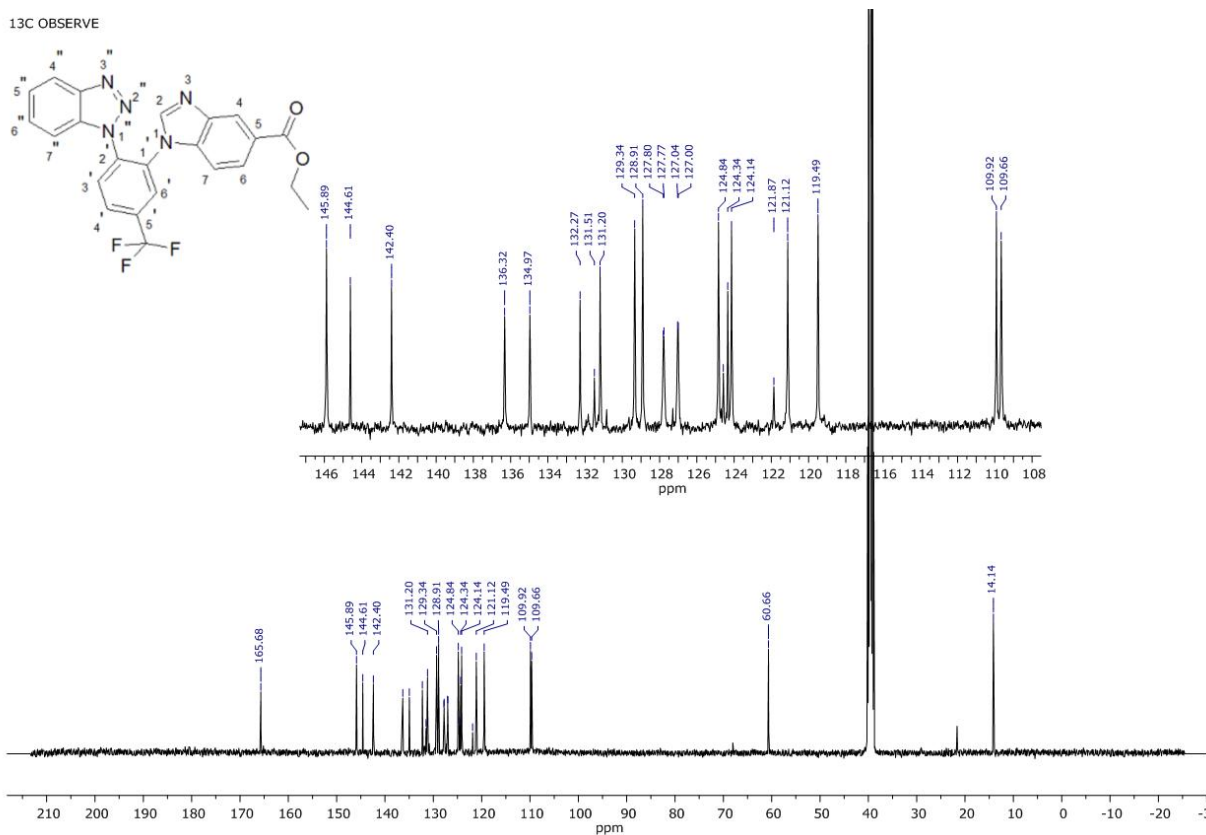
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¹H, DMSO



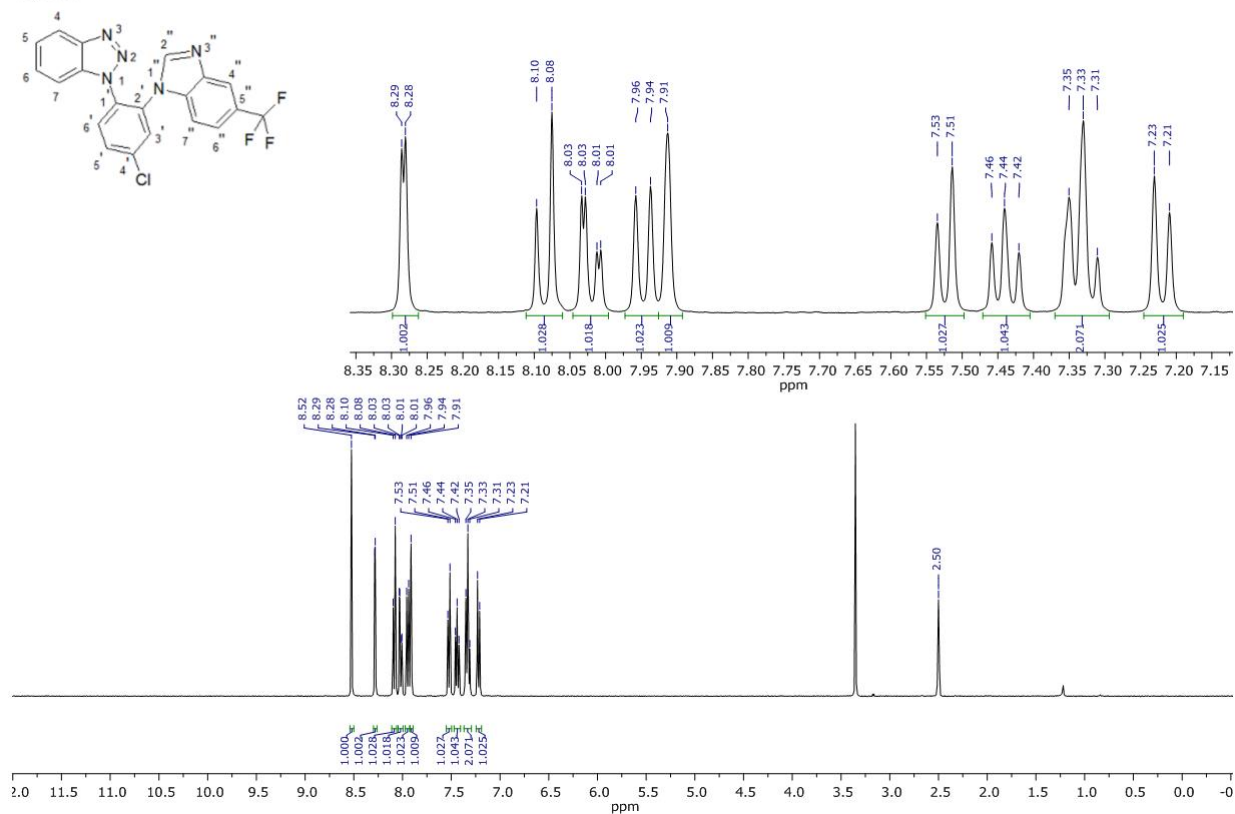
¹H NMR spectra of ethyl 1-[2-(1*H*-benzotriazol-1-yl)-5-(trifluoromethyl)phenyl]-1*H*-benzimidazole-5-carboxylate (**7b**) (DMSO-*d*₆)

¹³C OBSERVE



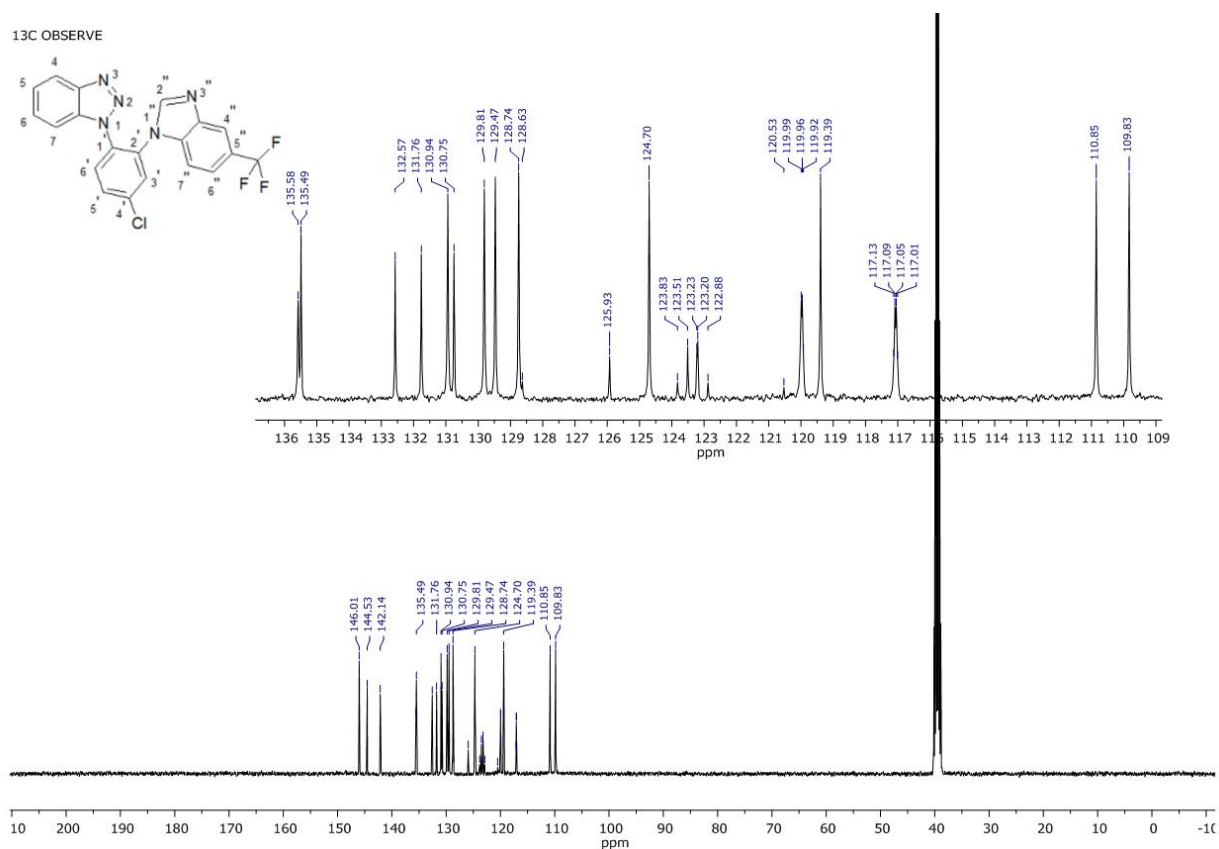
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¹H, DMSO

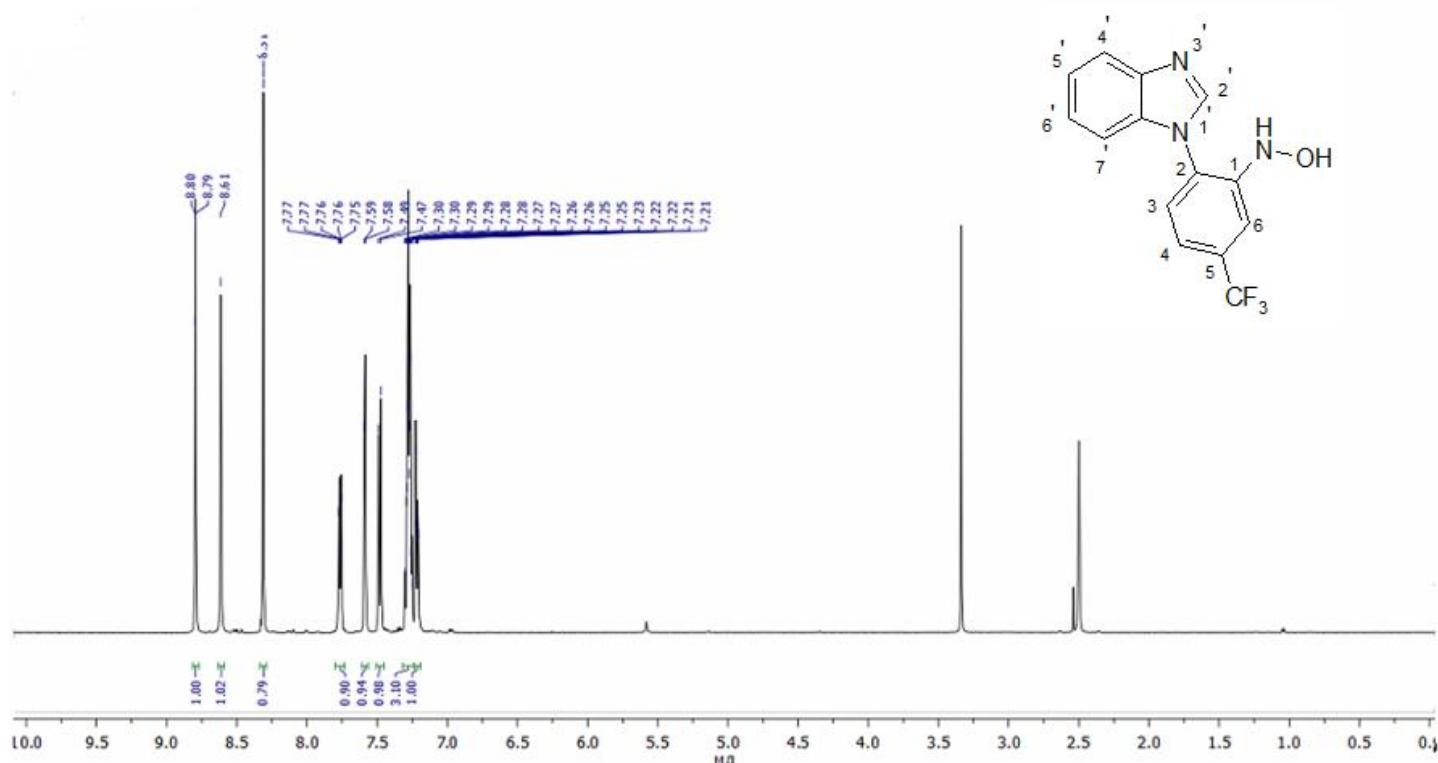


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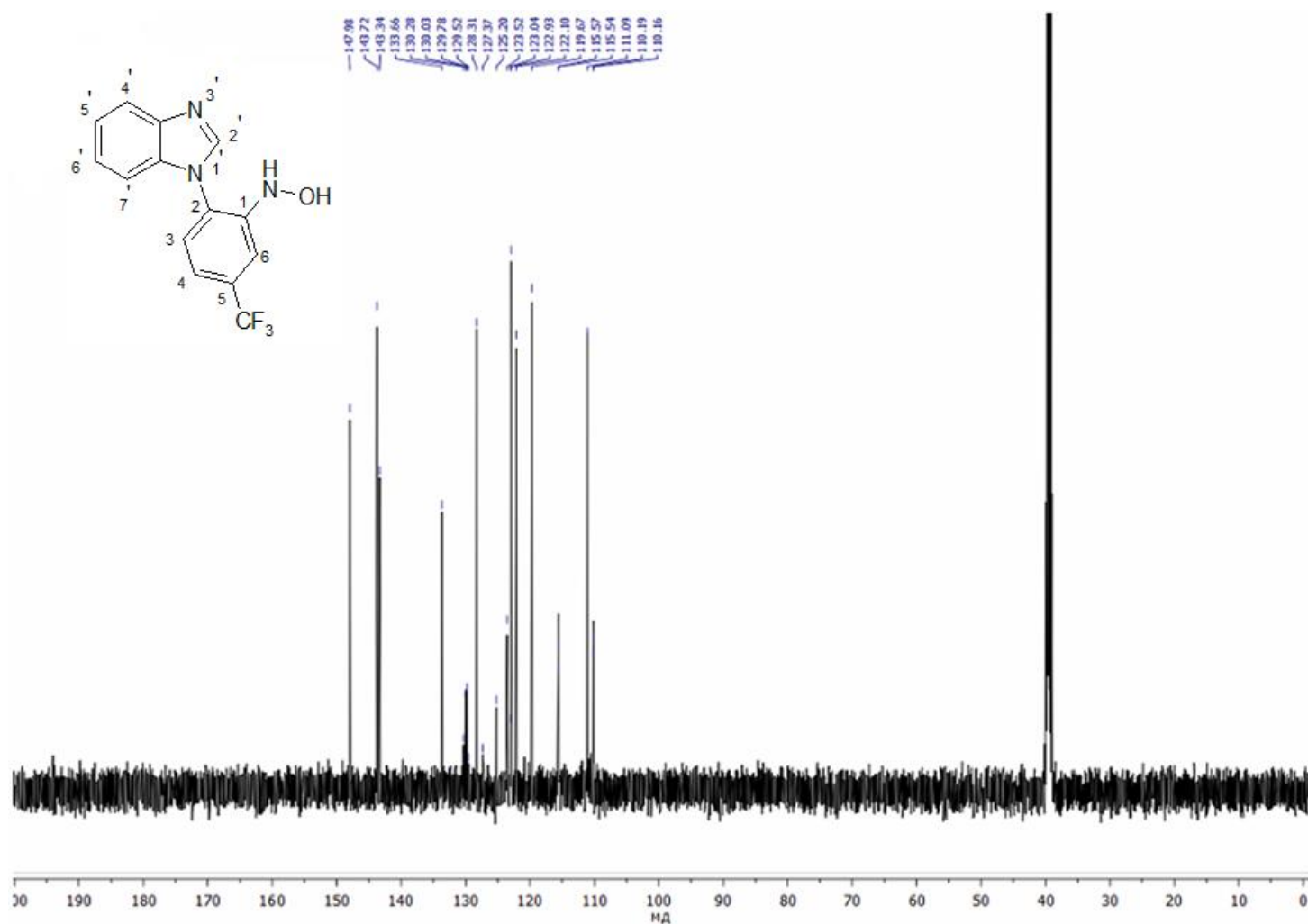
¹³C OBSERVE



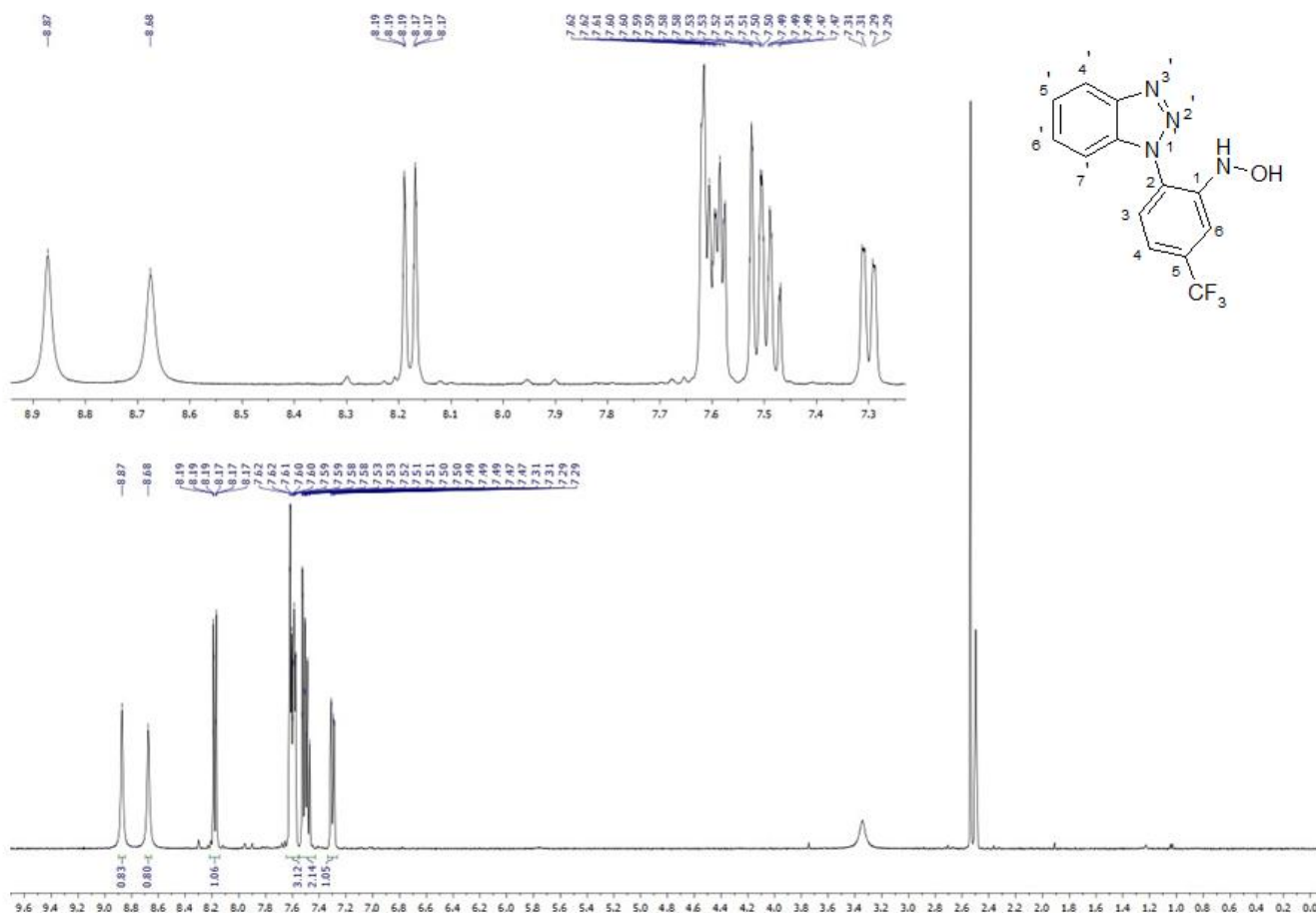
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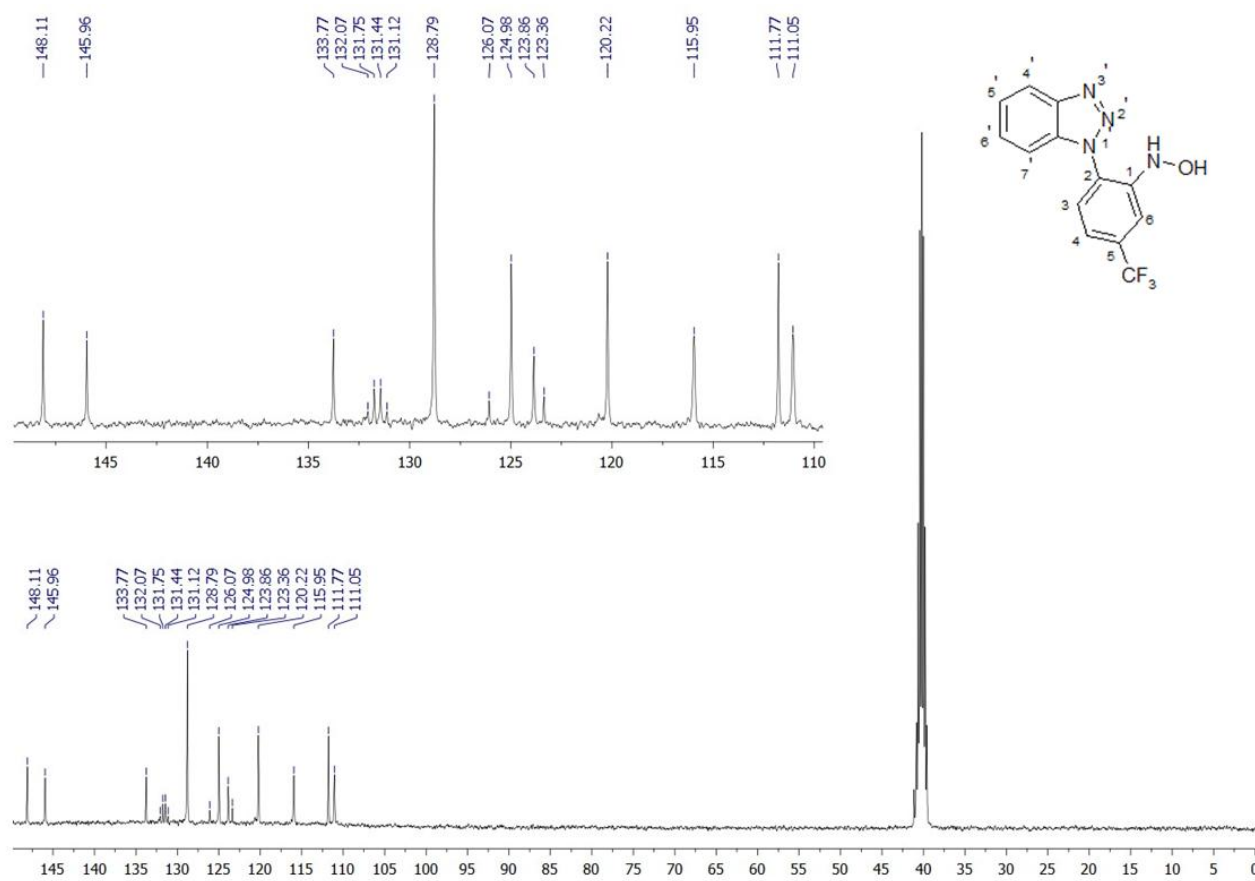
¹H NMR spectra of 1 N-(2-(1H-benzimidazol-1-yl)-5-(trifluoromethyl)phenyl)hydroxylamine (**8a**) (DMSO-*d*₆)



¹³C NMR spectra of 1 N-(2-(1H-benzimidazol-1-yl)-5-(trifluoromethyl)phenyl)hydroxylamine (**8a**) (DMSO-*d*₆)



¹H NMR spectra of 1 N-(2-(1H-benzotriazol-1-yl)-5-(trifluoromethyl)phenyl)hydroxylamine (**8b**) (DMSO-*d*₆)



^{13}C NMR spectra of 1 N-(2-(1*H*-benzotriazol-1-yl)-5-(trifluoromethyl)phenyl)hydroxylamine (**8b**) (DMSO-*d*₆)