

Supplementary Material

Bu₃SnH-mediated cyclopropyl radical cyclizations onto indole-3-carbaldehyde

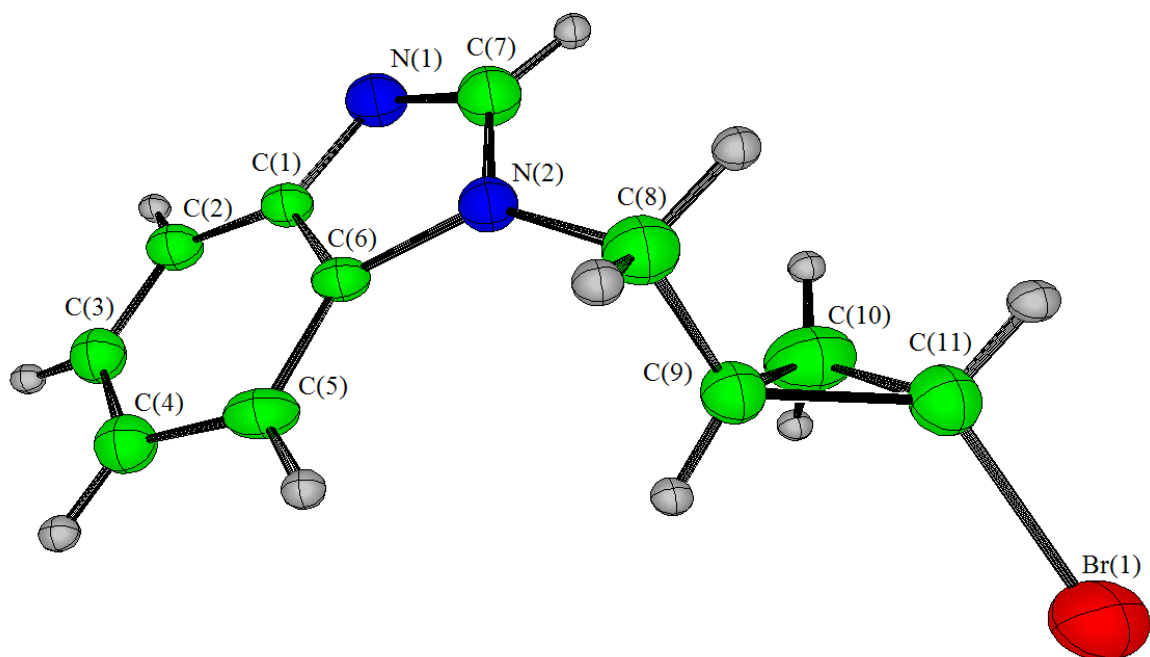
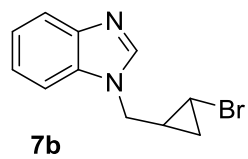
Karen Fahey, Robert Coyle, Patrick McArdle, and Fawaz Aldabbagh*

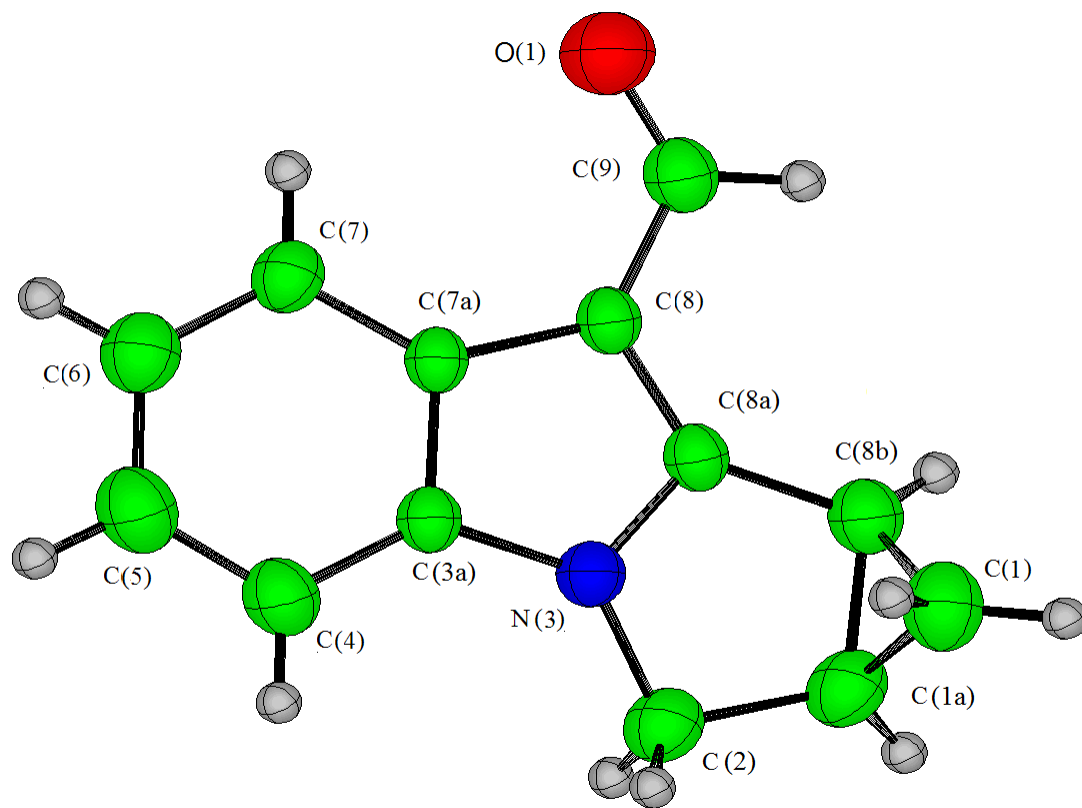
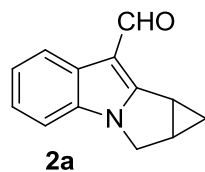
School of Chemistry, National University of Ireland Galway, University Road, Galway, Ireland

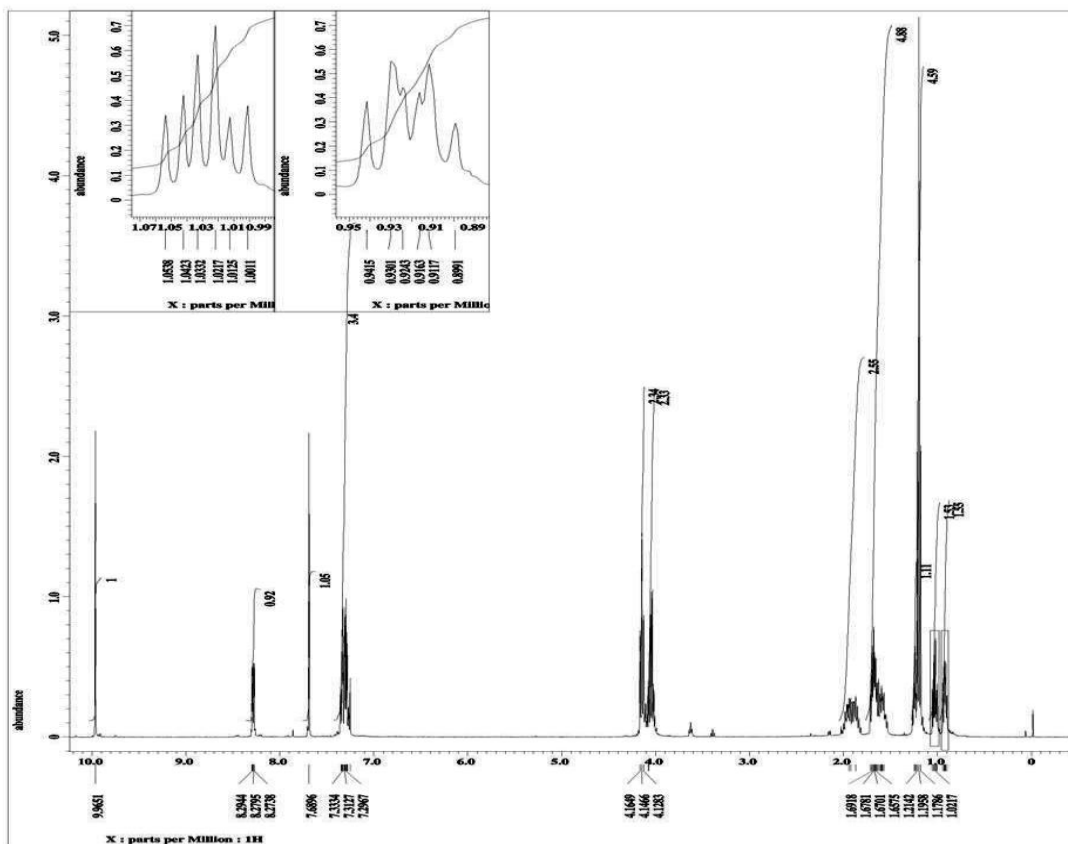
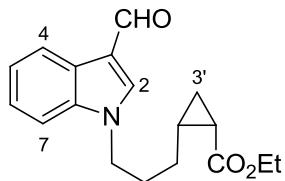
E-mail: fawaz.aldabbagh@nuigalway.ie

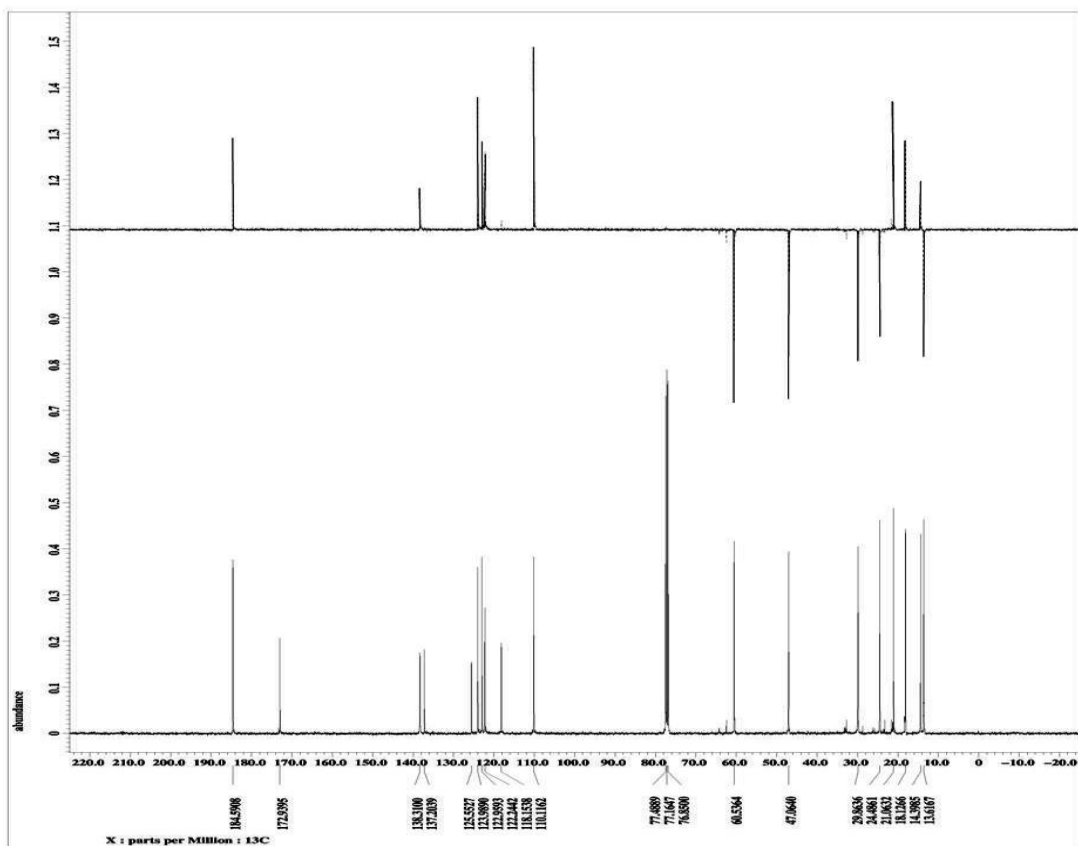
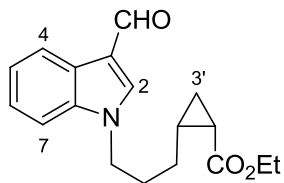
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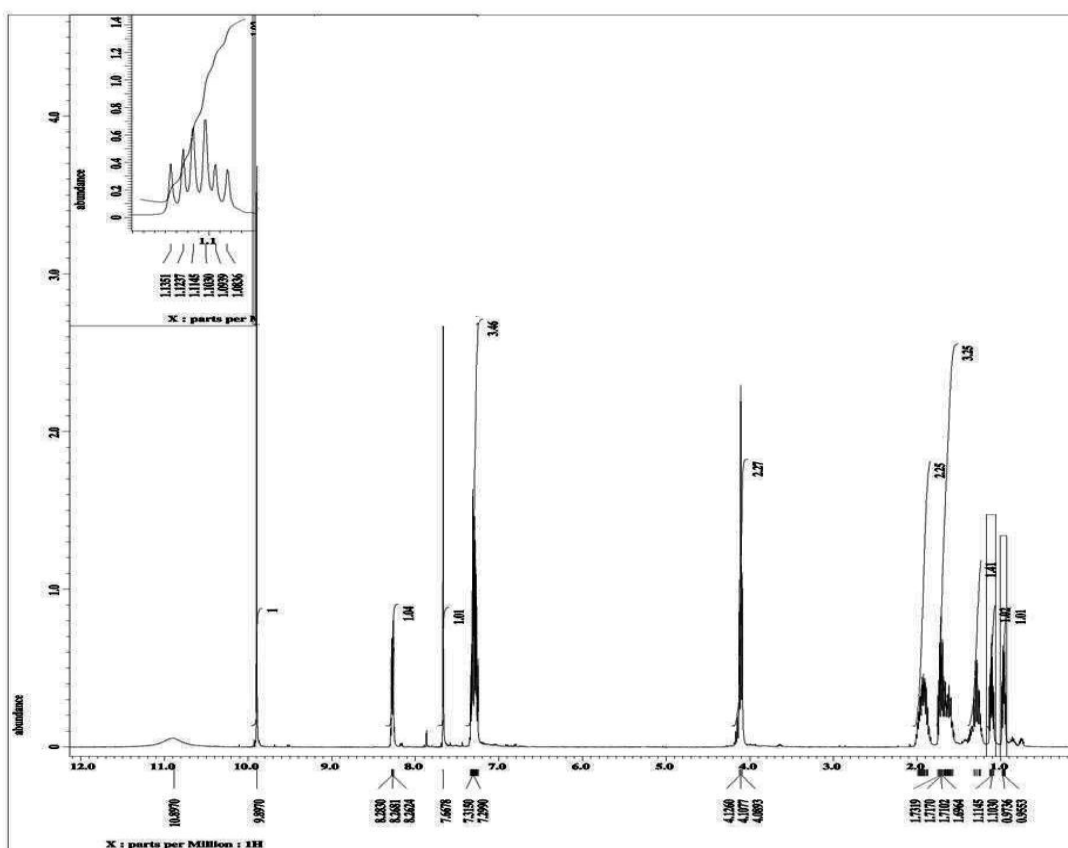
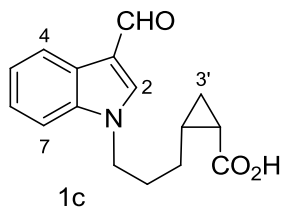
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|---|---------------|
| 1. X-ray Crystal Structures of Compounds 7b and 2a | S2-S3 |
| 2. NMR Spectra of compounds 1c , 4a , 4b , 5 , 6 , 6a , 7b , 8a , 8b , 2c , 3c | S4-S27 |

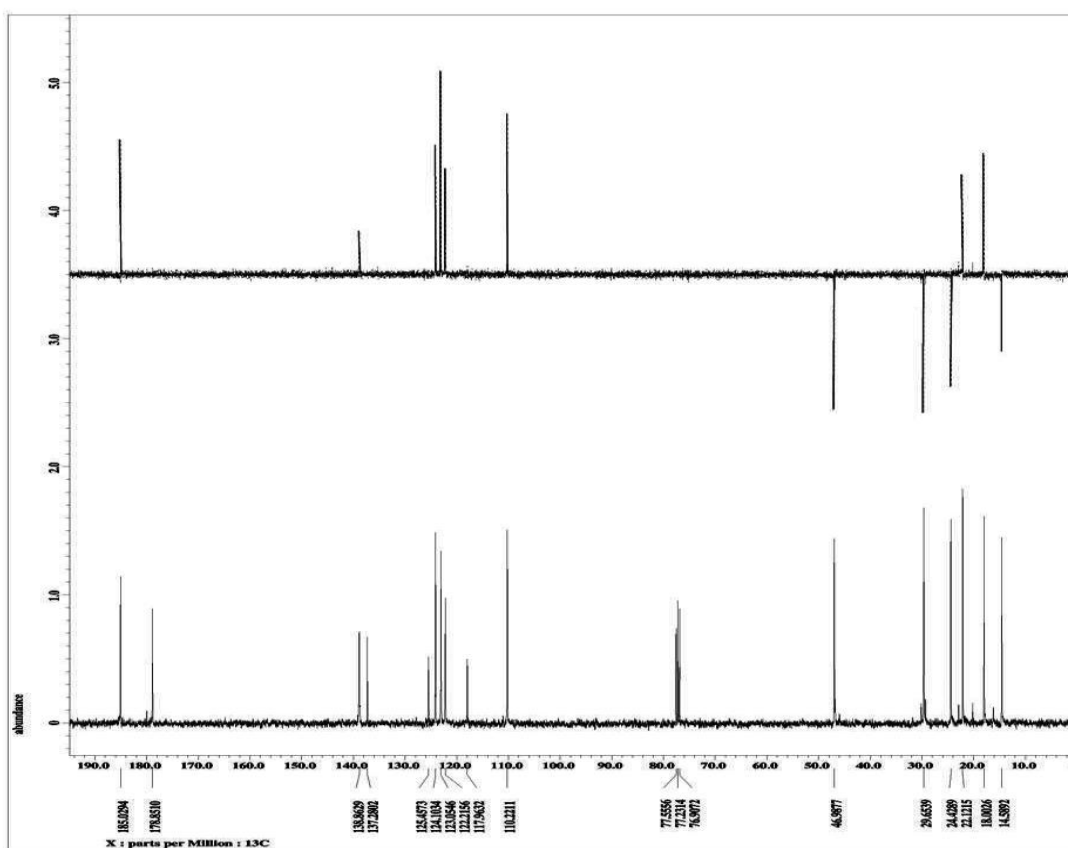
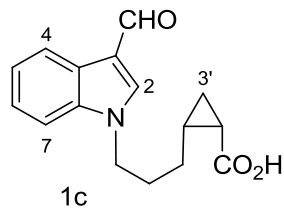
1-[(2'-bromocyclopropyl)-trans-methyl]-1H-benzimidazole (7b)

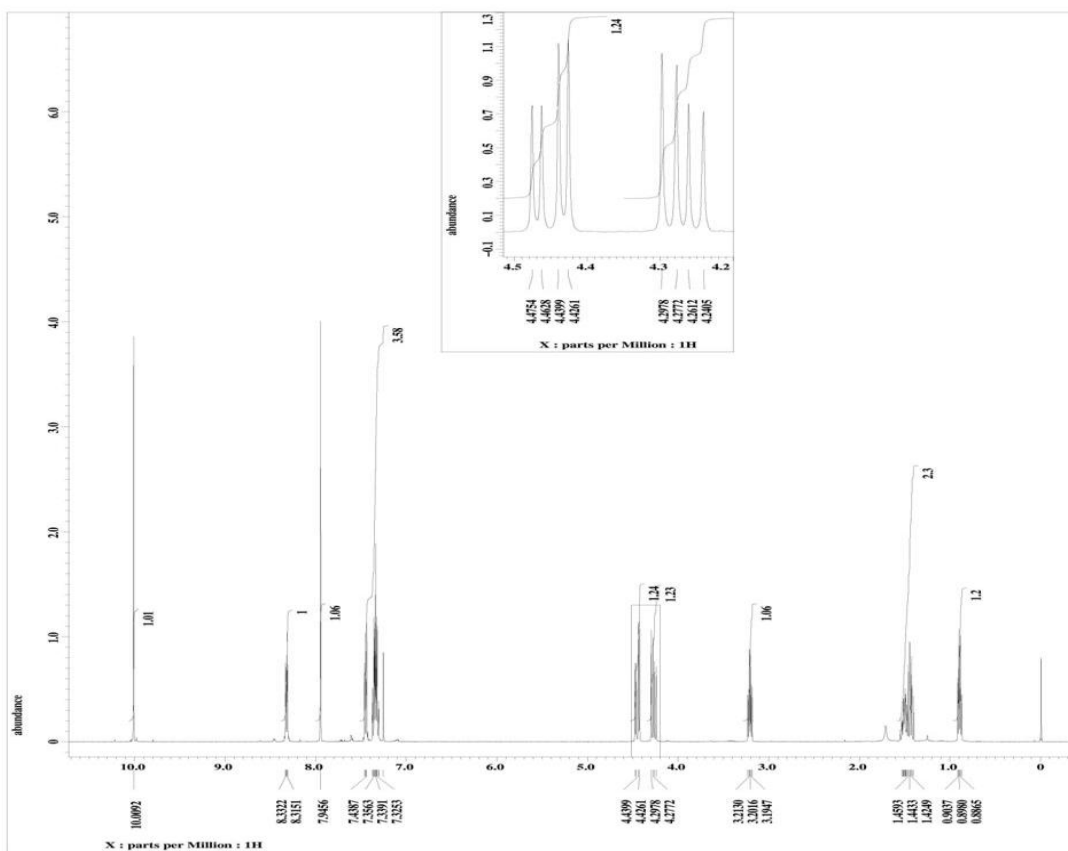
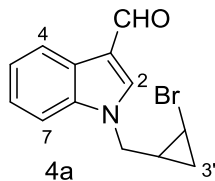
1,1a,2,8b-Tetrahydrocyclopropa[3,4]pyrrolo[1,2-a]indole-8-carbaldehyde (2a)

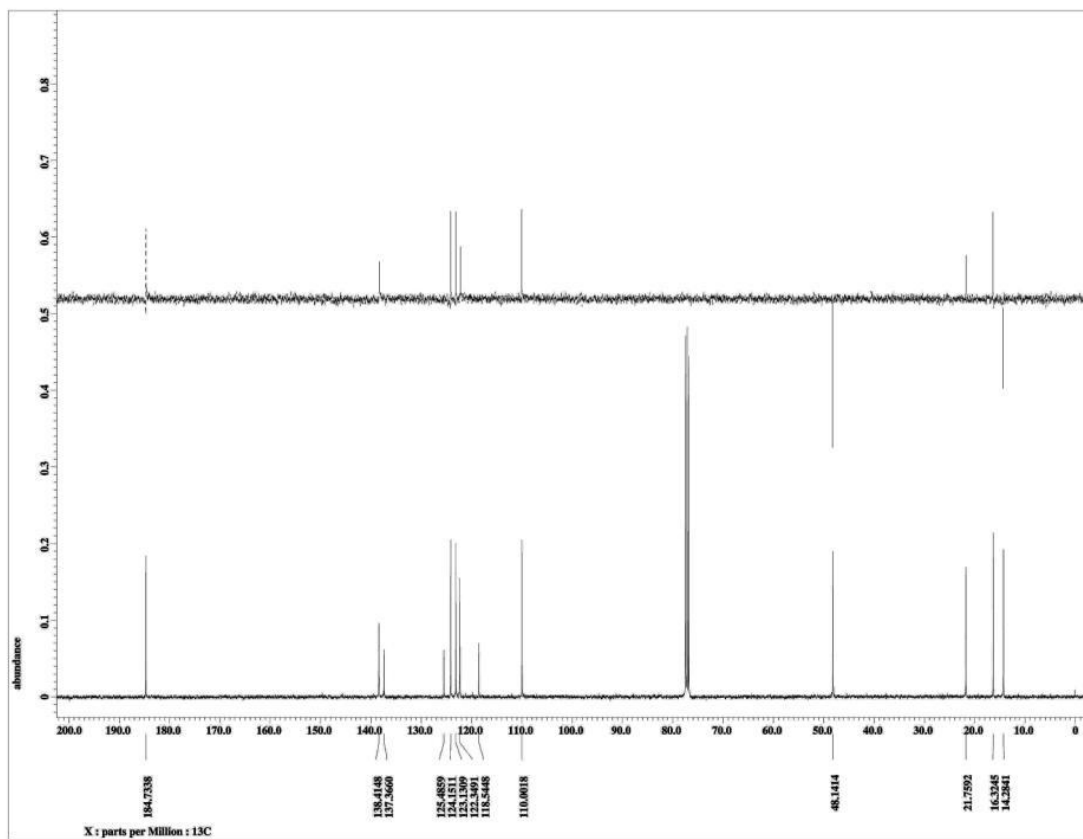
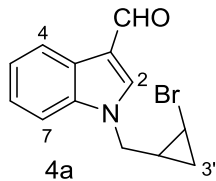
*Ethyl cis-2'-[3-(3-formyl-1H-indol-1-yl)propyl]cyclopropanecarboxylate*¹H NMR, 400 MHz, CDCl₃

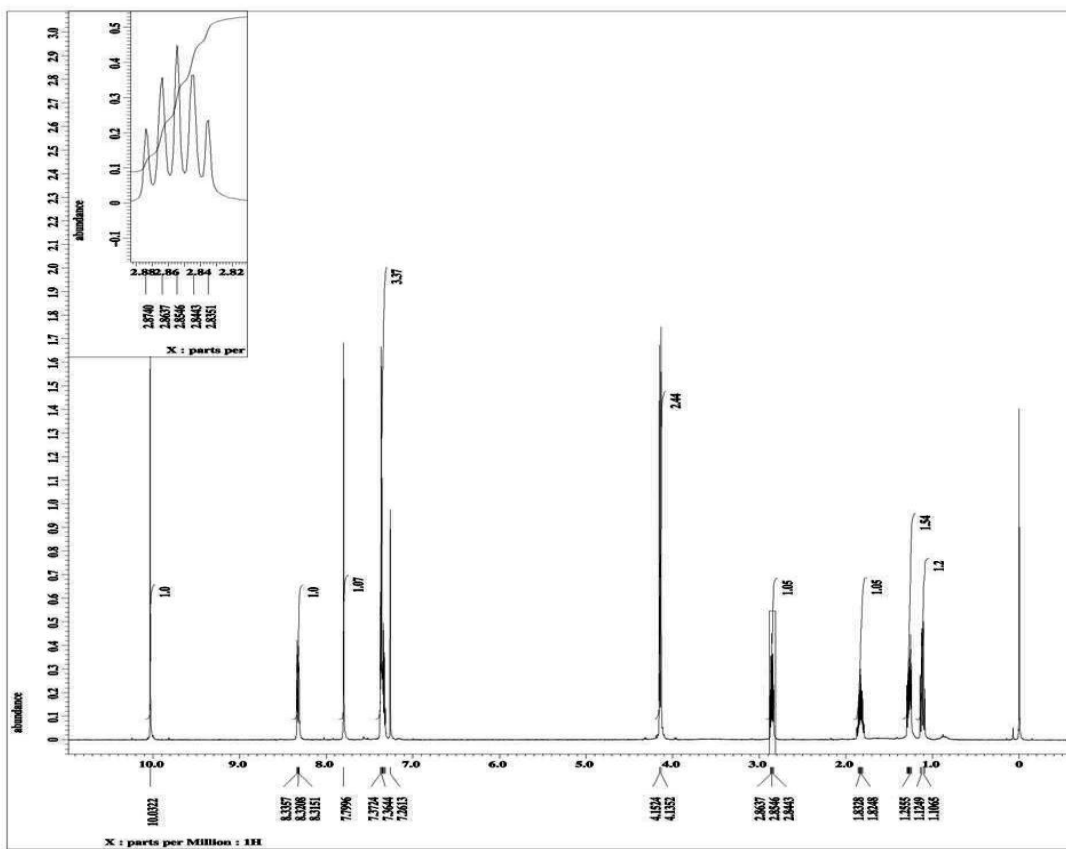
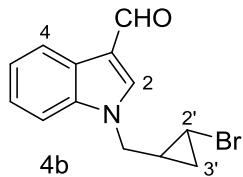
*Ethyl cis-2'-[3-(3-formyl-1H-indol-1-yl)propyl]cyclopropanecarboxylate*¹³C NMR, 100 MHz, CDCl₃

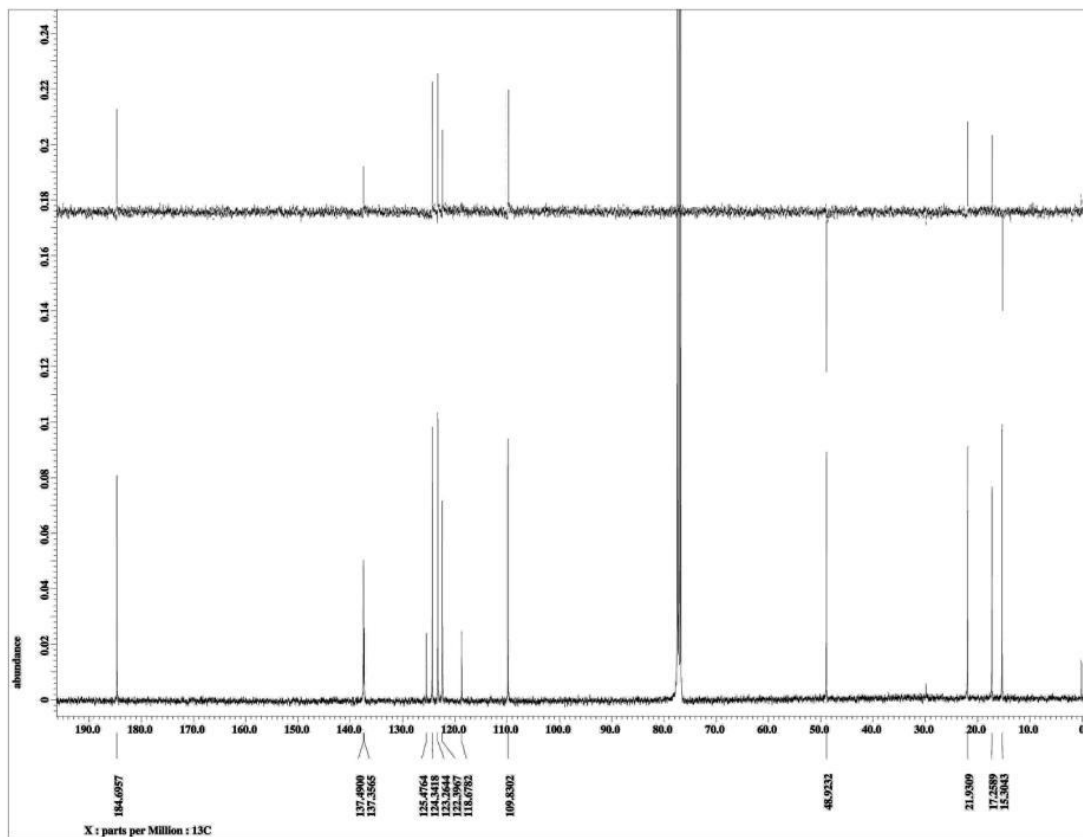
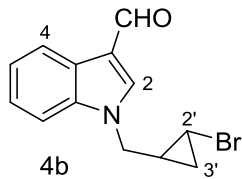
2'-[3-(3-Formyl-1H-indol-1-yl)propyl]-cis-cyclopropanecarboxylic acid (1c)**¹H NMR, 400 MHz, CDCl₃**

2'-[3-(3-Formyl-1H-indol-1-yl)propyl]-cis-cyclopropanecarboxylic acid (1c)**¹³C NMR, 100 MHz, CDCl₃**

*1-[(2'-Bromocyclopropyl)-cis-methyl]-1H-indole-3-carbaldehyde (4a)*¹H NMR, 400 MHz, CDCl₃

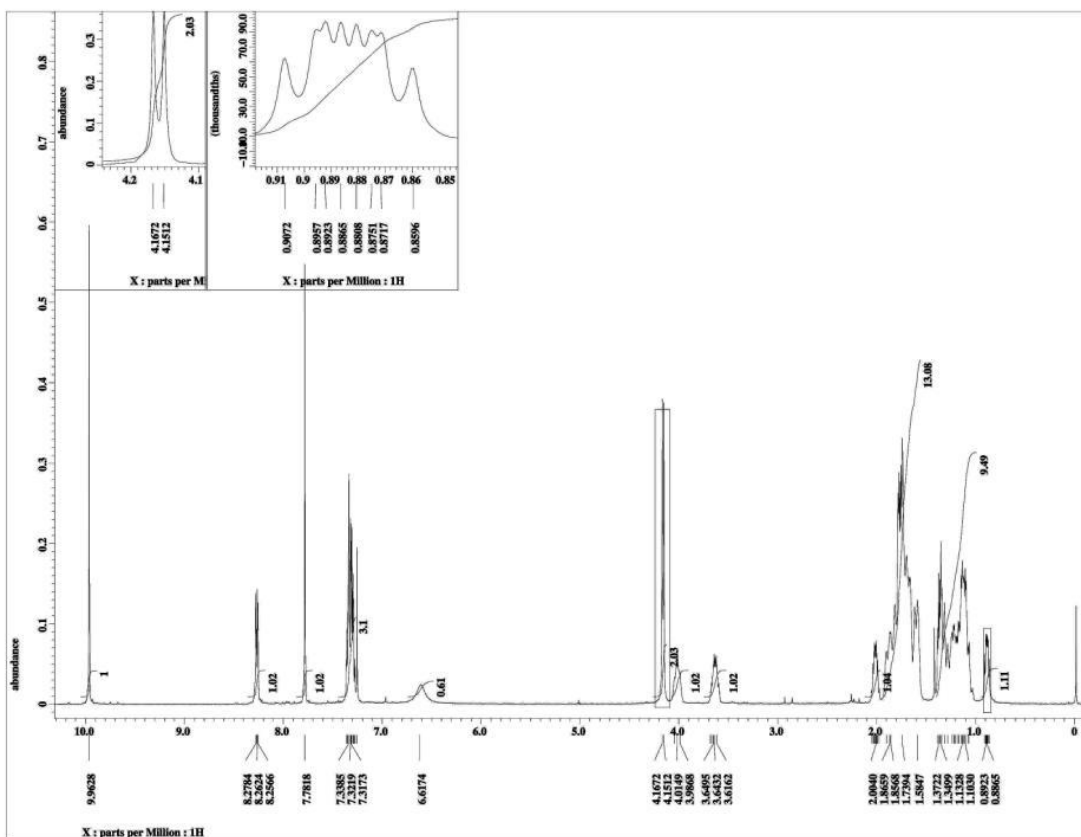
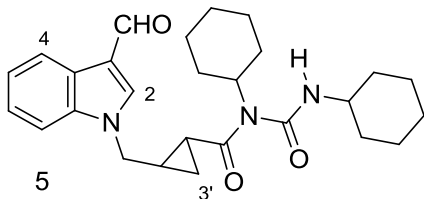
*1-[(2'-Bromocyclopropyl)-cis-methyl]-1H-indole-3-carbaldehyde (4a)*¹³C NMR, 100 MHz, CDCl₃

*1-[(2'-Bromocyclopropyl)-trans-methyl]-1H-indole-3-carbaldehyde (4b)*¹H NMR, 400 MHz, CDCl₃

*1-[(2'-Bromocyclopropyl)-trans-methyl]-1H-indole-3-carbaldehyde (4b)*¹³C NMR, 100 MHz, CDCl₃

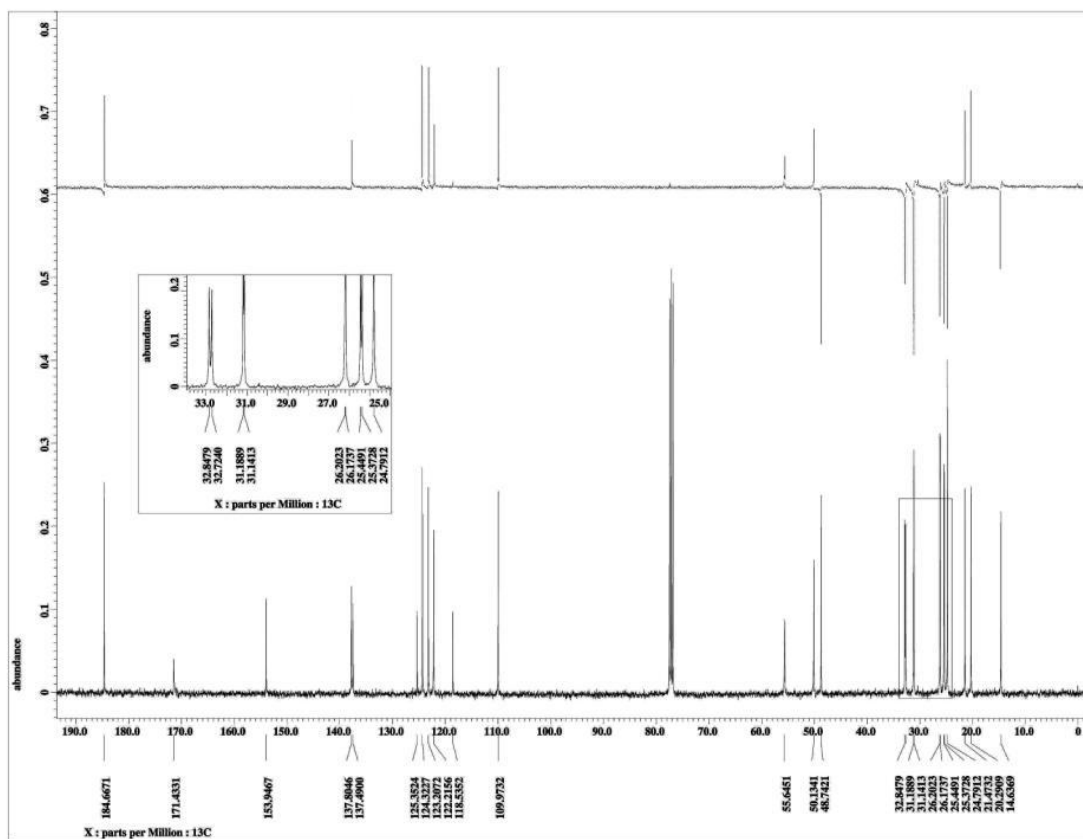
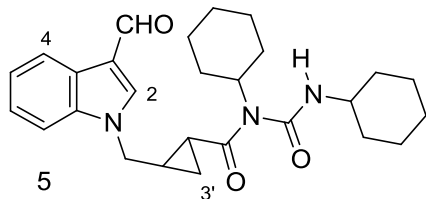
N-cyclohexyl-*N*-[(cyclohexylamino)carbonyl]-2'-*trans*-[(3-formyl-1*H*-indol-1-yl)methyl]cyclopropanecarboxamide (5)

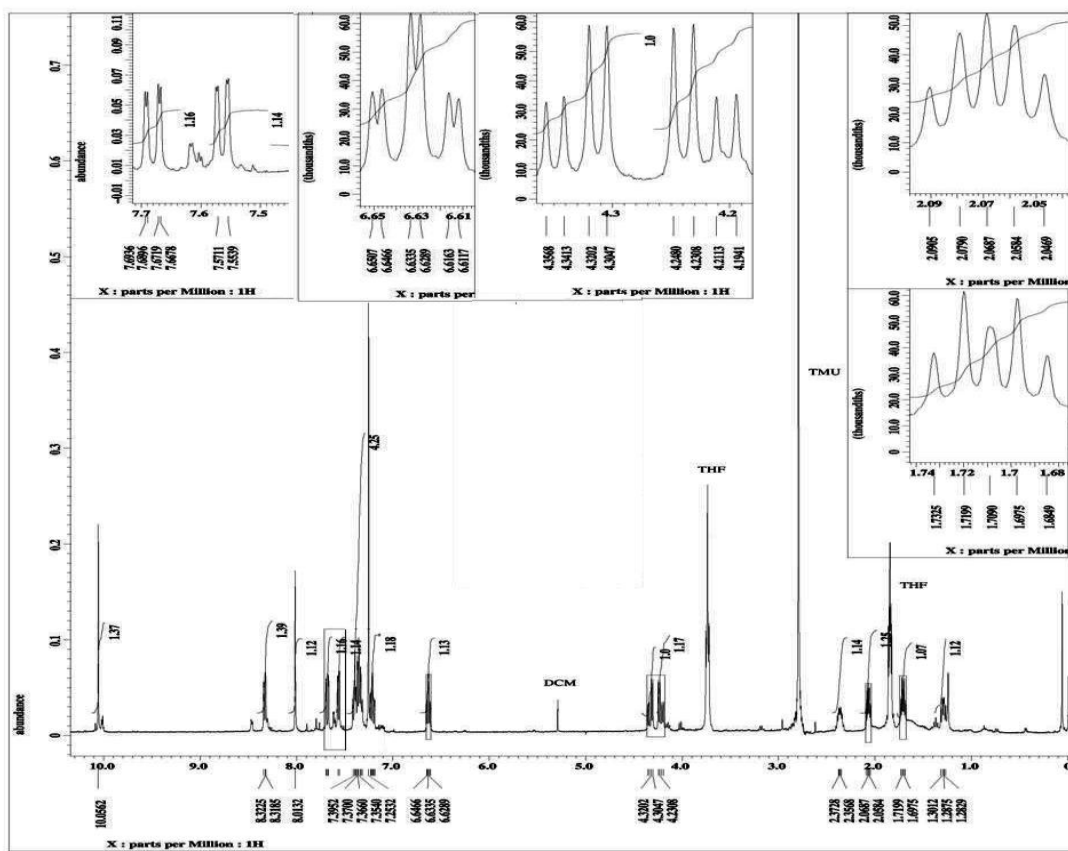
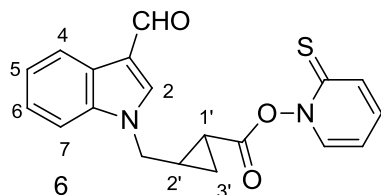
¹H NMR, 400 MHz, CDCl₃

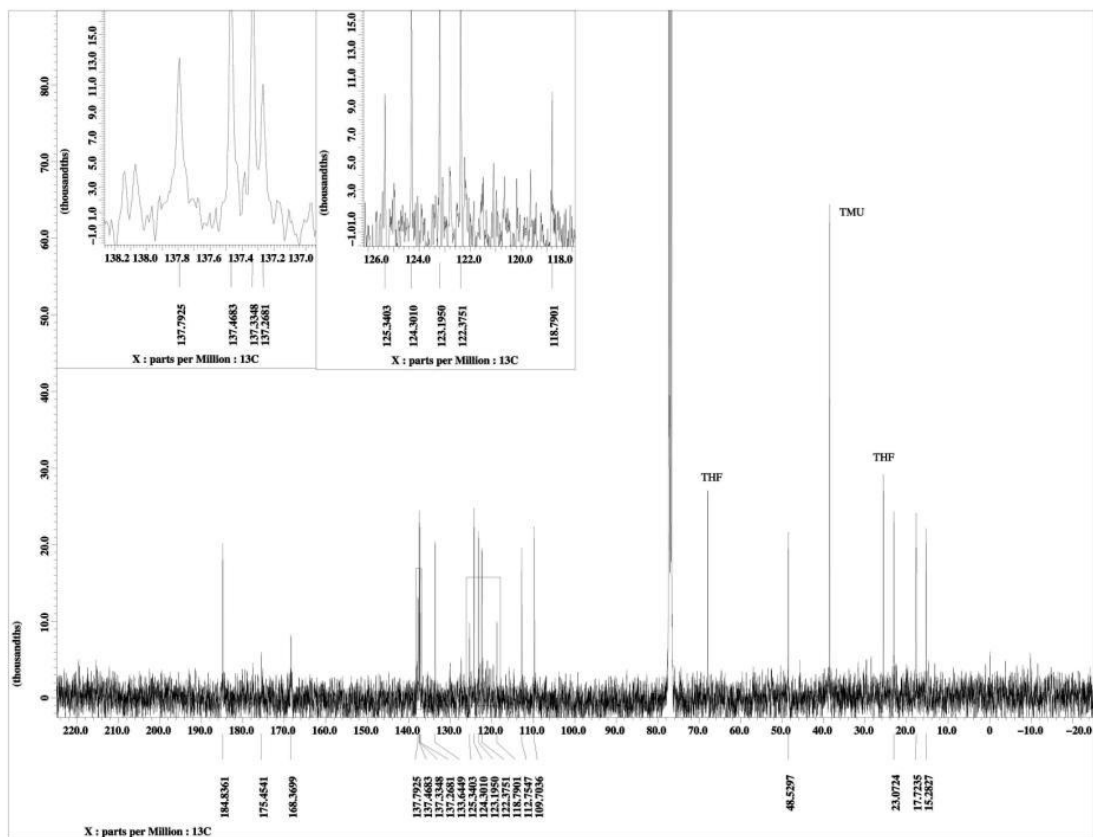
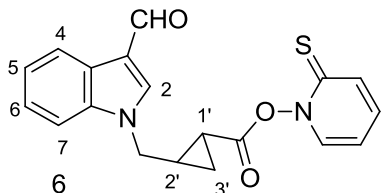


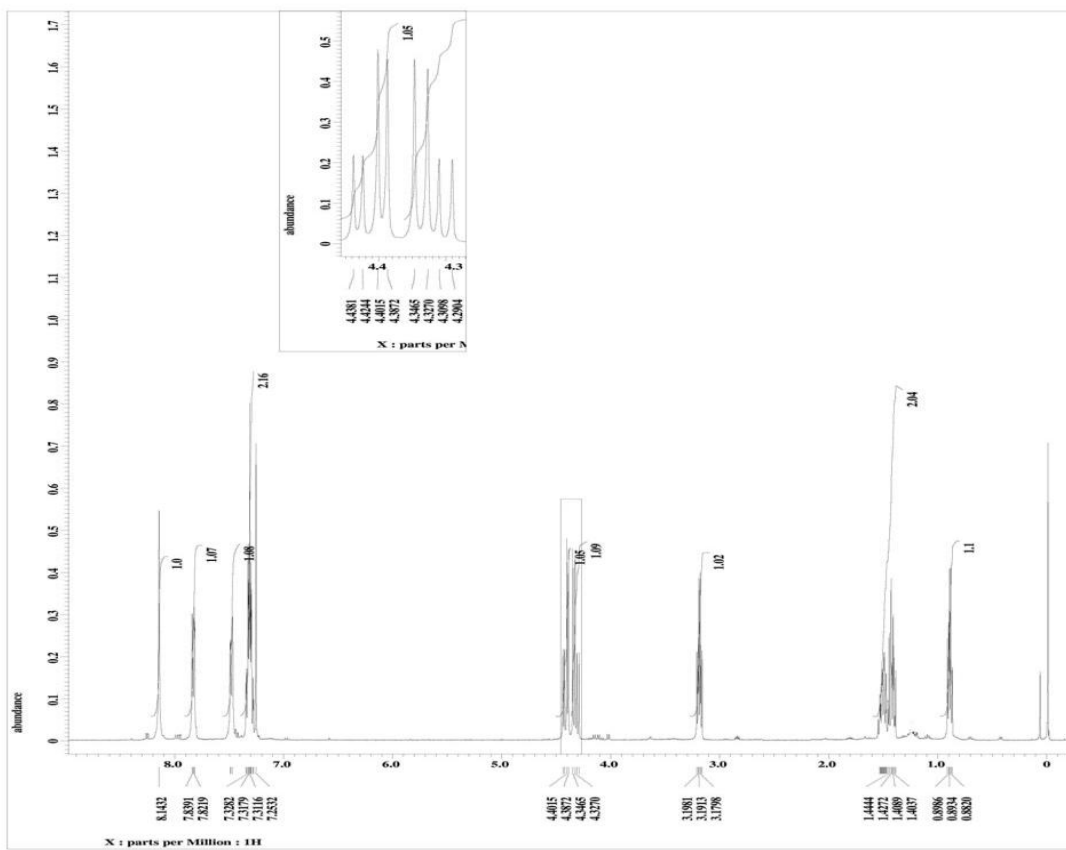
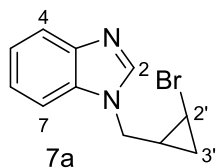
N-cyclohexyl-*N*-[(cyclohexylamino)carbonyl]-2'-*trans*-[(3-formyl-1*H*-indol-1-yl)methyl]cyclopropanecarboxamide (5)

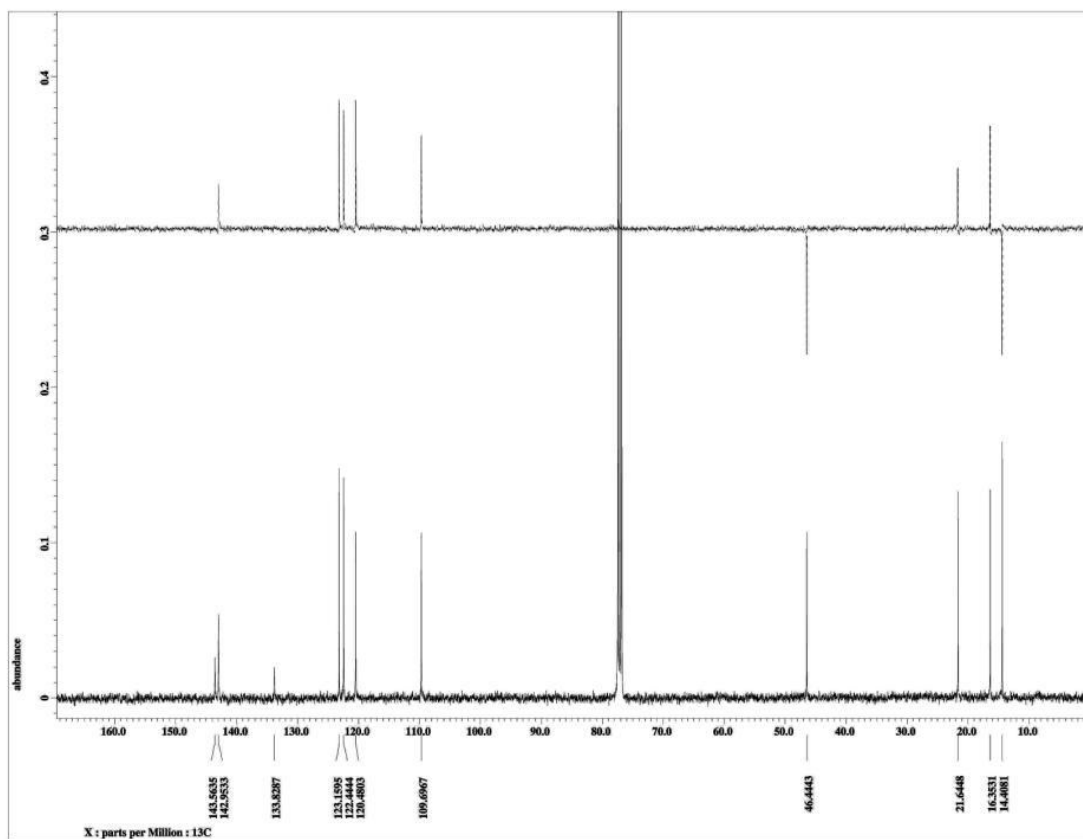
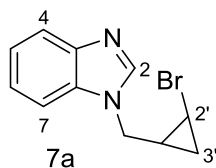
^{13}C NMR, 100 MHz, CDCl_3

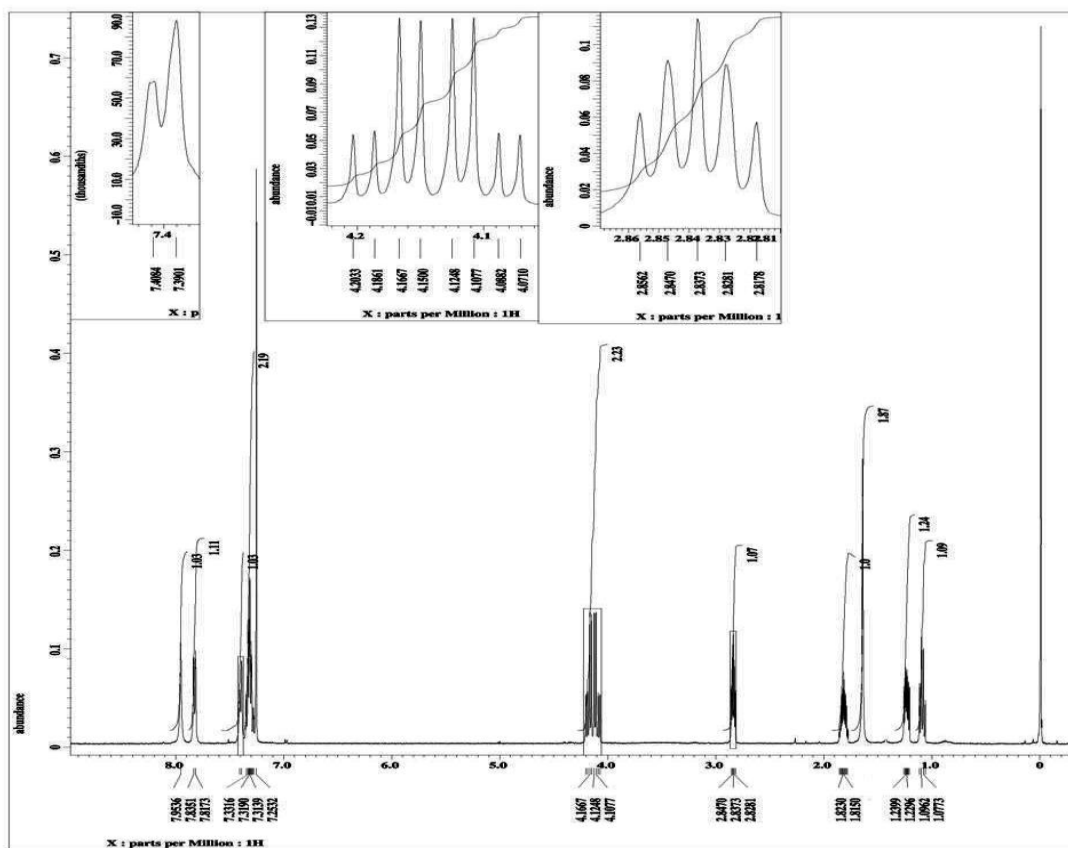
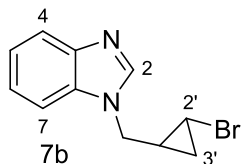


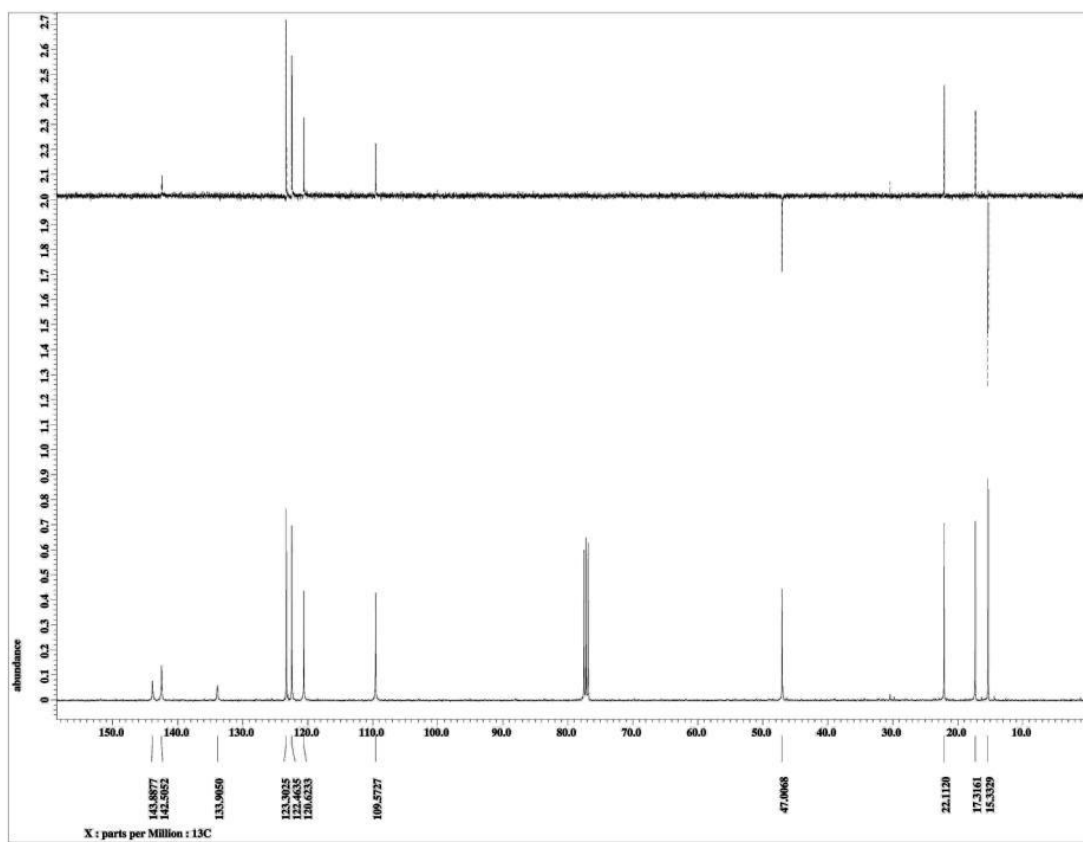
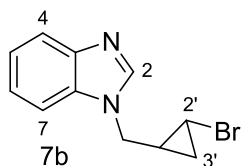
Barton Ester Intermediate (6)**¹H NMR, 400 MHz, CDCl₃**

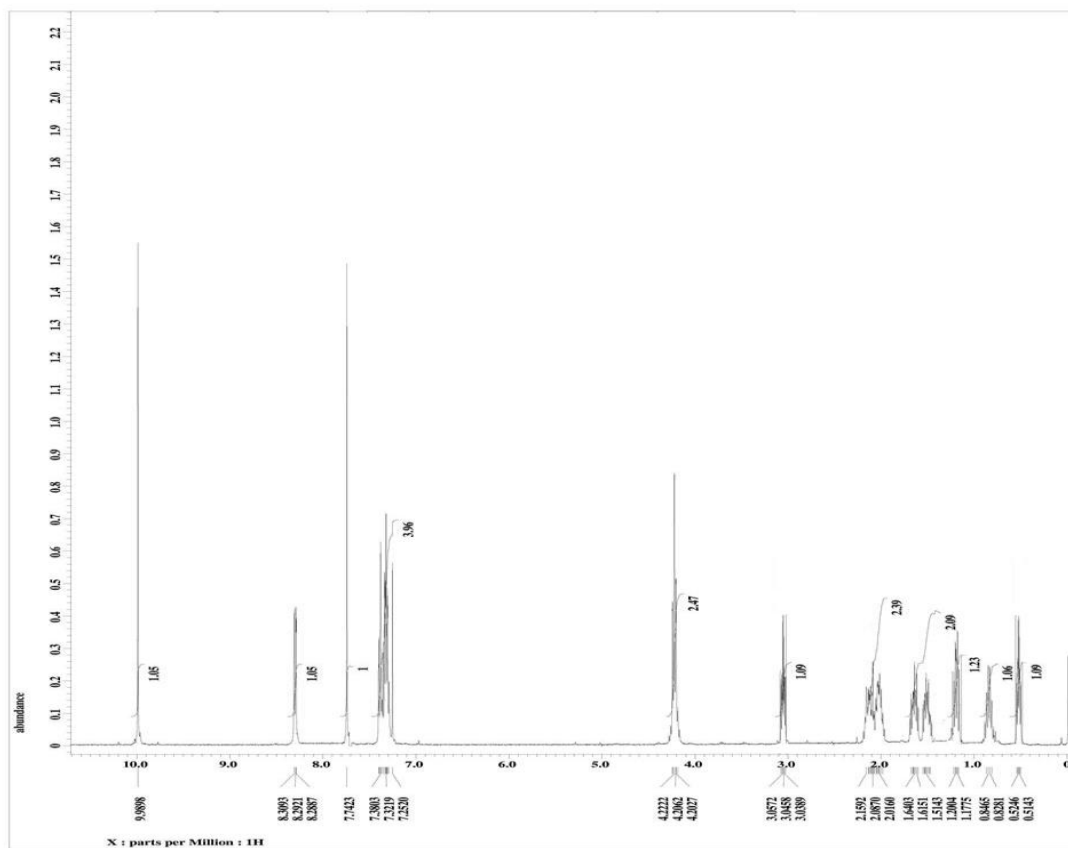
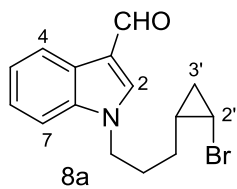
Barton Ester Intermediate (6)**¹H NMR, 400 MHz, CDCl₃**

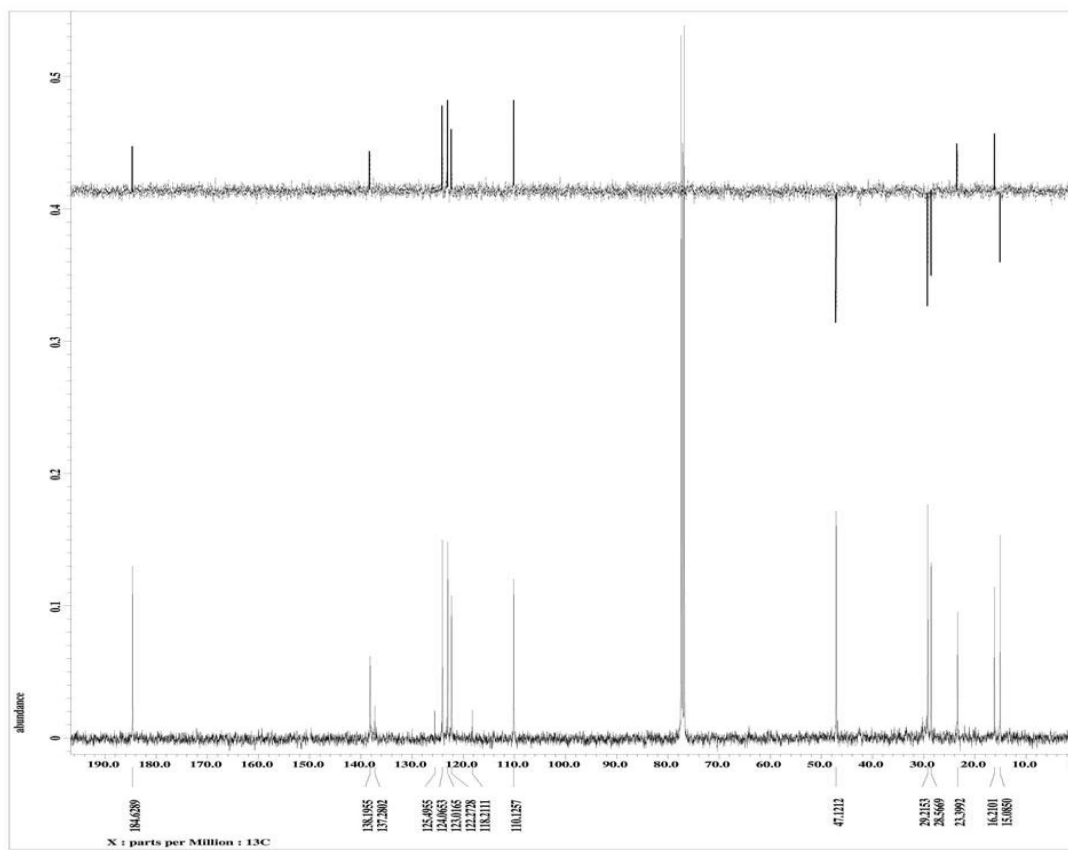
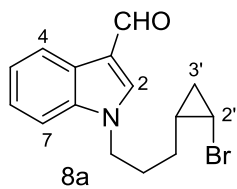
*1-[(2'-Bromocyclopropyl)-cis-methyl]-1H-benzimidazole (7a)*¹H NMR, 400 MHz, CDCl₃

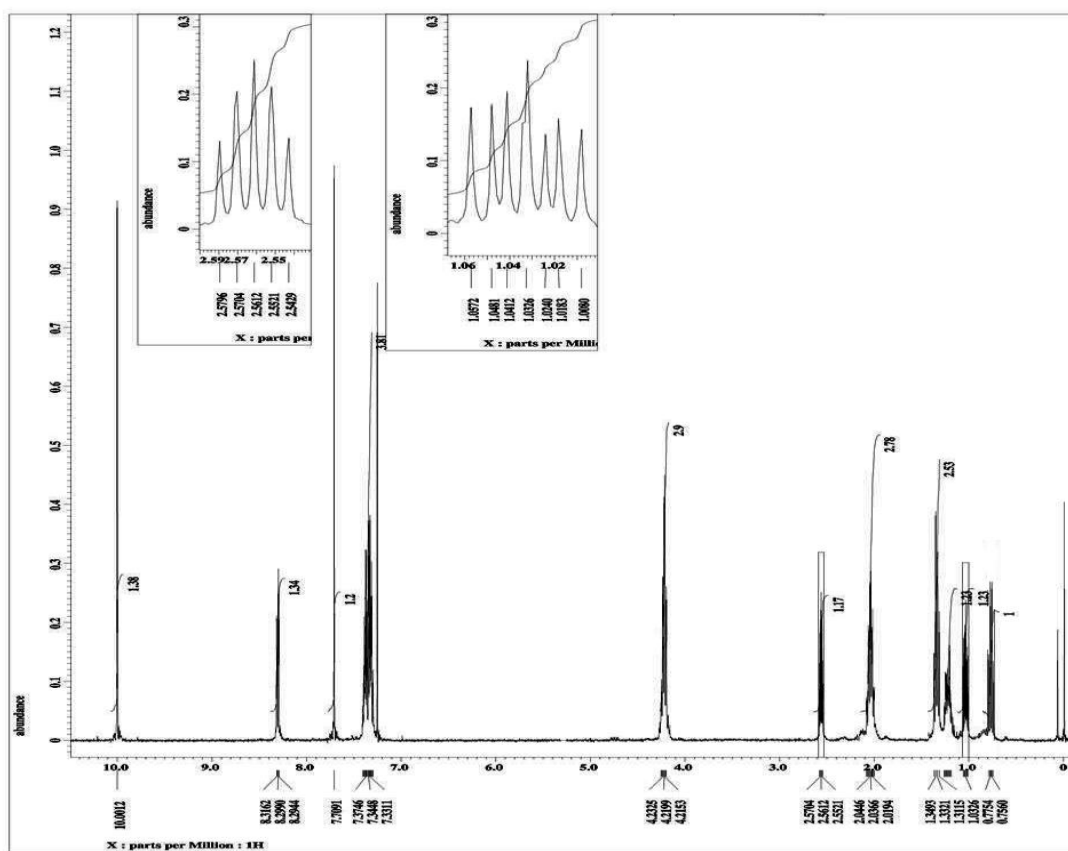
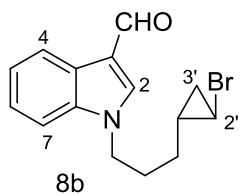
1-[(2'-Bromocyclopropyl)-cis-methyl]-1H-benzimidazole (7a) ^{13}C NMR, 100 MHz, CDCl_3 

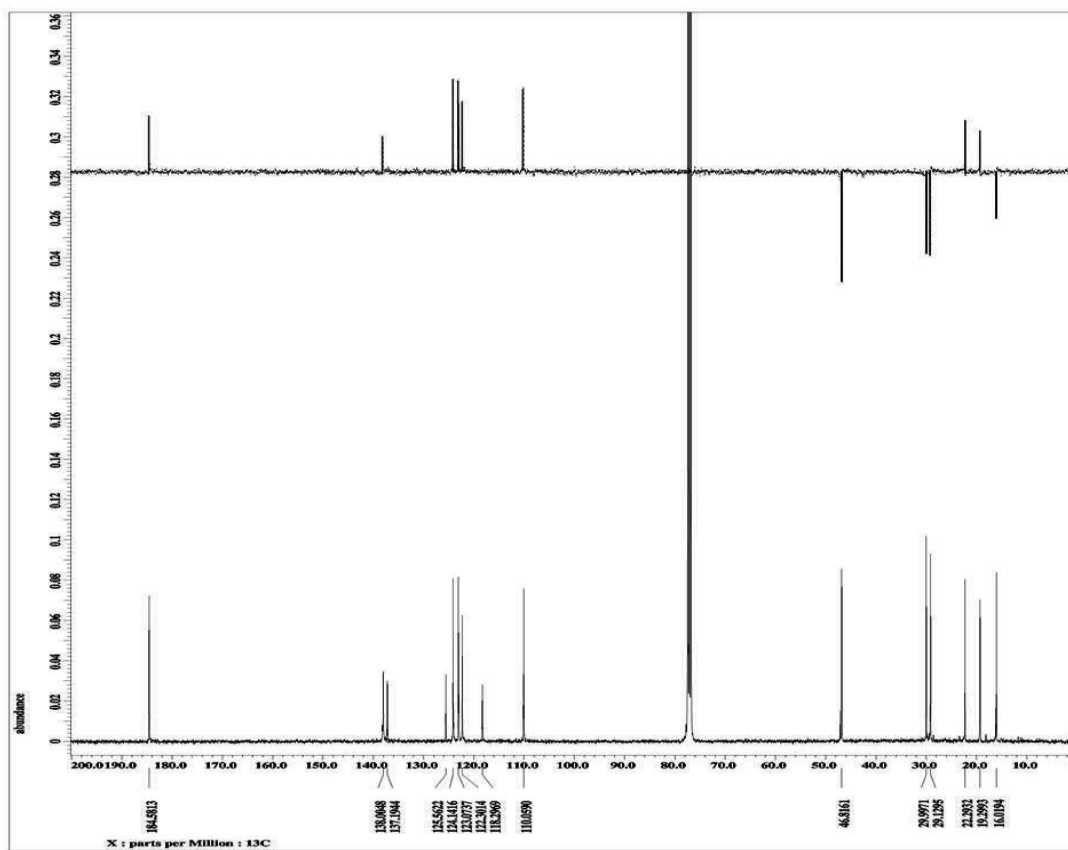
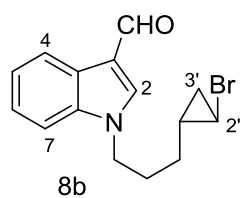
*1-[(2'-Bromocyclopropyl)-trans-methyl]-1H-benzimidazole (7b)*¹H NMR, 400 MHz, CDCl₃

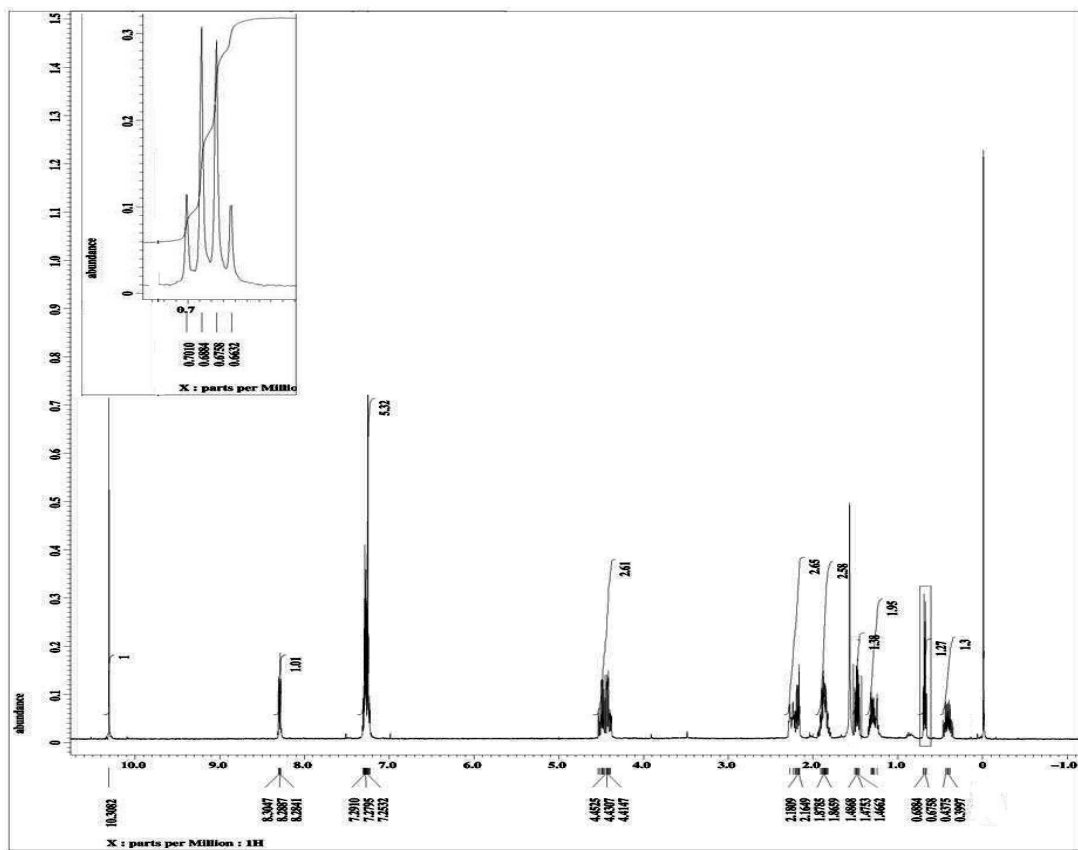
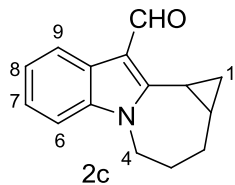
1-[(2'-Bromocyclopropyl)-trans-methyl]-1H-benzimidazole (7b) ^{13}C NMR, 100 MHz, CDCl_3 

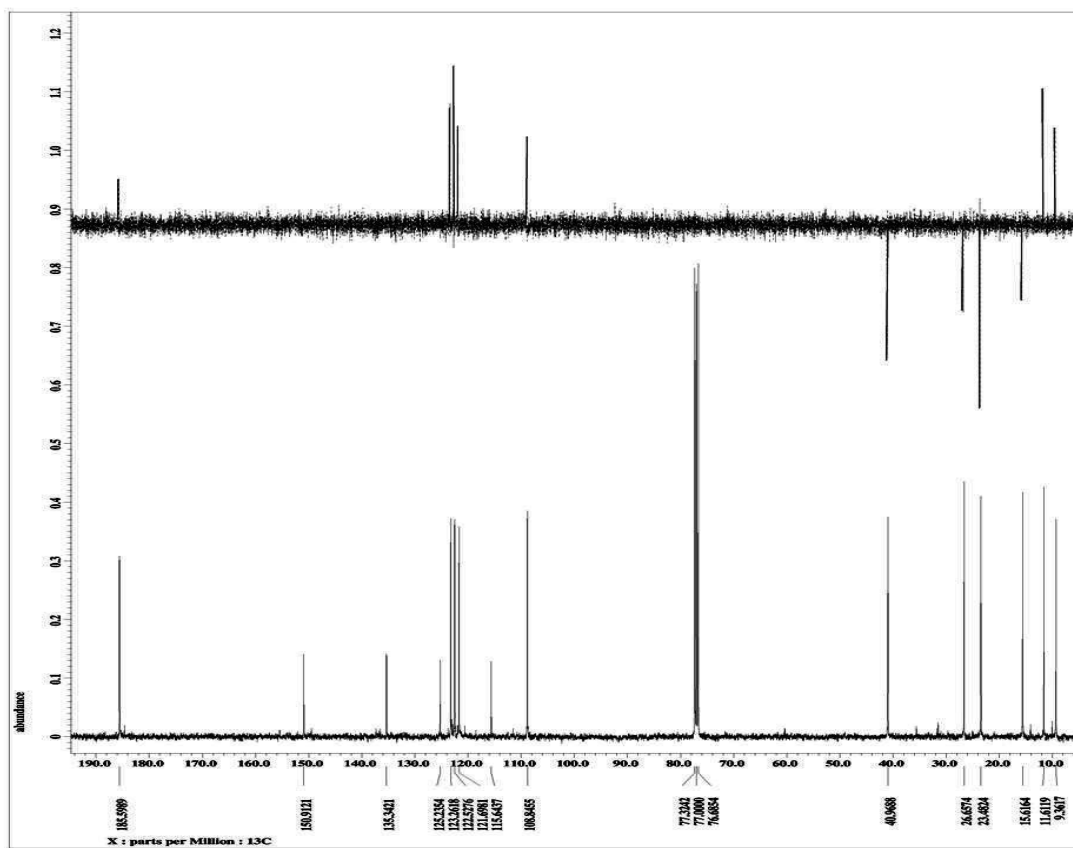
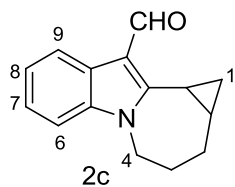
*1-[3-(2'-Bromocyclopropyl)-cis-propyl]-1H-indole-3-carbaldehyde (8a)*¹H NMR, 400 MHz, CDCl₃

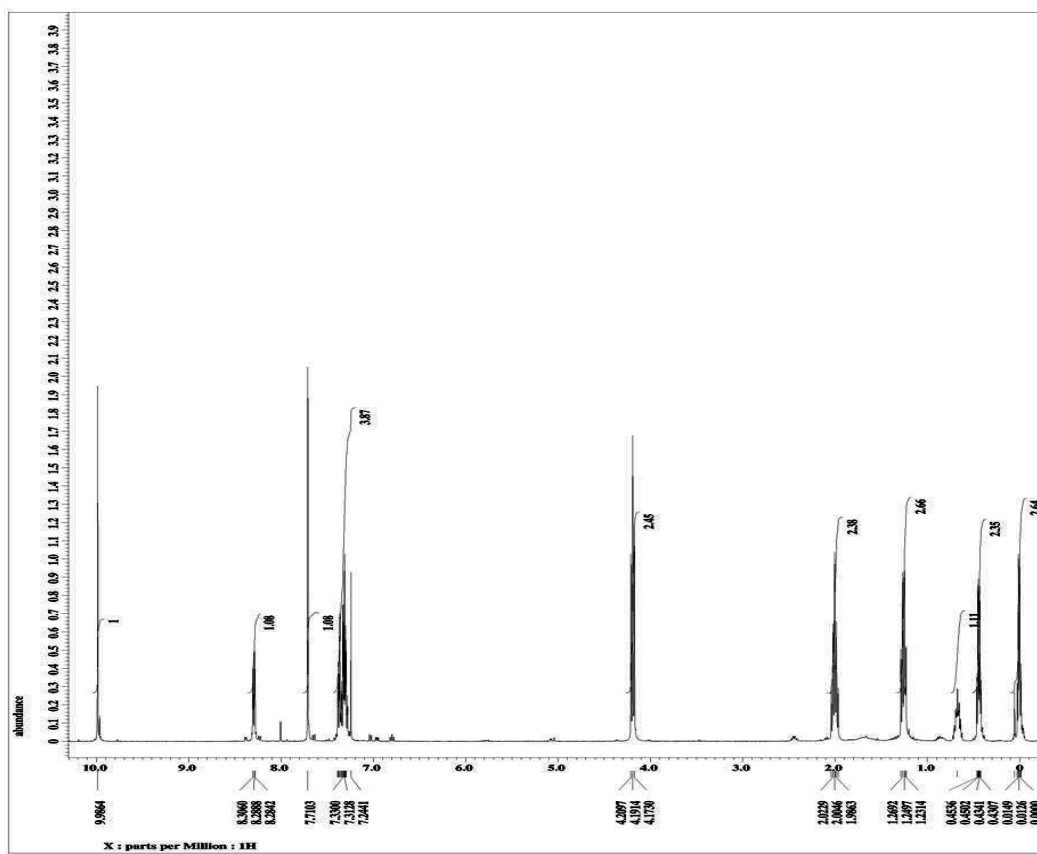
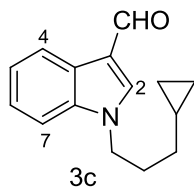
*1-[3-(2'-Bromocyclopropyl)-cis-propyl]-1H-indole-3-carbaldehyde (8a)*¹³C NMR, 100 MHz, CDCl₃

1-[3-(2'-Bromocyclopropyl)-trans-propyl]-1H-indole-3-carbaldehyde (8b) ^1H NMR, 400 MHz, CDCl_3 

1-[3-(2'-Bromocyclopropyl)-trans-propyl]-1H-indole-3-carbaldehyde (8b) ^{13}C NMR, 100 MHz, CDCl_3 

1,1a,2,3,4,10b-Hexahydrocyclopropa[3,4]azepino[1,2-*a*]indole-10-carbaldehyde (**2c**)¹H NMR, 400 MHz, CDCl₃

1,1a,2,3,4,10b-Hexahydrocyclopropa[3,4]azepino[1,2-*a*]indole-10-carbaldehyde (**2c**)¹³C NMR, 100 MHz, CDCl₃

*1-(3-Cyclopropylpropyl)-1H-indole-3-carbaldehyde (3c)*¹H NMR, 400 MHz, CDCl₃

*1-(3-Cyclopropylpropyl)-1H-indole-3-carbaldehyde (3c)*¹³C NMR, 100 MHz, CDCl₃