SUPPORTING INFORMATION

Platinum-catalyzed Cyclization Reaction of Alkynes: Synthesis of Azepino[3,4-b]indol-1-ones

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1-Methyl-1H-indole-2-carboxylic acid methyl-prop-2-ynyl-amide (4a)
1-Methyl-\(1H\)-indole-2-carboxylic acid methyl-(3-\(p\)-tolyl-prop-2-ynyl)-amide (5a)
1-Methyl-1H-indole-2-carboxylic acid [3-(3,4-dimethyl-phenyl)-prop-2-ynyl]-methyl-amide (5b)
1-Methyl-1H-indole-2-carboxylic acid [3-(4-methoxy-phenyl)-prop-2-ynyl]-methyl-amide (5c)

Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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1-Methyl-1H-indole-2-carboxylic acid [3-(4-chloro-phenyl)-prop-2-ynyl]-methyl-amide (5d)

**NMR Spectrum**

- **Chemical Shifts:**
  - 8.0-7.0 ppm
  - 7.4-7.3 ppm
  - 7.1-7.0 ppm
  - 6.8-6.7 ppm
  - 7.6-7.0 ppm

- **Resonance Assignments:**
  - 1H 8.02, 5.02, 3.07, 2.06
  - 13C 164.02, 31.18, 77.00, 84.16

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1-Methyl-1H-indole-2-carboxylic acid methyl-[3-(4-trifluoromethyl-phenyl)-prop-2-ynyl]-amide (5e)
1-Methyl-1H-indole-2-carboxylic acid [3-(4-cyano-phenyl)-prop-2-ynyl]-methyl-amide (5f)

![NMR spectrum of compound 5f](image)

**NMR Spectral Data**

- **Chemical Shifts (δ ppm):**
  - 3.5, 4.0, 4.5, 5.0, 5.5, 6.0, 6.5, 7.0, 7.5, 8.0 ppm
  - 3.31, 3.88, 4.64, 6.81, 7.13, 7.14, 7.16, 7.16, 7.16, 7.18, 7.19, 7.26, 7.30, 7.30, 7.32, 7.32, 7.33, 7.35, 7.35, 7.37, 7.40, 7.54, 7.54, 7.56, 7.57, 7.62, 7.63, 7.64, 7.65, 7.66, 13.26, 88.40, 109.91, 112.01, 118.30, 120.37, 121.70, 123.72, 126.21, 130.81, 132.07, 132.33, 138.11, 164.11

- **Resonance Assignments:**
  - 2.03, 2.07, 2.07, 4.98, 7.19, 7.66, 11.36
1-Methyl-1H-indole-2-carboxylic acid [3-(4-acetyl-phenyl)-prop-2-ynyl]-methyl-amide (5g)

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4-\{3-[Methyl-(1-methyl-1H-indole-2-carbonyl)-amino]-prop-1-ynyl\}-benzoic acid ethyl ester (5h)
1-Methyl-1H-indole-2-carboxylic acid methyl-(3-naphthalen-1-yl-prop-2-ynyl)-amide (5i)
1-Methyl-1H-indole-2-carboxylic acid (3-furan-2-yl-prop-2-ynyl)-methyl-amide (5j)

[Chemical structure image]

[1H NMR spectrum image]

[13C NMR spectrum image]
1-Methyl-1H-indole-2-carboxylic acid methyl-(3-thiophen-2-yl-prop-2-ynyl)-amide (5k)
1-Methyl-1H- indole-2-carboxylic acid methyl-(3-pyridin-2-yl-prop-2-ynyl)-amide (5l)
4-Methoxy-3-{3-[methyl-(1-methyl-1H-indole-2-carbonyl)-amino]-prop-1-ynyl}-benzoic acid methyl ester (5m)
Benzyl-(prop-2-ynyl)-amine

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Benzyl-(3-<i>p</i>-tolyl-prop-2-ynyl)-amine
1-Methyl-1H-indole-2-carboxylic acid benzyl-(3-p-tolyl-prop-2-ynyl)-amide (5o)
2,10-Dimethyl-5-\(p\)-tolyl-3,10-dihydro-2\(H\)-azepino[3,4-b]indol-1-one (6a)
2,6-Dimethyl-5-p-tolyl-3,6-dihydro-2H-azepino[4,3-b]indol-1-one (7a)
5-(3,4-Dimethylphenyl)-2,10-dimethyl-3,10-dihydro-2H-azepino[3,4-b]indol-1-one (6b)
5-(4-Methoxyphenyl)-2,10-dimethyl-3,10-dihydro-2H-azepino[3,4-b]indol-1-one (6c)
5-(4-Chlorophenyl)-2,10-dimethyl-3,10-dihydro-2H-azepino[3,4-b]indol-1-one (6d)
4-(4-Chlorobenzyl)-2,9-dimethyl-2,9-dihydro-β-carbolin-1-one (8d)

13 C-NMR: not enough product for good spectra!
2,10-Dimethyl-5-(4-trifluoromethylphenyl)-3,10-dihydro-2H-azepino[3,4-b]indol-1-one (6e)
2,9-Dimethyl-4-(4-trifluoromethyl-benzyl)-2,9-dihydro-β-carbolin-1-one (8e)
4-(2,9-Dimethyl-1-oxo-2,9-dihydro-1H-β-carboline-4-ylmethyl)-benzonitrile (8f)
5-(4-Acetylphenyl)-2,10-dimethyl-3,10-dihydro-2H-azepino[3,4-b]indol-1-one (6g)
4-(4-Acetylbenzyl)-2,9-dimethyl-2,9-dihydro-β-carbolin-1-one (8g)
4-(2,10-Dimethyl-1-oxo-1,2,3,10-tetrahydro-azepino[3,4-b]indol-5-yl)-benzoic acid ethyl ester (6h)
4-(2,9-Dimethyl-1-oxo-2,9-dihydro-1H-β-carbolin-4-ylmethyl)-benzoic acid ethyl ester (8h)
2,10-Dimethyl-5-naphthalen-1-yl-3,10-dihydro-2H-azepino[3,4-b]indol-1-one (6i)
5-Furan-2-yl-2,10-dimethyl-3,10-dihydro-2H-azepino[3,4-b]indol-1-one (6j)

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2,10-Dimethyl-5-thiophen-2-yl-3,10-dihydro-2H-azepino[3,4-b]indol-1-one (6k)
3-(2,10-Dimethyl-1-oxo-1,2,3,10-tetrahydro-azepino[3,4-b]indol-5-yl)-4-methoxy-benzoic acid methyl ester (6m)
3-(2,6-Dimethyl-1-oxo-1,2,3,6-tetrahydro-azepino[4,3-b]indol-5-yl)-4-methoxy-benzoic acid methyl ester (7m)
2,4,9-Trimethyl-2,9-dihydro-β-carbolin-1-one (8n)
2-Benzyl-10-methyl-5-\(p\)-tolyl-3,10-dihydro-2\(H\)-azepino[3,4-b]indol-1-one (6o)

6o / 7o = 5.7 : 1