Supporting Information

A Gold(I)-Catalyzed Substituent-Controlled Cycloisomerization of Propargyl Vinyl Ethers to Multi-Substituted Furofuran and Furopyran Derivatives

Yongxiang Liu, * Shengfei Jin, Yanshi Wang, Shanshan Cui, Xiaoshi Peng, Yuanyuan Niu, Chuan Du and Maosheng Cheng*

* Key Laboratory of Structure-Based Drug Design and Discovery (Shenyang Pharmaceutical University), Ministry of Education, Shenyang 110016, P. R. China. Institute of Drug Research in Medicine Capital of China, Benxi, 117000, P. R. China
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1. General Information

Unless otherwise noted, reagents were obtained commercially and used without further purification. Tetrahydrofuran was distilled from sodium under a nitrogen atmosphere. Dichloroethane was distilled from calcium chloride under a nitrogen atmosphere. TLC analysis of reaction mixtures was performed on Dynamic absorbents silica gel F-254 TLC plates. Flash chromatography was carried out on Zeoprep 60 (200-300 mesh) silica gel. $^1$H and $^{13}$C NMR spectra were recorded with Bruker Avance-III 600 spectrometers and referenced to CDCl$_3$ and DMSO-d$_6$. HR-ESI-MS was recorded on a Bruker micro-TOFQ-Q instrument. IR spectra were recorded on a Bruker IFS 55 spectrometer. Melting points were tested on Thomas Hoover capillary melting point apparatus.

2. Detailed Information for the Reaction Condition Screening

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3. General Procedures for the Preparation of Propargylic Alcohols (A1-A8) and Characterization Data

To a stirring solution of alkyne (5 mmol) in THF (5 mL) was added dropwise $n$-BuLi (1.0 M in THF, 5.5 mL) at $-78 \degree C$. Paraformaldehyde (6 mmol, 180 mg) was added portionwise after 0.5 h. The solution was warmed to room temperature after 1.0 h. The reaction was monitored by TLC till the consumption of the starting material; the reaction mixture was quenched by addition of saturated aqueous ammonium chloride (20 mL) and extracted with ethyl acetate three times (20 mL). The combined organic layers were washed with brine, dried over anhydrous Na$_2$SO$_4$, and concentrated in vacuo. The crude material was purified by a flash column chromatography on silica gel using petroleum ether/ethyl acetate as eluent to obtain the propargylic alcohols A1-A3, A5-A6. A4, A7 and A8 are commercially available.

4. General Procedures for the Preparation of Propargyl γ-Butyrolactone-2-enol Ether (1, 1a-1c, 3a-3d) and Characterization Data

$$
\text{R} = \equiv + \overset{n\text{-BuLi}}{\underset{-78 \degree C, THF}{\overset{\text{O}}{\underset{\text{H}}{\underset{\text{H}}{\text{H}}}}} \rightarrow \text{R} = \equiv \overset{\text{OH}}{\text{OH}}}
$$

A1-A8

$$
\text{MeO-} + \overset{\text{OH}}{\underset{\text{Me}}{\underset{\text{OH}}{\underset{\text{OH}}{\text{OH}}}}}
$$

A1$^1$

$$
\text{PentylO-} + \overset{\text{OH}}{\underset{\text{O}}{\underset{\text{OH}}{\underset{\text{OH}}{\text{OH}}}}}
$$

A4

$$
\text{A7}
$$

$$
\text{A8}
$$

4. General Procedures for the Preparation of Propargyl γ-Butyrolactone-2-enol Ether (1, 1a-1c, 3a-3d) and Characterization Data
A solution of diisopropyl azodicarboxylate (3 mmol, 606 mg) in dry THF was added dropwise to a solution of propargylic alcohol A1-A8 (2 mmol), 3-hydroxy-2,5-dihydrofuran-2-one B (2 mmol, 200 mg) and triphenylphosphine (3 mmol, 787 mg) in THF at 0 °C for 15 min under a nitrogen atmosphere. The reaction was stirred at room temperature overnight. The crude mixture was evaporated to dryness and purified by a flash column chromatography to afford the products 1, 1a-1c, 3a-3d.

3-((3-(4-Methoxyphenyl)prop-2-yn-1-yl)oxy)furan-2(5H)-one (1)

![Image](https://via.placeholder.com/150)

[Chemical structure image]

White solid in 40% yield (EtOAc/petroleum ether = 1:8): Mp 96.3–98.4 °C; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 7.36 (d, \(J = 8.7\) Hz, 2H), 6.84 (d, \(J = 8.7\) Hz, 2H), 6.40 (t, \(J = 2.0\) Hz, 1H), 4.87 (s, 2H), 4.81 (d, \(J = 2.0\) Hz, 2H), 3.81 (s, 3H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)) \(\delta\) 168.11, 160.32, 144.90, 133.50, 115.22, 114.16, 113.79, 88.84, 80.36, 67.70, 59.45, 55.44; IR (thin film, cm\(^{-1}\)) 3444, 3095, 1775, 1758, 1650, 1604, 1510, 1330, 1246, 1137, 1048, 1022, 829; HRMS (ESI): \(m/z\): Calcd. for C\(_{14}\)H\(_{13}\)O\(_4\) [M+H\(^+\)] 245.0808, Found 245.0817.

3-((3-(4-Methoxyphenyl)prop-2-yn-1-yl)oxy)furan-2(5H)-one (1a)

White solid in 29% yield (EtOAc/petroleum ether = 1:8): Mp 66.8–68.3 °C; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 7.32 – 7.21 (m, 4H), 6.47 (t, \(J = 2.1\) Hz, 1H), 4.95 (s, 2H), 4.89 (d, \(J = 2.1\) Hz, 2H), 3.89 (s, 3H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)) \(\delta\) 168.08, 144.90, 133.50, 115.22, 114.16, 113.79, 88.84, 80.36, 67.70, 59.45, 55.44; IR (thin film, cm\(^{-1}\)) 3444, 3095, 1775, 1758, 1650, 1604, 1510, 1330, 1246, 1137, 1048, 1022, 829; HRMS (ESI): \(m/z\): Calcd. for C\(_{14}\)H\(_{13}\)O\(_4\) [M+H\(^+\)] 245.0808, Found 245.0817.
3-((3-(4-((tert-Butyl)phenyl)prop-2-yn-1-yl)oxy)furan-2(5H)-one (1b)

White solid in 45% yield (EtOAc/petroleum ether = 1:15): Mp 98.2–99.6 °C; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta = 7.40 – 7.29 (m, 4H), 6.41 (t, J = 2.1 Hz, 1H), 4.89 (s, 2H), 4.82 (d, J = 2.1 Hz, 2H), 1.30 (s, 9H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)) \(\delta = 168.12, 152.65, 144.92, 131.70, 125.57, 118.75, 115.26, 89.03, 80.99, 67.71, 59.42, 34.98, 31.25; \) IR (thin film, cm\(^{-1}\)) 3456, 3091, 2918, 1755, 1647, 1584, 1324, 1115, 1045, 831, 560; HRMS (ESI): \(m/z\): Calcd. for C\(_{14}\)H\(_{12}\)O\(_3\)Na [M+Na]\(^+\) 251.0679, Found 251.0679.

3-((3-(4-(Pentyloxy)phenyl)prop-2-yn-1-yl)oxy)furan-2(5H)-one (1c)

Colorless oil in 39% yield (EtOAc/petroleum ether = 1:15): \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta = 7.38 – 7.31 (m, 2H), 6.86 – 6.78 (m, 2H), 6.40 (t, J = 2.1 Hz, 1H), 4.88 (s, 2H), 4.82 (d, J = 2.1 Hz, 2H), 3.95 (t, J = 6.6 Hz, 2H), 1.82 – 1.73 (m, 2H), 1.47 – 1.34 (m, 4H), 0.92 (t, J = 7.2 Hz, 3H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)) \(\delta = 168.13, 159.95, 144.94, 133.48, 115.19, 114.69, 113.51, 89.00, 80.25, 68.23, 67.71, 59.49, 28.95, 28.26, 22.55, 14.13; IR (thin film, cm\(^{-1}\)) 3461, 2932, 2229, 1770, 1652, 1509, 1470, 1324, 1115, 1045, 832; HRMS (ESI): \(m/z\): Calcd. for C\(_{18}\)H\(_{20}\)O\(_4\)Na [M+Na]\(^+\) 323.1254, Found 323.1252.

3-((3-(Thiophen-2-yl)prop-2-yn-1-yl)oxy)furan-2(5H)-one (3a)
Yellow oil in 41% yield (EtOAc/petroleum ether = 1:8): $^1$H NMR (600 MHz, CDCl$_3$) $\delta$ = 7.31 (dd, $J = 5.1, 1.0$ Hz, 1H), 7.25 (d, $J = 3.6$ Hz, 1H), 6.99 (dd, $J = 5.1, 3.7$ Hz, 1H), 6.39 (t, $J = 2.1$ Hz, 1H), 4.91 (s, 2H), 4.83 (d, $J = 2.1$ Hz, 2H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ = 167.98, 144.89, 133.38, 128.40, 127.25, 121.52, 115.35, 85.65, 82.25, 67.69, 59.33; IR (thin film, cm$^{-1}$) 3450, 3087, 2231, 1760, 1652, 1391, 1326, 1129, 1047, 832, 710; HRMS (ESI): $m/z$: Calcd. for C$_{11}$H$_8$SO$_3$Na [M+Na$^+$] 243.0086, Found 243.0095.

3-((3-(Furan-2-yl)prop-2-yn-1-yl)oxy)furan-2(5H)-one (3b)

![Image of 3b]

Yellow solid in 44% yield (EtOAc/petroleum ether = 1:8): Mp 94.3–96.0 °C; $^1$H NMR (600 MHz, CDCl$_3$) $\delta$ = 7.40 (dd, $J = 1.8, 0.6$ Hz, 1H), 6.65 (d, $J = 3.3$ Hz, 1H), 6.47 – 6.32 (m, 2H), 4.91 (s, 2H), 4.82 (d, $J = 2.1$ Hz, 2H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ = 167.92, 144.77, 144.46, 135.78, 117.04, 115.55, 111.16, 86.38, 79.19, 67.68, 59.05; IR (thin film, cm$^{-1}$) 3424, 3098, 2919, 1758, 1655, 1331, 1251, 1132, 1051, 970, 833, 758; HRMS (ESI): $m/z$: Calcd. for C$_{11}$H$_9$O$_4$ [M+H$^+$] 205.0495, Found 205.0496.

3-((3-(5-Methylthiophen-2-yl)prop-2-yn-1-yl)oxy)furan-2(5H)-one (3c)

![Image of 3c]
Yellow solid in 40% yield (EtOAc/petroleum ether = 1:8): Mp 89.7–91.6 °C; $^1$H NMR (600 MHz, CDCl$_3$) $\delta =$ 7.05 (d, $J =$ 3.6 Hz, 1H), 6.73 – 6.56 (m, 1H), 6.38 (t, $J =$ 2.1 Hz, 1H), 4.89 (s, 2H), 4.82 (d, $J =$ 2.1 Hz, 2H), 2.46 (s, 3H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta =$ 168.03, 144.88, 143.43, 133.71, 125.55, 118.99, 115.31, 84.89, 82.73, 67.69, 59.43, 15.52; IR (thin film, cm$^{-1}$) 3439, 2921, 2853, 2220, 1767, 1651, 1767, 1651, 1384, 1116, 1049, 799; HRMS (ESI): $m/z$: Calcd. for C$_{12}$H$_{10}$SO$_3$Na [M+Na]$^+$ 257.0248, Found 257.0256.

3-((3-(5-Methylfuran-2-yl)prop-2-yn-1-yl)oxy)furan-2(5H)-one (3d)

Yellow solid in 40% yield (EtOAc/petroleum ether = 1:8): Mp 59.1–61.2 °C; $^1$H NMR (600 MHz, CDCl$_3$) $\delta =$ 6.56 (d, $J =$ 3.3 Hz, 1H), 6.40 (t, $J =$ 2.1 Hz, 1H), 5.99 (dd, $J =$ 3.2, 0.7 Hz, 1H), 4.91 (s, 2H), 4.83 (d, $J =$ 2.1 Hz, 2H), 2.30 (s, 3H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta =$ 167.97, 154.80, 144.83, 134.01, 118.39, 115.45, 107.36, 86.11, 79.78, 67.69, 59.17, 13.98; IR (thin film, cm$^{-1}$) 3417, 2946, 2837, 1763, 1652, 1451, 1348, 1119, 1022, 790; HRMS (ESI): $m/z$: Calcd. for C$_{12}$H$_{10}$O$_4$Na [M+Na]$^+$ 241.0471, Found 241.0469.

5. General Procedures for the Preparation of Furan Derivatives (2, 2a-2i) and Characterization Data

To a solution of the substrates 1, 1a-1c (0.05 mmol) in dry DCE Ph$_3$PAuNTf$_2$ (0.0025 mmol, 2 mg) was added under a nitrogen atmosphere. Then alcohols (0.005 mmol) were added into the mixture. The reaction mixture was reacted at 80 °C for 5 min. The
solvent was removed in vacuo and the residue was purified by a flash column chromatography to afford the products 2, 2a-2i.

2-Methoxy-3-(4-methoxyphenyl)-2-methyl-2,3-dihydrofuro[3,4-b]furan-6(4H)-one (2)

![Structural formula of 2](image)

Colorless oil in 78% yield (EtOAc/petroleum ether = 1:25): $^1$H NMR (600 MHz, DMSO-$d_6$) $\delta$ = 7.21 (d, $J = 8.8$ Hz, 2H), 6.95 (d, $J = 8.8$ Hz, 2H), 4.68 (dd, $J = 9.3, 8.0$ Hz, 1H), 4.35 (ddd, $J = 7.9, 3.4, 1.8$ Hz, 1H), 4.04 (dd, $J = 9.3, 3.4$ Hz, 1H), 3.75 (s, 3H), 3.46 (s, 3H), 2.03 (d, $J = 1.7$ Hz, 3H); $^{13}$C NMR (150 MHz, DMSO-$d_6$) $\delta$ = 170.42, 157.81, 148.05, 128.00, 124.63, 114.25, 111.35, 105.99, 70.74, 55.12, 51.36, 46.43, 12.74; IR (thin film, cm$^{-1}$) 3454, 2918, 2848, 1790, 1660, 1608, 1514, 1248, 1181, 948, 832, 601; HRMS (ESI): m/z: Calcd. for C$_{15}$H$_{16}$O$_5$Na [M+Na]$^+$ 299.0890, Found 299.0897.

2-Methoxy-2-methyl-3-(m-tolyl)-2,3-dihydrofuro[3,4-b]furan-6(4H)-one (2a)

![Structural formula of 2a](image)

Colorless oil in 70% yield (EtOAc/petroleum ether = 1:25): $^1$H NMR (600 MHz, DMSO-$d_6$) $\delta$ = 7.26 (t, $J = 7.6$ Hz, 1H), 7.15 – 6.88 (m, 3H), 4.71 (dd, $J = 9.3, 8.1$ Hz, 1H), 4.47 – 4.27 (m, 1H), 4.05 (dd, $J = 9.3, 3.5$ Hz, 1H), 3.47 (s, 3H), 2.31 (s, 3H), 2.07 (d, $J = 1.7$ Hz, 3H); $^{13}$C NMR (150 MHz, DMSO-$d_6$) $\delta$ = 170.31, 149.45, 137.90, 132.35, 128.63, 127.22, 127.07, 123.89, 111.78, 106.11, 70.84, 51.40, 46.23, 21.07, 12.94; IR (thin film, cm$^{-1}$) 3454, 2920, 2848, 1790, 1660, 1514, 1248, 1181, 948, 832, 601; HRMS (ESI): m/z: Calcd. for C$_{15}$H$_{16}$O$_4$Na [M+Na]$^+$ 283.0941, Found 283.0940.
2-(2-Methoxyethoxy)-2-methyl-3-(m-tolyl)-2,3-dihydrofuro[3,4-b]furan-6(4H)-one (2b)

Colorless oil in 65% yield (EtOAc/petroleum ether = 1:30): $^1$H NMR (600 MHz, DMSO-d$_6$) δ = 7.26 (t, $J$ = 7.6 Hz, 1H), 7.07 (dd, $J$ = 18.9, 10.4 Hz, 3H), 4.72 (dd, $J$ = 9.2, 8.1 Hz, 1H), 4.37 (ddd, $J$ = 7.8, 3.3, 1.7 Hz, 1H), 4.04 (dd, $J$ = 9.3, 3.5 Hz, 1H), 3.96 – 3.71 (m, 2H), 3.53 (t, $J$ = 4.7 Hz, 2H), 3.27 (s, 3H), 2.31 (s, 3H), 2.06 (d, $J$ = 1.6 Hz, 3H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) δ = 170.33, 149.38, 137.89, 132.32, 128.63, 127.23, 127.08, 123.87, 111.77, 105.81, 70.80, 70.55, 63.51, 58.04, 47.00, 21.07, 12.99; IR (thin film, cm$^{-1}$) 3454, 2918, 2849, 1788, 1655, 1455, 1383, 1225, 1121, 1102, 959, 838, 786, 703; HRMS (ESI): $m/z$: Calcd. for C$_{17}$H$_{20}$O$_5$Na [M+Na]$^+$ 327.1203, Found 327.1206.

2-Methyl-2-phenethoxy-3-(m-tolyl)-2,3-dihydrofuro[3,4-b]furan-6(4H)-one (2c)

Colorless oil in 52% yield (EtOAc/petroleum ether = 1:30): $^1$H NMR (600 MHz, DMSO-d$_6$) δ = 7.46 – 7.12 (m, 6H), 7.14 – 6.94 (m, 3H), 4.66 (dd, $J$ = 9.2, 8.1 Hz, 1H), 4.32 (ddd, $J$ = 7.8, 3.2, 1.7 Hz, 1H), 4.02 (dd, $J$ = 9.3, 3.4 Hz, 1H), 3.98 – 3.87 (m, 2H), 2.91 (t, $J = 7.1$ Hz, 2H), 2.30 (s, 3H), 2.04 (d, $J = 1.5$ Hz, 3H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) δ = 170.39, 149.42, 138.14, 137.90, 132.32, 128.92, 128.63, 128.32, 127.19, 127.06, 126.31, 123.85, 111.70, 105.86, 70.75, 64.91, 46.83, 35.37, 21.07, 12.99; IR (thin film, cm$^{-1}$) 3421, 2919, 2850, 1789, 1643, 1469, 1384, 1122, 618; HRMS (ESI): $m/z$: Calcd. for C$_{22}$H$_{22}$O$_4$Na [M+Na]$^+$ 373.1410, Found 373.1440.
3-(4-(tert-Butyl)phenyl)-2-methyl-2-phenethoxy-2,3-dihydrofuro[3,4-b]furan-6(4H)-one (2d)

![Structure 2d]

Colorless oil in 60% yield (EtOAc/petroleum ether = 1:30): $^1$H NMR (600 MHz, DMSO-d$_6$) $\delta$ = 7.44 – 7.34 (m, 2H), 7.28 (ddd, $J$ = 9.6, 8.2, 6.0 Hz, 4H), 7.22 (dd, $J$ = 11.3, 4.3 Hz, 1H), 7.20 – 7.17 (m, 2H), 4.66 (dd, $J$ = 9.3, 8.1 Hz, 1H), 4.30 (ddd, $J$ = 8.0, 3.5, 1.8 Hz, 1H), 4.04 (dd, $J$ = 9.3, 3.6 Hz, 1H), 3.98 – 3.86 (m, 2H), 2.91 (t, $J$ = 7.1 Hz, 2H), 2.04 (d, $J$ = 1.7 Hz, 3H), 1.27 (s, 9H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) $\delta$ = 170.35, 149.03, 148.72, 138.12, 129.46, 128.90, 128.31, 126.30, 125.49, 111.47, 105.77, 70.87, 64.86, 46.90, 40.05, 35.38, 34.19, 31.04, 12.96; IR (thin film, cm$^{-1}$) 3453, 2959, 2919, 1787, 1657, 1384, 1225, 1114, 949, 834, 699; HRMS (ESI): $m/z$: Calcd. for C$_{25}$H$_{29}$O$_4$ [M+H]$^+$ 393.2060, Found 393.2067.

3-(4-(tert-Butyl)phenyl)-2-methoxy-2-methyl-2,3-dihydrofuro[3,4-b]furan-6(4H)-one (2e)

![Structure 2e]

Colorless oil in 70% yield (EtOAc/petroleum ether = 1:25): $^1$H NMR (600 MHz, DMSO-d$_6$) $\delta$ = 7.47 – 7.34 (m, 2H), 7.29 – 7.07 (m, 2H), 4.72 (dd, $J$ = 9.3, 8.2 Hz, 1H), 4.36 (ddd, $J$ = 8.0, 3.5, 1.8 Hz, 1H), 4.06 (dd, $J$ = 9.3, 3.6 Hz, 1H), 3.46 (s, 3H), 2.07 (d, $J$ = 1.7 Hz, 3H), 1.27 (s, 9H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) $\delta$ = 170.29, 149.08, 148.75, 129.50, 126.35, 125.31, 111.56, 106.03, 70.97, 51.35, 46.31, 34.20, 31.05, 12.92; IR (thin film, cm$^{-1}$) 3453, 2961, 2920, 1793, 1660, 1462, 1384, 1226, 1112, 1086, 1008, 950, 835; HRMS (ESI): $m/z$: Calcd. for C$_{18}$H$_{23}$O$_4$ [M+H]$^+$ 303.1591, Found 303.1594.
3-(4-(tert-Butyl)phenyl)-2-(2-methoxyethoxy)-2-methyl-2,3-dihydrofuro[3,4-b]furan-6(4H)-one (2f)

Colorless oil in 68% yield (EtOAc/petroleum ether = 1:25): $^1$H NMR (600 MHz, DMSO-d$_6$) $\delta$ = 7.39 (d, $J = 8.5$ Hz, 2H), 7.21 (d, $J = 8.5$ Hz, 2H), 4.72 (dd, $J = 9.3$, 8.1 Hz, 1H), 4.35 (ddd, $J = 8.0$, 3.5, 1.8 Hz, 1H), 4.06 (dd, $J = 9.4$, 3.6 Hz, 1H), 3.92 – 3.76 (m, 2H), 3.52 (t, $J = 4.7$ Hz, 2H), 3.26 (s, 3H), 2.07 (d, $J = 1.6$ Hz, 3H), 1.27 (s, 9H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) $\delta$ = 170.31, 149.01, 148.75, 129.46, 126.34, 125.50, 111.54, 105.74, 70.90, 70.56, 63.46, 58.04, 47.07, 34.20, 31.04, 12.98; IR (thin film, cm$^{-1}$) 3451, 2962, 2920, 1790, 1660, 1463, 1384, 1227, 1113, 951, 835; HRMS (ESI): $m/z$: Calcd. for C$_{20}$H$_{27}$O$_5$ [M+H]$^+$ 347.1853, Found 347.1852.

2-Methoxy-2-methyl-3-(4-(pentyloxy)phenyl)-2,3-dihydrofuro[3,4-b]furan-6(4H)-one (2g)

Colorless oil in 73% yield (EtOAc/petroleum ether = 1:30): $^1$H NMR (600 MHz, DMSO-d$_6$) $\delta$ = 7.19 (d, $J = 8.8$ Hz, 2H), 6.93 (d, $J = 8.8$ Hz, 2H), 4.68 (dd, $J = 9.3$, 8.1 Hz, 1H), 4.40 – 4.27 (m, 1H), 4.03 (dd, $J = 9.3$, 3.4 Hz, 1H), 3.95 (t, $J = 6.5$ Hz, 2H), 3.46 (s, 3H), 2.03 (d, $J = 1.7$ Hz, 3H), 1.70 (dd, $J = 14.6$, 6.7 Hz, 2H), 1.47 – 1.28 (m, 4H), 0.89 (t, $J = 7.2$ Hz, 3H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) $\delta$ = 170.41, 157.25, 147.98, 127.97, 124.48, 114.73, 111.36, 105.98, 70.74, 67.42, 51.35, 46.41, 28.35, 27.70, 21.87, 13.91, 12.75; IR (thin film, cm$^{-1}$) 3448, 2920, 1790, 1638, 1609, 1514, 1468, 1384, 1247, 1179, 619; HRMS (ESI): $m/z$: Calcd. for C$_{19}$H$_{24}$O$_5$Na [M+Na]$^+$ 355.1516, Found 355.1528.
2-Methyl-3-(4-(pentyloxy)phenyl)-2-phenethoxy-2,3-dihydrofuro[3,4-b]furan-6(4H)-one (2h)

Colorless oil in 55% yield (EtOAc/petroleum ether = 1:30): $^1$H NMR (600 MHz, DMSO-$d_6$) $\delta = 7.32 - 7.26$ (m, 4H), 7.21 (t, $J = 7.0$ Hz, 1H), 7.16 (d, $J = 8.8$ Hz, 2H), 6.92 (d, $J = 8.8$ Hz, 2H), 4.63 (dd, $J = 9.2, 8.0$ Hz, 1H), 4.31 – 4.27 (m, 1H), 4.01 (dd, $J = 9.3, 3.4$ Hz, 1H), 3.98 – 3.90 (m, 4H), 2.91 (t, $J = 7.1$ Hz, 2H), 2.00 (d, $J = 1.6$ Hz, 3H), 1.75 – 1.65 (m, 2H), 1.46 – 1.31 (m, 4H), 0.89 (t, $J = 7.1$ Hz, 3H); $^{13}$C NMR (150 MHz, DMSO-$d_6$) $\delta = 170.48, 157.22, 147.93, 138.13, 128.90, 128.30, 127.93, 126.29, 124.45, 114.73, 111.28, 105.72, 70.65, 67.41, 64.85, 47.00, 40.06, 35.37, 28.35, 27.70, 21.87, 13.91, 12.79; IR (thin film, cm$^{-1}$) 3443, 2918, 1788, 1632, 1469, 1384, 1111, 949, 618; HRMS (ESI): $m/z$: Calcd. for C$_{26}$H$_{30}$O$_5$Na [M+Na]$^+$ 455.1985, Found 455.1987.

2-(2-Methoxyethoxy)-2-methyl-3-(4-(pentyloxy)phenyl)-2,3-dihydrofuro[3,4-b]furan-6(4H)-one (2i)

Colorless oil in 52% yield (EtOAc/petroleum ether = 1:30): $^1$H NMR (600 MHz, DMSO-$d_6$) $\delta = 7.19$ (d, $J = 8.8$ Hz, 2H), 6.93 (d, $J = 8.8$ Hz, 2H), 4.69 (dd, $J = 9.2, 8.1$ Hz, 1H), 4.33 (ddd, $J = 7.9, 3.3, 1.8$ Hz, 1H), 4.03 (dd, $J = 9.3, 3.4$ Hz, 1H), 3.95 (t, $J = 6.5$ Hz, 2H), 3.89 – 3.78 (m, 2H), 3.52 (t, $J = 4.7$ Hz, 2H), 3.26 (s, 3H), 2.02 (d, $J = 1.6$ Hz, 3H), 1.70 (dd, $J = 14.5, 6.7$ Hz, 2H), 1.45 – 1.29 (m, 4H), 0.89 (t, $J = 7.2$ Hz, 3H); $^{13}$C NMR (150 MHz, DMSO-$d_6$) $\delta = 170.43, 157.25, 147.91, 127.97, 124.44,
114.73, 111.35, 105.67, 70.70, 70.57, 67.41, 63.45, 58.03, 47.18, 28.35, 27.70, 21.87, 13.91, 12.81; IR (thin film, cm\(^{-1}\)) 3454, 2918, 2849, 1788, 1655, 1383, 1225, 1121, 1102, 959, 838, 786, 703; HRMS (ESI): \(m/z\): Calcd. for C\(_{21}\)H\(_{29}\)O\(_6\) [M+H]\(^+\) 377.1959, Found 377.1957.

6. General Procedures for the Preparation of Pyran Derivatives (4a-4l) and Characterization Data

![Chemical Reaction Diagram](attachment:attachment.png)

To a solution of the substrates 3a-3d (0.05 mmol) in dry DCE Ph\(_3\)PAuNTf\(_2\) (0.0025 mmol, 2 mg) was added under a nitrogen atmosphere. Then alcohols (0.005 mmol) were added into the mixture. The reaction mixture was reacted at 80 °C for 5 min. The solvent was removed in vacuo and the residue was purified by a flash column chromatography to afford the products 4a-4l.

7a-Hydroxy-4-(thiophen-2-yl)-4a,7a-dihydro-2H-furo[3,4-b]pyran-7(5H)-one (4a)

![Chemical Structure](attachment:attachment.png)

Colorless oil in 70% yield (EtOAc/petroleum ether = 1:8): \(^1\)H NMR (600 MHz, DMSO-d\(_6\)) \(\delta = 7.59\) (s, 1H), 7.46 (d, \(J = 4.9\) Hz, 1H), 7.23 (d, \(J = 3.3\) Hz, 1H), 7.04 (dd, \(J = 5.1, 3.6\) Hz, 1H), 6.26 (dd, \(J = 3.7, 2.1\) Hz, 1H), 4.78 (t, \(J = 8.4\) Hz, 1H), 4.44 (dt, \(J = 17.4, 4.1\) Hz, 1H), 3.87 (dd, \(J = 9.9, 8.6\) Hz, 1H), 3.40 (td, \(J = 10.0, 2.6\) Hz, 1H); \(^{13}\)C NMR (150 MHz, DMSO-d\(_6\)) \(\delta = 172.56, 142.30, 128.02, 125.56, 125.30, 123.87, 120.39, 92.26, 69.81, 60.00, 40.50; IR (thin film, cm\(^{-1}\)) 3368, 2918, 2851, 1791, 1633, 1378, 1286, 1136, 1103, 989, 706; HRMS (ESI): \(m/z\): Calcd. for C\(_{11}\)H\(_{10}\)SO\(_4\)Na [M+Na]\(^+\) 261.0192, Found 261.0186.

7a-Methoxy-4-(thiophen-2-yl)-4a,7a-dihydro-2H-furo[3,4-b]pyran-7(5H)-one (4b)
Colorless oil in 63% yield (EtOAc/petroleum ether = 1:10): $^1$H NMR (600 MHz, DMSO-d$_6$) $\delta = 7.47$ (d, $J = 5.0$ Hz, 1H), 7.24 (d, $J = 3.5$ Hz, 1H), 7.05 (dd, $J = 5.1$, 3.6 Hz, 1H), 6.32 – 6.19 (m, 1H), 4.78 (t, $J = 8.5$ Hz, 1H), 4.44 (dd, $J = 17.6$, 4.0 Hz, 1H), 4.33 (dt, $J = 17.6$, 2.4 Hz, 1H), 3.90 (dd, $J = 9.6$, 8.8 Hz, 1H), 3.53 (td, $J = 9.7$, 2.6 Hz, 1H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) $\delta = 170.60$, 141.73, 127.88, 125.39, 124.97, 123.96, 119.77, 94.20, 69.48, 61.15, 49.96, 39.90; IR (thin film, cm$^{-1}$) 3453, 2920, 2851, 1788, 1642, 1384, 1169, 1104, 1002, 620; HRMS (ESI): $m/z$: Calcd. for C$_{12}$H$_{12}$SO$_4$Na $[M+Na]^+$ 275.0349, Found 275.0347.

7a-Butoxy-4-(thiophen-2-yl)-4a,7a-dihydro-2H-furo[3,4-b]pyran-7(5H)-one (4c)

Colorless oil in 65% yield (EtOAc/petroleum ether = 1:20): $^1$H NMR (600 MHz, DMSO-d$_6$) $\delta = 7.48$ (d, $J = 5.1$ Hz, 1H), 7.25 (d, $J = 3.5$ Hz, 1H), 7.05 (dd, $J = 5.0$, 3.7 Hz, 1H), 6.28 (d, $J = 2.8$ Hz, 1H), 4.78 (t, $J = 8.5$ Hz, 1H), 4.42 (dd, $J = 17.6$, 3.9 Hz, 1H), 4.34 (dt, $J = 17.6$, 2.3 Hz, 1H), 4.19 (dt, $J = 9.7$, 6.7 Hz, 1H), 3.90 (t, $J = 9.1$ Hz, 1H), 3.78 (dt, $J = 9.7$, 6.6 Hz, 1H), 3.54 (t, $J = 9.0$ Hz, 1H), 1.54 – 1.48 (m, 2H), 1.37 – 1.29 (m, 2H), 0.88 (t, $J = 7.4$ Hz, 3H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) $\delta = 170.65$, 141.75, 127.87, 125.38, 125.10, 124.00, 119.77, 94.35, 69.52, 61.82, 61.04, 40.07, 31.43, 18.74, 13.71; IR (thin film, cm$^{-1}$) 3462, 2958, 2922, 1791, 1649, 1383, 1180, 1104, 1090, 1002, 701; HRMS (ESI): $m/z$: Calcd. for C$_{15}$H$_{18}$SO$_4$Na $[M+Na]^+$ 317.0818, Found 317.0828.

7a-Phenethoxy-4-(thiophen-2-yl)-4a,7a-dihydro-2H-furo[3,4-b]pyran-7(5H)-one (4d)
Colorless oil in 60% yield (EtOAc/petroleum ether = 1:20): $^1$H NMR (600 MHz, DMSO-d$_6$) δ = 7.47 (d, $J$ = 5.1 Hz, 1H), 7.34 – 7.15 (m, 6H), 7.04 (dd, $J$ = 5.1, 3.6 Hz, 1H), 6.20 (t, $J$ = 2.6 Hz, 1H), 4.77 (t, $J$ = 8.5 Hz, 1H), 4.38 (dt, $J$ = 9.6, 6.9 Hz, 1H), 4.33 (dd, $J$ = 17.5, 4.0 Hz, 1H), 4.09 (dt, $J$ = 17.5, 2.3 Hz, 1H), 3.98 (dt, $J$ = 9.7, 7.2 Hz, 1H), 3.88 (t, $J$ = 8.9 Hz, 1H), 3.53 (td, $J$ = 9.6, 2.5 Hz, 1H), 2.85 (td, $J$ = 7.0, 2.4 Hz, 2H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) δ = 170.56, 141.74, 138.58, 128.88, 128.25, 127.88, 126.22, 125.36, 124.91, 124.00, 119.71, 94.37, 69.60, 63.18, 60.83, 40.05, 35.68; IR (thin film, cm$^{-1}$) 3455, 2919, 2851, 1789, 1648, 1383, 1291, 1176, 1107, 1001, 699; HRMS (ESI): m/z: Calcd. for C$_{19}$H$_{18}$SO$_4$Na [M+Na]$^+$ 365.0818, Found 365.0815.

4-(Furan-2-yl)-7a-hydroxy-4a,7a-dihydro-2H-furo[3,4-b]pyran-7(5H)-one (4e)

Colorless oil in 65% yield (EtOAc/petroleum ether = 1:8): $^1$H NMR (600 MHz, DMSO-d$_6$) δ = 7.66 (d, $J$ = 1.4 Hz, 1H), 7.58 (s, 1H), 6.62 (d, $J$ = 3.3 Hz, 1H), 6.52 (dd, $J$ = 3.3, 1.8 Hz, 1H), 6.31 (t, $J$ = 2.4 Hz, 1H), 4.77 (t, $J$ = 8.4 Hz, 1H), 4.44 (dt, $J$ = 17.4, 2.2 Hz, 1H), 4.35 (dd, $J$ = 17.5, 4.1 Hz, 1H), 3.86 (dd, $J$ = 9.7, 8.6 Hz, 1H), 3.23 (t, $J$ = 9.1 Hz, 1H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) δ = 172.44, 151.58, 142.98, 121.59, 118.51, 111.56, 106.61, 91.96, 69.74, 59.59, 38.65; IR (thin film, cm$^{-1}$) 3412, 2919, 2851, 1789, 1648, 1383, 1291, 1176, 1107, 1001, 699; HRMS (ESI): m/z: Calcd. for C$_{11}$H$_{10}$O$_5$Na [M+Na]$^+$ 245.0420, Found 245.0420.

4-(Furan-2-yl)-7a-methoxy-4a,7a-dihydro-2H-furo[3,4-b]pyran-7(5H)-one (4f)
Colorless oil in 80% yield (EtOAc/petroleum ether = 1:15): $^1$H NMR (600 MHz, DMSO-d$_6$) $\delta = 7.67$ (s, 1H), 6.62 (d, $J = 3.3$ Hz, 1H), 6.52 (dd, $J = 3.3$, 1.8 Hz, 1H), 6.33 (t, $J = 2.8$ Hz, 1H), 4.78 (t, $J = 8.5$ Hz, 1H), 4.48 (dd, $J = 17.7$, 4.0 Hz, 1H), 4.35 (dt, $J = 17.7$, 2.3 Hz, 1H), 3.90 (t, $J = 8.8$ Hz, 1H), 3.61 (s, 3H), 3.5 (td, $J = 9.8$, 2.6 Hz, 1H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) $\delta = 170.58$, 151.19, 143.13, 121.05, 118.01, 111.58, 106.86, 93.95, 69.56, 60.94, 49.96, 38.16; IR (thin film, cm$^{-1}$) 3441, 2255, 2127, 1785, 1649, 1172, 1050, 1026, 1004, 825, 763; HRMS (ESI): $m/z$: Calcd. for C$_{12}$H$_{12}$O$_5$Na [M+Na]$^+$ 259.0569, Found 259.0575.

4-(Furan-2-yl)-7a-(2-methoxyethoxy)-4a,7a-dihydro-2H-furo[3,4-b]pyran-7(5H)-one (4g)

Colorless oil in 78% yield (EtOAc/petroleum ether = 1:15): $^1$H NMR (600 MHz, DMSO-d$_6$) $\delta = 7.67$ (d, $J = 1.4$ Hz, 1H), 6.63 (d, $J = 3.3$ Hz, 1H), 6.52 (dd, $J = 3.4$, 1.8 Hz, 1H), 6.33 (t, $J = 3.0$ Hz, 1H), 4.79 (t, $J = 8.5$ Hz, 1H), 4.44 (s, 2H), 4.25 (dd, $J = 7.7$, 4.1 Hz, 1H), 3.98 – 3.93 (m, 1H), 3.90 (dd, $J = 9.7$, 8.7 Hz, 1H), 3.47 (dd, $J = 5.6$, 3.8 Hz, 2H), 3.37 (t, $J = 9.1$ Hz, 1H), 3.23 (s, 3H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) $\delta = 170.59$, 151.19, 143.14, 120.99, 118.08, 111.59, 106.88, 93.99, 71.02, 69.70, 61.64, 60.53, 58.06, 38.33; IR (thin film, cm$^{-1}$) 3432, 2925, 1787, 1721, 1667, 1460, 1181, 1109, 1055, 1031, 1007, 737; HRMS (ESI): $m/z$: Calcd. for C$_{14}$H$_{16}$O$_6$Na [M+Na]$^+$ 303.0845, Found 303.0838.

4-(Furan-2-yl)-7a-phenethoxy-4a,7a-dihydro-2H-furo[3,4-b]pyran-7(5H)-one (4h)
Colorless oil in 63% yield (EtOAc/petroleum ether = 1:15): $^1$H NMR (600 MHz, DMSO-d$_6$) $\delta$ = 7.67 (s, 1H), 7.35 – 7.13 (m, 5H), 6.62 (d, $J = 3.3$ Hz, 1H), 6.52 (dd, $J = 3.3$, 1.8 Hz, 1H), 6.25 (s, 1H), 4.77 (t, $J = 8.5$ Hz, 1H), 4.41 – 4.31 (m, 2H), 4.09 (d, $J = 17.6$ Hz, 1H), 3.98 (dt, $J = 9.7$, 7.2 Hz, 1H), 3.88 (t, $J = 9.1$ Hz, 1H), 3.36 (t, $J = 7.5$ Hz, 1H), 2.84 (td, $J = 6.9$, 3.4 Hz, 2H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) $\delta$ = 170.54, 151.17, 143.11, 138.61, 128.87, 128.24, 126.21, 120.99, 117.97, 111.59, 106.89, 94.11, 69.68, 63.17, 60.61, 38.34, 35.67; IR (thin film, cm$^{-1}$) 3441, 2938, 2252, 2125, 1785, 1660, 1107, 1053, 1028, 1007, 823, 761; HRMS (ESI): $m/z$: Calcd. for C$_{19}$H$_{19}$O$_5$N [M+H]$^+$ 327.1232, Found 327.1230.

7a-Hydroxy-4-(5-methylthiophen-2-yl)-4a,7a-dihydro-2H-furo[3,4-b]pyran-7(5H)-one (4i)

Colorless oil in 72% yield (EtOAc/petroleum ether = 1:8): $^1$H NMR (600 MHz, DMSO-d$_6$) $\delta$ = 7.56 (s, 1H), 7.00 (d, $J = 3.5$ Hz, 1H), 6.72 (dd, $J = 3.5$, 1.1 Hz, 1H), 6.11 (dd, $J = 3.6$, 2.1 Hz, 1H), 4.75 (t, $J = 8.4$ Hz, 1H), 4.42 (d, $J = 17.4$ Hz, 1H), 4.29 (dd, $J = 17.4$, 4.1 Hz, 1H), 3.84 (dd, $J = 9.8$, 8.6 Hz, 1H), 3.35 (t, $J = 9.2$ Hz, 1H), 2.41 (s, 3H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) $\delta$ = 172.46, 139.92, 138.64, 126.05, 125.62, 123.72, 119.03, 92.21, 69.67, 59.77, 40.13, 15.06; IR (thin film, cm$^{-1}$) 3372, 2921, 1793, 1646, 1449, 1373, 1215, 1138, 1103, 1025, 1001, 795, 637; HRMS (ESI): $m/z$: Calcd. for C$_{12}$H$_{12}$O$_4$Na [M+Na]$^+$ 275.0349, Found 275.0351.

7a-(2-Methoxyethoxy)-4-(5-methylthiophen-2-yl)-4a,7a-dihydro-2H-furo[3,4-b]pyran-7(5H)-one (4j)
Colorless oil in 68% yield (EtOAc/petroleum ether = 1:15): $^1$H NMR (600 MHz, DMSO-d$_6$) δ = 7.02 (d, $J$ = 3.5 Hz, 1H), 6.73 (dd, $J$ = 3.5, 1.1 Hz, 1H), 6.12 (t, $J$ = 2.8 Hz, 1H), 4.77 (t, $J$ = 8.5 Hz, 1H), 4.47 – 4.33 (m, 2H), 4.28 – 4.22 (m, 1H), 3.98 – 3.91 (m, 1H), 3.87 (dd, $J$ = 9.6, 8.7 Hz, 1H), 3.52 (t, $J$ = 8.6 Hz, 1H), 3.50 – 3.46 (m, 2H), 3.24 (s, 3H), 2.41 (s, 3H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) δ = 170.61, 139.43, 138.87, 126.10, 125.07, 123.99, 118.59, 94.27, 71.01, 69.62, 61.60, 60.67, 58.03, 39.74, 15.05; IR (thin film, cm$^{-1}$) 3428, 2925, 1787, 1648, 1452, 1374, 1213, 1182, 1108, 1056, 1027, 822, 760; HRMS (ESI): m/z: Calcd. for C$_{15}$H$_{18}$O$_5$Na [M+Na]$^+$ 333.0733, Found 333.0762.

7a-Methoxy-4-(5-methylfuran-2-yl)-4a,7a-dihydro-2H-furo[3,4-b]pyran-7(5H)-one (4k)

Colorless oil in 70% yield (EtOAc/petroleum ether = 1:15): $^1$H NMR (600 MHz, DMSO-d$_6$) δ = 6.48 (d, $J$ = 3.2 Hz, 1H), 6.20 (s, 1H), 6.12 (dd, $J$ = 3.1, 0.9 Hz, 1H), 4.76 (t, $J$ = 8.5 Hz, 1H), 4.45 (dd, $J$ = 17.6, 4.0 Hz, 1H), 4.33 (d, $J$ = 17.6 Hz, 1H), 3.88 (t, $J$ = 8.8 Hz, 1H), 3.60 (s, 3H), 3.29 (td, $J$ = 9.1, 2.0 Hz, 1H), 2.27 (s, 3H); $^{13}$C NMR (150 MHz, DMSO-d$_6$) δ = 170.62, 152.04, 149.68, 121.05, 116.43, 107.87, 107.67, 93.97, 69.61, 60.91, 49.96, 38.02, 13.33; IR (thin film, cm$^{-1}$) 3423, 2949, 2845, 1789, 1657, 1383, 1211, 1170, 1031, 999, 1096, 738; HRMS (ESI): m/z: Calcd. for C$_{13}$H$_{14}$O$_5$Na [M+Na]$^+$ 273.0733, Found 273.0733.

7a-Hydroxy-4-(5-methylfuran-2-yl)-4a,7a-dihydro-2H-furo[3,4-b]pyran-7(5H)-one (4l)
Colorless oil in 72% yield (EtOAc/petroleum ether = 1:8): $^1$H NMR (600 MHz, DMSO-$d_6$) δ = 7.54 (s, 1H), 6.47 (d, $J = 3.1$ Hz, 1H), 6.19 (s, 1H), 6.11 (dd, $J = 3.1$, 0.9 Hz, 1H), 4.75 (t, $J = 8.4$ Hz, 1H), 4.43 (d, $J = 17.5$ Hz, 1H), 4.32 (dd, $J = 17.4$, 4.1 Hz, 1H), 3.84 (dd, $J = 9.7$, 8.6 Hz, 1H), 3.18 (t, $J = 8.5$ Hz, 1H), 2.27 (s, 3H); $^{13}$C NMR (150 MHz, DMSO-$d_6$) δ = 172.48, 151.85, 150.06, 121.58, 116.94, 107.63, 107.60, 91.98, 69.78, 59.56, 38.50, 13.34; IR (thin film, cm$^{-1}$) 3407, 2942, 2852, 1789, 1658, 1383, 1283, 1283, 1142, 1104, 1025, 764, 738; HRMS (ESI): m/z: Calcd. for C$_{12}$H$_{12}$O$_5$Na$^{[M+Na]^+}$ 259.0576, Found 259.0577.

7. General Procedures for the Antifungal Bioassay

The in vitro minimum inhibitory concentrations (MICs) of the synthesized compounds were determined according to the National Committee for Clinical Laboratory Standards (NCCLS)$^6$ using the serial dilution method in 96-well microtest plates. The tested microorganism strains including *M. gypseum*, *A. fumigatus*, *Aspergillus*, *R. rubra*, *C. neoformans* were provided by Department of Microbiology of Shenyang Pharmaceutical University. Fluconazole was used as the standard drug. The strains were retrieved from the storage tube of potato dextrose agar (PDA) slants to sterilized PDA Petri dishes and incubated at 35 °C for the antifungal assay. The fungal suspension was adjusted with sterile saline to a concentration of 0.5 × 10$^3$ – 1.0 × 10$^5$ cfu·mL$^{-1}$. All of test compounds and fluconazole were dissolved in dimethyl sulfoxide (DMSO), serially diluted to obtain the required concentrations of 200, 100, 50, 25, 12.5, 6.25, 3.125, 1.5 and 0.75 mg/L. The MIC values were determined at 48 h for all the strains.

8. References


9. NMR Spectra
Parameter | Value
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2 Owner | nmr
3 Spectrometer | spect
4 Solvent | CDCl3
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8 Nucleus | 13C
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Owner | nmr
Spectrometer | spect
Solvent | CDCl3
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Number of Scans | 16
Spectrometer Frequency | 600.13
Nucleus | 1H

Chemical structure of compound 1b

1,4-Dioxane-2-carboxylic acid 4-phenylbut-2-ynyl ester

S27
Parameter | Value
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Spectrometer | spect
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<tr>
<td>Spectrometer Frequency</td>
<td>(600.13, 150.90)</td>
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<tr>
<td>Spectrometer Spectral Width</td>
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</tr>
<tr>
<td>Lowest Frequency</td>
<td>(-612.2, -3008.1)</td>
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<tr>
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<td>(1H, 13C)</td>
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<tr>
<td>Acquired Size</td>
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<td>Parameter</td>
<td>Value (f2, f1)</td>
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<tr>
<td>Origin</td>
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<tr>
<td>Owner</td>
<td>nmr</td>
</tr>
<tr>
<td>Spectrometer</td>
<td>spect</td>
</tr>
<tr>
<td>Solvent</td>
<td>DMSO</td>
</tr>
<tr>
<td>Temperature</td>
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</tr>
<tr>
<td>Number of Scans</td>
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<tr>
<td>Spectrometer Frequency</td>
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<td>Spectral Width</td>
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**Diagram:**

![NMR spectrum diagram](image-url)
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>Origin</td>
<td>Bruker BioSpin GmbH</td>
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<tr>
<td>Owner</td>
<td>nmr</td>
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<tr>
<td>Spectrometer</td>
<td>spect</td>
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<tr>
<td>Solvent</td>
<td>DMSO</td>
</tr>
<tr>
<td>Temperature</td>
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</tr>
<tr>
<td>Number of Scans</td>
<td>16</td>
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<tr>
<td>Spectrometer Frequency</td>
<td>600.13</td>
</tr>
<tr>
<td>Nucleus</td>
<td>1H</td>
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</table>

8 Nucleus
7 Spectrometer Frequency 600.13
6 Number of Scans 16
5 Temperature 297.9
4 Solvent DMSO
3 Spectrometer spec
2 Number 2
1 Origin Bruker Biospin GmbH

Parameter Value

![Diagram of chemical structure]
f1 (ppm)

Parameter
Value
1 Origin
Bruker BioSpin GmbH
2 Owner
tnr
3 Spectrometer
spect
4 Solvent
DMSO
5 Temperature
297.9 K
6 Number of Scans
16
7 Spectrometer Frequency
600.13 MHz
8 Nucleus
1H
**Parameter** | **Value**
--- | ---
1 Origin | Bruker BioSpin GmbH
2 Owner | nmr
3 Spectrometer | spect
4 Solvent | DMSO
5 Temperature | 297.9
6 Number of Scans | 16
7 Spectrometer Frequency | 600.13
8 Nucleus | 1H

```latex
\begin{align*}
\text{H}_1 & \quad 129.9 \\
\text{H}_2 & \quad 39.10 \\
\text{H}_3 & \quad 39.24 \\
\text{H}_4 & \quad 39.38 \\
\text{H}_5 & \quad 39.52 \\
\text{H}_6 & \quad 39.66 \\
\text{H}_7 & \quad 39.80 \\
\text{H}_8 & \quad 46.83 \\
\text{H}_9 & \quad 64.91 \\
\text{H}_{10} & \quad 70.75 \\
\text{H}_{11} & \quad 105.86 \\
\text{H}_{12} & \quad 111.70 \\
\text{H}_{13} & \quad 123.85 \\
\text{H}_{14} & \quad 126.31 \\
\text{H}_{15} & \quad 127.06 \\
\text{H}_{16} & \quad 127.19 \\
\text{H}_{17} & \quad 128.32 \\
\text{H}_{18} & \quad 128.63 \\
\text{H}_{19} & \quad 128.92 \\
\text{H}_{20} & \quad 132.32 \\
\text{H}_{21} & \quad 137.90 \\
\text{H}_{22} & \quad 149.42 \\
\text{H}_{23} & \quad 170.39
\end{align*}
```
Parameter | Value
--- | ---
1 Origin | Bruker BioSpin GmbH
2 Owner | nmr
3 Spectrometer | spect
4 Solvent | DMSO
5 Temperature | 297.9
6 Number of Scans | 16
7 Spectrometer Frequency | 600.13
8 Nucleus | 1H

Chemical shift values (ppm):
- 30.0
- 31.05
- 34.20
- 39.10
- 39.24
- 39.38
- 39.52
- 39.66
- 39.94
- 46.31
- 51.35
- 70.97
- 106.03
- 111.56
- 125.51
- 126.35
- 129.50
- 148.75
- 149.08
- 170.29

Structural formula:

![Chemical Structure Image]
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
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<tr>
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<td>nmr</td>
</tr>
<tr>
<td>Spectrometer</td>
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<tr>
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<tr>
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<td>Spectrometer Frequency</td>
<td>600.13 MHz</td>
</tr>
<tr>
<td>Nucleus</td>
<td>1H</td>
</tr>
</tbody>
</table>

![Chemical structure image]
**Parameter**

1. Origin: Bruker BioSpin GmbH

2. Owner: nmr

3. Spectrometer: spect

4. Solvent: DMSO

5. Temperature: 297.9

6. Number of Scans: 16

7. Spectrometer Frequency: 600.13

8. Nucleus: 1H
f1 (ppm)

Parameter | Value
--- | ---
1 | Origin
2 | Owner
3 | Spectrometer
4 | Solvent
5 | Temperature
6 | Number of Scans
7 | Spectrometer Frequency
8 | Nucleus
Sample parameters:

1. **Origin**: Bruker BioSpin GmbH
2. **Owner**: nmr
3. **Spectrometer**: spect
4. **Solvent**: DMSO
5. **Temperature**: 297.9 K
6. **Number of Scans**: 1196
7. **Spectrometer Frequency**: 150.90 MHz
8. **Nucleus**: 13C

Sample molecule structure: ![Chemical Structure Image]
**Parameter**

<table>
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<tbody>
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<tr>
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<td>Solvent</td>
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<tr>
<td>5</td>
<td>Temperature</td>
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<tr>
<td>6</td>
<td>Number of Scans</td>
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<td>7</td>
<td>Spectrometer Frequency</td>
</tr>
<tr>
<td>8</td>
<td>Nucleus</td>
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</tbody>
</table>

**Value**

- Bruker Biospin GmbH
- nmr
- spect
- DMSO
- 297.9
- 16
- 600.13
- 1H
- 1H Spectrometer Frequency
- $6$ Scans
- $13$
Parameter | Value
--- | ---
1 | Origin
2 | Owner
3 | Spectrometer
4 | Solvent
5 | Temperature
6 | Number of Scans
7 | Spectrometer Frequency
8 | Nucleus

Bruker Biospin GmbH