Supporting Information for

Dual gold-catalyzed regioselective synthesis of benzofulvenes *via* 5-*endo dig* cyclization [†]

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Electronic Supplementary Material (ESI) for Chemical Communications

1. Copies of 1H and 13C NMR spectra (2a-2v)



















































2. X-ray Crystallography

X-ray data for the compound was collected at room temperature on a Bruker D8 QUEST instrument with an I μ S Mo microsource ($\lambda = 0.7107$ A) and a PHOTON-III detector. The raw data frames were reduced and corrected for absorption effects using the Bruker Apex 3 software suite programs.¹ The structure was solved using intrinsic phasing method [2] and further refined with the SHELXL.² program and expanded using Fourier techniques. Anisotropic displacement parameters were included for all non-hydrogen atoms. All C bound H atoms were positioned geometrically and treated as riding on their parent C atoms [C-H = 0.93-0.97 Å, and Uiso(H) = 1.5Ueq(C) for methyl H or 1.2Ueq(C) for other H atoms].

Crystal structure determination of 2s [KB418_0m_a]

Crystal Data for $C_{19}H_{15}ClO_2$ (M=310.76 g/mol): monoclinic, space group $P2_1/c$ (no. 16.4838(4) Å, b = 11.3226(3) Å, c = 8.5334(2) Å, $\beta = 98.0460(10)^{\circ}$, V = 11.3226(3) Å, c = 8.5334(2) Å, $\beta = 11.3226(3)$ Å, $\beta = 11.32$ 14), *a* = 1576.99(7) Å³, Z = 4, T = 294.15 K, μ (MoK α) = 0.246 mm⁻¹, Dcalc = 1.309 g/cm³, 21052 reflections measured (4.378° $\leq 2\Theta \leq 56.538°$), 3888 unique ($R_{int} = 0.0415$, $R_{sigma} = 0.0388$) which were used in all calculations. The final R_1 was 0.0460 (I > 2 σ (I)) and wR_2 was 0.1462 (all data). CCDC 2254463 deposition numbers contains the supplementary crystallographic data for this paper which can be obtained free of charge at https://www.ccdc.cam.ac.uk/structures/



Figure 3: ORTEP diagram of **2s** (KB418) compound with the atom-numbering. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius.

- 1. Bruker (2016). APEX3, SAINT and SADABS. Bruker AXS, Inc., Madison, Wisconsin, USA.
- 2. Sheldrick G. M. (2015). ActaCrystallogr C71: 3-8.