Supplementary Material (ESI) for Chemical Communications

Ni(II)-Catalyzed Enantioselective Nazarov Cyclizations

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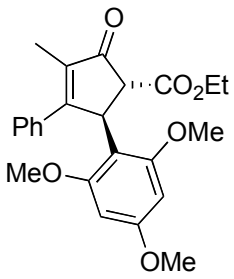
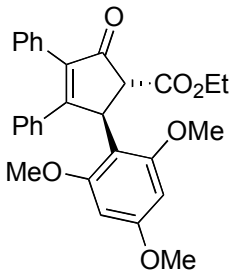
General: All catalysis experiments were conducted under an atmosphere of argon or nitrogen using standard Schlenk techniques or in a glove box. All solvents were stored over activated 4 Å molecular sieves unless otherwise indicated. In the case of freshly distilled solvents, the following drying agents were used: Na/benzophenone for THF and Et_2O; Na for toluene; CaH_2 for CH_2Cl_2. Chromatography was carried out with Merck silica gel 60. The NMR spectra were recorded at 25 °C on Brucker Avance 250 (250.1 MHz, ^1H; 62.9 MHz, ^{13}C), 300 (300.1 MHz, ^1H; 75.5 MHz, ^{13}C) spectrometers. ^1H and ^{13}C chemical shifts (δ) were referenced internally by the residual solvent signal. High-resolution MALDI mass spectra were measured by the analytical service of the Organic Chemistry Laboratory of the ETH Zürich on an IonSpec ultima FT MALDI mass spectrometer. Elemental analyses were obtained on a Leco CHN-900 analyzer. All commercially available chemicals were used without further purification.

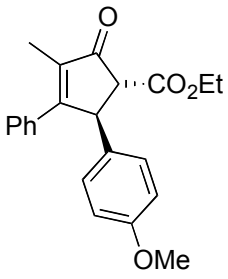
General procedure for the nickel(II)-catalyzed Nazarov cyclization: $[Ni(H_2O)_6][ClO_4]_2$ (5 µmol, 0.1 equiv.) und Pigiphos **2a** (0.01 mmol, 0.2 equiv.) were dissolved in dry THF (1 mL) under argon. After stirring for 16 h at room temperature, the solvent was evaporated to dryness and the residue was dried under vacuo for 3 h. Afterwards, the Nazarov substrate **1** (0.05 mmol, 1 equiv.) and dry CH_2Cl_2 (1 mL) were added. After the cyclization completed, the solvent was evaporated and the residue was purified by column chromatography.



(1*R*,5*R*)-Ethyl 3-methyl-2-oxo-4-phenyl-5-(2,4,6-trimethoxyphenyl)-cyclopent-3-enecarboxylate (4a): beige solid, yield 84%, 86% ee (DP, *n*Hex:*i*PrOH 70:30, 1 mL/min, 11.64 min (major), 13.32 min (minor)); $[\alpha]_D$ = –55.65 enantiopure (*c* = 0.1, $CHCl_3$); δ_H (300.1 MHz; $CDCl_3$) 1.31 (3H, t, *J* 7.2, CH_2CH_3), 1.96 (3H, d, *J* 2.2, CH_3), 3.55 (1H, s, OCH_3), 3.69 (1H, d, *J* 3.3, C(O)*CH*C(O)), 3.72 (1H, s, OCH_3), 3.84 (1H, s, OCH_3), 4.18–4.32 (2H, m, CH_2CH_3), 5.42 (1H, t, *J* 2.5, *CH*), 5.89 (1H, d, *J* 2.0, *CH*Ar), 6.06 (1H, d, *J* 2.0, *CH*Ar), 7.25–7.35 (5H, m, *CH*Ar); δ_C (75.5 MHz; $CDCl_3$) 10.03, 14.25, 40.50, 55.14, 55.17, 56.13, 58.31, 61.18, 90.62, 90.87, 108.14, 127.90, 127.91, 128.85, 133.17, 135.11, 158.77, 159.41, 160.34, 170.13, 171.50, 202.86; EA $C_{24}H_{26}O_6$ (410.47): calcd. C 70.23, H 6.38, found C 70.42, H 6.49; MS (HR MALDI) *m/z* 411.1808 (calcd. for $C_{24}H_{27}O_6$), found 411.1802 [MH^+].

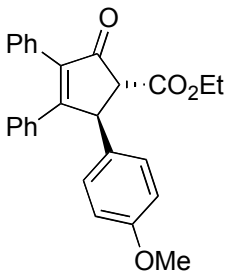


(1*R*,5*R*)-Ethyl 2-oxo-3,4-diphenyl-5-(2,4,6-trimethoxyphenyl)cyclo-pent-3-enecarboxylate (4b): yellowish solid, yield 85%, 87% ee (DP, *n*Hex:*i*PrOH 40:60, 1 mL/min, 9.25 min (minor), 20.83 min (major)); $[\alpha]_D$ = –45.41 @ 87% ee (*c* = 0.1, $CHCl_3$); δ_H (250.1 MHz; $CDCl_3$) 1.30 (3H, t, *J* 7.2, CH_2CH_3), 3.61 (3H, s, OCH_3), 3.74 (3H, s, OCH_3), 3.79 (1H, d, *J* 3.2, *CH*), 3.90 (3H, s, OCH_3), 4.13–4.31 (2H, m, CH_2CH_3), 5.53 (1H, d, *J* 3.2, C(O)*CH*C(O)), 5.94 (1H, d, *J* 2.0, *CH*Ar), 6.12 (1H, d, *J* 2.0, *CH*Ar), 7.09–7.33 (m, 1H, *CH*Ar); δ_C (75.5 MHz; $CDCl_3$) 14.27, 40.45, 55.17, 55.23, 56.20, 59.17, 61.31, 90.70, 90.87, 107.98, 127.58, 127.72, 128.20, 128.52, 129.07, 129.72, 132.21, 134.61, 136.62, 158.78, 159.37, 160.49, 169.77, 173.05, 200.57; EA $C_{29}H_{28}O_6$ (472.53): calcd. C 73.71, H 5.97, found C 73.56, H 6.07; MS (HR MALDI) *m/z* 473.1964 (calcd. for $C_{29}H_{29}O_6$), found 473.1963 [MH^+].

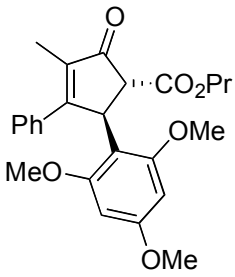


(1*R*,5*R*)-Ethyl 3-methyl-2-oxo-4-phenyl-5-(4-methoxyphenyl)cyclo-pent-3-enecarboxylate (4c): yellowish oil, yield 32%, 71% ee (DP, *n*Hex:*i*PrOH 90:10, 1 mL/min, 19.96 min (major), 22.70 min (minor)); $[\alpha]_D$ = –33.38 @ 71% ee (*c* = 0.1, $CHCl_3$); δ_H (300.1 MHz; $CDCl_3$) 1.34 (3H, t, *J* 7.2, CH_2CH_3), 2.03 (3H, d, *J* 1.8, CH_3), 3.45 (1H, d, *J* 2.7, C(O)*CH*C(O)), 3.73 (3H, s, OCH_3), 4.24–4.32 (2H, m, CH_2CH_3), 4.86 (1H, t, *J* 1.8, *CH*), 6.75 (2H, d, *J* 8.7, *CH*Ar), 7.00 (2H, d, *J* 8.7, *CH*Ar), 7.30–7.36 (5H, m, *CH*Ar); δ_C (75.5 MHz; $CDCl_3$) 10.21, 14.23, 50.34, 55.15, 61.79, 61.88, 113.68, 114.30, 127.59, 127.90, 128.31, 128.38, 128.65, 129.32, 132.72, 134.64, 135.72, 158.57, 168.69,

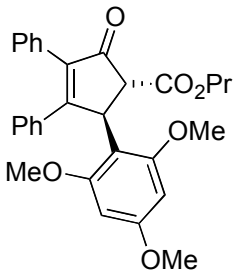
169.19, 201.72; EA $C_{22}H_{22}O_4$ (350.41): calcd. C 75.41, H 6.33; found C 74.86, H 6.20; MS (HR MALDI) *m/z* 351.1596 (calcd. for $C_{22}H_{23}O_4$), found 351.1591 [MH^+].



(1*R*,5*R*)-Ethyl 2-oxo-3,4-diphenyl-5-(4-methoxyphenyl)cyclopent-3-enecarboxylate (4d): yellowish oil, yield 96%, 83% ee (OD-H, *n*Hex:*i*PrOH 80:20, 1 mL/min, 14.60 min (minor), 17.93 min (major)); $[\alpha]_D$ = –20.07 @ 83% ee (*c* = 0.1, $CHCl_3$); δ_H (300.1 MHz; $CDCl_3$) 1.34 (3H, t, *J* 6.9, CH_2CH_3), 3.64 (1H, d, *J* 3.0, *CH*), 3.74 (3H, s, OCH_3), 4.21–4.38 (2H, m, CH_2CH_3), 4.99 (1H, d, *J* 2.7, C(O)*CH*C(O)), 6.79 (2H, d, *J* 8.7, *CH*Ar), 7.10 (2H, d, *J* 8.7, *CH*Ar), 7.12–7.37 (10H, m, *CH*Ar); δ_C (75.5 MHz; $CDCl_3$) 14.24, 50.35, 55.17, 61.87, 62.71, 114.46, 128.20, 128.23, 128.37, 128.78, 128.97, 129.57, 129.90, 131.31, 132.44, 134.21, 138.57, 158.70, 168.44, 170.28, 199.61; EA $C_{27}H_{24}O_4$ (412.48): calcd. for C 78.62, H 5.86; found C 78.27, H 5.93; MS (HR MALDI) *m/z* 413.1753 (calcd. for $C_{27}H_{25}O_4$), found 413.1747 [MH^+].

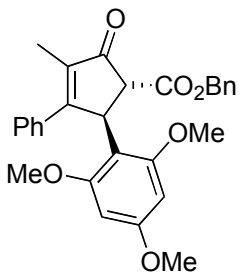


(1*R*,5*R*)-Propyl 3-methyl-2-oxo-4-phenyl-5-(2,4,6-trimethoxyphenyl)-cyclopent-3-enecarboxylate (4e): yellowish solid, yield 80%, 82% ee (DP, *n*Hex:*i*PrOH 70:30, 1mL/min, 11.04 min (major), 12.43 min (minor)); δ_H (250.1 MHz, $CDCl_3$) 0.96 (3H, t, *J* 7.2, $OCH_2CH_2CH_3$), 1.62–1.76 (2H, m, $OCH_2CH_2CH_3$), 1.94 (3H, d, *J* 1.7, CH_3), 3.52 (3H, s, OCH_3), 3.67 (1H, br, *CH*), 3.70 (3H, s, OCH_3), 3.81 (3H, s, OCH_3), 4.03–4.24 (2H, m, $OCH_2CH_2CH_3$), 5.40 (1H, s, *CH*), 5.86 (1H, br, *CH*Ar), 6.02 (1H, br, *CH*Ar), 7.20–7.30 (5H, m, *CH*Ar, *CH*); δ_C (75.5 MHz, $CDCl_3$) 10.13, 10.43, 22.15, 40.63, 55.25, 55.29, 56.20, 58.47, 66.90, 90.71, 90,97, 108,25, 128.02, 133.33, 135.25, 158.86, 159.54, 160.44, 170.32, 171.59, 203.02; MS (HR MALDI) *m/z* 425.1959 (calc. $C_{25}H_{29}O_6$), found 425.1964 [MH^+].

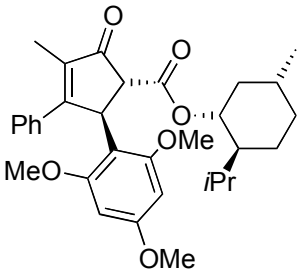


(1*R*,5*R*)-Propyl 2-oxo-3,4-diphenyl-5-(2,4,6-trimethoxyphenyl)cyclopent-3-enecarboxylate (4f): yellowish solid, yield 82%, 88 % ee (DP, *n*Hex:*i*PrOH 40:60, 1mL/min, 9.05 min (minor), 19.57 min (major)); δ_H (250.1 MHz, $CDCl_3$) 0.99 (3H, t, *J* 7.2, $OCH_2CH_2CH_3$), 1.66–1.78 (2H, m, $OCH_2CH_2CH_3$), 3.60 (3H, s, OCH_3), 3.73 (3H, s, OCH_3), 3.86–3.87 (4H, m, OCH_3, *CH*), 4.06–4.28 (2H, m, $OCH_2CH_2CH_3$), 5.43 (1H, d, *J* 3.3, *CH*), 5.90 (1H, d, *J* 2.1, *CH*Ar), 6.07 (1H, d, *J* 2.4, *CH*Ar), 7.07–7.28 (10H, m, *CH*Ar); δ_C (75.5 MHz, $CDCl_3$) 10.47, 22.16, 40.57, 55.27, 55.34, 56.26, 59.30, 67.03, 90.77, 90.95, 108.10, 127.67, 127.81, 128.31, 128.62, 129.15, 129.81, 132.33, 134.74, 136.78, 158.87,

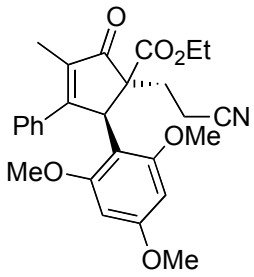
159.49, 160.58, 169.95, 173.12, 200.70; MS (HR MALDI) *m/z* 487.2121 (calc. for $C_{30}H_{31}O_6$), found 487.2115 [MH^+].



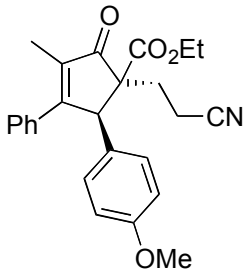
(1*R*,5*R*)-Benzyl 3-methyl-2-oxo-4-phenyl-5-(2,4,6-trimethoxyphenyl)-cyclopent-3-enecarboxylate (4g): yellowish solid, yield 58%, 45% ee (OD-H, *n*Hex:*i*PrOH 80:20, 0.5 mL/min, 13.54 min (minor), 17.20 min (major)); δ_H (300.1 MHz; $CDCl_3$) 1.97 (3H, d, *J* 2.4, *CH*$_3$), 3.54 (3H, s, O*CH*$_3$), 3.72 (3H, s, O*CH*$_3$), 3.75 (3H, s, O*CH*$_3$), 3.79 (1H, d, *J* 3.3, *CH*), 5.19 (1H, d, *J* 12.6, C(O)*CH*$_2$Ph), 5.30 (1H, d, *J* 12.6, C(O)*CH*$_2$Ph), 5.42–5.47 (1H, m, C(O)*CH*C(O)), 5.87 (1H, d, *J* 2.1, *CH*Ar), 6.03 (1H, d, *J* 1.8, *CH*Ar), 7.25–7.46 (10H, m, *CH*Ar); δ_C (75.5 MHz; $CDCl_3$) 10.05, 40.49, 55.15, 56.07, 58.24, 66.82, 90.61, 90.83, 108.03, 127.90, 127.91, 127.93, 127.99, 128.00, 128.44, 128.86, 133.22, 135.08, 136.01, 158.74, 159.39, 160.35, 170.00, 202.59; MS (HR MALDI) *m/z* 473.1964 (calcd. for $C_{29}H_{29}O_6$), found 473.1959 [MH^+].



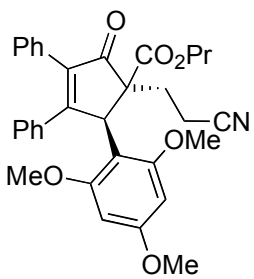
(1*R*,5*R*)-((1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl) 3-methyl-2-oxo-4-phenyl-5-(2,4,6-trimethoxyphenyl)cyclopent-3-enecarboxylate (5): In a two-neck round bottom flask, equipped with a micro-distillation apparatus, enantiopure **4a** (26.7 mg, 0.06 mmol, 1 equiv.), (Dr. Maisch ReproSil Chiral DP, 8 μm, 250 x 20 mm, *n*Hex:*i*PrOH 70:30, 19 mL/min), $NaBO_3 \cdot 4H_2O$ (4.6 mg, 0.03 mmol, 0.4 equiv.) and (1*R*)-(–)-Menthol (9.7 mg, 0.06 mmol, 0.95 equiv.) were dissolved in toluene (2 mL) at 90 °C. After 24 h at this temperature the reaction mixture was cooled and filtered over celite. The crude material was purified by column chromatography (*c*Hex:EtOAc, 85:15, R_f 0.26) to give 19.4 mg (56%) of a white solid. δ_H (300.1 MHz, $CDCl_3$) 0.76 (3H, d, *J* 6.0, *CH*$_3$), 0.84 (3H, d, *J* 6.0, *CH*$_3$), 0.94 (3H, d, *J* 6.0, *CH*$_3$), 1.01–1.17 (2H, m, *CH*$_2$), 1.36–1.85 (6H, m, *CH*$_2$, *CH*), 1.96 (3H, d, *J* 1.8, *CH*$_3$), 2.06–2.11 (1H, m, *CH*), 3.54 (3H, s, O*CH*$_3$), 3.62 (1H, d, *J* 3.3, C(O)*CH*C(O)), 3.73 (3H, s, O*CH*$_3$), 3.82 (3H, s, O*CH*$_3$), 4.78 (1H, dt, J_1 4.2, J_2 10.8, CO_2*CH*), 5.37 (1H, m, *CH*), 5.88 (1H, s, *CH*Ar), 6.04 (1H, s, *CH*Ar), 7.26–7.34 (5H, m, *CH*Ar); δ_C (75.5 MHz; $CDCl_3$) 10.16, 16.50, 20.80, 22.20, 23.72, 26.22, 31.58, 34.45, 40.88, 40.98, 46.95, 55.29, 56.16, 58.86, 75.20, 90.62, 90.94, 108.40, 128.03, 128.08, 128.93, 133.41, 133.35, 158.87, 159.56, 160.43, 170.10, 171.49, 203.19; MS (HR MALDI) *m/z* 543.2723 (calc. for $C_{32}H_{40}NaO_6$), found 543.2717 [MNa^+].



Ethyl 1-(2-cyanoethyl)-3-methyl-2-oxo-4-phenyl-5-(2,4,6-trimethoxyphenyl)cyclopent-3-enecarboxylate (6a): For the Michael addition, the solvent was evaporated after the Nazarov cyclization completed, as monitored by TLC. Acrylonitrile (1 mL) and DBU (5 μmol, 0.1 equiv.) were then added and the mixture was stirred for 3 h, after which time the reaction was complete. After evaporation of the solvent, the residue was purified by column chromatography (*c*Hex:EtOAc (8:2), R_f 0.25) to give **6a** as a white solid (84%), 87% ee (DP, *n*Hex:*i*PrOH 80:20, 1 mL/min, 22.67 min (minor), 24.83 min (major)); $[\alpha]_D$ = –23.67 @ 87% ee (*c* = 0.75, $CHCl_3$); δ_H (300.1 MHz, $CDCl_3$) 0.95 (3H, t, *J* 7.2, CH_2CH_3), 2.04 (3H, s, CH_3), 2.15–2.27 (1H, m, CH_2), 2.40–2.53 (1H, m, CH_2), 2.73–2.91 (2H, m, CH_2CN), 3.37 (3H, s, OCH_3), 3.60–3.81 (2H, m, CH_2CH_3), 3.72 (3H, s, OCH_3), 3.92 (3H, s, OCH_3), 4.94 (1H, s, *CH*), 5.75 (1H, s, *CH*Ar), 6.09 (1H, s, *CH*Ar), 7.28–7.33 (5H, m, Ph); δ_C (75.5 MHz; $CDCl_3$) 10.16, 12.70, 13.63, 32.25, 47.52, 54.83, 55.13, 56.01, 60.90, 61.13, 90.08, 90.40, 105.47, 119.87, 127.83, 127.99, 129.06, 133.43, 135.13, 159.27, 159.41, 160.69, 169.02, 169.59, 205.09; $C_{20}H_{24}NO_6$ (463.52): calc. C 69.96, H 6.31, N 3.02; found C 69.72, H 6.51, N 2.80; MS (HR MALDI) *m/z* 464.2073 (calc. for $C_{27}H_{29}NO_6$), found 464.2068 [MH^+].



Ethyl-1-(2-cyanoethyl)-2-(4-methoxyphenyl)-5-oxo-3,4-diphenylcyclopent-3-encarboxylate (6c): yield 63%, 72% ee (DP, *n*Hex:*i*PrOH 40:60, 1 mL/min, 19.12 min (minor), 21.10 min (major)); $[\alpha]_D$ = –33.84 @ 72% ee (*c* = 1, $CHCl_3$).δ_H (300.1 MHz, $CDCl_3$) 0.92 (3H, t, *J* 7.2, CH_2CH_3), 2.1 (3H, d, J 1.8, CH_3), 2.14–2.23 (1H, m, CH_2), 2.51–2.61 (1H, m, CH_2), 2.71–3.89 (2H, m, CH_2CN), 3.43–3.54 (1H, m, OCH_2CH_3), 3.61–3.69 (1H, m, OCH_2CH_3), 3.70 (3H, m, OCH_3), 4.24 (1H, d, J 1.8, *CH*), 6.70 (2H, d, *J* 8.7, *CH*Ar), 6.94 (2H, d, *J* 8.4, *CH*Ar), 7.26–7.38 (5H, m, Ph); δ_C (75.5 MHz; $CDCl_3$) 10.47, 12.91, 13.71, 32.14, 55.29, 57.99, 61.50, 62.45, 113.73, 119.67, 128.33, 128.51, 128.75, 129.80, 130.61, 134.47, 137.23, 159.12, 166.29, 169.26, 204.91; MS (HR MALDI) *m/z* 426.1681 (calc. $C_{25}H_{25}NNaO_4$), found 426.1676 [MNa^+].



Propyl 1-(2-cyanoethyl)-2-oxo-3,4-diphenyl-5-(2,4,6-trimethoxyphenyl)cyclopent-3-enecarboxylate (6f): white solid, yield 97%, 88% ee (DP, *n*Hex:*i*PrOH 40:60, 1mL/min, 11.74 min (minor), 15.29 min (major)); δ_H (300.1 MHz, $CDCl_3$) 0.87 (3H, t, *J* 7.5, $OCH_2CH_2CH_3$),

1.39–1.52 (2H, m, $OCH_2CH_2CH_3$), 2.26–2.56 (2H, m, CH_2CH_2CN), 2.78–2.95 (2H, m, CH_2CH_2CN), 3.38 (3H, s, OCH_3), 3.55–3.60 (1H, m, $OCH_2CH_2CH_3$), 3.62–3.79 (4H, m, $OCH_2CH_2CH_3$, OCH_3), 3.96 (3H, s, OCH_3), 5.09 (1H, s, *CH*), 5.77 (1H, d, *J* 2.1, *CH*), 6.11 (1H, d, *J* 2.1, *CH*Ar), 7.12–7.38 (10H, m, Ph); δ_C (75.5 MHz, $CDCl_3$) 10.35, 12.76, 21.59, 32.76, 47.54, 54.86, 55.15, 56.04, 61.86, 66.56, 90.17, 90.39, 105.24, 119.80, 127.71, 127.83, 128.39, 128.46, 129.28, 129.61, 132.15, 134.42, 136.96, 159.26, 160.84, 169.49, 202.99; MS (HR MALDI) *m/z* 562.2206 (calc. for $C_{33}H_{33}NNaO_6$), found 562.2203 [MNa^+].

Fig. 1 Monitoring of the catalytic reaction involving substrate **3a** by ^{31}P-NMR spectroscopy.

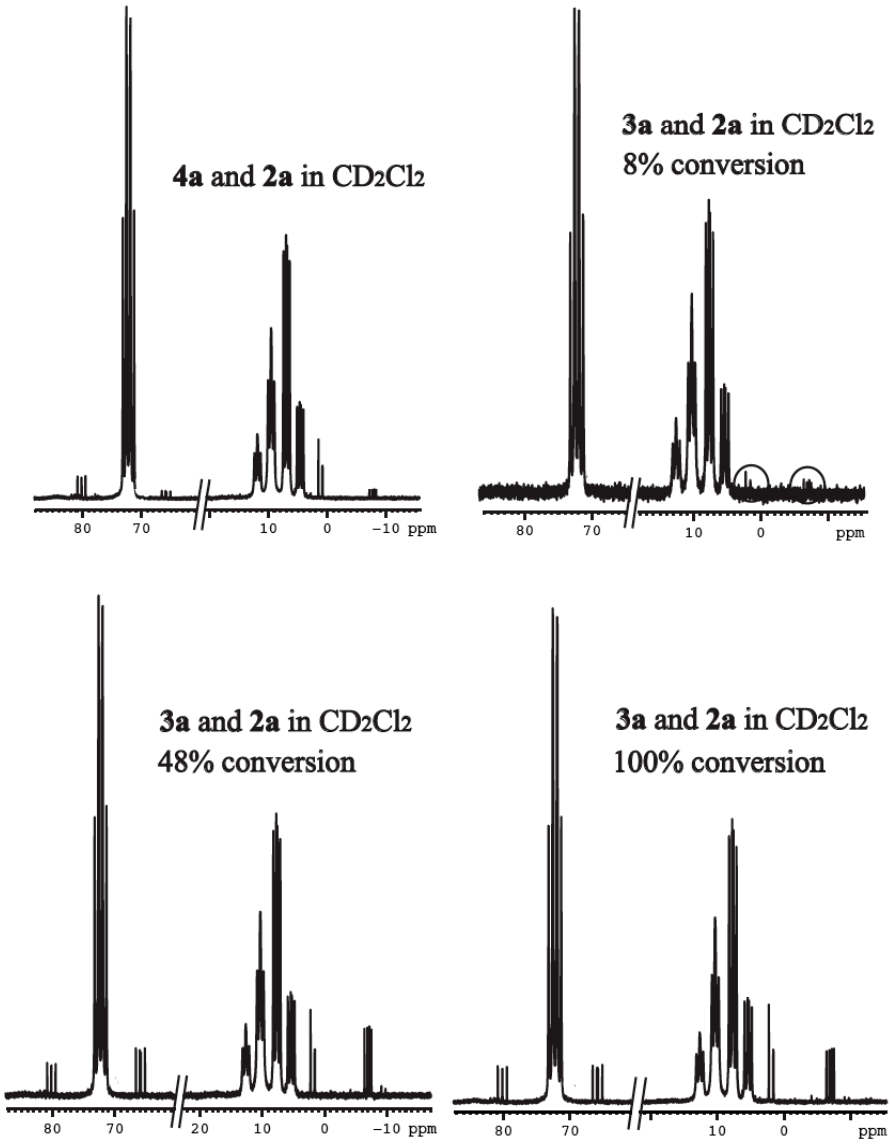
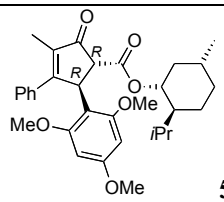


Table 1 Crystallographic data of **5**.



5

Empirical formula	$C_{32}H_{40}O_6$
Formula weight	520.64
Temperature (K)	200(2)
Wavelength (Å)	0.71073
Crystal system	orthorhombic
Space group	P 21 21 21
a (Å), α (°)	10.0389(5), 90
b (Å), β (°)	15.9508(7), 90
c (Å), γ (°)	18.4174(8), 90
V (Å^3)	2949.2(2)
Z, ρ_{calc} (g/cm^{-3})	4, 1.173
Abs. coefficient (mm^{-1})	0.080
F(000)	1120
Crystal size (mm)	0.51×0.44×0.40
θ range (°)	1.69–36.35
Reflections collected	120948
Reflections unique	14329 [R_{int} = 0.0493]
GOF in F^2	1.037
R_1 [I>2σ(I)], wR_2	0.0440, 0.1089
(all data)	0.0503, 0.1140
Largest diff. peak and hole (eA^{-3})	0.444/–0.135

Refinement method: Full-matrix least-squares on F^2

Table 2 Atom coordinates ($\times 10^4$) und equivalent isotrope temperature factors U_{eq} ($Å^2 \times 10^3$) of **5**.

Atom	**x**	**y**	**z**	**U_{eq}**
O(1)	4405(1)	5306(1)	-1238(1)	39(1)
O(2)	5679(1)	3068(1)	-30(1)	33(1)
O(3)	4522(1)	1330(1)	2030(1)	48(1)
O(4)	3108(1)	4164(1)	1849(1)	32(1)
O(5)	1341(1)	4652(1)	-111(1)	40(1)
O(6)	2564(1)	5778(1)	194(1)	31(1)
C(1)	3729(1)	4558(1)	-143(1)	21(1)
C(2)	4500(1)	4463(1)	579(1)	20(1)
C(3)	5910(1)	4737(1)	385(1)	21(1)
C(4)	6005(1)	5046(1)	-296(1)	24(1)
C(5)	4696(1)	5021(1)	-645(1)	25(1)
C(6)	7193(1)	5396(1)	-677(1)	38(1)
C(7)	6959(1)	4670(1)	938(1)	25(1)
C(8)	8242(1)	4393(1)	781(1)	38(1)
C(9)	9182(1)	4317(1)	1334(1)	51(1)
C(10)	8861(1)	4517(1)	2042(1)	51(1)
C(11)	7604(1)	4826(1)	2195(1)	55(1)
C(12)	6663(1)	4893(1)	1651(1)	43(1)
C(13)	4442(1)	3606(1)	928(1)	21(1)
C(14)	5108(1)	2920(1)	629(1)	24(1)
C(15)	5171(1)	2140(1)	974(1)	28(1)
C(16)	4520(1)	2054(1)	1636(1)	30(1)
C(17)	3791(1)	2709(1)	1939(1)	29(1)
C(18)	3769(1)	3479(1)	1586(1)	23(1)
C(19)	6630(2)	2484(1)	-294(1)	54(1)
C(20)	5399(2)	686(1)	1805(1)	56(1)
C(21)	2374(1)	4071(1)	2503(1)	34(1)
C(22)	2405(1)	4990(1)	-34(1)	23(1)
C(23)	1396(1)	6209(1)	491(1)	29(1)
C(24)	1342(1)	7096(1)	185(1)	28(1)
C(25)	161(1)	7544(1)	553(1)	38(1)
C(26)	268(2)	7541(1)	1376(1)	49(1)
C(27)	377(2)	6652(1)	1680(1)	51(1)
C(28)	1538(1)	6201(1)	1313(1)	41(1)
C(29)	1298(1)	7129(1)	-652(1)	29(1)
C(30)	1367(1)	8032(1)	-926(1)	41(1)
C(31)	90(1)	6683(1)	-980(1)	40(1)

Atom	**x**	**y**	**z**	**U_{eq}**
C(32)	542(3)	6665(1)	2504(1)	80(1)