Supplementary Material (ESI) for Chemical Communications

Lead(IV) acetate: intriguing reactivity profile

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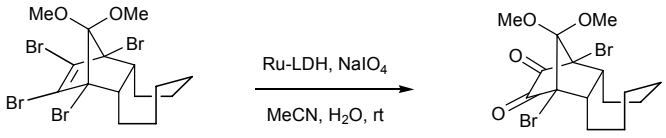
General Methods

NMR spectra were recorded at 400 MHz (^{1}H) and 100 MHz (^{13}C) on a 400 MHz FT-NMR spectrometer. Samples for NMR were made in $CDCl_3$ and TMS was used as the internal standard. Melting points were recorded on JSGW melting point apparatus and are uncorrected. TLC was performed on silica gel coated on microscopic slides. Visualization of spots was effected by exposure to iodine or spraying with 4% ethanolic H_2SO_4 and charring. Column chromatography was performed using silica gel (100-200 mesh), and ethyl acetate-hexane was used as eluent. Solvents and reagents were purified by standard methods. X-ray data were collected on a Bruker SMART APEX diffractometer. The structures were solved using SIR-92[1] and refined using SHELXL-97.[2]

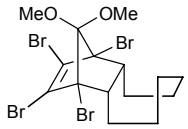
Procedure for the preparation of compound **4b**



4e **4b**

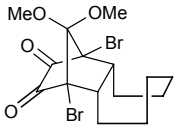
To a stirred solution of **4e** (1 mmol) in acetonitrile (12 mL), were added $NaIO_4$, Ru-LDH (0.86 mol% of $RuCl_3.3H_2O$, 40 mg) and distilled H_2O (2 mL) and the mixture was allowed to stir at room temperature until the completion of the reaction (monitored by TLC). The mixture was filtered and the residue was washed with MeCN. The filtrate (along with MeCN washings) was concentrated under reduced pressure and the crude mixture was dissolved in EtOAc (10 mL), washed first with $Na_2S_2O_3$ solution (3 mL) and then with brine (3 mL). EtOAc was dried over anhyd. Na_2SO_4 and concentrated to obtain the crude product, which after silica gel column chromatography (hexane and EtOAc) furnished the pure diketone **4b**.

Compound **4e**: yield 91%; white solid; mp 78 – 80 ^oC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.62 (s, 3H, OMe), 3.55 (s, 3H, OMe), 2.54 (dd, 2H, J = 7.4, 2.1 Hz), 1.91 (dd, 2H, J = 11.0, 4.5 Hz), 1.67 – 1.64 (m, 2H), 1.37 – 1.36 (m, 4H), 1.25 – 1.15 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 124.2 (olefin C, 2C), 111.3 (ketal C), 75.8 (Bridge head C-Br, 2C),



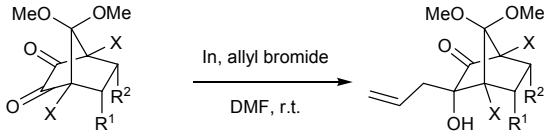
53.1, 52.7 (2C), 51.7, 30.4 (2C), 25.9 (2C), 22.9 (2C); IR (KBr) 2850, 1550, 1450, 1430, 1170 cm^{-1}; Anal. calcd. for $C_{15}H_{20}Br_4O_2$: C, 32.64; H, 3.65, found: C, 32.79; H, 3.66.

Compound **4b**: yield 96%; yellow solid; mp 114 – 116 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ



3.73 (s, 3H, OMe), 3.53 (s, 3H, OMe), 2.63 (dd, 2H, *J* = 7.9, 2.6 Hz), 1.74 – 1.62 (m, 4H), 1.33 –1.30 (m, 4H), 1.21 – 1.05 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.4 (C=O, 2C), 101.5 (ketal C), 75.3 (C-Br, 2C), 52.9 (OMe), 52.2 (OMe), 48.2 (2C), 30.2 (2C), 25.6 (2C), 22.8 (2C); IR (KBr) 2850,1730, 1550, 1450, 1420, 1170 cm^{-1}; Anal. calcd. for $C_{15}H_{20}Br_2O_4$: C, 42.48; H, 4.75, found: C, 42.49; H, 4.72.

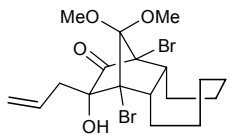
General procedure for the preparation of compounds **4a** and **10a**



b **a**

A mixture of diketone **b** (1 mmol), indium metal (2 mmol, cut into small pieces) and allyl bromide (4 mmol) in DMF (1.2 mL) was stirred at room temperature for 6h. After completion of the reaction, as monitored by tlc, the reaction was quenched with few drops of 10% HCl (saturated NH_4Cl was used for acid sensitive substrate **10b**) and extracted with diethyl ether (5x5 mL). The combined organic layers were washed with brine, dried over anhyd. Na_2SO_4 and concentrated. The resulting residue was purified by silica gel column chromatography to provide the pure homoallylic alcohols.

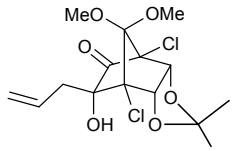
Compound **4a**: yield 84%; white solid; mp 82 – 84 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ



6.14 – 6.03 (m, 1H, olefin CH), 5.36 – 5.25 (m, 2H, olefin CH_2), 3.73 (s, 3H, OMe), 3.60 (s, 3H, OMe), 2.91 – 2.83 (m, 2H), 2.76 (s, 1H, D_2O exchangeable), 2.6 – 2.5 (m, 2H), 1.98 –1.49 (m, 7H), 1.34 – 1.25 (m, 2H), 1.08 – 1.06 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.0 (C=O), 131.8

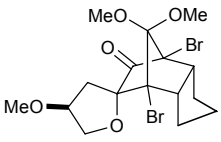
(olefin CH), 122.7 (olefin CH_2), 102.7 (ketal C), 80.9 (C-OH), 76.0 (C-Br), 73.9 (C-Br), 52.2, 51.6, 50.6, 49.5, 43.4, 31.6, 30.8, 25.7, 24.9, 24.4, 22.0; IR (KBr) 2850, 1760, 1450, 1430, 1180 cm^{-1}; Anal. calcd. for $C_{18}H_{26}Br_2O_4$: C, 46.37; H, 5.62, found: C, 46.49; H, 5.77.

Compound **10a**: yield 80%; white solid; mp 176 – 177 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 6.13 – 6.06 (m, 1H, olefin CH), 6.04 (s, 1H, D_2O exchangeable), 5.11 – 5.03 (m, 3H), 4.72 (d, 1H, *J* = 8.1 Hz), 3.57 (s, 3H, OMe), 3.55 (s, 3H, OMe), 2.74 (d, 2H, *J* = 7.1 Hz), 1.48 (s, 3H, Me), 1.31 (s, 3H, Me); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.4 (C=O), 131.9 (olefin CH), 118.1 (olefin CH_2), 115.4 (ketal C), 105.0 (ketal C), 86.3, 83.0, 80.5, 71.9, 51.8 (OMe), 51.3 (OMe), 40.6, 25.1, 23.1; IR (KBr) 2850, 1770, 1450, 1430, 1180 cm^{-1}; Anal. calcd. for $C_{15}H_{20}Cl_2O_6$: C, 49.06; H, 5.49; found: C, 49.14; H, 5.61.

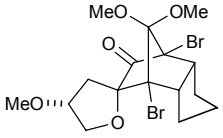


Spectral and analytical data for compounds **c** and **d:**

Compound **1c**: white solid; mp 82 – 84 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 4.18 – 4.14 (m, 2H), 3.99 – 3.96 (m, 1H), 3.71 (s, 3H, OMe), 3.62 (s, 3H, OMe), 3.54 – 3.50 (m, 1H), 3.34 (s, 3H, OMe), 2.99 – 2.97 (m, 1H), 2.55 – 2.50 (m, 3H), 1.84 – 1.70 (m, 2H), 1.62 – 1.52 (m, 2H), 1.42 – 1.38 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.7 (C=O), 105.8 (ketal C), 92.0, 79.7, 73.3, 72.9 (C-Br), 69.1 (C-Br), 57.1 (OMe), 54.1, 51.8, 51.5, 50.7, 43.0, 26.1, 26.0, 25.5; IR (KBr) 2850, 1760, 1440, 1180, 1050 cm^{-1}; Anal. calcd. for $C_{16}H_{22}Br_2O_5$: C, 42.31; H, 4.88, found: C, 42.57; H, 4.88; ESI-HRMS: calcd. for $C_{16}H_{22}Br_2O_5$+H 452.9913, found 452.9918.

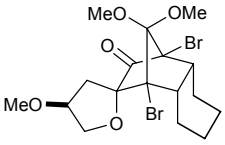


Compound **1d**: white crystals (CH_2Cl_2 / Hexane); mp 126 – 128 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 4.12 (dd, 1H, *J* = 8.3, 4.6 Hz), 4.09 – 4.02 (m, 2H), 3.70 (s, 3H, OMe), 3.62 (s, 3H, OMe), 3.47 – 3.42 (m, 1H), 3.33 (s, 3H, OMe), 3.10 –2.98 (m, 1H), 2.77 (dd, 1H, *J* = 14.6, 6.8 Hz), 2.48 – 2.46 (m, 1H), 2.30 (dd, 1H, 14.6, 3.4 Hz), 1.89 – 1.85 (m, 1H), 1.73



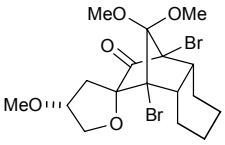
– 1.69 (m, 2H), 1.59 – 1.43 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.9 (C=O), 105.7 (ketal C), 92.0, 79.7, 73.8, 72.8 (C-Br), 69.9 (C-Br), 57.1 (OMe), 53.8, 51.9, 51.5, 50.8, 43.6, 26.0, 25.9, 25.4; IR (KBr) 2850, 1760, 1440, 1200, 1060, 960 cm^{-1}; Anal. calcd. for $C_{16}H_{22}Br_2O_5$: C, 42.31; H, 4.88, found: C, 42.39; H, 4.94.

Compound **2c**: white solid; mp 81 – 82 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.14 – 4.09 (m, 2H), 3.98 – 3.94 (m, 1H), 3.67 (s, 3H, OMe), 3.58 (s, 3H, OMe), 3.29 (s, 3H, OMe), 3.0 (dt, 1H, *J* = 12.0, 6.5 Hz), 2.55 – 2.37 (m, 3H), 2.28 – 2.19 (m,1H), 1.67 – 1.62 (m, 2H),



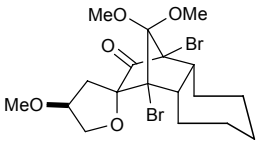
1.61 – 1.49 (m, 2H), 1.39 – 1.30 (m, 1H), 1.22 – 1.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.0 (C=O), 103.2 (ketal C), 92.1, 80.0, 74.4 (C-Br), 73.6, 71.0 (C-Br), 57.0 (OMe), 52.0 (OMe), 51.7 (OMe), 47.4, 43.6, 42.6, 20.3, 19.8, 19.7, 18.8; IR (KBr) 2850, 1760, 1440, 1180, 1060, 940 cm^{-1}; Anal. calcd. for $C_{17}H_{24}Br_2O_5$: C, 43.61; H, 5.17, found: C, 43.44; H, 5.13; ESI-HRMS: calcd. for $C_{17}H_{24}Br_2O_5$+H 467.0069, found 467.0068.

Compound **2d**: white solid; mp 108 – 109 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.12 – 4.04 (m, 2H), 3.96 (dd, 1H, *J* = 8.2, 3.8 Hz), 3.70 (s, 3H, OMe), 3.59 (s, 3H, OMe), 3.32 (s, 3H, OMe), 2.98 (dt, 1H, *J* = 12.0, 6.6 Hz), 2.79 (dd, 1H, *J* = 14.4, 6.8 Hz), 2.47 (ddd, 1H,



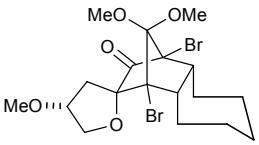
J = 14.2, 12.4, 4.6 Hz), 2.29 – 2.19 (m, 2H), 1.67 – 1.60 (m, 2H), 1.58 – 1.50 (m, 2H), 1.41 – 1.33 (m, 1H), 1.22 – 1.09 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.3 (C=O), 103.1 (ketal C), 92.2, 79.6, 74.3 (C-Br), 73.7, 71.9 (C-Br), 57.2 (OMe), 52.0 (OMe), 51.8 (OMe), 47.0, 43.9, 43.4, 20.3, 19.9, 19.6, 18.6; IR (KBr) 2850, 1760, 1440, 1180, 1060, 940 cm^{-1}; Anal. calcd. for $C_{17}H_{24}Br_2O_5$: C, 43.61; H, 5.17, found: C, 43.69; H, 5.41.

Compound **3c**: white solid; mp 94 – 96 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.19 – 4.12 (m, 2H), 3.98 – 3.96 (m, 1H), 3.74 (s, 3H, OMe), 3.62 (s, 3H, OMe), 3.32 (s, 3H, OMe), 3.07 (dd, 1H, *J* = 12.4, 8.2 Hz), 2.56 – 2.52 (m, 2H), 2.44 – 2.41 (m, 1H), 2.14 – 1.97 (m, 4H), 1.79 – 1.71 (m, 2H), 1.2 – 0.97 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.6 (C=O), 102.8 (ketal C), 92.2, 80.1, 75.4 (C-Br), 73.6, 72.2 (C-Br), 57.0 (OMe), 52.1, 51.7, 51.6,



49.2, 42.6, 30.6, 30.5, 29.1, 25.7, 25.1; IR (KBr) 2850, 1760, 1440, 1180, 1060 cm^{-1}; Anal. calcd. for $C_{18}H_{26}Br_2O_5$: C, 44.83; H, 5.43, found: C, 44.89; H, 5.41.

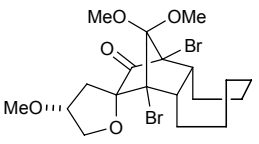
Compound **3d**: white solid; mp 88 – 89 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 4.11 – 4.06 (m, 2H), 3.99 – 3.96 (m, 1H), 3.72 (s, 3H, OMe), 3.61 (s, 3H, OMe), 3.33 (s, 3H, OMe),



3.04 – 2.98 (m, 1H,), 2.81 (dd, 1H, *J* = 14.5, 7.4 Hz), 2.52 (dt, 1H, *J* = 12.3, 1.9 Hz), 2.23 (dd, 1H, *J* = 14.3, 4.3 Hz), 2.17 – 2.14 (m, 1H), 2.0 – 1.96 (m, 3H), 1.79 – 1.70 (m, 2H), 1.21 – 0.95 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.8 (C=O), 102.8 (ketal C), 92.4, 79.7, 75.2 (C-Br), 73.7, 73.1 (C-Br), 57.2 (OMe), 52.1, 51.7, 51.3, 49.5, 43.4, 30.6, 30.5, 29.1, 25.4, 25.0; IR (KBr) 2850, 1760, 1430, 1180, 1050, 980, 930 cm^{-1}; Anal. calcd. for $C_{18}H_{26}Br_2O_5$: C, 44.83; H, 5.43, found: C, 44.85; H, 5.41.

Compound **4c**: colorless viscous liquid; ^1H NMR (400 MHz, $CDCl_3$) δ 4.18 – 4.11 (m, 1H), 4.08 – 4.03 (m, 1H), 3.92 – 3.89 (m, 1H), 3.71 (s, 3H, OMe), 3.56 (s, 3H, OMe), 3.28 (s, 3H, OMe), 2.85 – 2.79 (m, 1H), 2.52 – 2.44 (m, 2H), 2.34 (dd, 1H, *J* = 14.2, 6.6 Hz), 1.93 – 1.75 (m, 3H), 1.69 – 1.65 (m, 2H), 1.59 – 1.47 (m, 2H), 1.36 – 1.23 (m, 2H), 1.12 – 1.01 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.1 (C=O), 102.3 (ketal C), 91.6, 80.3, 76.2 (C-Br), 73.5, 73.3 (C-Br), 56.9 (OMe), 52.1, 51.7, 50.0, 49.0, 42.1, 31.4, 30.6, 25.7, 24.9, 24.4, 21.6; IR (neat) 2850, 1750, 1440, 1240, 1180, 1060, 940 cm^{-1}; Anal. calcd. for $C_{19}H_{28}Br_2O_5$: C, 45.99; H, 5.69, found: C, 45.76; H, 5.69.

Compound **4d**: white solid; 110 – 112 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 4.10 – 4.02 (m,



2H), 3.95 – 3.90 (m, 1H), 3.71 (s, 3H, OMe), 3.57 (s, 3H, OMe), 3.30 (s, 3H, OMe), 2.80 - 2.71 (m, 2H), 2.54 – 2.48 (m, 1H), 2.18 (dd, 1H, *J* = 14.5, 4.6 Hz), 2.04 – 1.79 (m, 3H), 1.72 – 1.61 (m, 2H), 1.57 – 1.46 (m, 2H), 1.39 – 1.22 (m, 2H), 1.12 - 1.02 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.4 (C=O), 102.3 (ketal C), 91.8, 79.9, 76.1 (C-Br), 74.5 (C-Br), 73.8, 57.2 (OMe), 52.1, 51.8, 49.6, 49.5, 43.1, 31.4, 30.7, 25.7, 24.9, 24.4, 21.5; IR (KBr) 2860,

1770, 1440, 1180, 1080 cm^{-1}; Anal. calcd. for $C_{19}H_{28}Br_2O_5$: C, 45.99; H, 5.69, found: C, 45.86; H, 5.71.

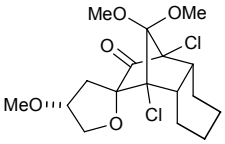
Compound **5c**: colorless solid; mp 90 – 92 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.26 (m, 5H), 4.34 – 4.28 (m, 2H), 4.09 (dd, 1H, *J* = 9.0, 3.4 Hz), 3.81 (s, 3H, OMe), 3.74 – 3.68 (m, 1H, buried under OMe peak), 3.68 (s, 3H, OMe), 3.37 (s, 3H, OMe), 3.16 (dd, 1H, *J* = 13.0, 5.7 Hz), 2.92 (t, 1H, *J* = 12.7 Hz), 2.51 – 2.48 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.4 (C=O), 136.0 (Aromatic C), 129.4 (Aromatic CH, 2C), 128.1 (Aromatic CH, 2C), 127.8 (Aromatic CH), 103.6 (ketal C), 89.9, 80.9, 76.4, 73.1, 66.9, 57.3 (OMe), 52.0 (OMe), 51.9 (OMe), 49.7, 40.6, 39.6; IR (KBr) 2850, 1750, 1480, 1430, 1200 cm^{-1}; Anal. calcd. for $C_{19}H_{22}Br_2O_5$: C, 46.55; H, 4.52, found: C, 46.66; H, 4.71.

Compound **5d**: colorless solid; mp 98 – 99 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.23 (m, 5H), 4.28 (dd, 1H, *J* = 8.5, 5.4 Hz), 4.25 – 4.19 (m, 1H), 4.13 (dd, 1H, *J* = 8.6, 4.6 Hz), 3.81 (s, 3H, OMe), 3.78 – 3.69 (m, 1H, buried under OMe peak), 3.69 (s, 3H, OMe), 3.37 (s, 3H, OMe), 3.11 (dd, 1H, *J* = 12.9, 5.6 Hz), 2.86 (t, 1H, *J* = 12.7 Hz), 2.78 (dd, 1H, *J* = 14.2, 7.1 Hz), 2.3 (dd, 1H, *J* = 14.2, 4.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.1 (C=O), 135.9 (Aromatic C), 129.6 (Aromatic CH, 2C), 128.2 (Aromatic CH, 2C), 127.7 (Aromatic CH), 103.6 (ketal C), 89.9, 80.2, 76.4, 73.9, 67.9, 57.4 (OMe), 52.0 (OMe), 51.9 (OMe), 49.7, 41.1, 39.1; IR (KBr) 2850, 1750, 1480, 1430, 1200 cm^{-1}; Anal. calcd. for $C_{19}H_{22}Br_2O_5$: C, 46.55; H, 4.52, found: C, 46.57; H, 4.59.

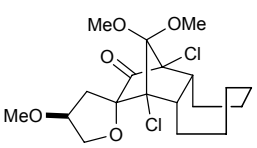
Compound **6c** : white crystals (CH_2Cl_2 / Hexane); mp 87 – 88 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 4.11 – 4.04 (m, 2H), 3.95 – 3.91 (m, 1H), 3.62 (s, 3H, OMe), 3.50 (s, 3H, OMe), 3.26 (s, 3H, OMe), 2.93 (td, 1H, *J* = 11.2, 7.0 Hz), 2.54 – 2.49 (m, 1H), 2.43 – 2.29 (m, 2H), 2.23 – 2.19 (m, 1H), 1.65 – 1.60 (m, 2H), 1.55 – 1.46 (m, 2H), 1.39 – 1.31 (m, 1H), 1.14 – 1.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.6 (C=O), 103.3 (ketal C), 91.9, 80.5 (C-Cl), 80.1, 76.0 (C-Cl), 73.7, 57.0 (OMe), 51.9 (OMe), 51.6 (OMe), 45.4, 42.3, 40.5, 20.2, 20.0,

19.4, 18.3; IR (KBr) 2850, 1760, 1440, 1180, 1060 cm^{-1}; Anal. calcd. for $C_{17}H_{24}Cl_2O_5$: C, 53.83; H, 6.38, found: C, 53.79; H, 6.55; ESI-HRMS: calcd. for $C_{17}H_{24}Cl_2O_5$+H 379.1079, found 379.1073.

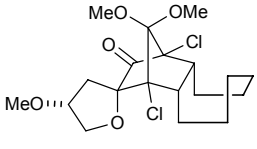
Compound **6d**: colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.09 – 4.04 (m, 2H), 4.0 – 3.97 (m, 1H), 3.67 (s, 3H, OMe), 3.56 (s, 3H, OMe), 3.34 (s, 3H, OMe), 2.98 – 2.91 (m, 1H), 2.87 – 2.82 (m, 1H), 2.52 – 2.43 (m, 1H), 2.29 – 2.20 (m, 1H), 2.21 (dd, 1H, *J* = 14.4, 4.2 Hz), 1.73 – 1.67 (m, 2H), 1.59 – 1.53 (m, 2H), 1.42 – 1.32 (m, 1H), 1.27 – 1.09 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.5 (C=O), 103.1 (ketal C), 91.9, 80.4 (C-Cl), 79.8, 76.8 (C-Cl), 73.7, 57.2 (OMe), 51.8 (OMe), 51.6 (OMe), 44.8, 42.5, 41.3, 20.2, 19.9, 19.2, 18.0; IR (neat) 2850, 1740, 1440, 1200, 1060, 960 cm^{-1}; Anal. calcd. for $C_{17}H_{24}Cl_2O_5$: C, 53.83; H, 6.38, found: C, 53.85; H, 6.63.



Compound **7c**: colorless viscous liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.13 – 4.10 (m, 1H), 4.04 (dd, 1H, *J* = 9.3, 4.8 Hz), 3.91 – 3.88 (m, 1H), 3.66 (s, 3H, OMe), 3.51 (s, 3H, OMe), 3.28 (s, 3H, OMe), 2.79 –2.72 (m, 1H), 2.50 – 2.45 (m, 2H), 2.29 (dd, 1H, *J* = 14.4, 6.8 Hz), 1.89 – 1.81 (m, 3H), 1.70 – 1.67 (m, 2H), 1.58 – 1.50 (m, 2H), 1.32 – 1.25 (m, 2H), 1.09 – 1.03 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.7 (C=O), 102.4 (ketal C), 91.3, 81.1 (C-Cl), 80.3, 77.2 (C-Cl), 73.6, 56.9 (OMe), 51.9 (OMe), 51.5 (OMe), 48.6, 48.3, 39.9, 31.4, 30.6, 25.7, 25.0, 23.8, 20.7; IR (neat) 2850, 1770, 1440, 1200, 1050, 960 cm^{-1}; Anal. calcd. for $C_{19}H_{28}Cl_2O_5$: C, 56.02; H, 6.93, found: C, 55.89; H, 6.77.

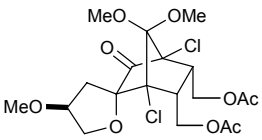


Compound **7d**: white solid; mp 104 – 105 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.07 – 4.02 (m, 1H), 3.99 (dd, 1H, *J* = 9.0, 5.4 Hz), 3.66 (dd, 1H, *J* = 9.0, 4.4 Hz), 3.66 (s, 3H, OMe), 3.52 (s, 3H, OMe), 3.31 (s, 3H, OMe), 2.77 (dd, 1H, *J* = 14.4, 7.1 Hz), 2.72 – 2.67 (m, 1H), 2.49 – 2.44 (m, 1H), 2.14 (dd, 1H, *J* = 14.4, 4.6 Hz), 1.99 – 1.95 (m, 1H), 1.81 – 1.67 (m, 4H), 1.58 – 1.46 (m, 2H), 1.38 – 1.22 (m, 2H), 1.12 – 1.02 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.8 (C=O), 102.3 (ketal C), 91.5, 81.2 (C-Cl), 80.1, 78.4 (C-Cl), 73.9, 57.1 (OMe),



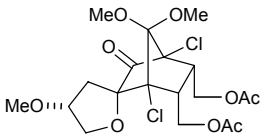
51.9 (OMe), 51.6 (OMe), 48.6, 48.2, 40.9, 31.4, 30.6, 25.7, 25.0, 23.8, 20.5; IR (KBr) 2850, 1770, 1440, 1200, 1050, 960 cm^{-1}; Anal. calcd. for $C_{19}H_{28}Cl_2O_5$: C, 56.02; H, 6.93, found: C, 56.12; H, 6.84.

Compound **8c**: colorless viscous liquid; ^1H NMR (400 MHz, $CDCl_3$) δ 4.48 – 4.39 (m, 2H), 4.18 – 4.07 (m, 3H), 4.02 – 3.96 (m, 2H), 3.66 (s, 3H, OMe), 3.53 (s, 3H, OMe),



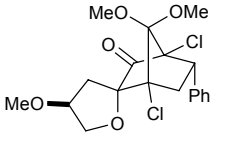
3.31 – 3.25 (m, 1H, buried under OMe peak), 3.26 (s, 3H, OMe), 2.99 – 2.95 (m, 1H), 2.48 – 2.43 (m ,1H), 2.31 (dd , 1H, J = 14.4, 6.6 Hz), 2.01 (s, 3H, Me), 1.95 (s, 3H, Me); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.2 (C=O), 170.4 (O-C=O), 170.1 (O-C=O), 102.2 (ketal C), 90.8, 80.4, 77.9 (C-Cl), 75.5 (C-Cl), 73.7, 60.9, 59.7, 56.9 (OMe), 52.1 (OMe), 51.9 (OMe), 46.4, 43.0, 39.4, 20.9, 20.5; IR (neat) 2850, 1760 – 1720 (broad), 1440,1350, 1200, 1020 cm^{-1}; Anal. calcd. for $C_{19}H_{26}Cl_2O_9$: C, 48.63; H, 5.58, found: C, 48.81; H, 5.76.

Compound **8d**: colorless viscous liquid; ^1H NMR (400 MHz, $CDCl_3$) δ 4.47 – 4.41 (m, 2H), 4.22 – 4.10 (m, 2H), 4.08 – 4.01 (m, 2H), 3.89 – 3.86 (m, 1H), 3.67 (s, 3H, OMe), 3.54 (s, 3H, OMe), 3.32 (s, 3H, OMe), 3.26 – 3.2 (m, 1H), 3.01 – 2.97 (m, 1H), 2.75 –



2.69 (m, 1H), 2.17 (dd, 1H, J = 14.2, 5.2 Hz), 2.03 (s, 3H, Me), 1.96 (s, 3H, Me); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.6 (C=O), 170.5 (O-C=O), 170.1 (O-C=O), 102.0 (ketal C), 90.7, 80.2 (C-Cl), 79.6, 77.9 (C-Cl), 73.7, 60.7, 59.5 (OMe), 57.4, 52.0, 51.9, 46.1, 43.1, 39.9, 20.9, 20.5; IR (neat) 2850, 1770 – 1720 (broad), 1440,1350, 1200, 1020 cm^{-1}; Anal. calcd. for $C_{19}H_{26}Cl_2O_9$: C, 48.63; H, 5.58, found: C, 48.68; H, 5.61.

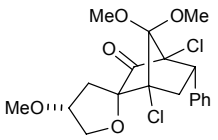
Compound **9c**: white solid; mp 120 – 122 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.25 (m, 5H), 4.32 – 4.23 (m, 2H), 4.11 – 4.08 (m, 1H), 3.77 (s, 3H, OMe), 3.7 (dd, 1H, J =



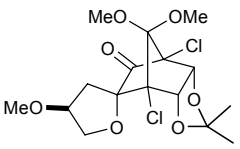
12.6, 5.8 Hz), 3.64 (s, 3H, OMe), 3.36 (s, 3H, OMe), 3.08 (dd, 1H, J = 13.1, 5.8 Hz), 2.8 (t, 1H, J = 12.8 Hz), 2.57 – 2.54 (m, 1H), 2.42 (dd, 1H, J = 14.0, 6.7 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.1 (C=O), 135.5 (Aromatic C), 129.3 (Aromatic CH, 2C), 128.2 (Aromatic CH, 2C), 127.8 (Aromatic CH), 103.4 (ketal C), 89.5, 82.0 (C-Cl), 80.8, 73.2, 73.0 (C-Cl), 57.1 (OMe),

51.8 (OMe), 51.7 (OMe), 48.3, 38.4, 37.2; IR (KBr) 2850, 1760, 1480, 1430, 1200 cm^{-1}; Anal. calcd. for $C_{19}H_{22}Cl_2O_5$: C, 56.87; H, 5.53, found: C, 57.06; H, 5.43.

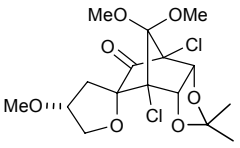
Compound **9d:** colorless viscous liquid; ^1H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.22 (m, 5H), 4.22 – 4.14 (m, 2H), 4.11 – 4. 08 (m, 1H), 3.75 (s, 3H, OMe), 3.71 – 3.64 (m, 1H, partially buried under OMe peak), 3.62 (s, 3H, OMe), 3.35 (s, 3H, OMe), 3.0 (dd, 1H, J = 12.9, 5.6 Hz), 2.81 – 2.70 (m, 2H), 2.24 (dd, 1H, J = 14.3, 4.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.4 (C=O), 135.5 (Aromatic C), 129.5 (Aromatic CH, 2C), 128.3 (Aromatic CH, 2C), 127.7 (Aromatic CH), 103.4 (ketal C), 89.6, 82.1, 80.3, 74.01, 73.96, 57.3 (OMe), 51.86 (OMe), 51.81 (OMe), 48.4, 39.0, 36.9; IR (neat) 2850, 1770, 1480, 1430, 1200 cm^{-1}; Anal. calcd. for $C_{19}H_{22}Cl_2O_5$: C, 56.87; H, 5.53, found: C, 56.89; H, 5.51.



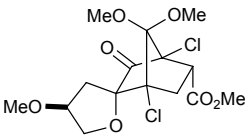
Compound **10c**: white crystals (CH_2Cl_2 / Hexane); mp 124 – 125 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 5.08 (d, 1H, J = 8.3 Hz), 4.75 (d, 1H, J = 8.3 Hz), 4.17 – 4.13 (m, 2H), 4.03 – 4.02 (m, 1H), 3.63 (s, 3H, OMe), 3.56 (s, 3H, OMe), 3.29 (s, 3H, OMe), 2.49 – 2.47 (m, 2H), 1.5 (s, 3H, Me), 1.3 (s, 3H, Me); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.7 (C=O), 115.5 (ketal C), 105.2 (ketal C), 90.8, 84.1, 81.0, 79.2, 78.0 (C-Cl), 73.6 (C-Cl), 73.0, 57.2 (OMe), 52.1 (OMe), 51.5 (OMe), 41.6, 24.9, 24.5; IR (KBr) 2850, 1770, 1440, 1360, 1250, 1180, 1110 cm^{-1}; Anal. calcd. for $C_{16}H_{22}Cl_2O_7$: C, 48.38; H, 5.58, found: C, 48.49; H, 5.67.



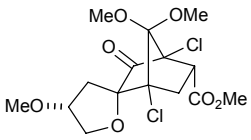
Compound **10d**: white solid; mp 136 – 138 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 5.05 (d, 1H, J = 8.3 Hz), 4.76 (d, 1H, J = 8.3 Hz), 4.18 – 4.15 (m, 1H), 4.06 – 4.0 (m, 2H), 3.62 (s, 3H, OMe), 3.56 (s, 3H, OMe), 3.32 (s, 3H, OMe), 2.78 (dd, 1H, J = 14.4, 7.3 Hz), 2.24 – 2.2 (m, 1H), 1.51 (s, 3H, Me), 1.29 (s, 3H, Me); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9 (C=O), 115.5 (ketal C), 105.2 (ketal C), 90.9, 83.9, 81.3, 79.3, 78.0 (C-Cl), 74.1 (C-Cl), 73.7, 57.4 (OMe), 52.1 (OMe), 51.6 (OMe), 41.7, 24.9, 24.5; IR (KBr) 2850, 1760, 1440, 1360, 1260, 1180 cm^{-1}; Anal. calcd. for $C_{16}H_{22}Cl_2O_7$: C, 48.38; H, 5.58, found: C, 48.42; H, 5.59.



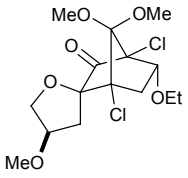
Compound **11c**: colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.24 – 4.22 (m, 1H), 4.05 (dd, 1H, *J* = 9.6, 4.8 Hz), 3.98 – 3.95 (m, 1H), 3.7 (s, 3H, OMe), 3.69 (s, 3H, OMe), 3.55 (s, 3H, OMe), 3.41 (dd, 1H, *J* = 12.8, 4.8 Hz) 3.3 (s, 3H, OMe), 2.95 (dd, 1H, *J* = 12.5, 4.8 Hz), 2.65 (t, 1H, *J* = 12.7 Hz), 2.42 – 2.35 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.4 (C=O), 170.0 (O=C-O), 102.9 (ketal C), 89.2, 81.1, 77.4 (C-Cl), 73.3, 72.4 (C-Cl), 57.0 (OMe), 52.5 (OMe), 51.92 (OMe), 51.87 (OMe), 47.1, 38.1, 34.1; IR (neat) 2850, 1760, 1750, 1430, 1350, 1290 cm^{-1}; Anal. calcd. for $C_{15}H_{20}Cl_2O_7$: C, 47.01; H, 5.26, found: C, 46.94; H, 5.28.



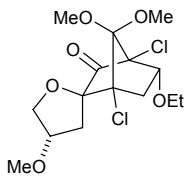
Compound **11d**: colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.13 – 4.06 (m, 2H), 3.94 – 3.89 (m, 1H), 3.67 (s, 3H, OMe), 3.66 (s, 3H, OMe), 3.55 (s, 3H, OMe), 3.39 (dd, 1H, *J* = 12.8, 4.8 Hz), 3.33 (s, 3H, OMe), 2.91 (dd, 1H, *J* = 12.8, 4.9 Hz), 2.71 – 2.66 (m, 1H), 2.58 (t, 1H, *J* = 12.7 Hz), 2.27 – 2.22 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.1 (C=O), 169.9 (O=C-O), 102.9 (ketal C), 89.2, 80.0, 73.5, 73.3 (C-Cl), 57.4 (OMe), 52.5 (OMe), 52.0 (OMe), 51.9 (OMe), 47.0, 38.7, 33.5; IR (neat) 2850, 1770, 1750, 1430, 1350, 1290 cm^{-1}; Anal. calcd. for $C_{15}H_{20}Cl_2O_7$: C, 47.01; H, 5.26, found: C, 47.18; H, 5.36.



Compound **13c**: white crystals (CH_2Cl_2 / Hexane); mp 86 – 88 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.28 – 4.22 (m, 2H), 3.98 (dd, 1H, *J* = 10.0, 1.9 Hz), 3.84 – 3.81 (m, 1H), 3.63 – 3.54 (m, 1H), 3.56 (s, 3H, OMe), 3.53 (s, 3H, OMe), 3.46 – 3.38 (m, 1H), 3.29 (s, 3H, OMe), 2.84 (dd, 1H, *J* = 13.4, 10.0 Hz), 2.36 (dd, 1H, *J* = 13.0, 6.8 Hz), 1.92 (dd, 1H, *J* = 13.0, 6.6 Hz), 1.89 (dd, 1H, *J* = 13.4, 1.9 Hz), 1.05 (t, 3H, *J* = 7.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.6 (C=O), 104.7 (ketal C), 88.4, 81.2 (C-Cl), 79.0, 78.1, 73.7, 71.4 (C-Cl), 66.3, 57.7 (OMe), 52.0, 51.3, 42.2, 36.2, 15.2; IR (KBr) 2850, 1760, 1440, 1180,1100, 1060, 970 cm^{-1}; Anal. calcd. for $C_{15}H_{22}Cl_2O_6$: C, 48.79; H, 6.01, found: C, 48.76; H, 6.18.

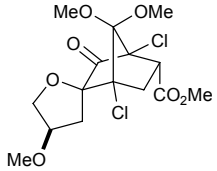


Compound **13d**: colorless viscous liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.18 – 4.15 (m, 1H), 4.06 – 4.01 (m, 2H), 3.97 (dd, 1H, *J* = 9.8, 1.8 Hz), 3.64 – 3.6 (m, 1H), 3.56 (s, 3H,



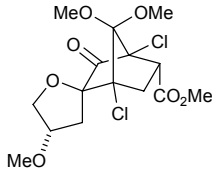
OMe), 3.53 (s, 3H, OMe), 3.43 – 3.37 (m, 1H), 3.27 (s, 3H, OMe), 2.83 (dd ,1H, J = 13.5, 10.0 Hz), 2.28 – 2.24 (m, 1H), 2.15 – 2.09 (m, 1H), 1.91 (dd, 1H, J = 13.6, 1.8 Hz), 1.04 (t, 3H, J = 7.1 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.7 (C=O), 104.7 (ketal C), 88.7, 81.5 (C-Cl), 80.1, 78.2, 75.3, 72.7 (C-Cl), 66.3, 56.7 (OMe), 52.0 (OMe), 51.3 (OMe), 41.9, 35.8, 15.2; IR (neat) 2850, 1760, 1440, 1250, 1100, 1080, 970 cm^{-1}; Anal. calcd. for $C_{15}H_{22}Cl_2O_6$: C, 48.79; H, 6.01, found: C, 48.88; H, 6.25.

Compound **14c**: white solid; mp 120 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.26 – 4.22 (m, 2H), 3.87 – 3.85(m, 1H), 3.65 (s, 3H, OMe), 3.58 (s, 3H, OMe), 3.57 (s, 3H, OMe), 3.3



(s, 3 H, OMe), 3.25 (dd, 1H, J = 12.4, 4.8 Hz), 2.71 (t, 1H, J = 3.6 Hz), 2.69 – 2.65 (m, 1H), 2.17 (dd, 1H, J = 13.3, 4.7 Hz), 2.0 (dd, 1H, J = 13.1, 5.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.9 (C=O), 171.4 (O=C-O), 104.7 (ketal C), 88.9, 79.3, 78.1 (C-Cl), 74.0, 71.1 (C-Cl), 57.6 (OMe), 52.8 (OMe), 52.4 (OMe), 51.1 (OMe), 46.1, 36.8, 35.8; IR (KBr) 2850, 1770, 1730, 1440, 1350, 1290 cm^{-1}; Anal. calcd. for $C_{15}H_{20}Cl_2O_7$: C, 47.01; H, 5.26, found: C, 47.05; H, 5.43.

Compound **14d**: white crystals (CH_2Cl_2 / Hexane); mp 124 – 125 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.20 – 4.17 (m, 1H), 4.11 – 4.08 (m, 2H), 3.68 (s, 3H, OMe), 3.63 (s, 3H,



OMe), 3.60 (s, 3H, OMe), 3.33 (s, 3H, OMe), 3.28 (dd, 1H, J = 12.3, 4.8 Hz), 2.69 (t, 1H, J = 12.9 Hz), 2.63 (dd, 1H, J = 13.2, 2.2 Hz), 2.28 – 2.22 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.9 (C=O), 171.3 (O=C-O), 104.6 (ketal C), 89.1, 80.0, 78.3 (C-Cl), 75.4, 72.4 (C-Cl), 56.7 (OMe), 52.8 (OMe), 52.3 (OMe), 51.1 (OMe), 46.1, 36.3, 35.3; IR (KBr) 2850, 1780, 1710, 1430, 1360, 1290 cm^{-1}; Anal. calcd. for $C_{15}H_{20}Cl_2O_7$: C, 47.01; H, 5.26, found: C, 47.26; H, 5.37.

X-ray crystal structure of 1d: White crystals (CH_2Cl_2 / Hexane). $C_{16}H_{22}Br_2O_5$, M_r = 454.16, 0.18 x 0.15 x 0.13 mm^3, monoclinic, space group P121/n1 with a = 8.9742 (8) Å, b = 17.9301 (16) Å, c = 10.6917 (10) Å, $\alpha = 90^{o}$ β = 106.031 (2) °, $\gamma = 90^{o}$, V = 1653.5 (3) $Å^3$, Z = 4, $\rho_{calcd.}$ = 1.824 g cm^{-3}, F (000) = 912, Absorption coefficient = 4.925 mm^{-1}, $Mo_{k\alpha}$ radiation, λ = 0.71073 Å, T= 100 K, Number of measured and independent reflections = 10726 / 4062, $R_{int.}$ = 0.0533, R1= 0.048, $wR2$ = 0.0980, maximum and minimum residual electron density is 1.512 and -1.341 $eÅ^{-3}$, respectively.

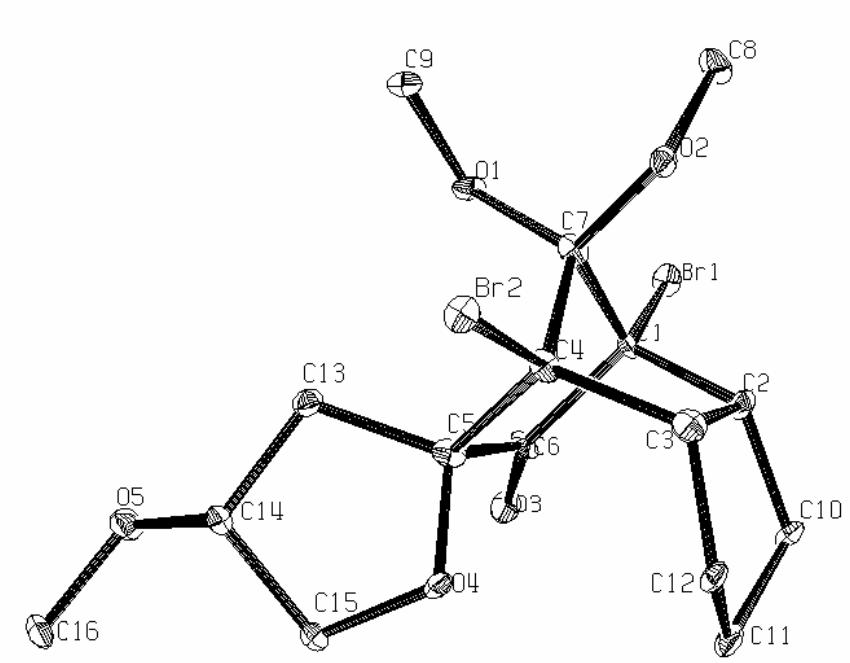


Fig. S1 X-ray crystal structure of **1d** (ORTEP diagram). Displacement ellipsoids are drawn at 30% probability level for non-hydrogen atoms. Hydrogen atoms are omitted for clarity.

X-ray crystal structure of 6c: White crystals (CH_2Cl_2 / Hexane). $C_{17}H_{24}Cl_2O_5$, M_r = 379.26, 0.18 x 0.15 x 0.13 mm^3, orthorhombic, space group Pca21 with a = 11.5727 (9) Å, b = 11.7784 (10) Å, c = 25.579 (2) Å, $\alpha = 90^{o}$ $\beta = 90^{o}$, $\gamma = 90^{o}$, V = 3486.6 (5) $Å^3$, Z = 8, $\rho_{calcd.}$ = 1.445 g cm^{-3}, F (000) = 1600, Absorption coefficient = 0.397 mm^{-1}, $Mo_{k\alpha}$ radiation, λ = 0.71073 Å, T= 100 K, Number of measured and independent reflections = 22182 / 7292, $R_{int.}$ = 0.0482, R1= 0.0494, $wR2$ = 0.1069, maximum and minimum residual electron density is 0.486 and -0.470 $eÅ^{-3}$, respectively.

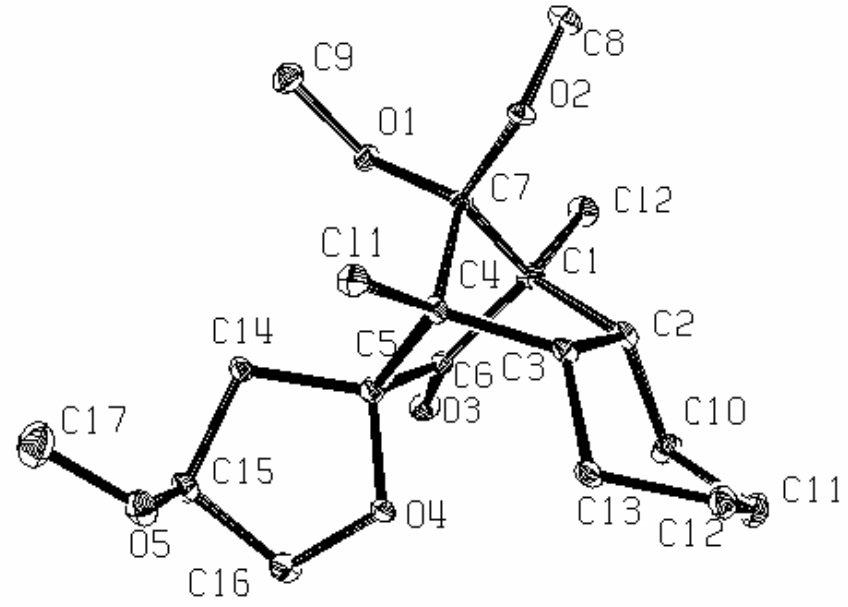


Fig. S2 X-ray crystal structure of **6c** (ORTEP diagram). Displacement ellipsoids are drawn at 30% probability level for non-hydrogen atoms. Hydrogen atoms are omitted for clarity.

X-ray crystal structure of 10c: White crystals (CH_2Cl_2 / Hexane). $C_{16}H_{22}Cl_2O_7$, M_r = 397.24, 0.19 x 0.07 x 0.05 mm^3, monoclinic, space group P121/c1 with a = 8.2163 (7) Å, b = 8.1296 (7) Å, c = 26.697 (2) Å, $\alpha = 90^{o}$ $\beta = 94.502$ (2) °, $\gamma = 90^{o}$, V = 1777.7 (3) $Å^3$, Z = 4, $\rho_{calcd.}$ = 1.484 g cm^{-3}, F (000) = 832, Absorption coefficient = 0.401 mm^{-1}, $Mo_{k\alpha}$ radiation, λ = 0.71073 Å, T= 100 K, Number of measured and independent reflections = 11386 / 4356, $R_{int.}$ = 0.0502, R1= 0.0595, $wR2$ = 0.1500, maximum and minimum residual electron density is 0.674 and -0.685 $eÅ^{-3}$, respectively.

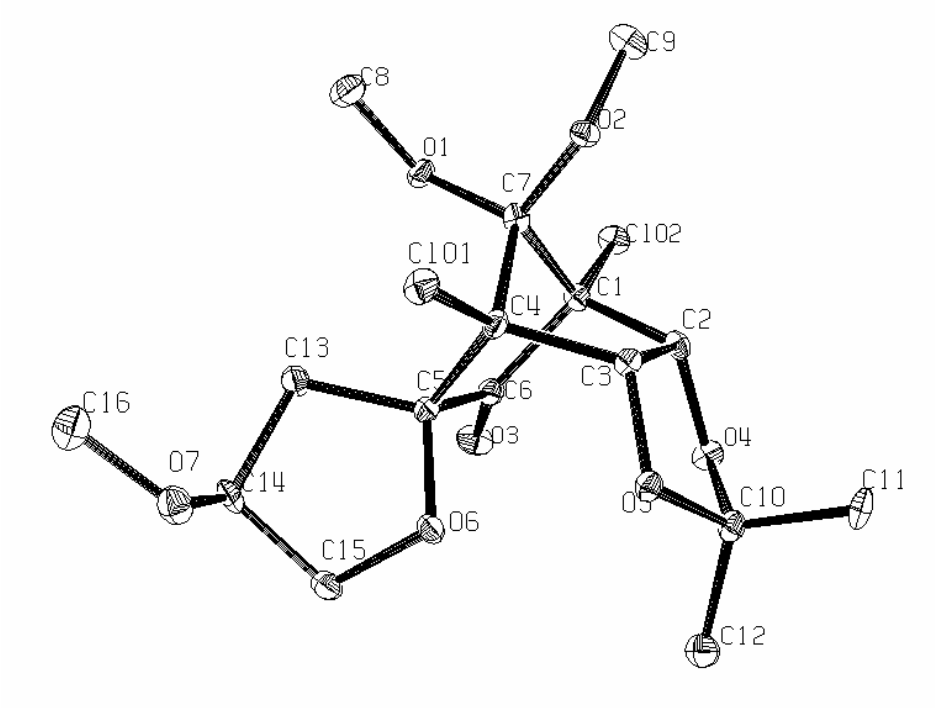


Fig. S3 X-ray crystal structure of **10c** (ORTEP diagram). Displacement ellipsoids are drawn at 30% probability level for non-hydrogen atoms. Hydrogen atoms are omitted for clarity.

X-ray crystal structure of 13c: White crystals (CH_2Cl_2 / Hexane). $C_{15}H_{22}Cl_2O_6$, M_r = 369.23, 0.10 x 0.08 x 0.06 mm^3, trigonal, space group R-3 with a = 34.375 (2) Å, b = 34.375 (2) Å, c = 7.2354 (6) Å, $\alpha = 90\ ^{o}\beta = 90\ °$, $\gamma = 120\ ^{o}$, V = 7404.0 (9) $Å^3$, Z = 18, $\rho_{calcd.}$ = 1.491 g cm^{-3}, F (000) = 3492, Absorption coefficient = 0.422 mm^{-1}, $Mo_{k\alpha}$ radiation, λ = 0.71073 Å, T= 100 K, Number of measured and independent reflections = 16448 / 4096, $R_{int.}$ = 0.0415, R1= 0.0475, $wR2$ = 0.1242, maximum and minimum residual electron density is 0.717 and -0.585 $eÅ^{-3}$, respectively.

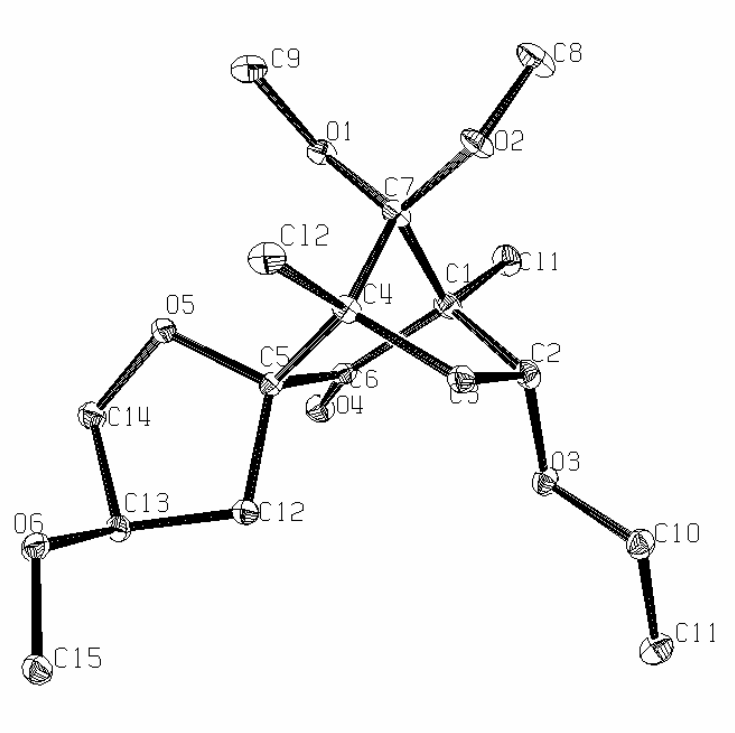


Fig. S4 X-ray crystal structure of **13c** (ORTEP diagram). Displacement ellipsoids are drawn at 30% probability level for non-hydrogen atoms. Hydrogen atoms are omitted for clarity.

X-ray crystal structure of 14d: White crystals (CH_2Cl_2 / Hexane). $C_{15}H_{20}Cl_2O_7$, M_r = 383.21, 0.13 x 0.07 x 0.06 mm^3, monoclinic, space group P121/c1 with a = 7.3266 (6) Å, b = 21.5800 (17) Å, c = 11.0281 (9) Å, $\alpha = 90^{o}$ $\beta = 101.9950\ (10)^{o}$, $\gamma = 90^{o}$, V = 1705.6 (2) $Å^3$, Z = 4, $\rho_{calcd.}$ = 1.492 g cm^{-3}, F (000) = 800, Absorption coefficient = 0.415 mm^{-1}, $Mo_{k\alpha}$ radiation, λ = 0.71073 Å, T= 100 K, Number of measured and independent reflections = 11005 / 4161, $R_{int.}$ = 0.0299, R1= 0.0502, $wR2$ = 0.1117, maximum and minimum residual electron density is 0.644 and -0.668 $eÅ^{-3}$, respectively.

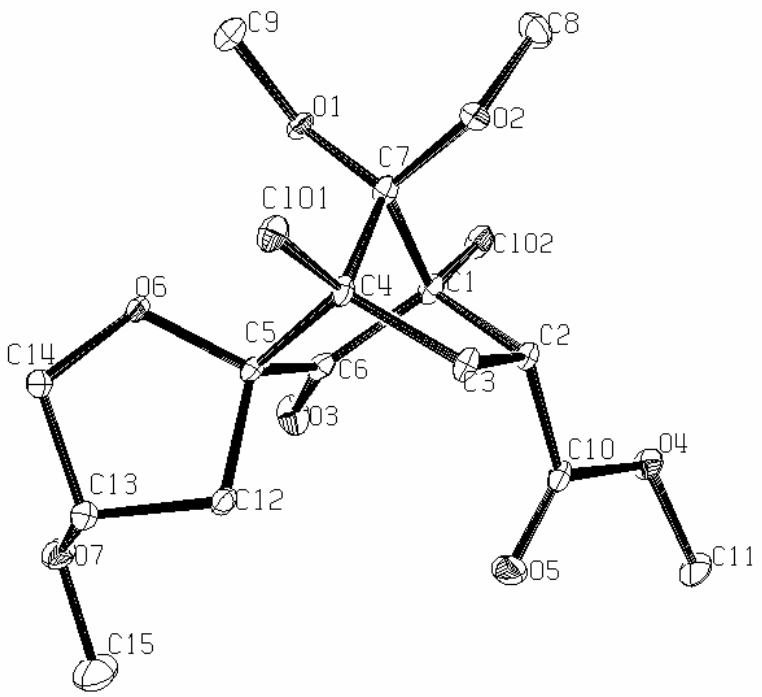
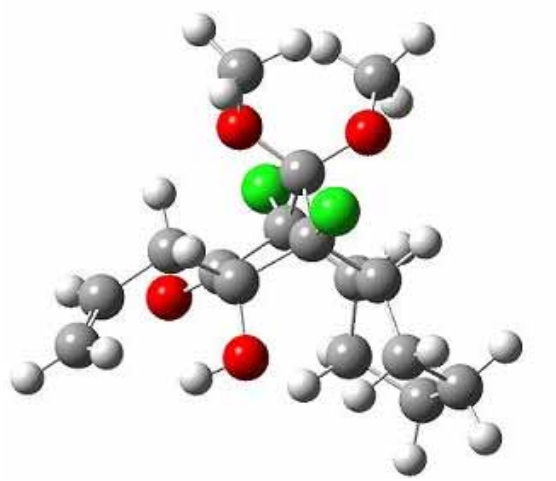


Fig. S5 X-ray crystal structure of **14d** (ORTEP diagram). Displacement ellipsoids are drawn at 30% probability level for non-hydrogen atoms. Hydrogen atoms are omitted for clarity.

Computational details

All theoretical calculations were performed with GAUSSIAN-03,[3] using the density functional/Hartee-Fock hybrid model BeckeLYP[4] and the basis set 6-31G(d). Reported compounds are optimized as being true minima by the absence of negative eigenvalues in the vibrational frequency analysis.

Cartesian Coordinates of Compound **6a.**



Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
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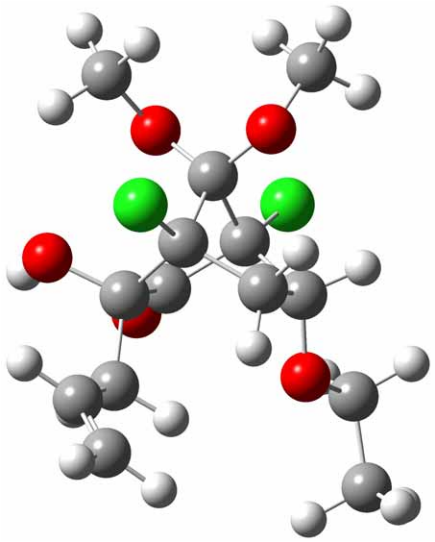
3	6	1.163587	-0.681044	1.058293
4	6	1.778511	-0.312358	-0.345159
5	6	-0.491692	-0.213828	-1.390914
6	6	0.708664	0.633520	-0.965328
7	6	0.116408	1.343479	0.304419
8	8	1.011689	2.006230	1.138024
9	6	1.656785	3.184510	0.636936
10	8	-0.928147	2.170963	-0.124204
11	6	-1.622710	2.944366	0.865452
12	8	-0.833786	-0.498350	-2.511748
13	8	-1.107799	-2.121452	-0.004041
14	6	-2.685379	-0.292941	-0.043468
15	6	-3.503158	-1.022301	-1.079397
16	6	-4.315202	-2.046832	-0.797893
17	17	1.323182	1.666007	-2.294702
18	17	-0.995442	0.076012	2.634412

19	6	1.388495	-2.151356	1.449651
20	6	2.154161	-1.554381	-1.158772
21	6	2.854664	-2.502215	1.139441
22	6	3.170663	-2.418559	-0.380469
23	1	1.687273	-0.079873	1.804750
24	1	2.676845	0.295116	-0.190643
25	1	1.953877	3.755785	1.519665
26	1	2.545006	2.927628	0.051687
27	1	0.981622	3.781334	0.017992
28	1	-2.095925	3.763233	0.318925
29	1	-0.934574	3.344388	1.613646
30	1	-2.388598	2.348929	1.371383
31	1	-1.843681	-2.468324	-0.542496
32	1	-3.053602	-0.535027	0.958432
33	1	-2.769640	0.783638	-0.194547
34	1	-3.383605	-0.699102	-2.110909
35	1	-4.885426	-2.552785	-1.572542
36	1	-4.459536	-2.399127	0.221985
37	1	0.717688	-2.823732	0.917395
38	1	1.184661	-2.273362	2.519671
39	1	2.563297	-1.263519	-2.132883
40	1	1.254489	-2.146173	-1.359073
41	1	3.087937	-3.503927	1.517964
42	1	3.506580	-1.810658	1.691402
43	1	4.181696	-2.016119	-0.521928
44	1	3.178440	-3.422695	-0.820733

E(RB+HF-LYP) = -1844.16169589 a.u.

Cartesian Coordinates of Compound **13a.**



Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
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3	6	0.121869	0.566517	-1.553452
4	6	1.273556	-0.330960	-1.016986
5	6	0.479918	-0.007440	1.328894
6	6	0.613984	-1.041707	0.211157
7	6	-0.904261	-1.133666	-0.208857
8	8	-1.189360	-1.796629	-1.402277
9	6	-1.088063	-3.225873	-1.421520
10	8	-1.579091	-1.649270	0.888666
11	6	-3.014953	-1.629557	0.871084
12	17	1.400487	-2.559048	0.737989
13	17	-2.576125	1.005793	-1.120235
14	8	0.985448	-0.006329	2.423604
15	6	0.125912	2.454140	0.808947
16	8	-1.641409	1.088643	1.751818
17	6	-0.760014	3.555282	0.296237
18	6	-0.378459	4.471269	-0.595035
19	8	2.373639	0.491295	-0.699139
20	6	4.715978	0.876595	-0.471829
21	6	3.616419	-0.170804	-0.430912
22	1	0.451587	1.597192	-1.680442

23	1	-0.242508	0.192284	-2.509695
24	1	1.564852	-1.096223	-1.748353
25	1	-0.057241	-3.545727	-1.604564
26	1	-1.438487	-3.663433	-0.483346
27	1	-1.724505	-3.556484	-2.245658
28	1	-3.401778	-1.870290	-0.123088
29	1	-3.326678	-2.396100	1.584547
30	1	-3.379695	-0.650520	1.187138
31	1	1.070153	2.419593	0.258075
32	1	0.394916	2.650543	1.858025
33	1	-1.260679	1.001501	2.643504
34	1	-1.765172	3.586635	0.711930
35	1	-1.047693	5.262832	-0.921026
36	1	0.619756	4.470292	-1.029397
37	1	5.686414	0.412678	-0.264408
38	1	4.537659	1.650906	0.281441
39	1	4.760536	1.355288	-1.455412
40	1	3.784226	-0.949030	-1.191261
41	1	3.581435	-0.662679	0.548360

E(RB+HF-LYP) = -1841.95516431 a.u.

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2. G. M. Sheldrick, SHELXL97, Program for the Refinement of Crystal Structures, University of Göttingen, Germany, 1997.

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