Designing bifunctional alkene isomerization catalysts using predictive modelling

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This supplemanetary information contains the VIP plot for the 308 descriptors, the mass balance deviation plot, characterisation data for catalysts **9** and **13**, and a table containing the entire dataset (308 descriptor values for each of the 39 experimental cases, separate excel file).

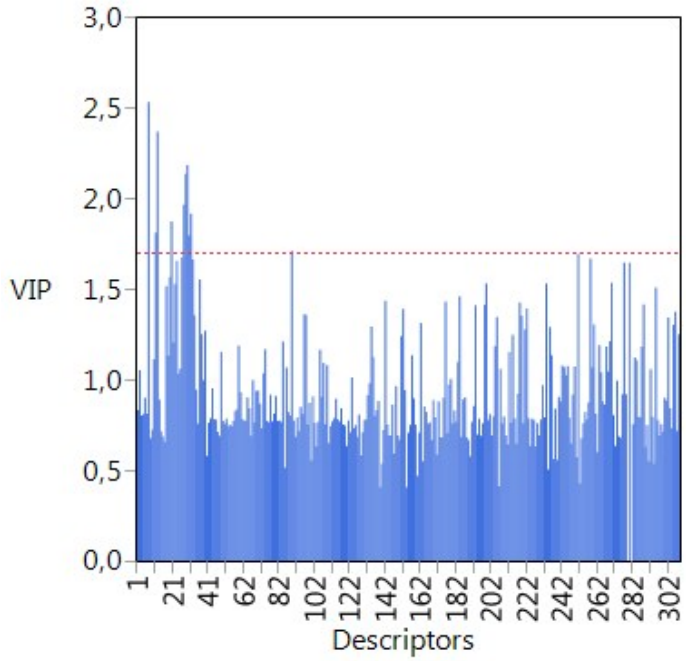

Figure S1. Variable Importance Plot vs. 308 descriptors for the FOM yield of 3-alkene.

The threshold of VIP (see Figure S1) is set to separate the most outstanding descriptors from the less relevant descriptors with lower VIP values. For each FOM, the most outstanding descriptors were selected based on the VIP plot.

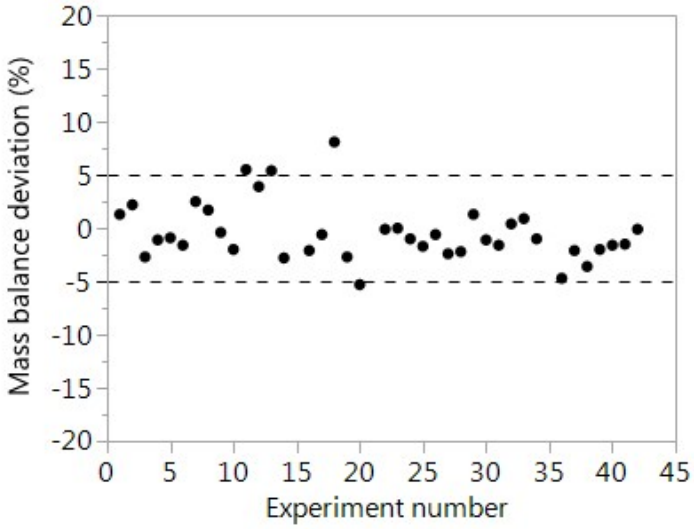

Figure S2. Mass balance deviation plot.

The data points had a 5% deviation centred on 100%, and were spread randomly (see Figure S2), confirming that there was no systemic error in the reaction mass balance.

Experimental data

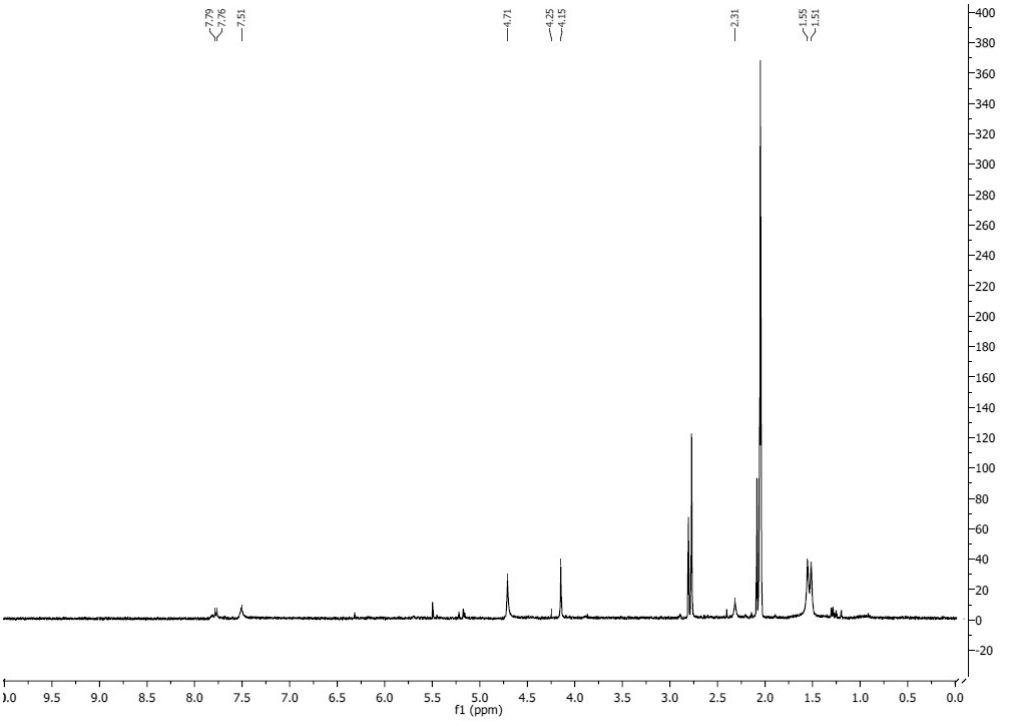

Figure S3. Catalyst **9**, ^{1}H NMR spectrum.

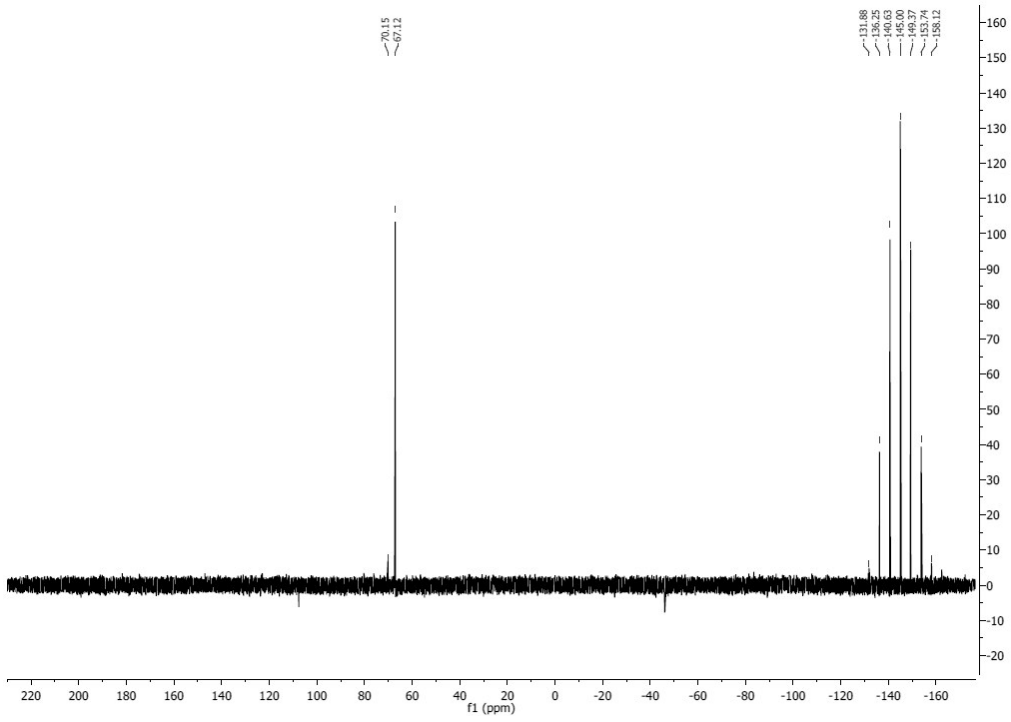

Figure S4. Catalyst **9**, ^{31}P NMR spectrum.

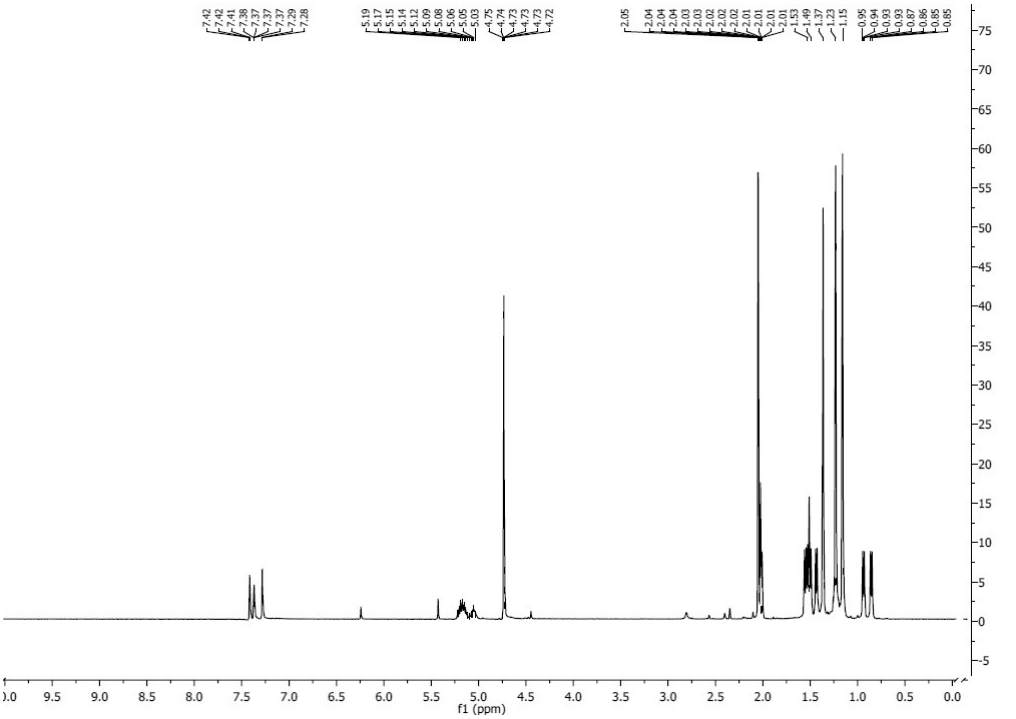

Figure S5. Catalyst **13**, ^{1}H NMR spectrum.

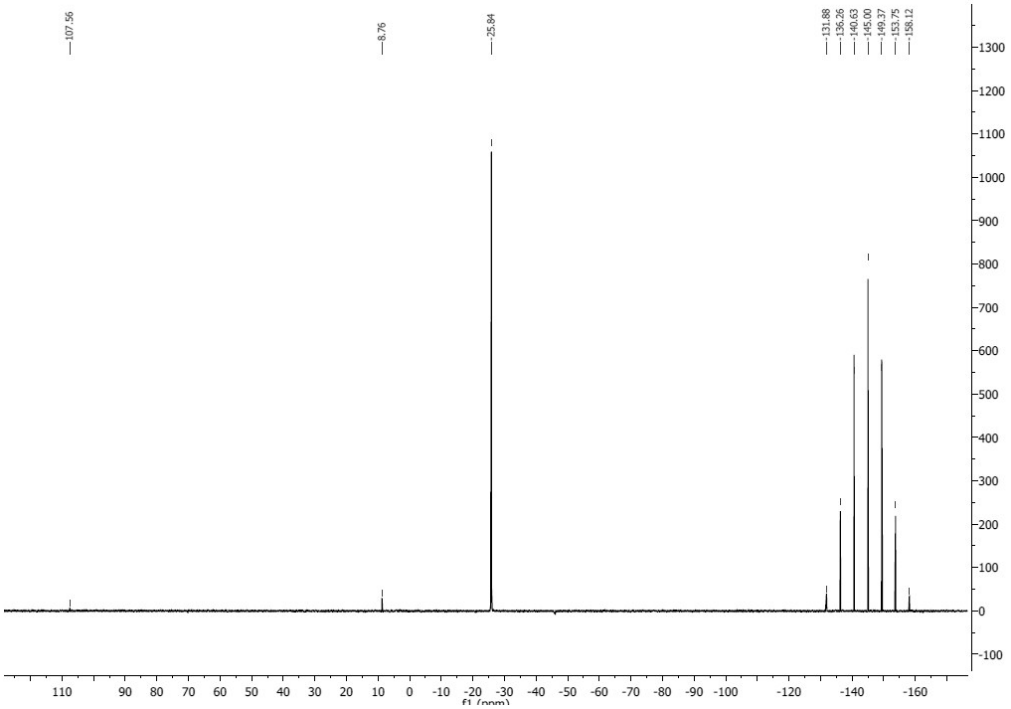

Figure S6. Catalyst **13**, ^{31}P NMR spectrum.

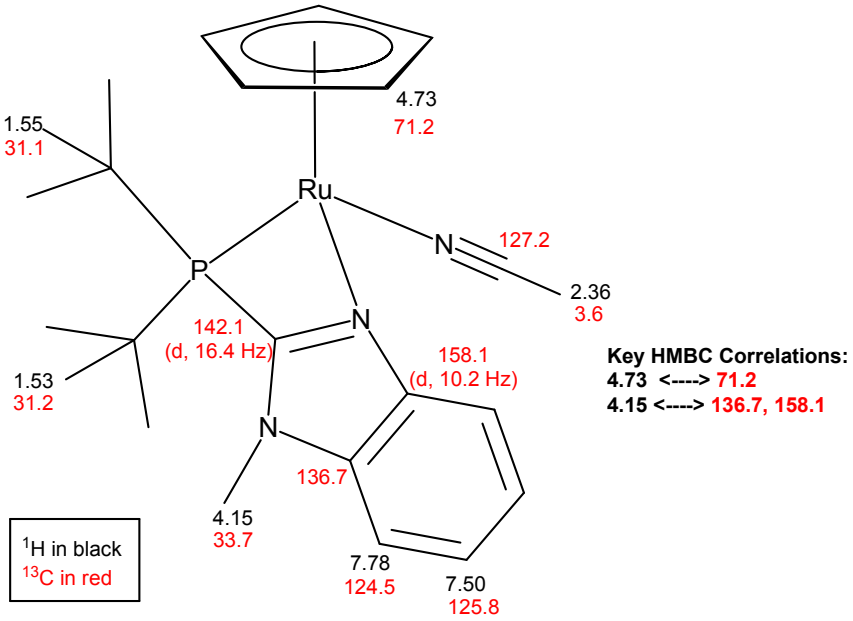

Figure S7. Catalyst **9**, $^{1}H - ^{13}C$ NMR peak assignments for the cation (from 2D NMR data).

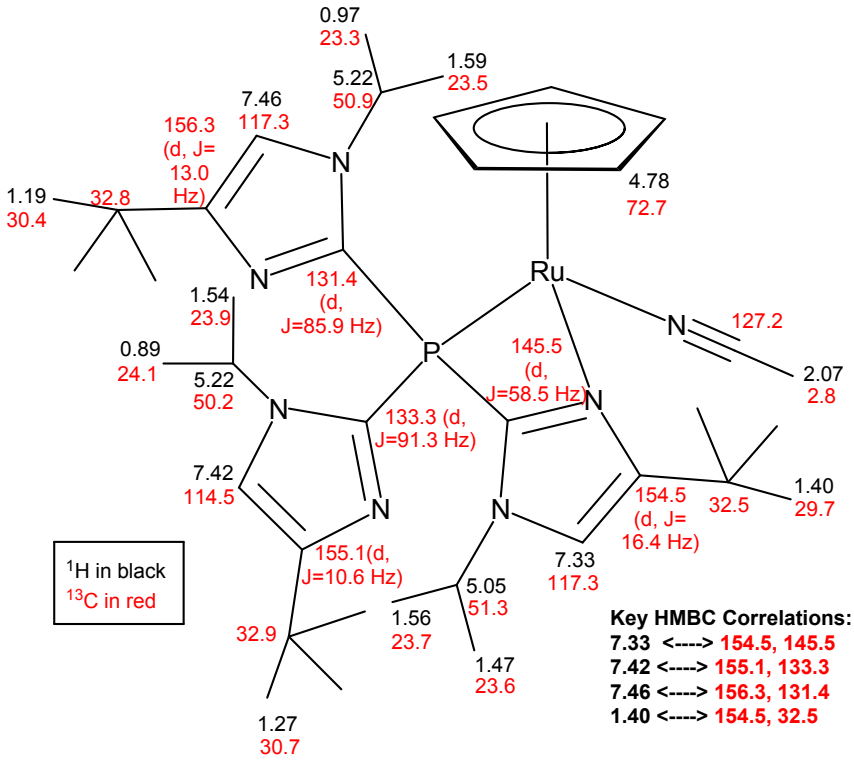

Figure S8. Catalyst **13**, $^{1}H - ^{13}C$ NMR peak assignments for the cation (from 2D NMR data).

Predictive models

Listed below are the prediction formulas for each FOM. The FOM is described by 2 descriptors with corresponding coefficients. Note that the values are based on scaled and centred data.

Pred Formula log(TOF) =

0.46143749364052*(“q(e)_N*”) + -7.34083838383433*(“E(HOMO)”) + (

-88.8747316618149)

Pred Formula log(TON) =

-0.0393080389325798*(“d_Ru-P”) + 120.333537225117*(“d_Ru-Cp”) + (

-213.304077054034)

Pred Formula Yield 2-E-alkene (%) =

-0.816015493792368*(“d_Ru-N”) + -1.27919272688913*(“PSA”) + 59.3493452372081

Pred Formula Yield 3-alkene (%) =

-3.18084933075505*(“E(HOMO)”) + -271.930106960903*(“d_Ru-Cp”)

+456.35543760031

Complete list of the 308 computed descriptors and the entire dataset (see separate excel file)

The descriptors can be categorized by different types of descriptors. Within the Spartan and MarvinSketch programs we calculated electrostatic, constitutional and topological descriptors. Using ChemDes we calculated constitutional, topological, connectivity, Kappa, E-state, Moran autocorrelation, Geary autocorrelation, molecular property, Moreau-Broto autocorrelation, charge, MOE-type descriptors.