SUPPLEMENTARY MATERIAL

New *fac*-[Re(CO)$_3$(OO)(L)] and [Re(CO)$_2$(OO)(L)$_2$] complexes bearing two natural food additives, maltol and kojic acid, as OO ligands

Angeliki Panagiotopoulou [1,*], Patricia Kyprianidou [2], Charalampos Tsoukalas [2], Vassilis Psycharis [3], Catherine P. Raptopoulou [3], Ioannis Pirmettis [2], Minas S. Papadopoulos [2] and Maria Pelecanou [1]

[1] Institute of Biosciences and Applications, National Centre for Scientific Research "Demokritos", Aghia Paraskevi, 15310 Athens, Greece
[2] Institute of Nuclear & Radiological Sciences & Technology, Energy & Safety, National Center for Scientific Research "Demokritos", Aghia Paraskevi, 15310 Athens, Greece
[3] Institute of Nanoscience and Nanotechnology, National Centre for Scientific Research "Demokritos", Aghia Paraskevi, 15310 Athens, Greece
* Correspondence: apanagio@bio.demokritos.gr (A.P.)

Supplementary crystallographic data for this paper. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html (or from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: +44 1223 336033; E-mail: deposit@ccdc.cam.ac.uk).

FT-IR spectra of Re complexes (**1 – 10**)

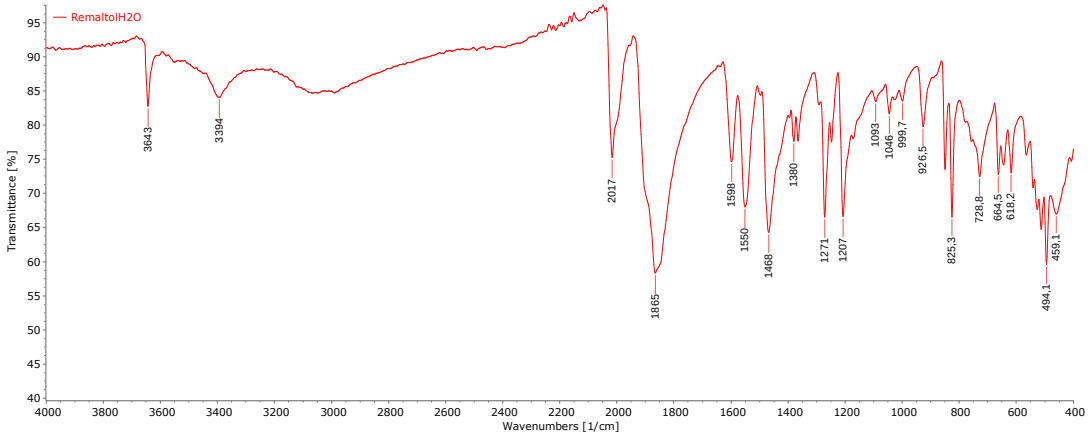


Figure S1 FT-IR of *fac*-[Re(CO)$_3$(OO^1)H$_2$O] (**1**)

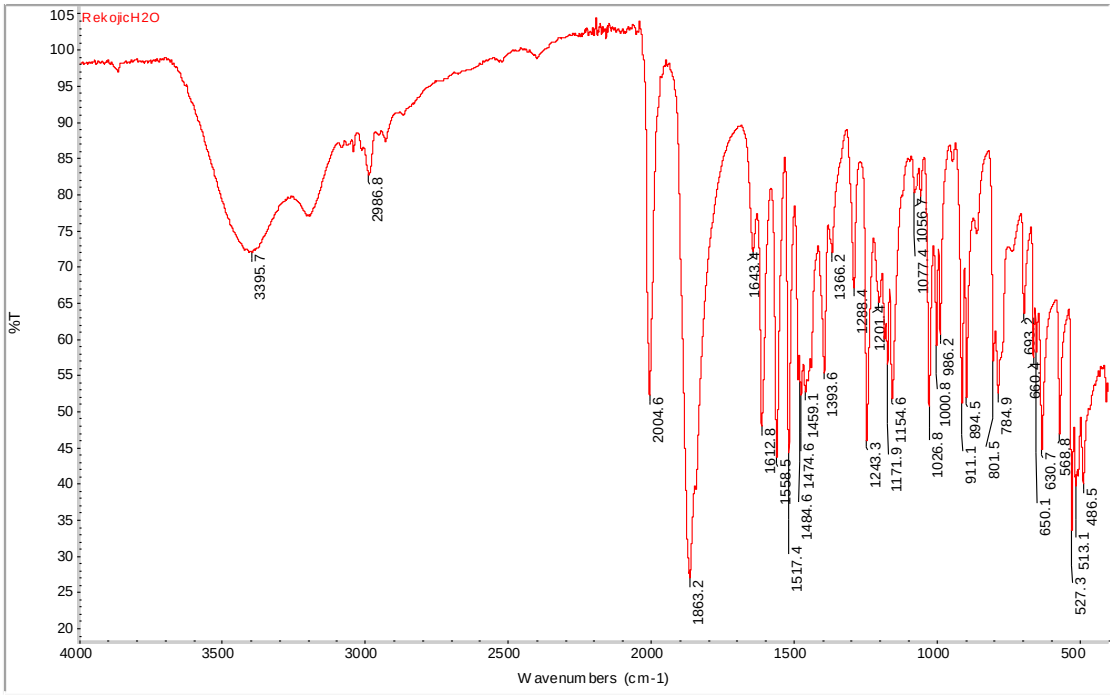


Figure S2 FT-IR of *fac*-[Re(CO)$_3$(OO^2)H$_2$O] (**2**)

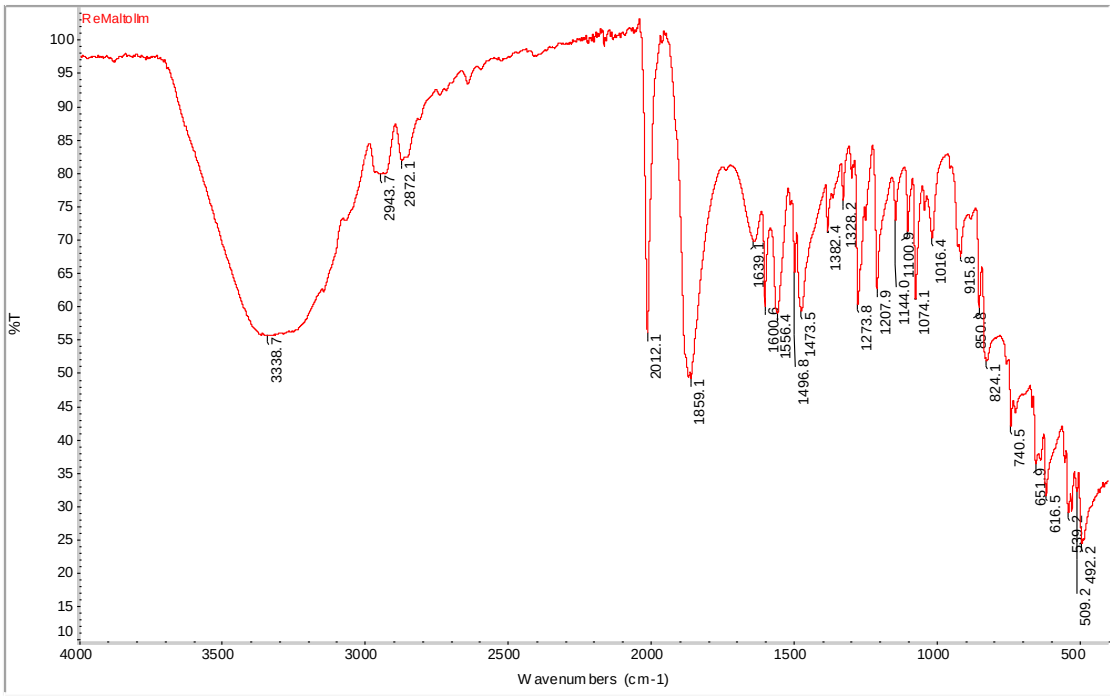


Figure S3 FT-IR of *fac*-[Re(CO)$_3$(OO^1)L$_1$] (**3**)

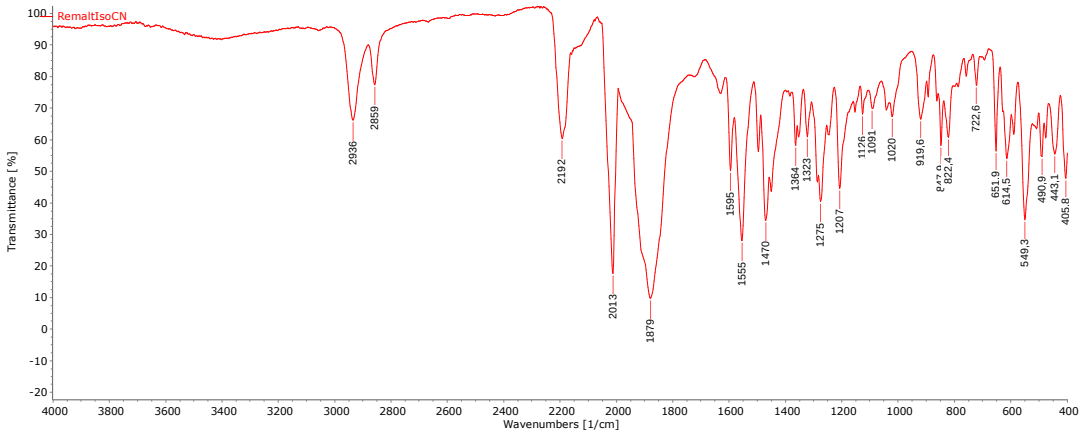


Figure S4 FT-IR of *fac*-[Re(CO)$_3$(OO^1)L$_2$] (4)

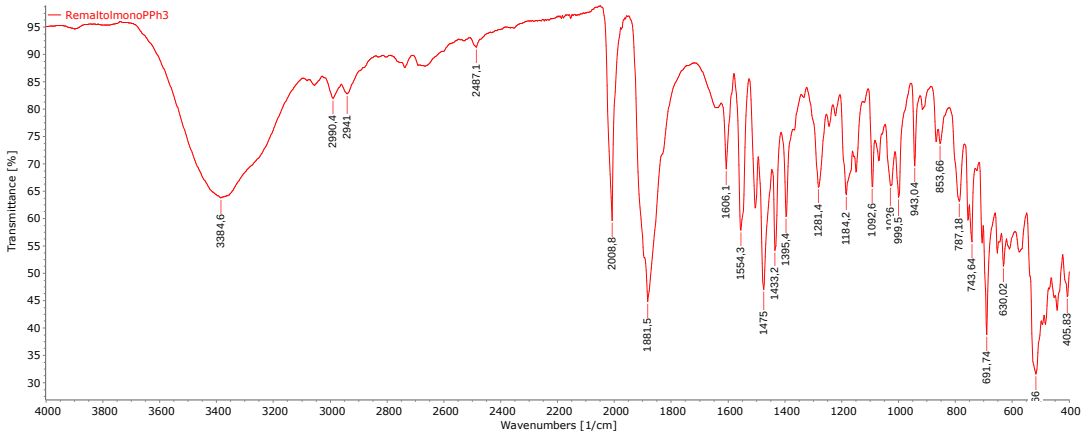


Figure S5 FT-IR of *fac*-[Re(CO)$_3$(OO^1)L$_3$] (5)

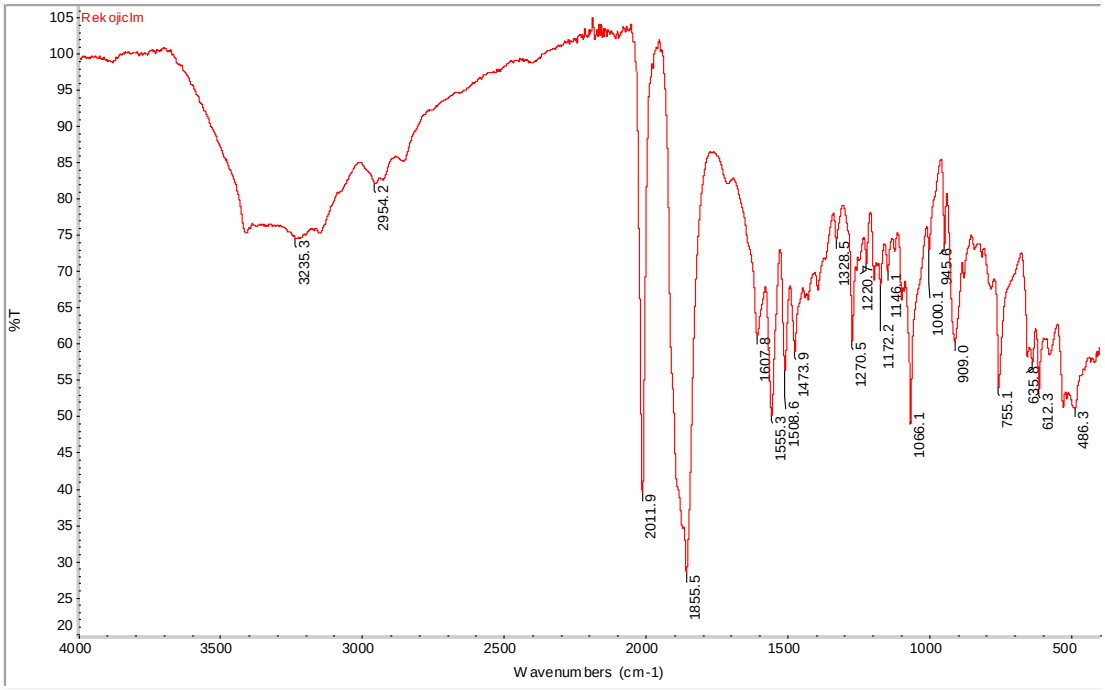


Figure S6 FT-IR of *fac*-[Re(CO)$_3$(OO^2)L$_1$] (**6**)

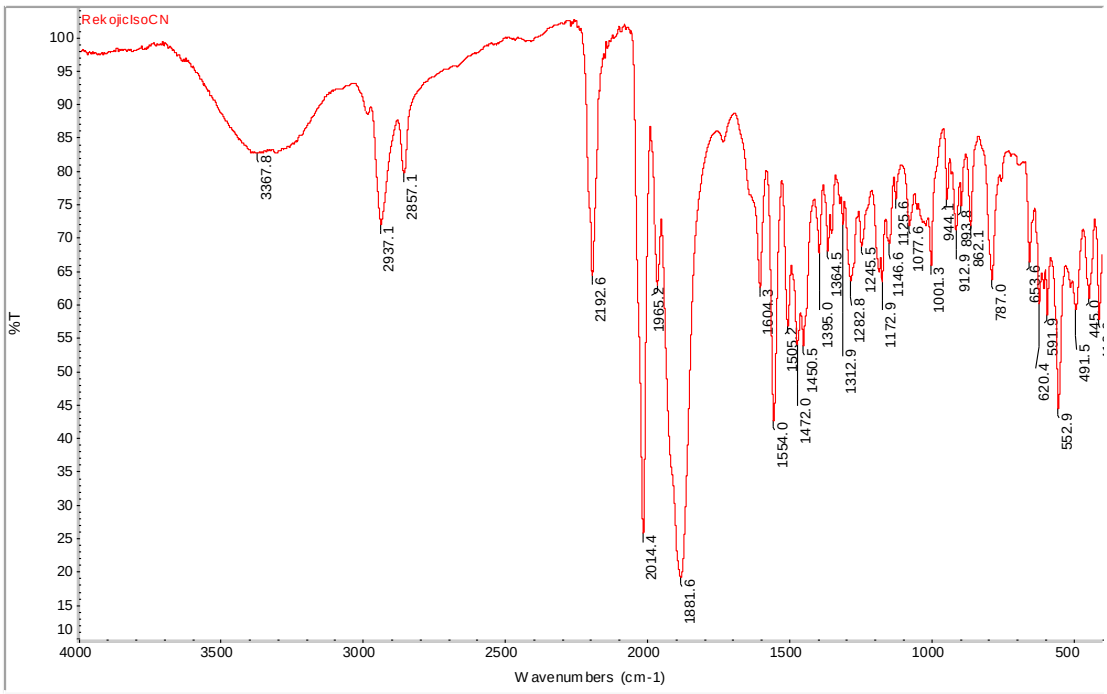


Figure S7 FT-IR of *fac*-[Re(CO)$_3$(OO^2)L$_2$] (**7**)

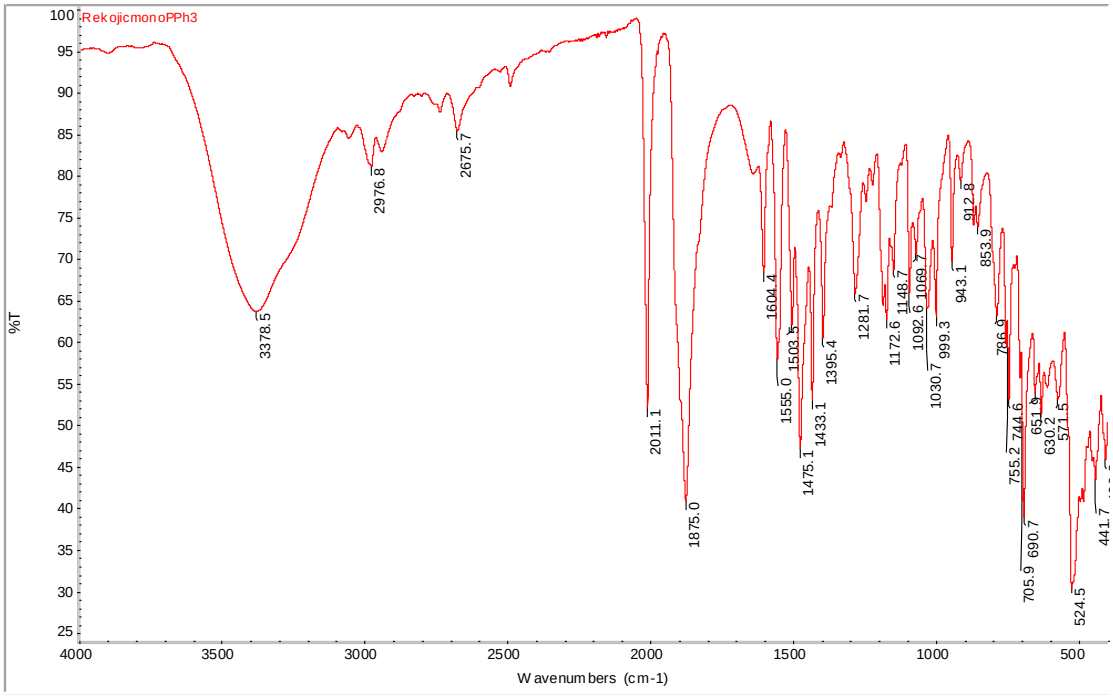


Figure S8 FT-IR of *fac*-[Re(CO)$_3$(OO^2)L$_3$] (**8**)

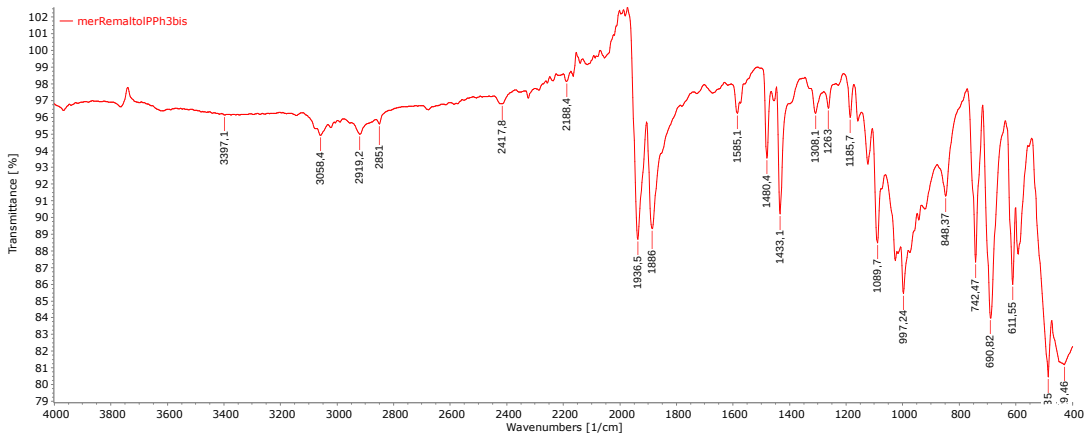


Figure S9 FT-IR of [Re(CO)$_2$(OO^1)(L$_3$)$_2$] (**9**)

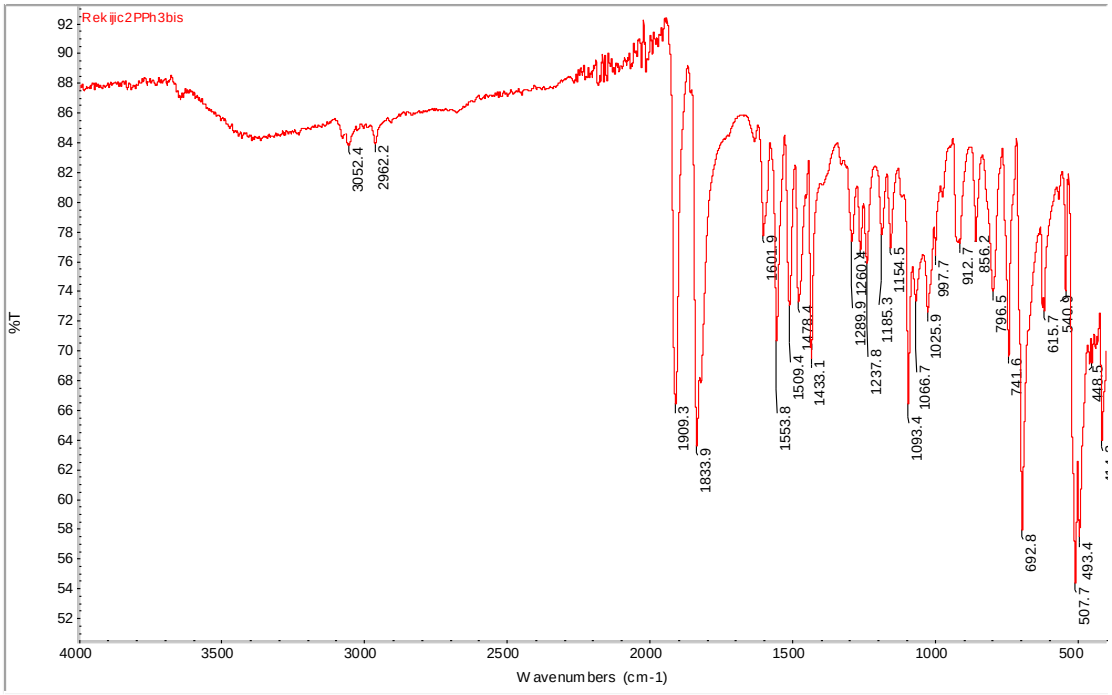


Figure S10 FT-IR of $[Re(CO)_2(OO^2)(L_3)]$ (**10**)

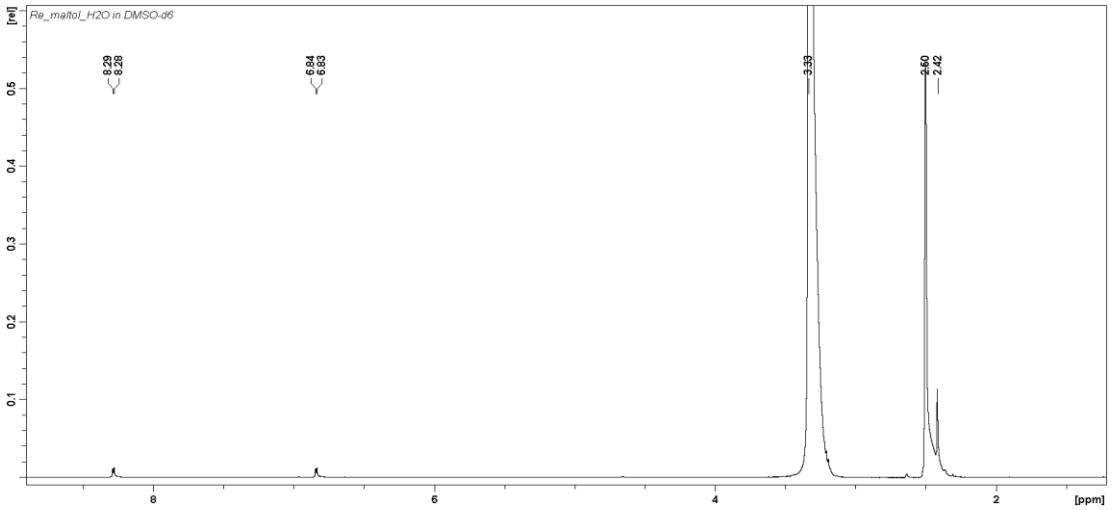


Figure S11 ^{1}H NMR of *fac*-$Re[(CO)_3(OO^1)H_2O]$ (**1**) in DMSO-d_6 at 25 °C

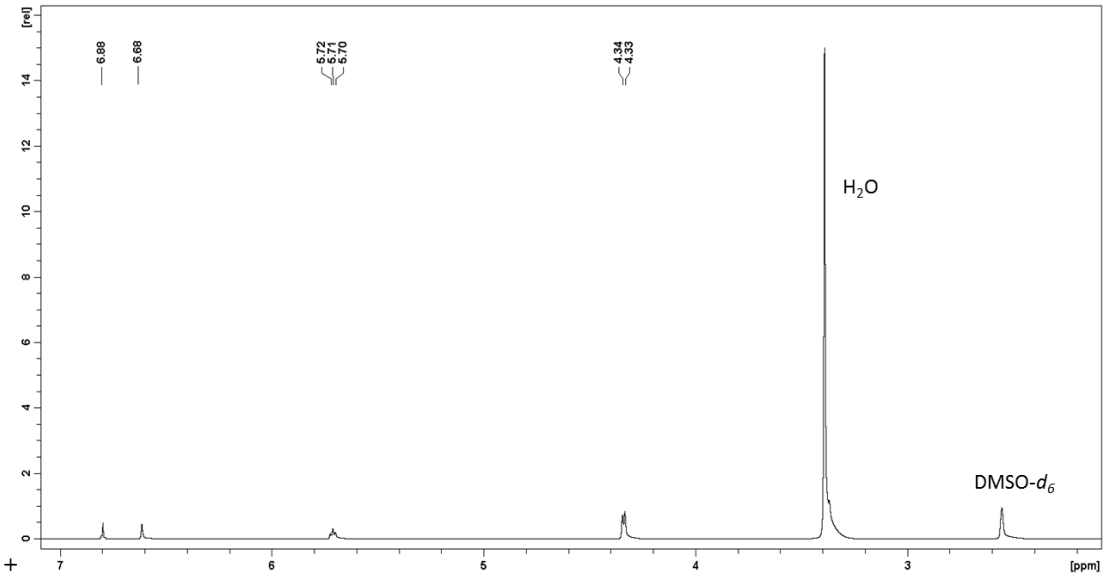


Figure S12 ^{1}H NMR of *fac*-Re[(CO)$_3$(OO^2)H$_2$O] (**2**) in DMSO-d_6 at 25 °C

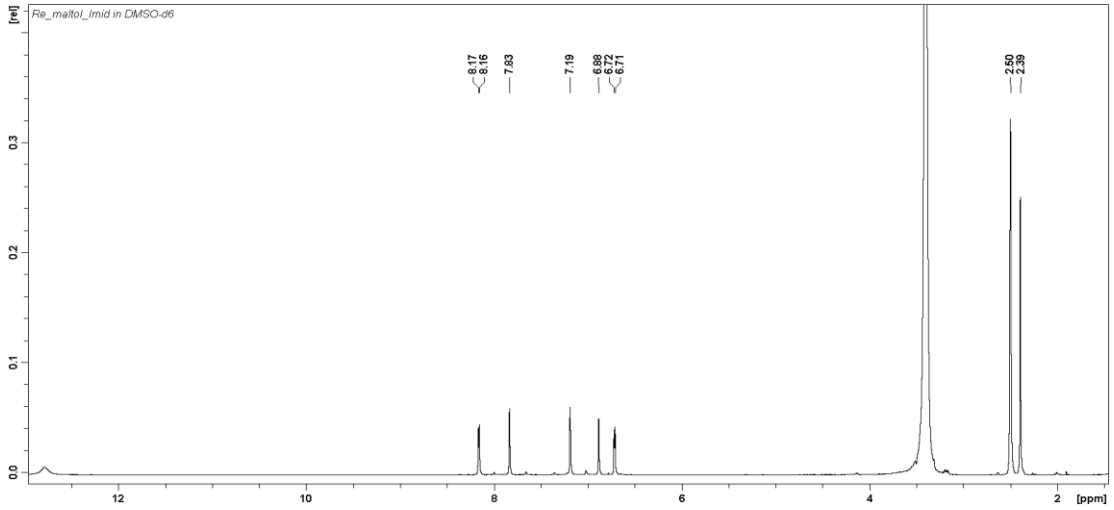


Figure S13 ^{1}H NMR of *fac*-Re[(CO)$_3$(OO^1)L$_1$] (**3**) in DMSO-d_6 at 25 °C

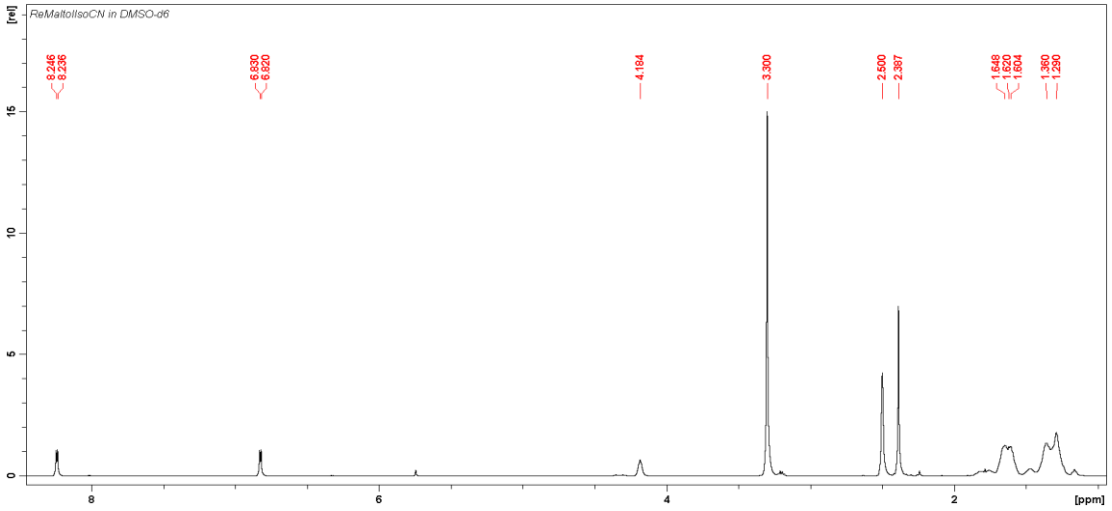


Figure S14 ^{1}H NMR of *fac*-Re[(CO)$_3$(OO^1)L$_2$] (**4**) in DMSO-d_6 at 25 °C

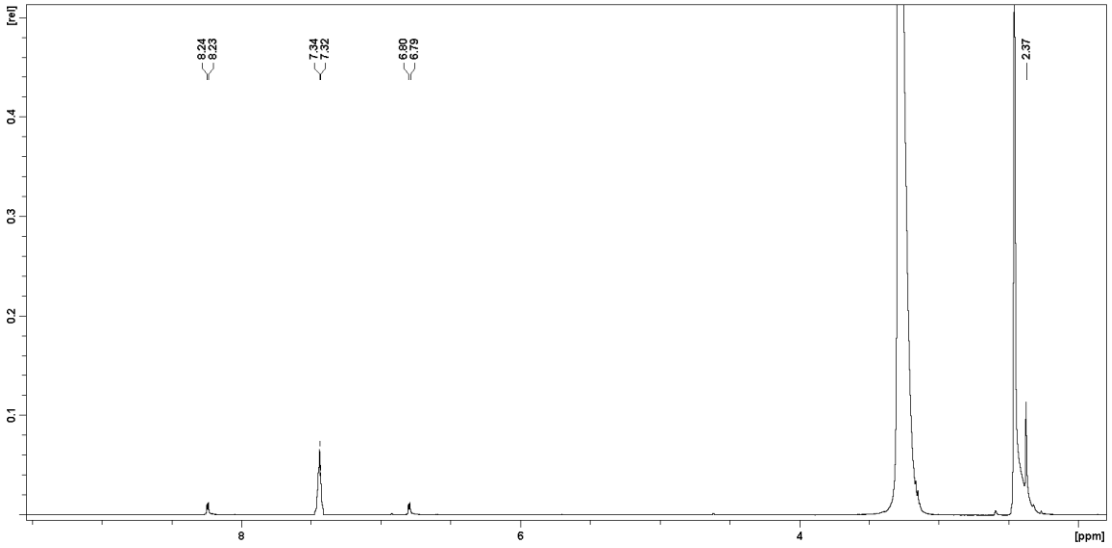


Figure S15 ^{1}H NMR of *fac*-Re[(CO)$_3$(OO^1)L$_3$] (**5**) in DMSO-d_6 at 25 °C

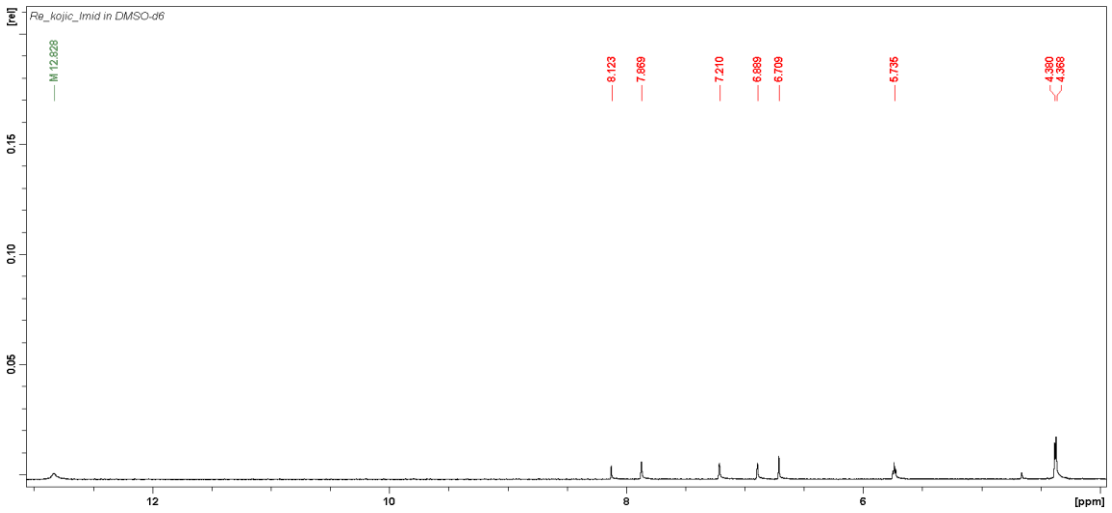


Figure S16 ^{1}H NMR of *fac*-Re[(CO)$_3$(OO^2)L$_1$] (**6**) in DMSO-d_6 at 25 °C

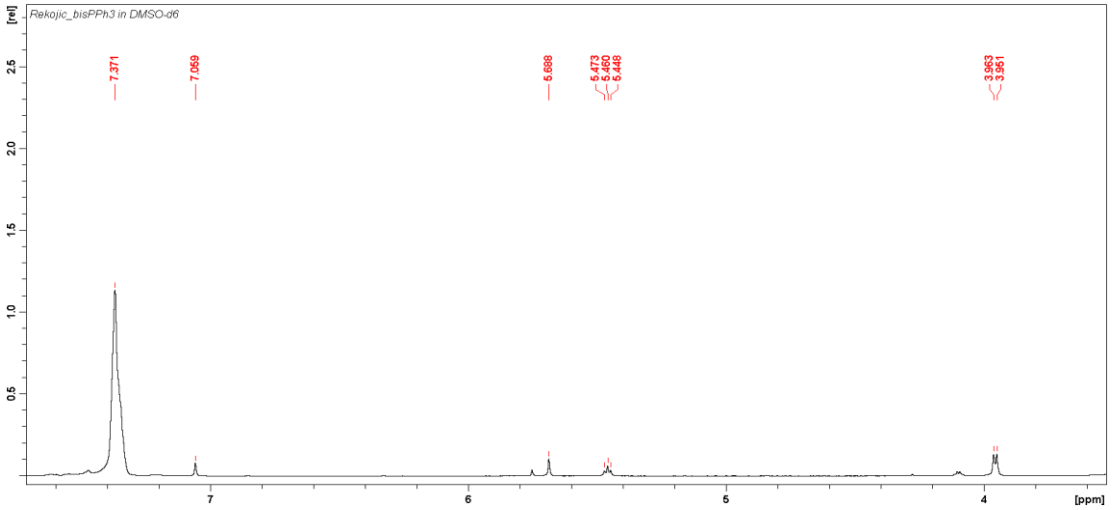


Figure S17 ^{1}H NMR of [Re(CO)$_2$(OO^2)(L$_3$)$_2$] (**10**) in DMSO-d_6 at 25 °C

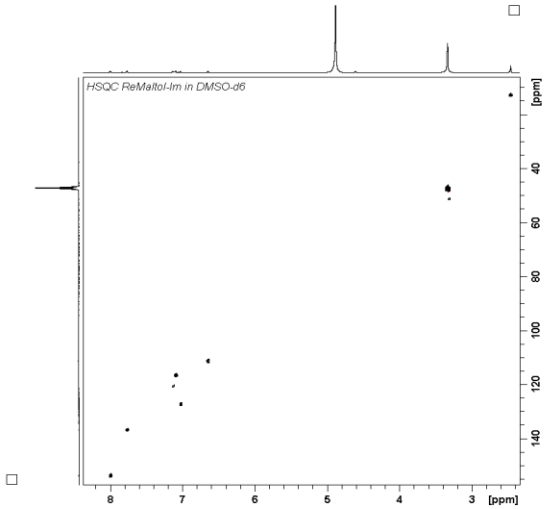


Figure S18 ^{1}H – ^{13}C HSQC NMR of [Re(CO)$_3$(OO^1)(L$_1$] (**3**) in DMSO-d_6 at 25 °C.

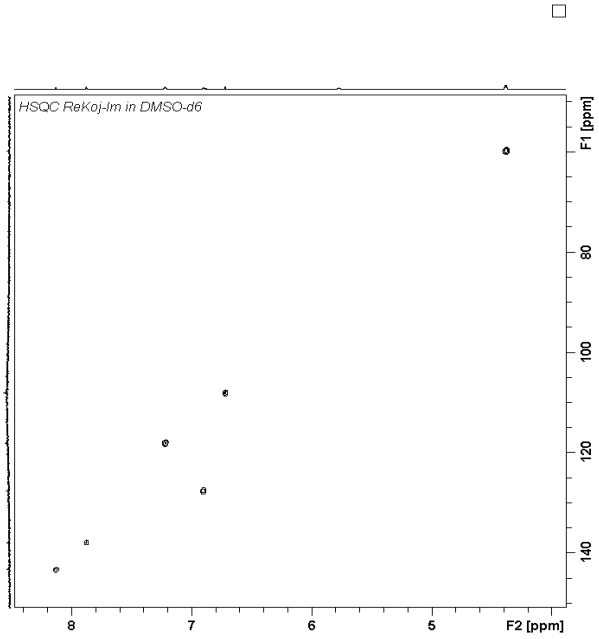


Figure S19 ^{1}H – ^{13}C HSQC NMR of $[Re(CO)_3(OO^2)(L_1]$ (**6**) in DMSO-d_6 at 25 °C

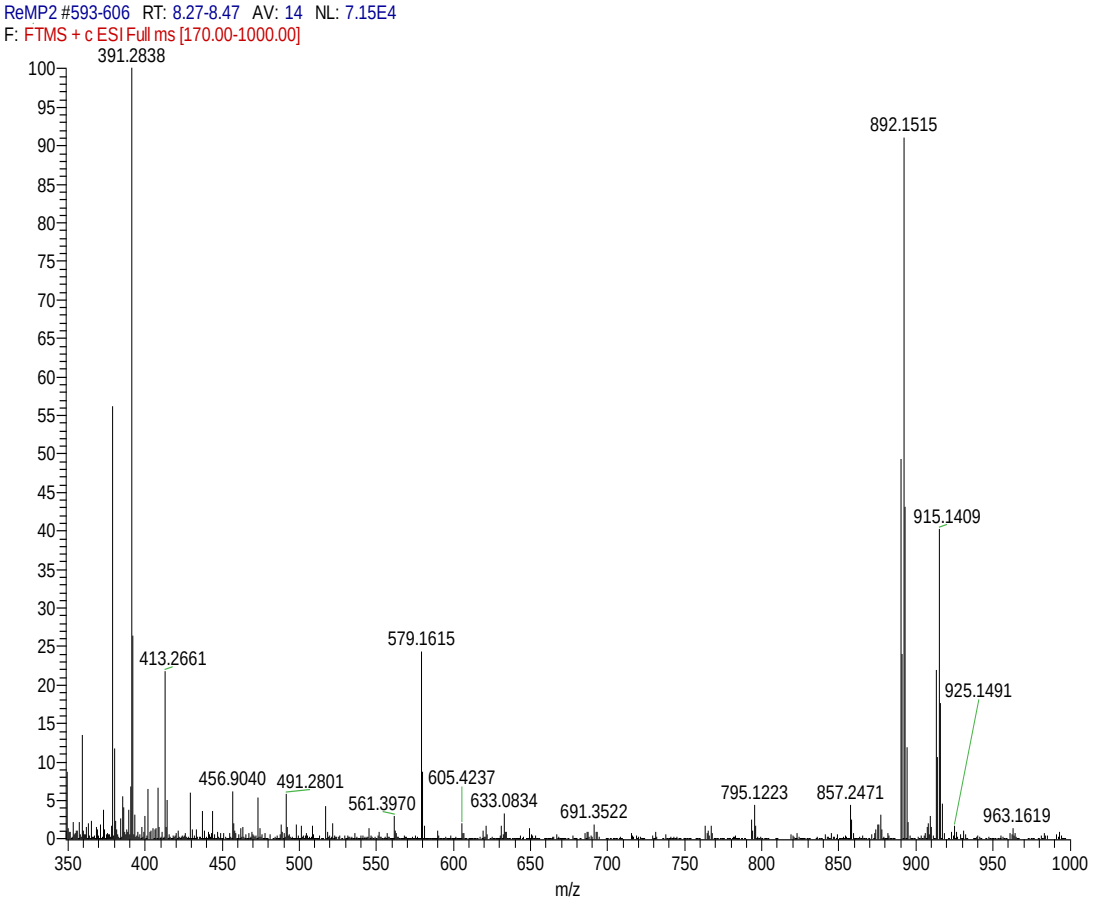


Figure S20 (ESI-MS) spectrum of $[Re(CO)_2(OO^1)(L_3)_2]$ (**9**)

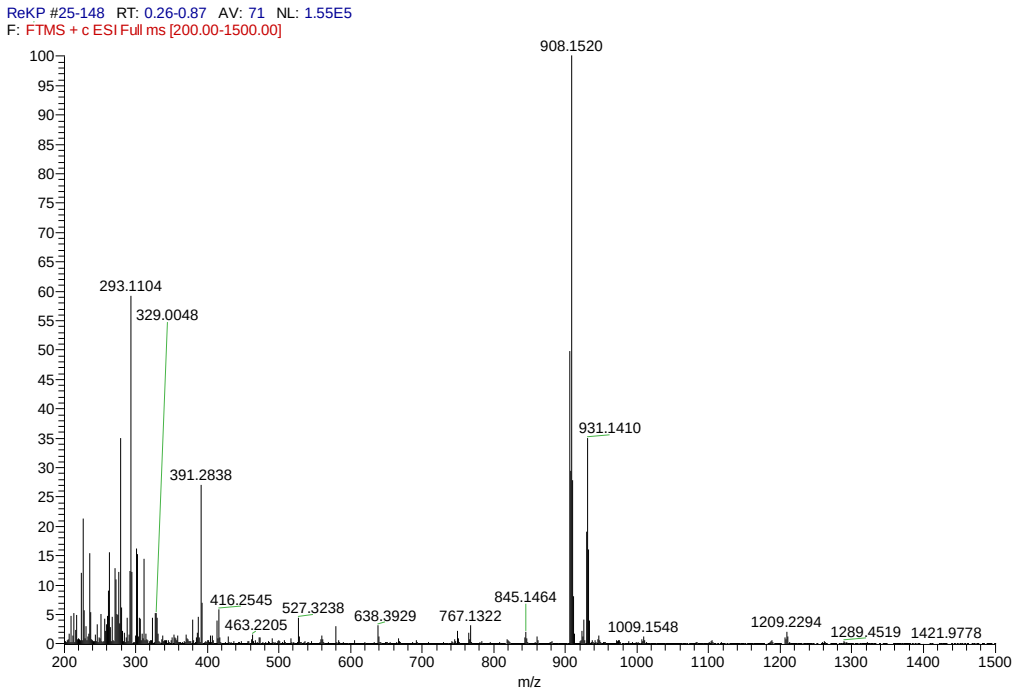


Figure S21 (ESI-MS) spectrum of $[Re(CO)_2(OO^2)(L_3)_2]$ (**10**)

HPLC / Autoscaled Chromatograms (OO^1, OO^2, **1-10)**

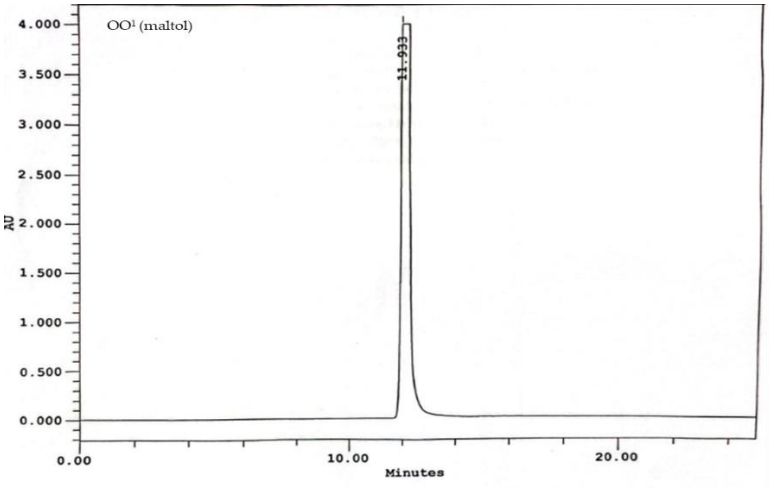


Figure S22: HPLC / Autoscaled Chromatogram of maltol, OO^1, *RT* = 11.9 min

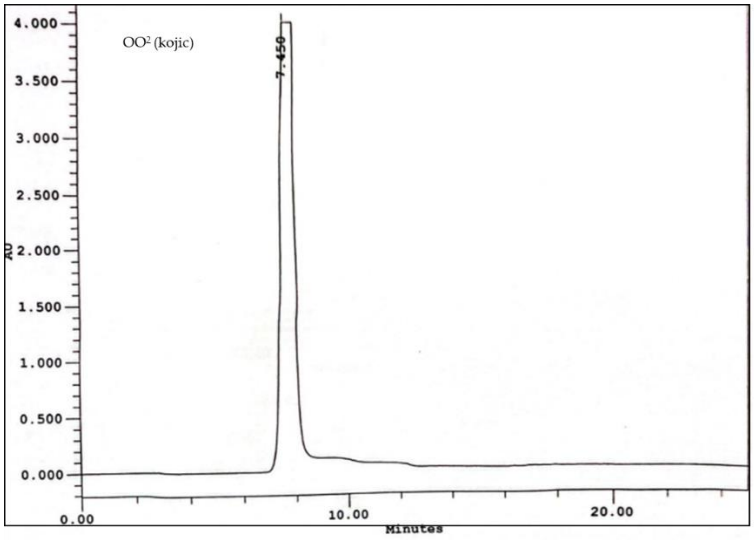


Figure S23: HPLC / Autoscaled Chromatogram of kojic, OO^2, *RT* = 7.5 min

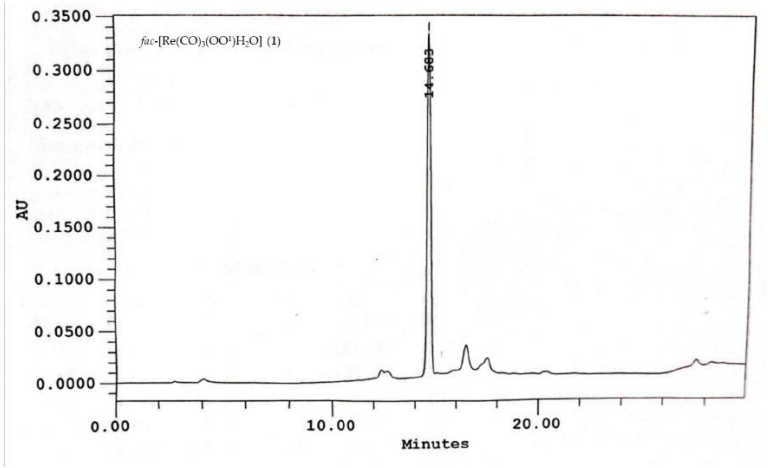


Figure S24: HPLC / Autoscaled Chromatogram of *fac*-$[Re(CO)_3(OO^1)H_2O]$ (**1**), *RT* = 14.7 min

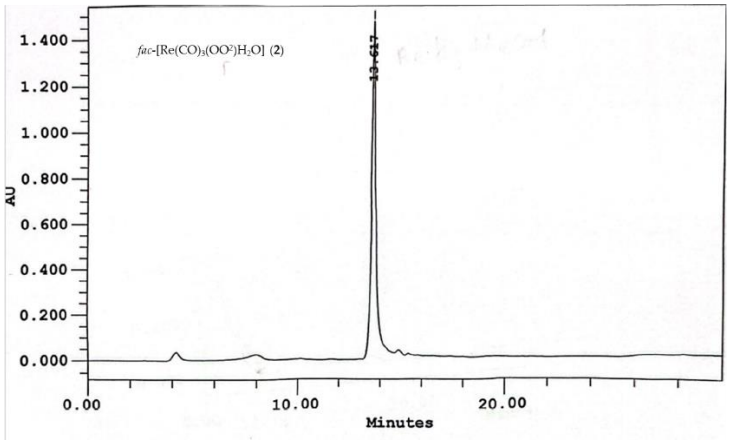


Figure S25: HPLC / Autoscaled Chromatogram of *fac*-$[Re(CO)_3(OO^2)H_2O]$ (**2**), *RT* = 13.6 min

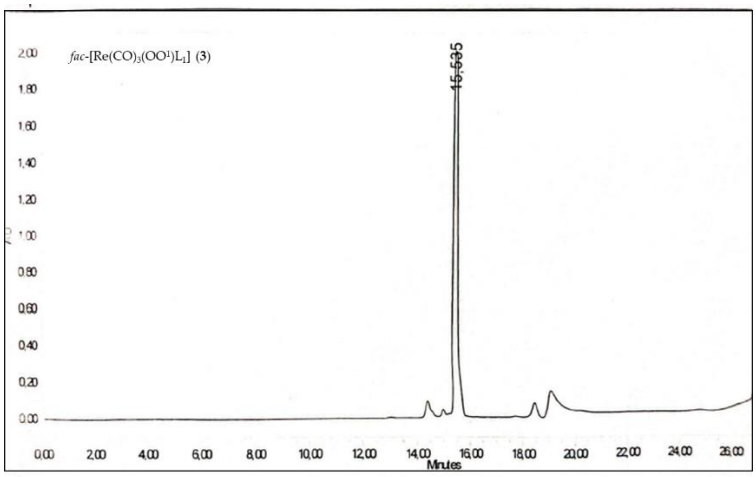


Figure S26: HPLC / Autoscaled Chromatogram of *fac*-[Re(CO)$_3$(OO^1)L$_1$] (**3**), *RT* = 15.5 min

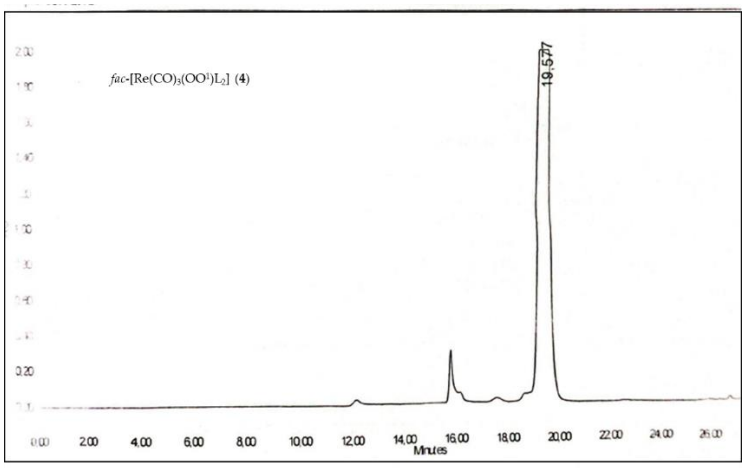


Figure S27: HPLC / Autoscaled Chromatogram of *fac*-[Re(CO)$_3$(OO^1)L$_2$] (**4**), *RT* = 19.6 min

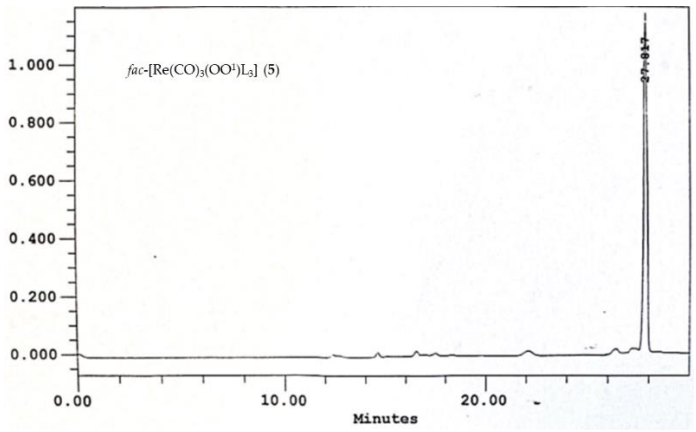


Figure S28: HPLC / Autoscaled Chromatogram of *fac*-[Re(CO)$_3$(OO^1)L$_3$] (**5**), *RT* = 27.8 min

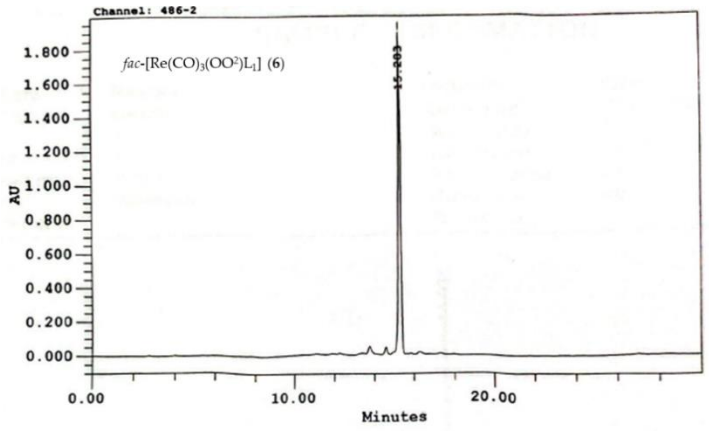


Figure S29: HPLC / Autoscaled Chromatogram of *fac*-[Re(CO)$_3$(OO^2)L$_1$] (**6**), *RT* = 15.3 min

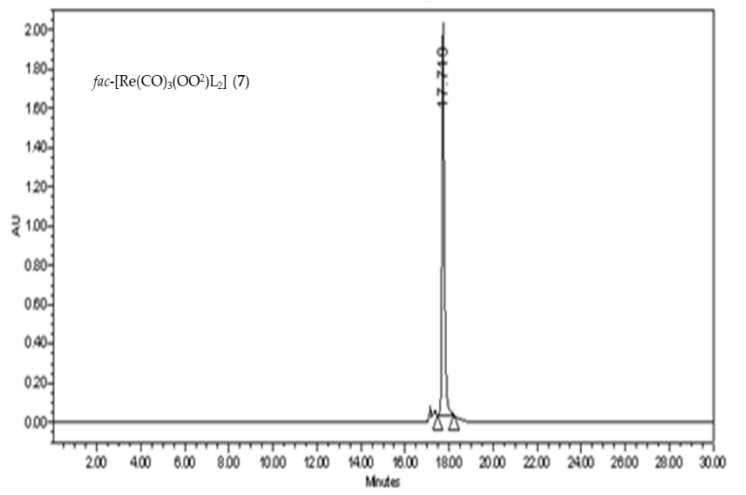


Figure S30: HPLC / Autoscaled Chromatogram of *fac*-[Re(CO)$_3$(OO^2)L$_2$] (**7**), *RT* = 17.7 min

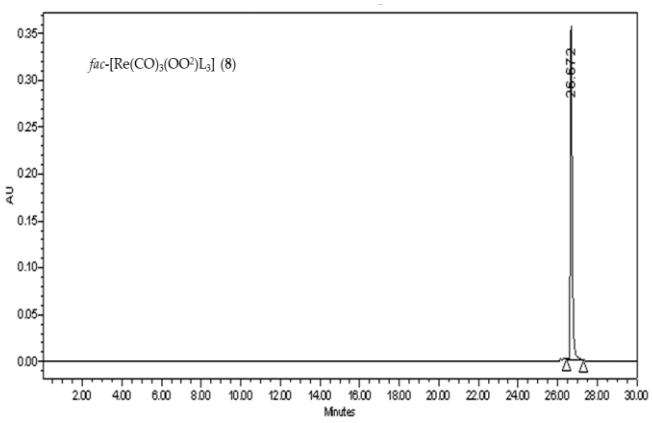


Figure S31: HPLC / Autoscaled Chromatogram of *fac*-[Re(CO)$_3$(OO^2)L$_3$] (**8**), *RT* = 26.6 min

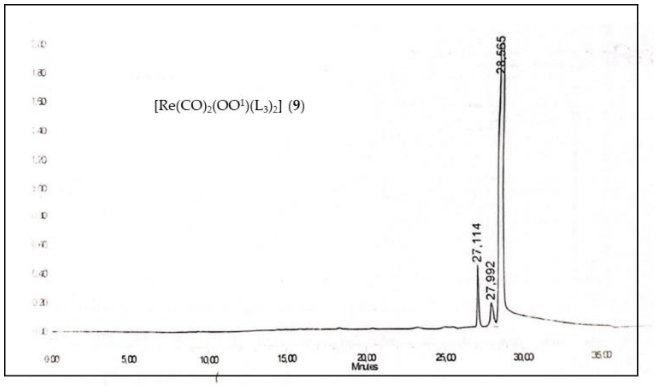


Figure S32: HPLC / Autoscaled Chromatogram of $[Re(CO)_2(OO^1)(L_3)_2]$ (**9**), *RT* = 28.6 min

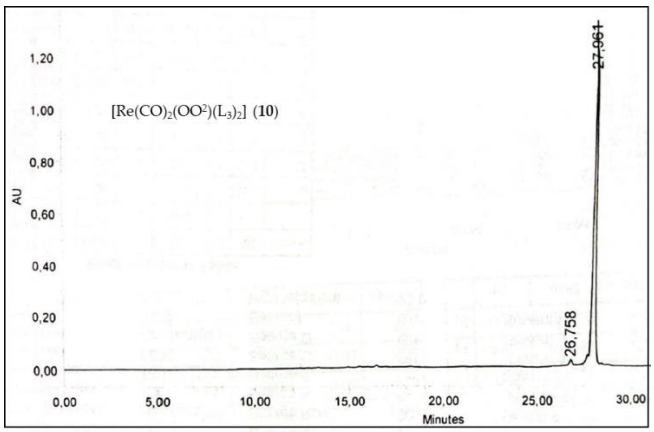


Figure S33: HPLC / Autoscaled Chromatogram of $[Re(CO)_2(OO^2)(L_3)_2]$ (**10**), *RT* = 28.0 min

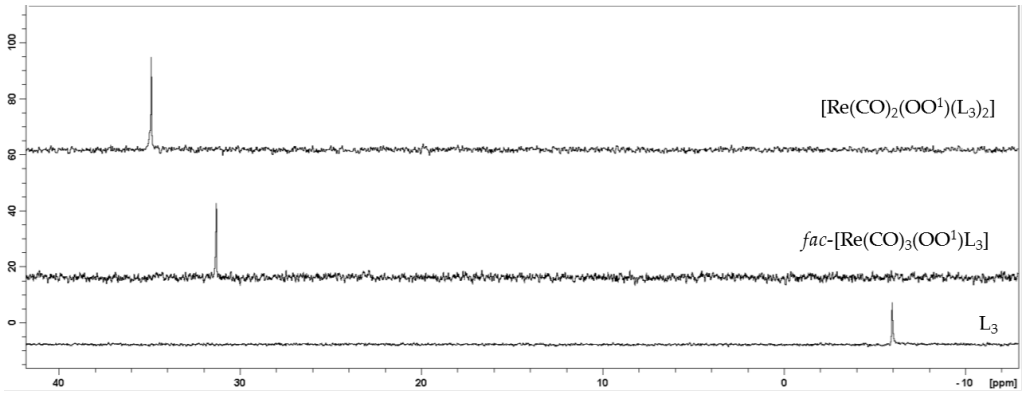


Figure S34: Characteristic ^{31}P NMR of L_3, *fac*-$[Re(CO)_3(OO^1)(L_3)]$ (**5**) and $[Re(CO)_2(OO^1)(L_3)_2]$ (**9**)