# Supporting Information

## Synthesis, cytotoxicity and cellular uptake studies of N3 functionalized $Re(CO)_3$ thymidine complexes

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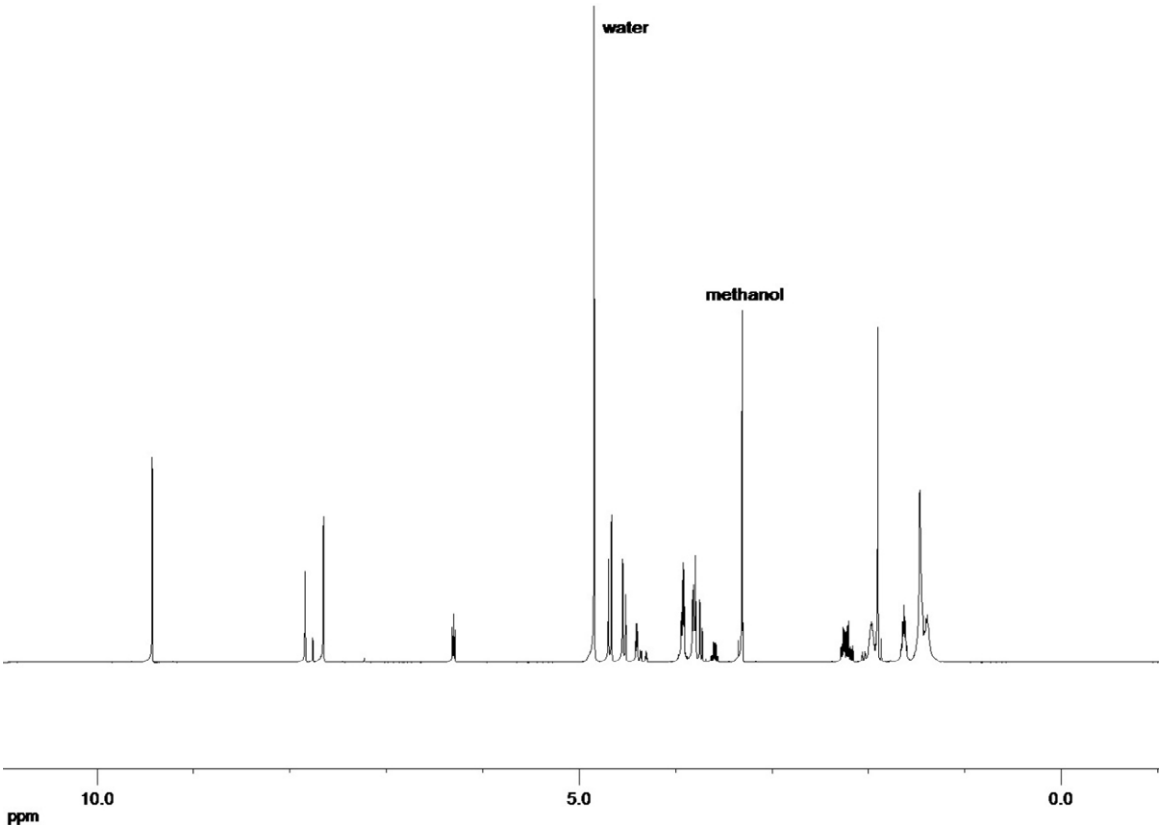
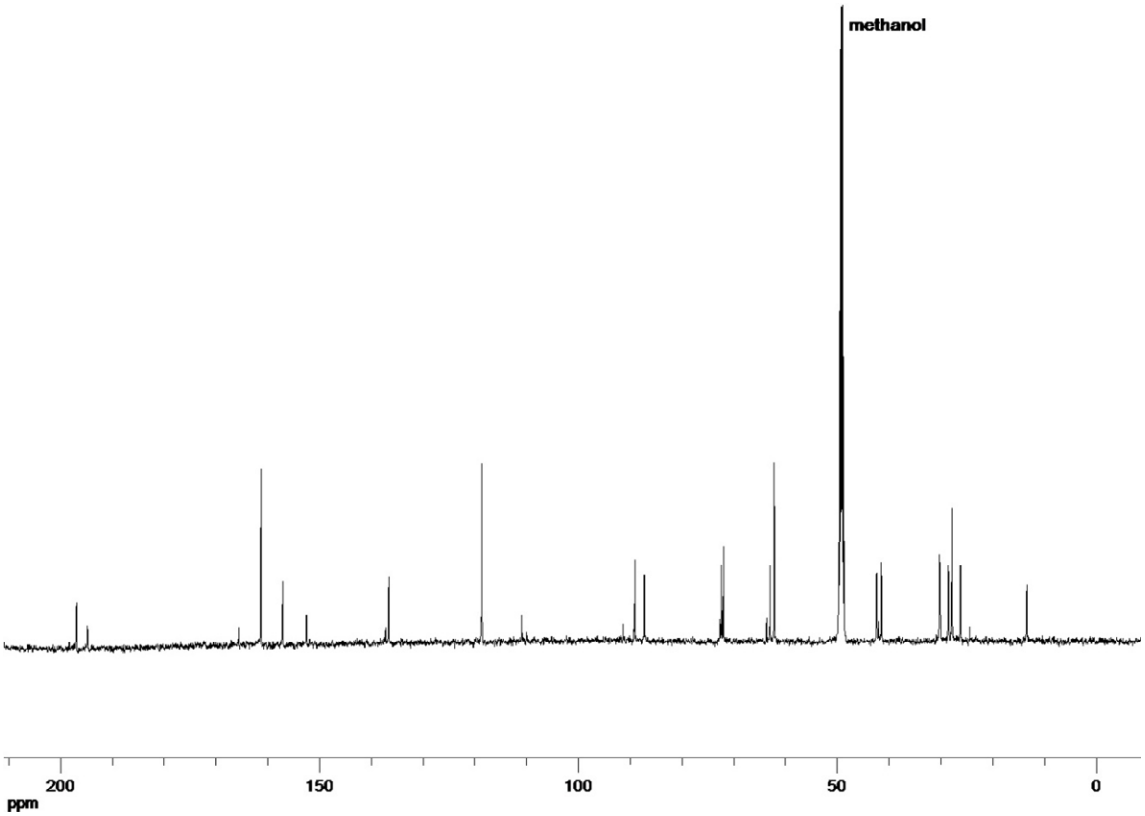
**Contents:**

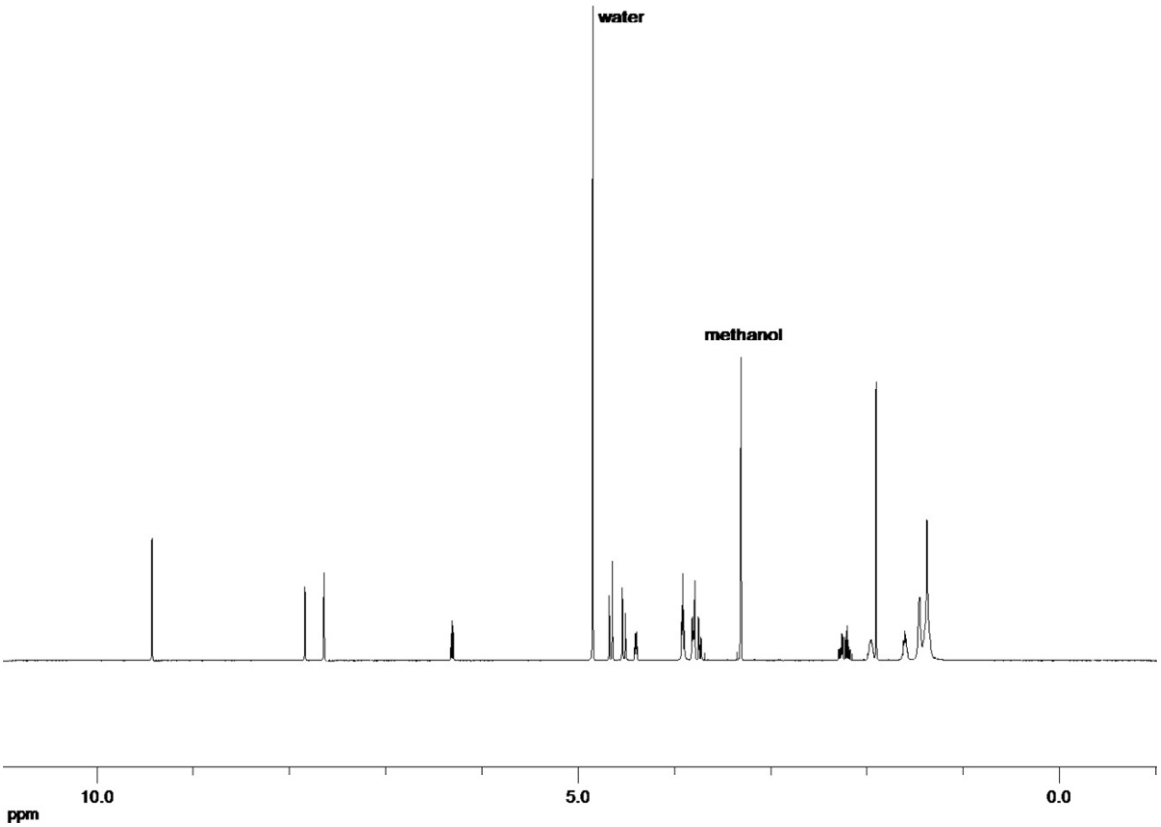
## 1. NMR spectra of $Re(CO)_3$ complexes



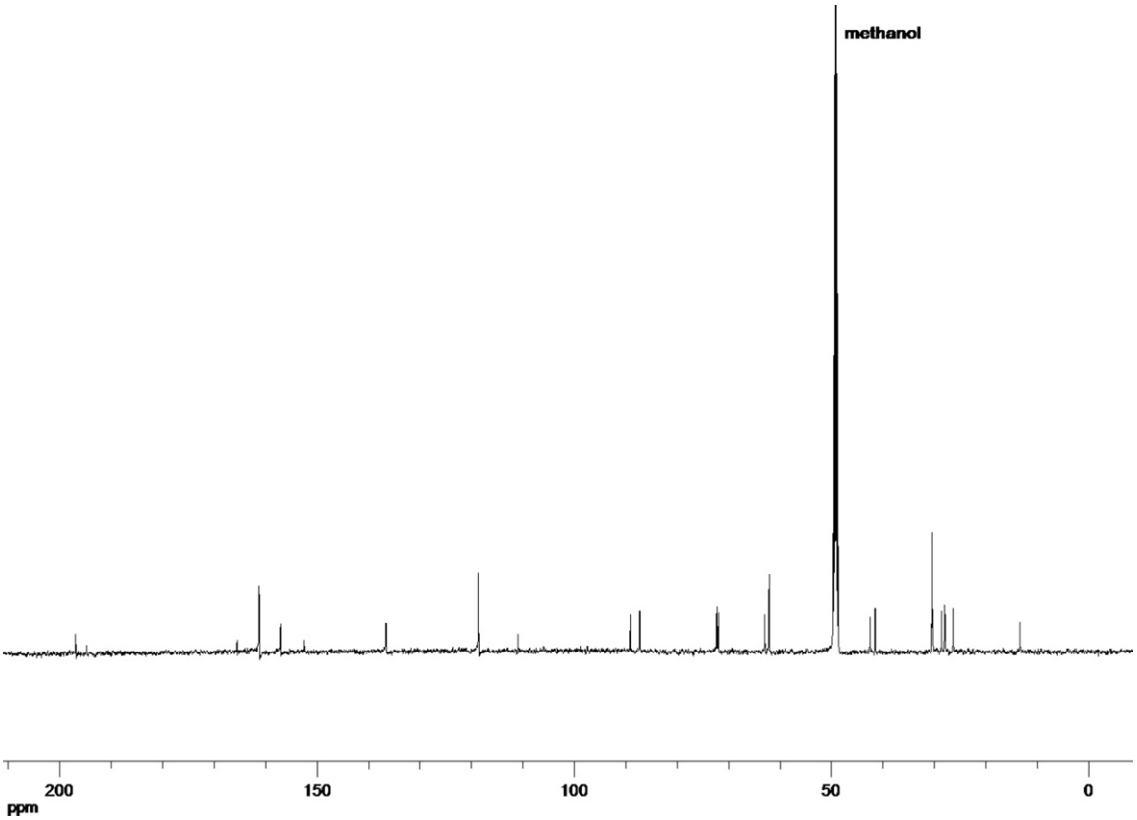

$^1$H NMR $[Re(CO)_3(15)]Br$ **(19)**



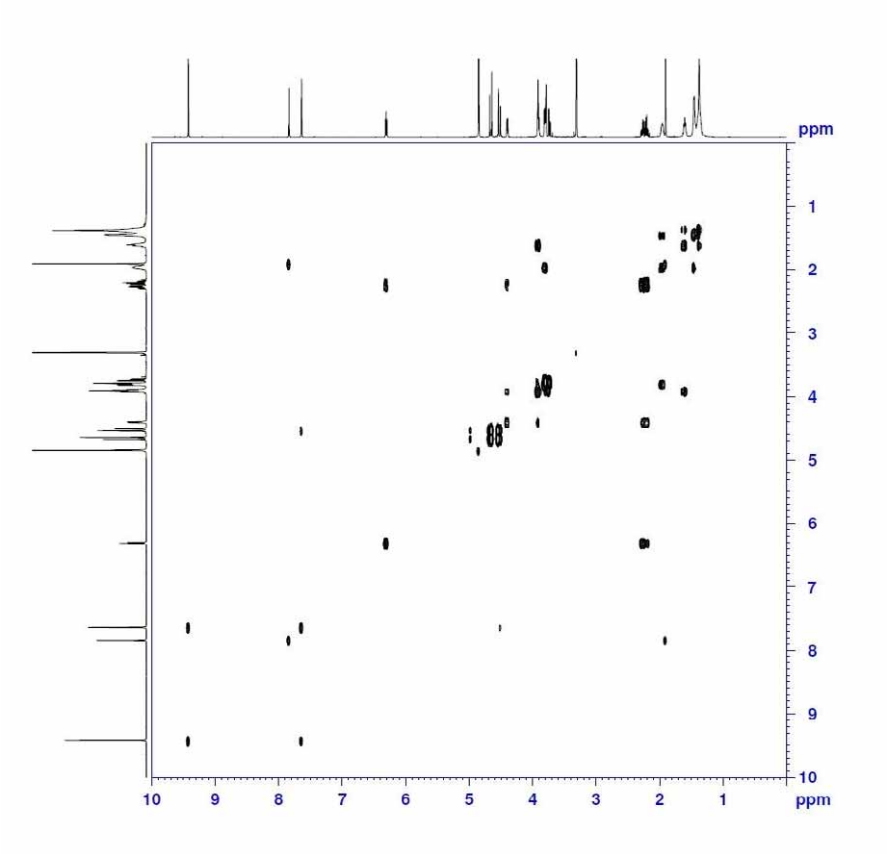
$^{13}$C NMR [Re(CO)$_3$(15)]Br **(19)**



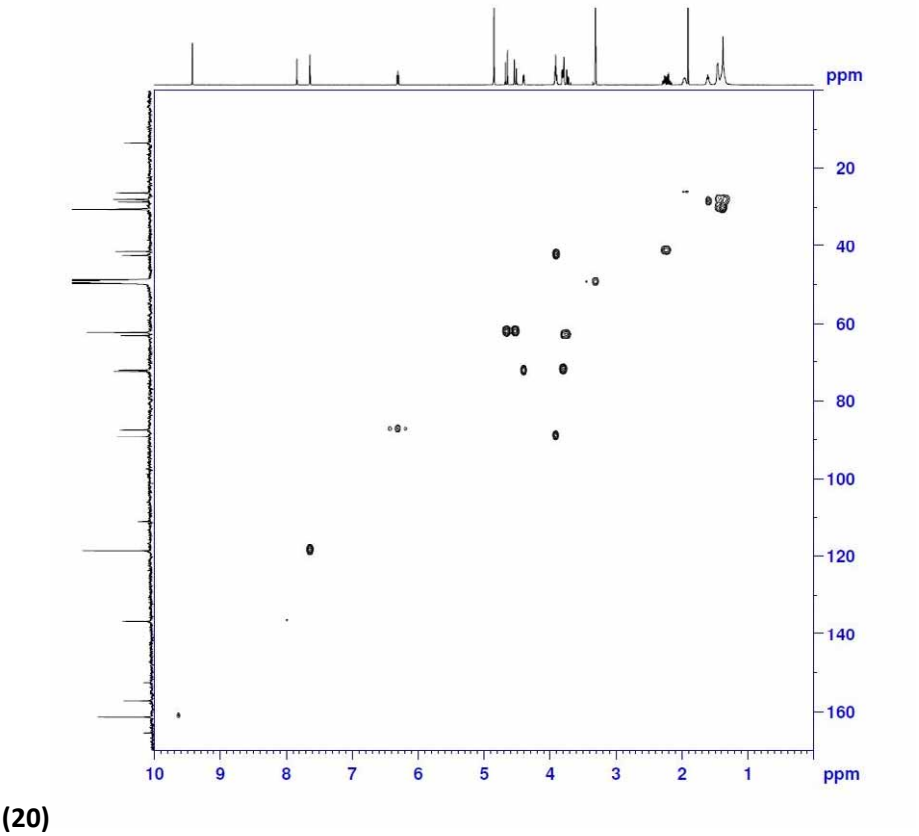

$^{1}$H NMR [Re(CO)$_3$(16)]Br **(20)**




$^{13}$C NMR [Re(CO)$_3$(16)]Br **(20)**

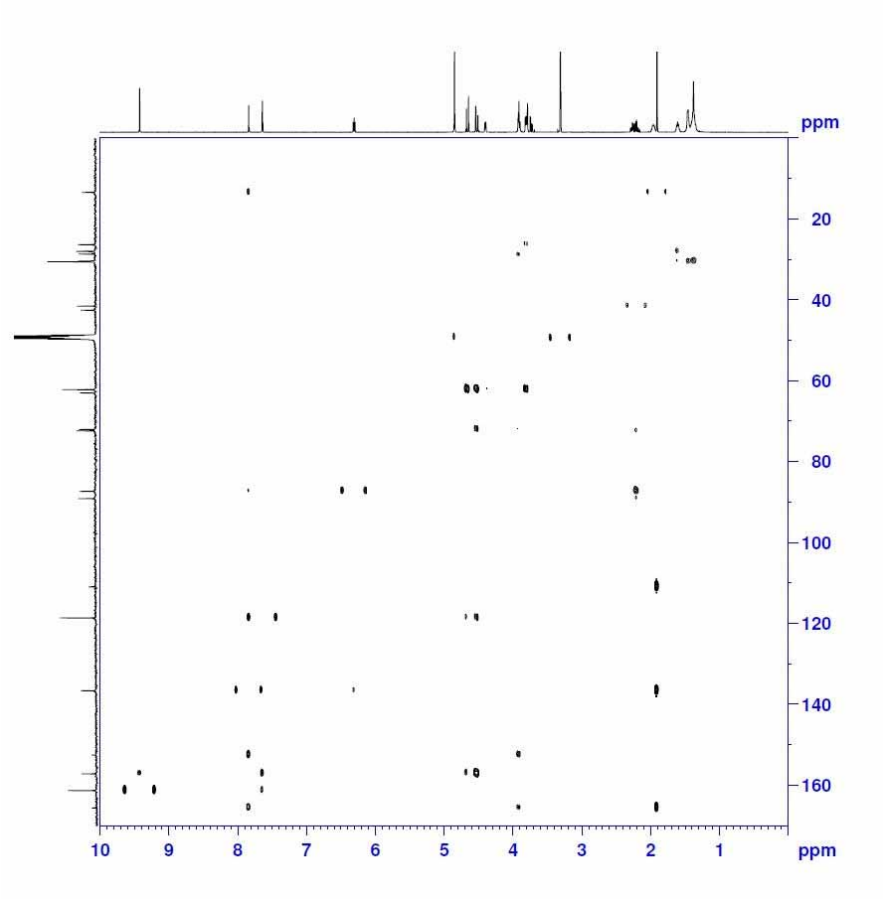



HH COSY [Re(CO)$_3$(16)]Br

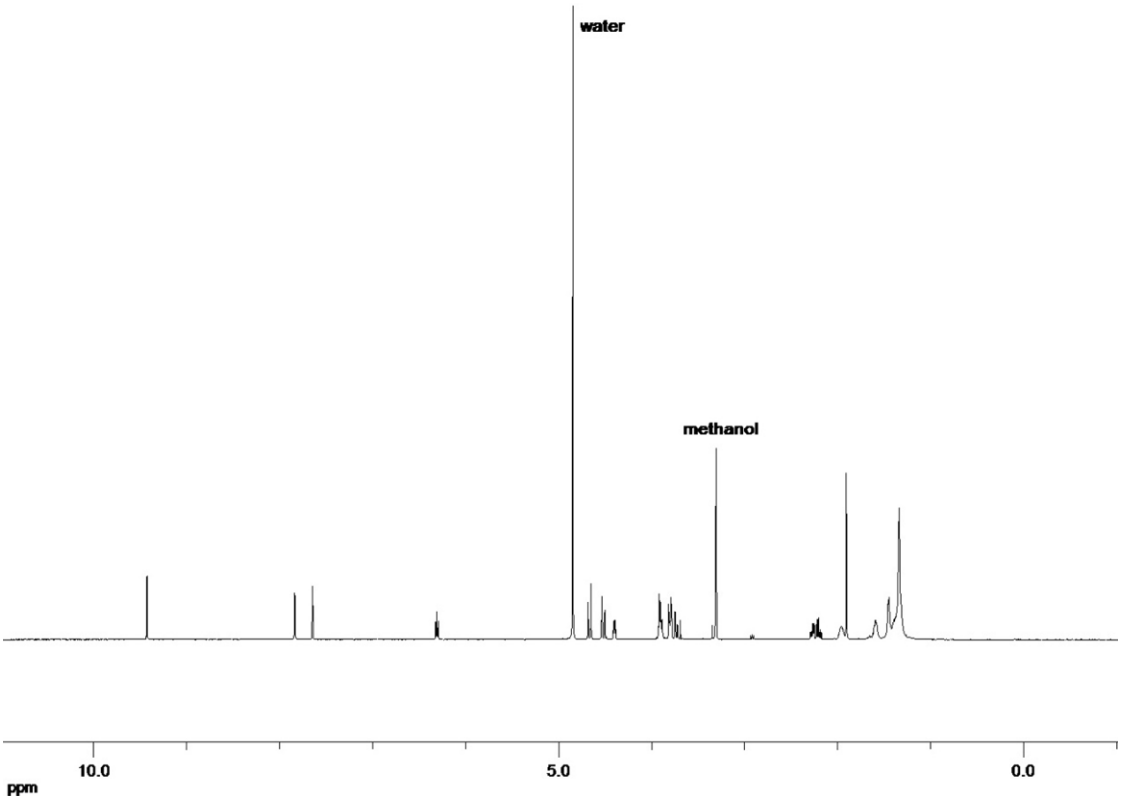



**(20)**

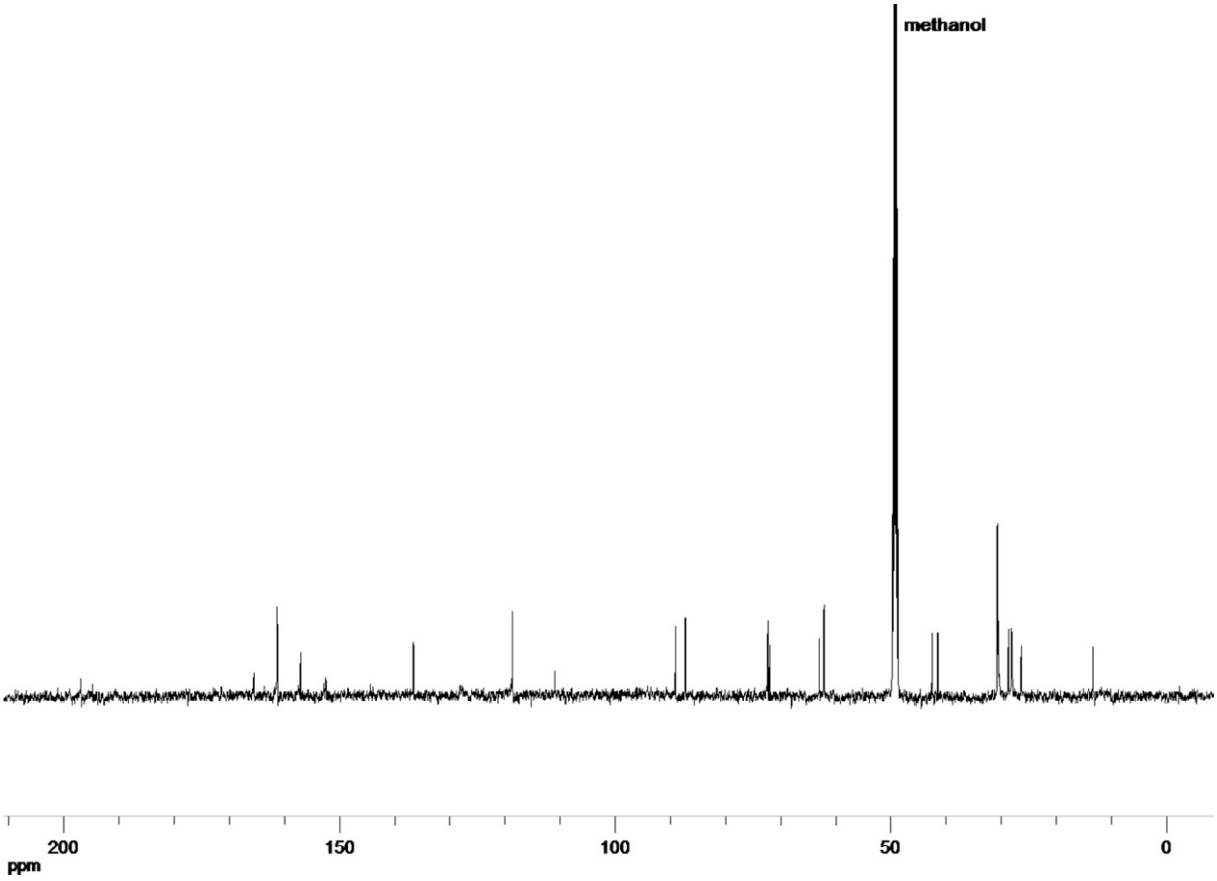
CH COSY [Re(CO)$_3$(16)]Br **(20)**



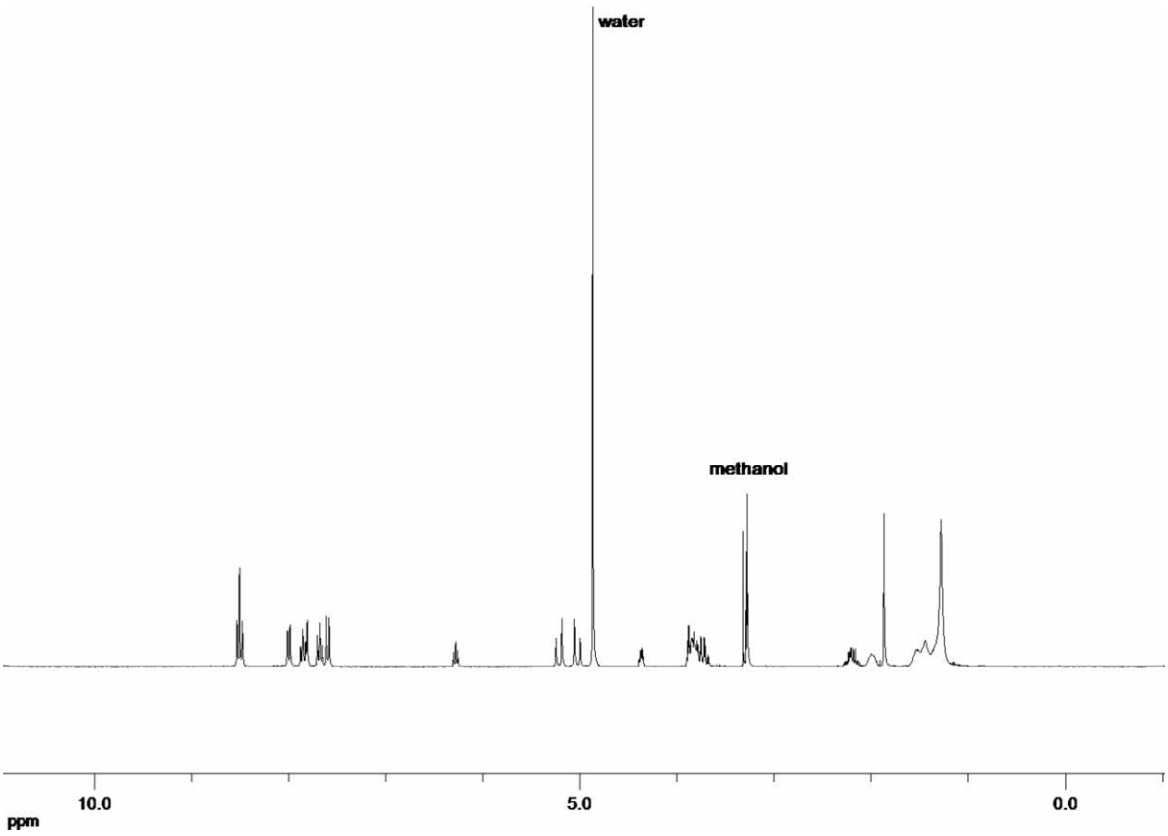

CH long-range COSY $[Re(CO)_3(16)]Br$ **(20)**



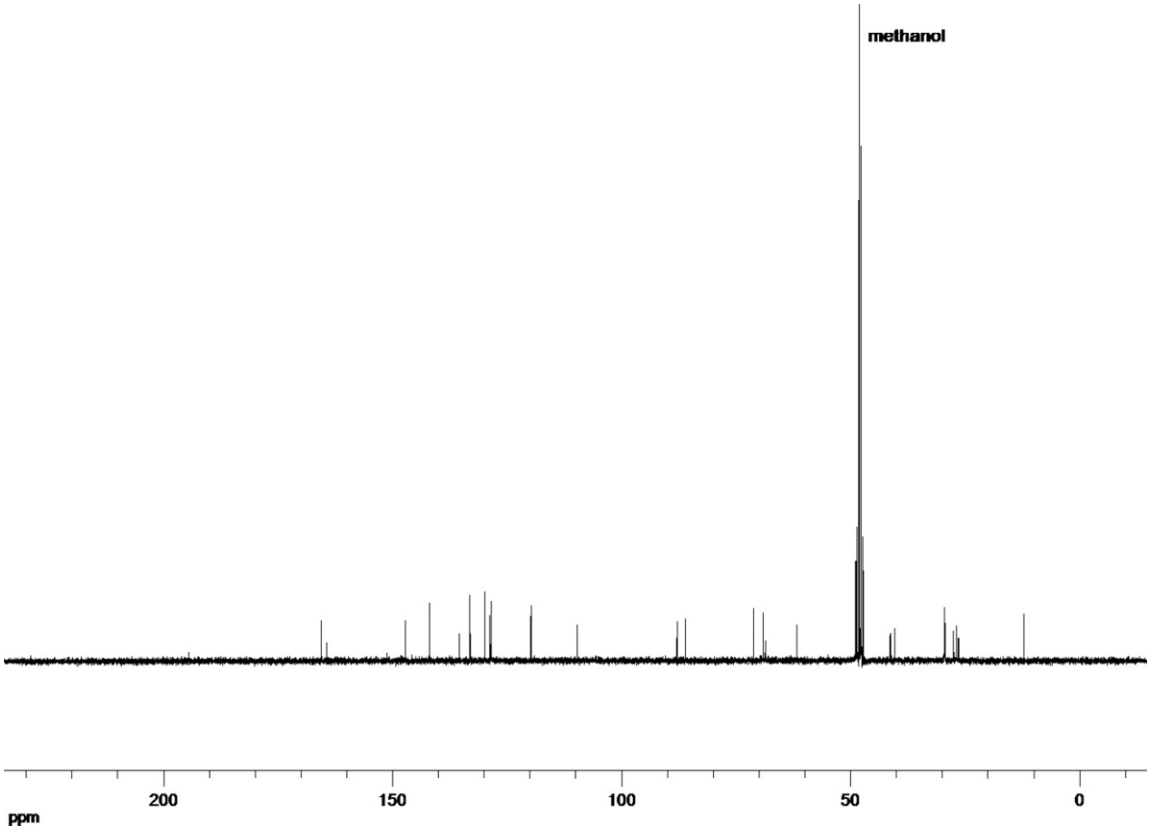

$^1H$ NMR $[Re(CO)_3(17)]Br$ **(21)**




$^{13}C$ NMR $[Re(CO)_3(17)]Br$ **(21)**

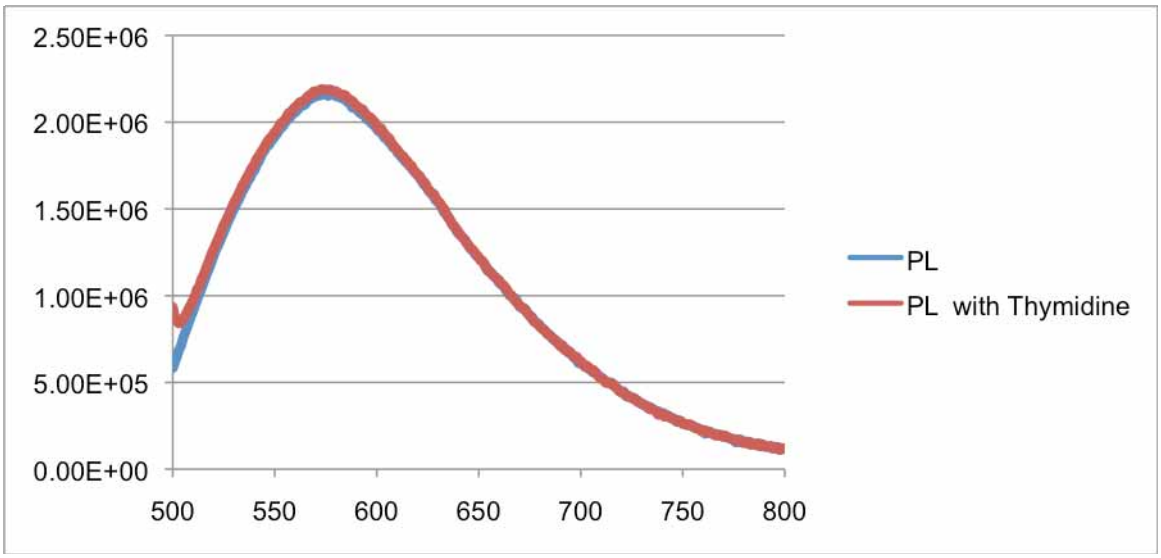



$^{1}H$ NMR $[Re(CO)_3(18)]Br$ **(22)**



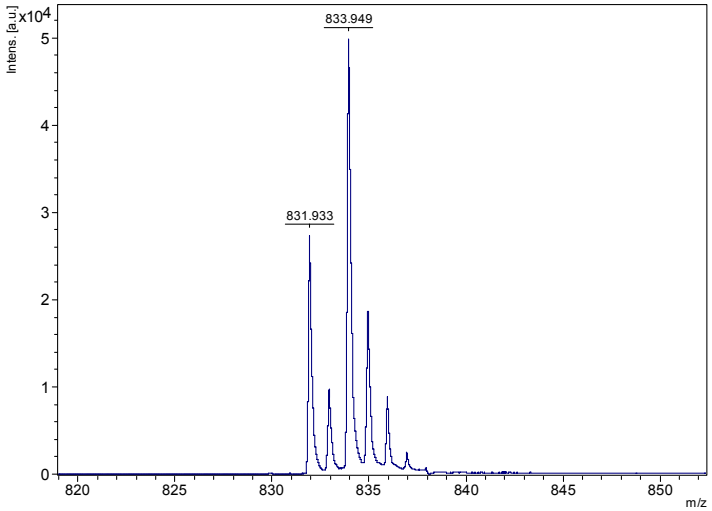

$^{13}C$ NMR $[Re(CO)_3(18)]Br$ **(22)**

**2. Emission Spectrum for compound 22.**

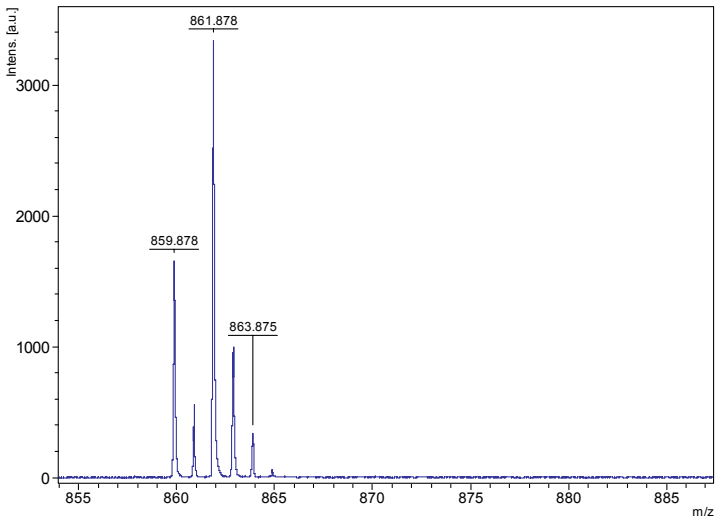



Emission profile of $[Re(CO)_3(18)]Br$ **(22)** excited at 488 nm (blue) and 100-fold dT challenge (red).

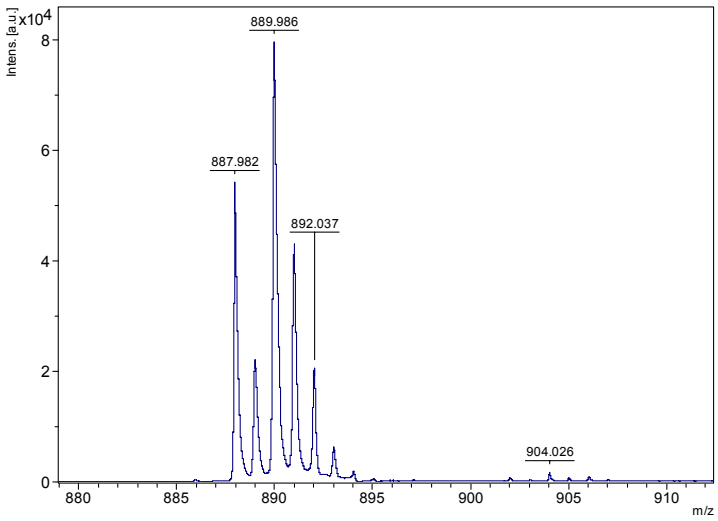
## 3. Mass spectra for 19-22.



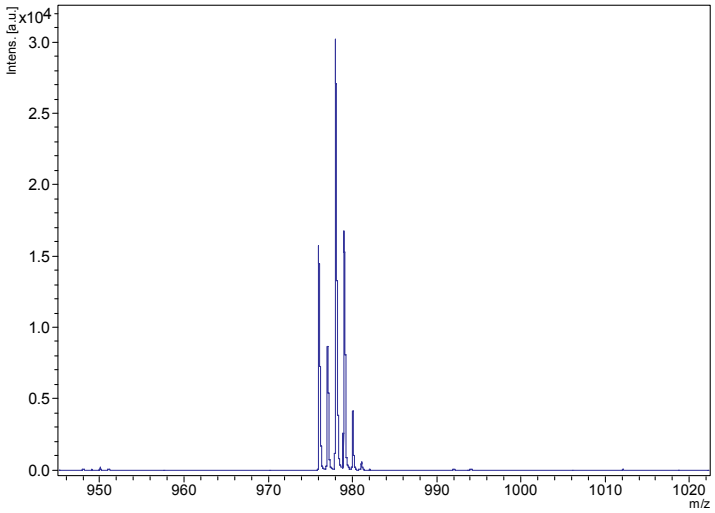

Mass spec $[Re(CO)_3(15)]Br$ **(19)**



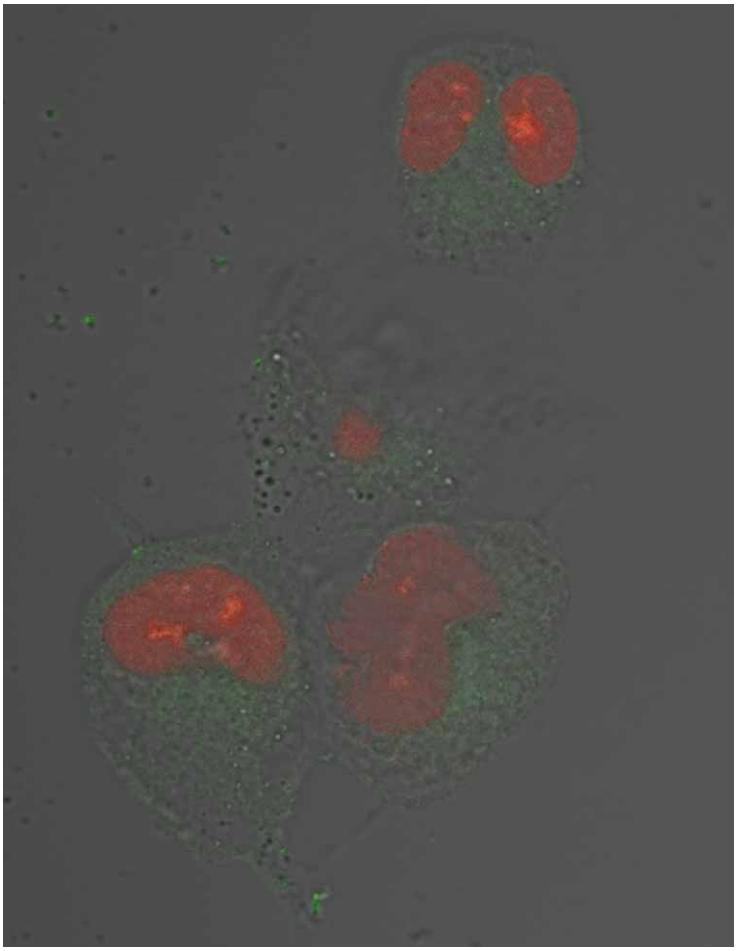

Mass spec $[Re(CO)_3(16)]Br$ **(20)**




Mass spec $[Re(CO)_3(17)]Br$ **(21)**




Mass spec $[Re(CO)_3(18)]Br$ **(22)**



**4.** Nuclear counterstaining of Nuclear-ID Red and **22** indicating no incorporation of **22** into the nucleus.