Supporting Information

Synthesis, cytotoxicity and cellular uptake studies of N3 functionalized Re(CO)₃ thymidine complexes

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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)₅(16)]Br

CH COSY [Re(CO)₅(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).

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.