SUPPLEMENTARY INFORMATION FOR

Synthesis of Tripeptide Derivatized Cyclopentadienyl Complexes of Technetium and Rhenium as Radiopharmaceutical Probes

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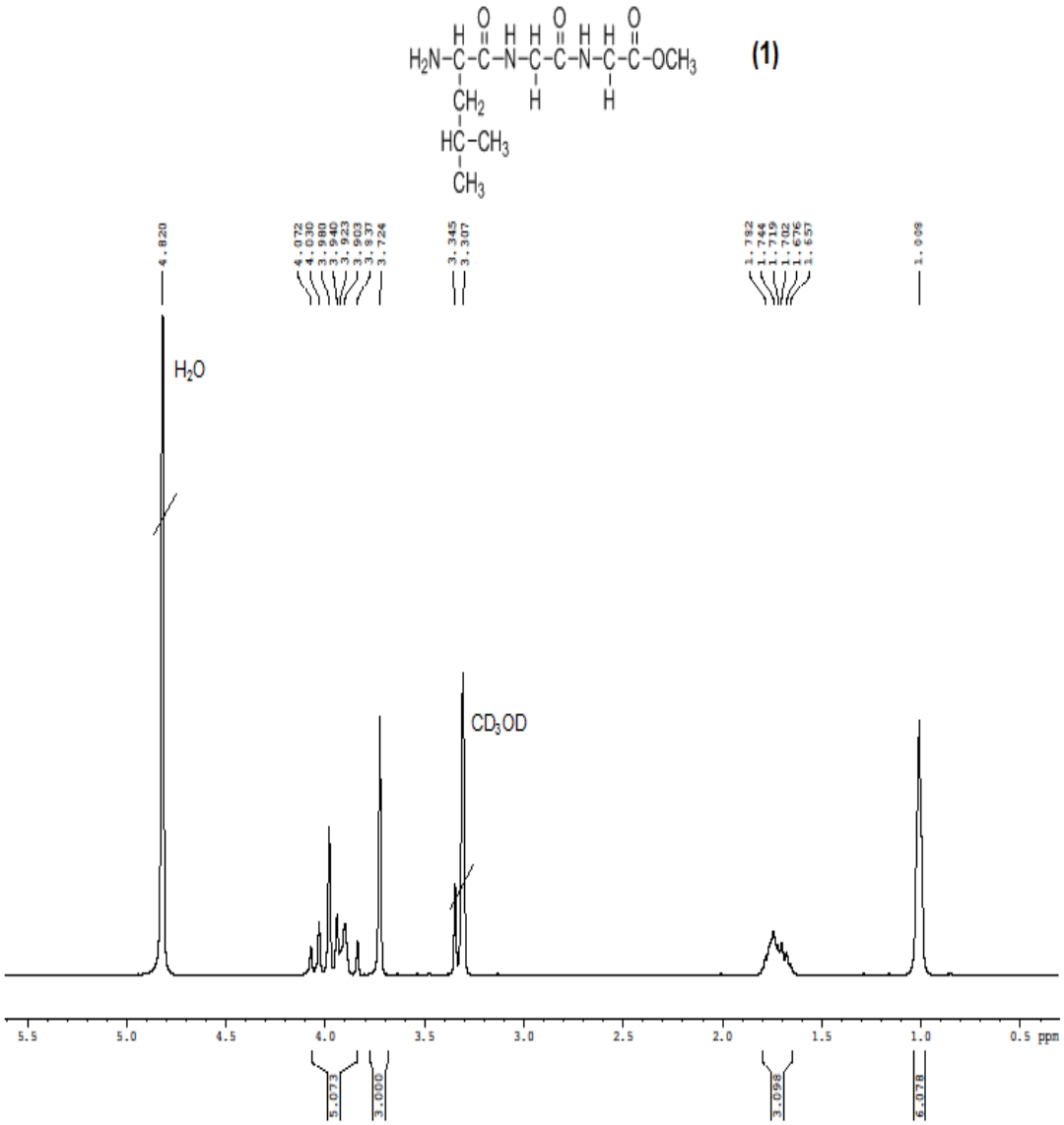
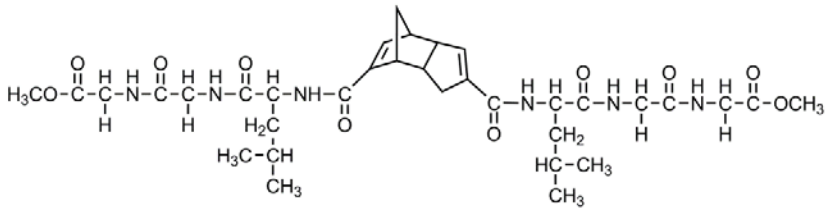
General Experimental Conditions:

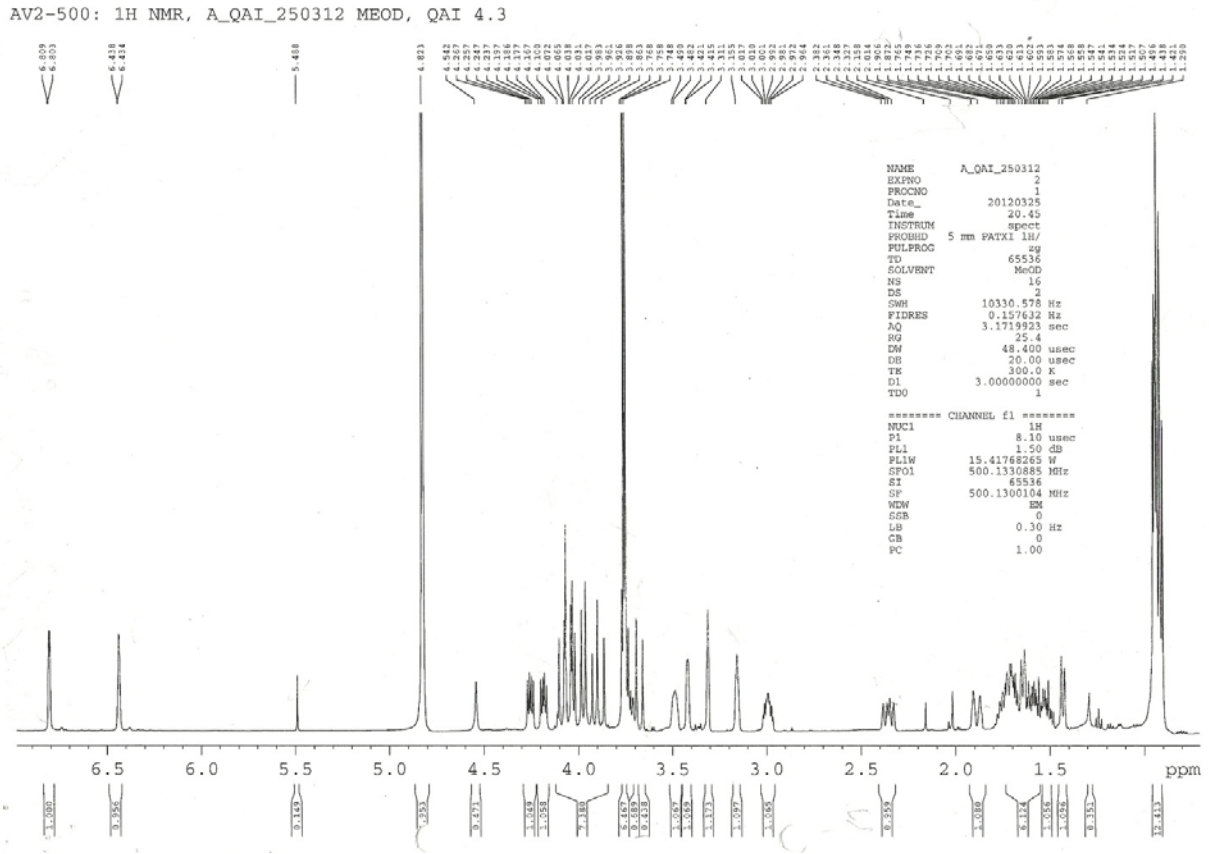
Reactions were carried out in dried glassware under nitrogen environment. Solvents were dried using standard techniques. IR spectra were recorded as KBr pellets on a Perkin-Elmer BX II IR spectrometer. Some chemical reactions were monitored by TLC, using silica gel plates MERCK 60 F_{254} with 0.25 mm of thickness, in an aluminum support; the plates were analyzed with UV radiation. UV/vis detection was performed at 250 nm. The detection of radioactive ^{99m}Tc complexes was performed with a Berthold LB 507 radiodetector equipped with a NaI(Tl) scintillation detector. The elementary analyses for some compounds were not performed due to various contents of trifluoroacetate after purification with the preparative HPLC.

SI 1-^{1}H NMR (CD_3OD) spectra of [(HCl·H-Leu-Gly-Gly-OCH_3)] **1**

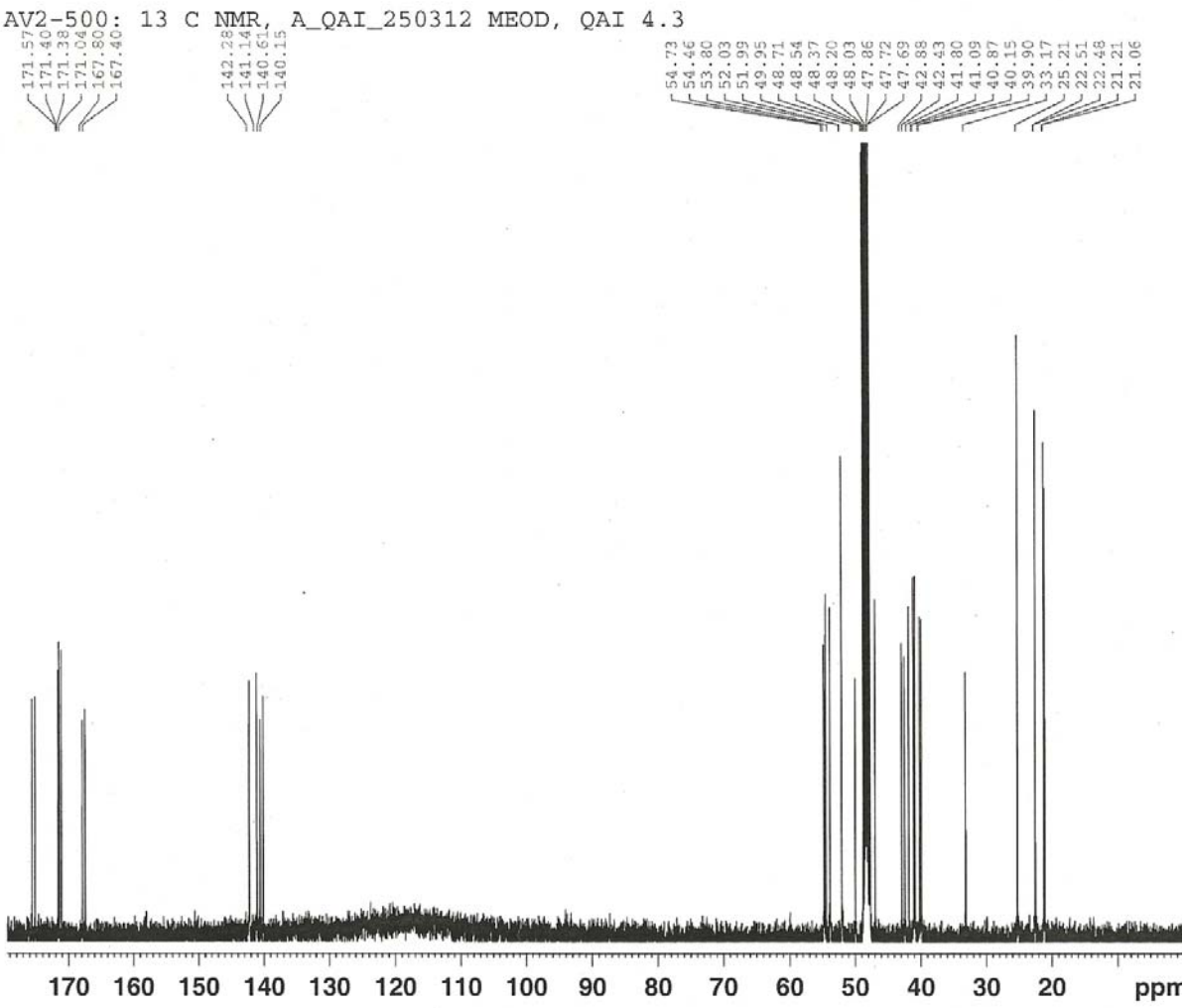


SI 2-^{1}H NMR (CD_3OD) spectra of [(HCpCONH-Leu-Gly-Gly-$OCH_3)_2$] **2**

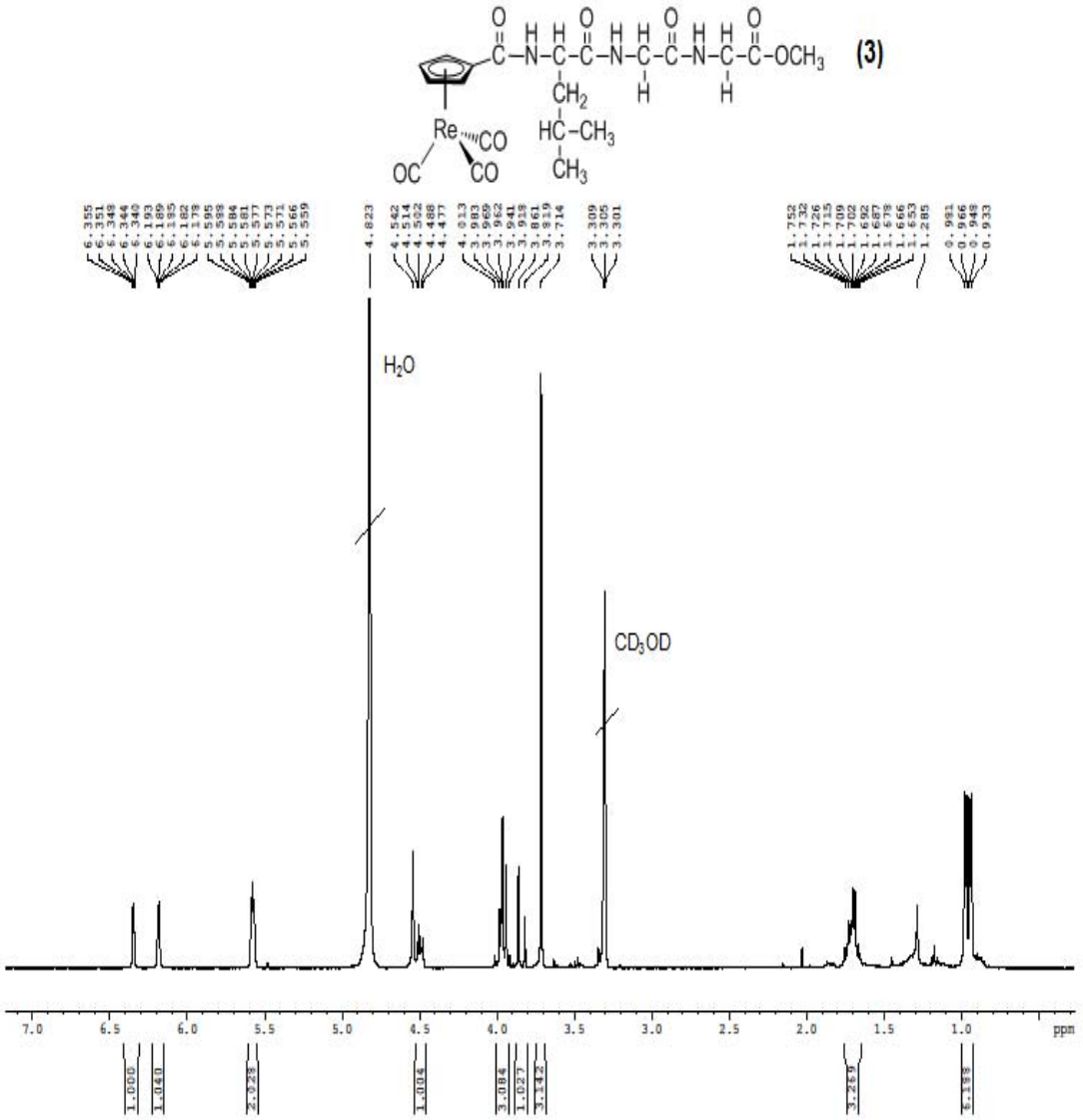




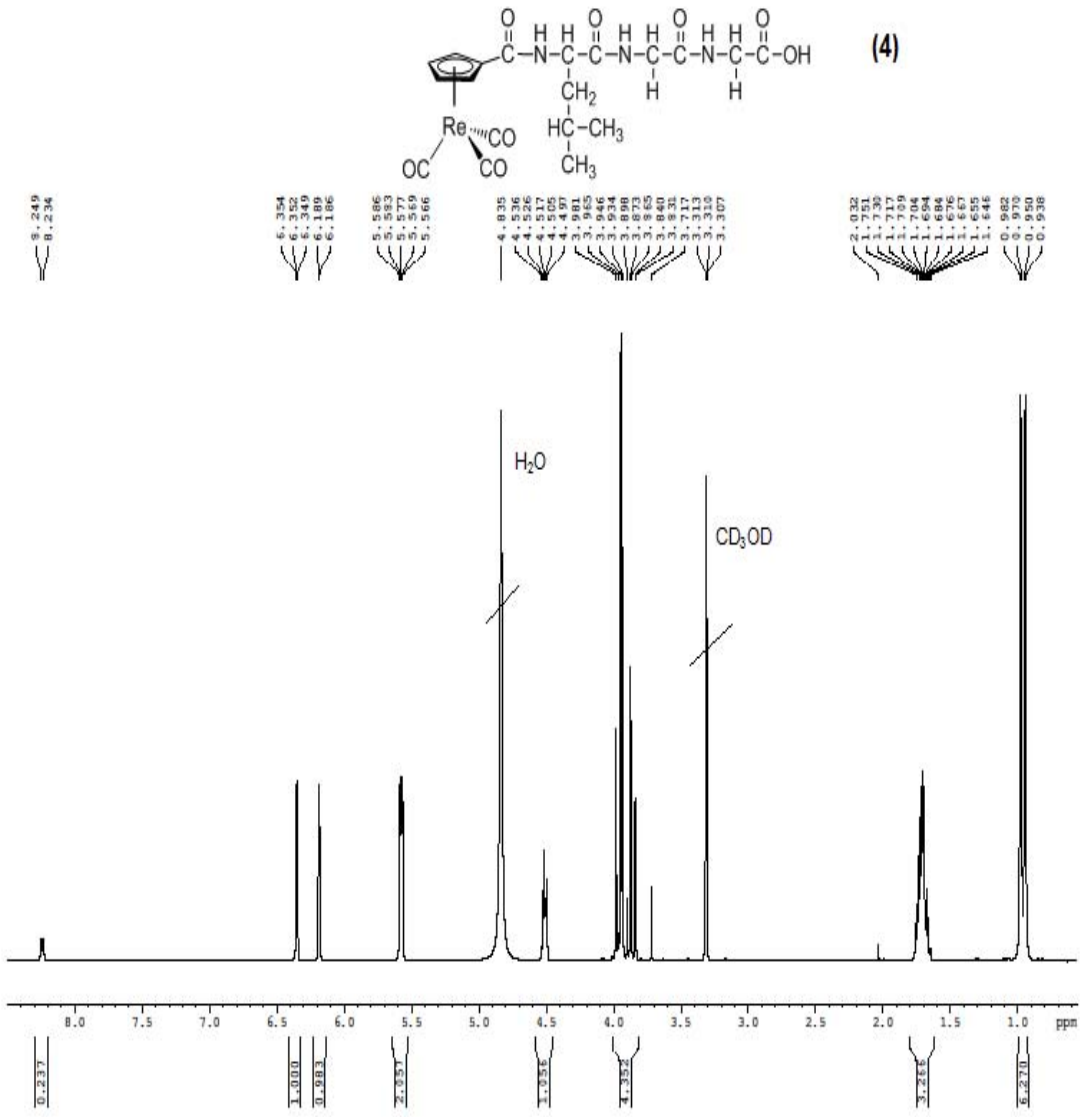
SI 3-^{13}C NMR (CD_3OD) spectra of [(HCpCONH-Leu-Gly-Gly-$OCH_3)_2$] **2**



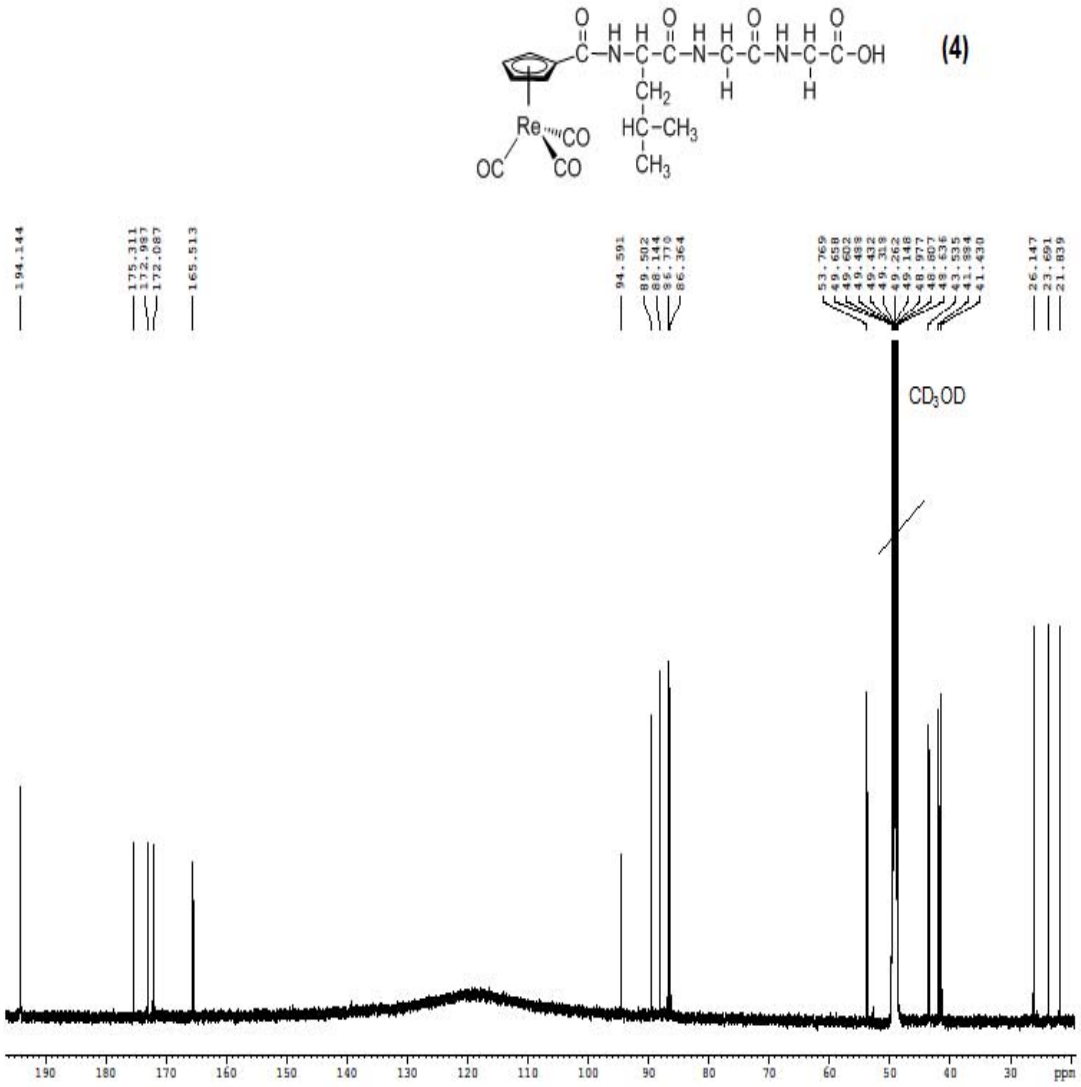
SI 4-^{1}H NMR (CD_3OD) spectra of [(CpCO-Leu-Gly-Gly-OCH_3)Re$(CO)_3$] **3**



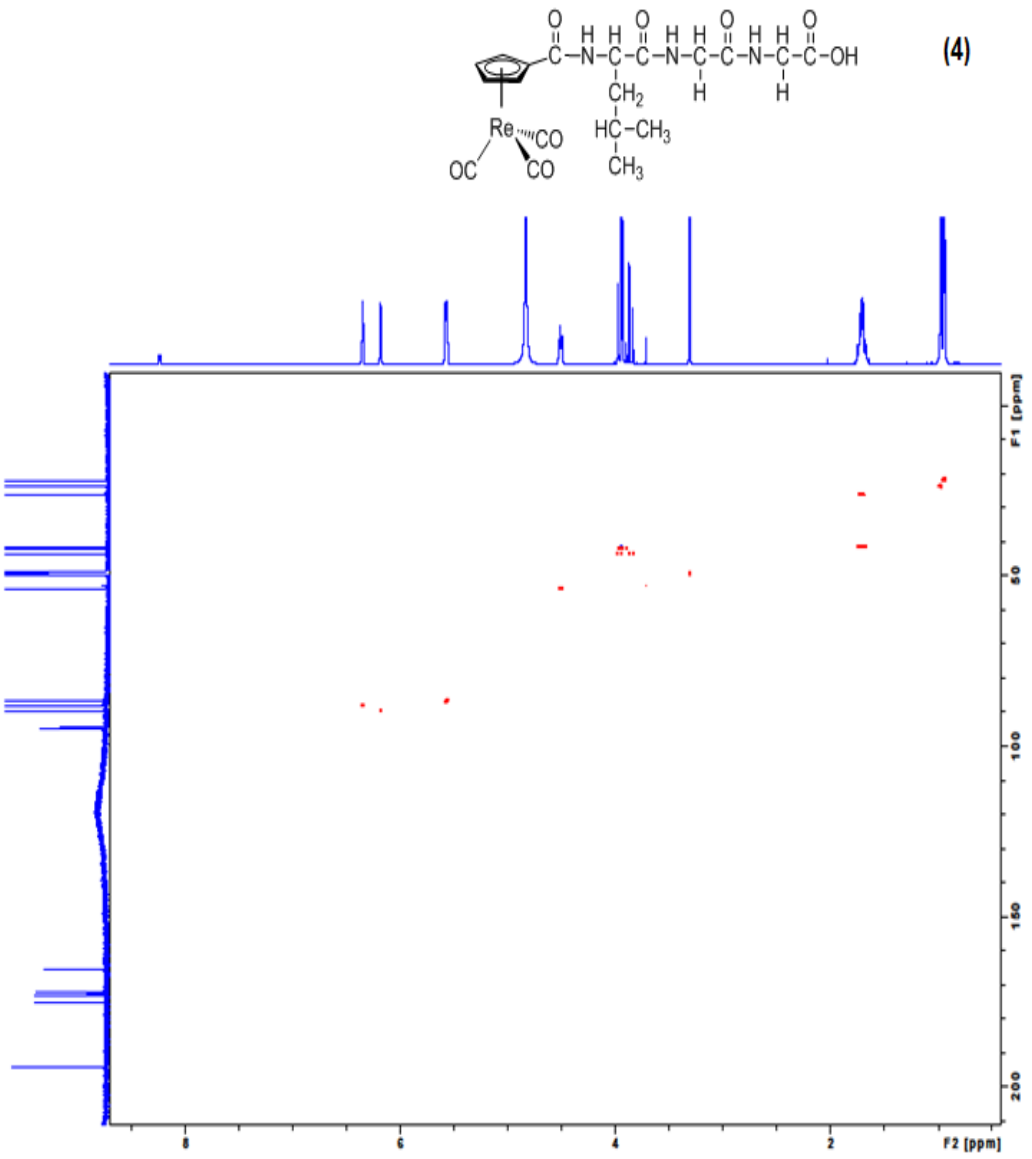
SI 5-^{1}H NMR (CD_3OD) spectra of [(CpCO-Leu-Gly-Gly-OH)Re(CO)$_3$] **4**



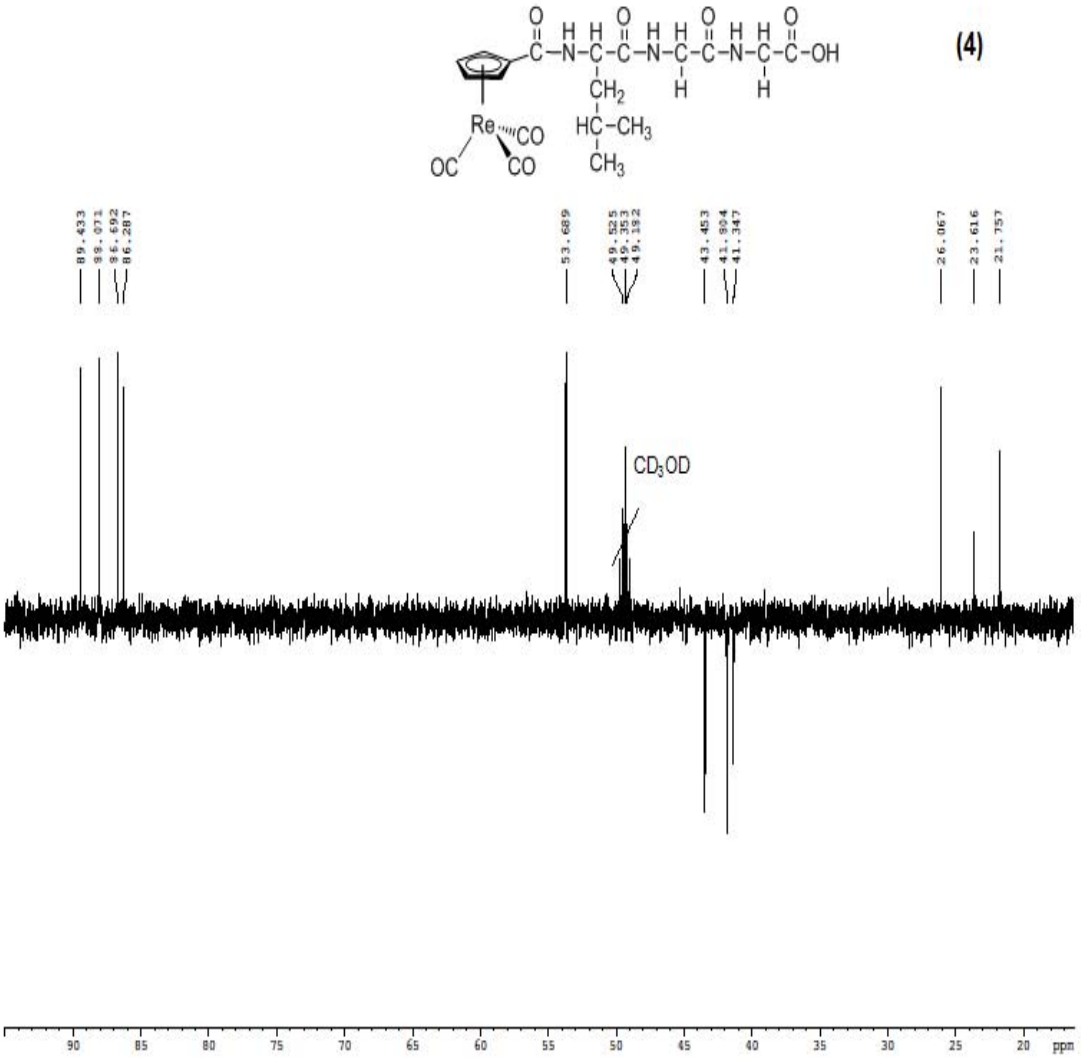
SI 6-^{13}C NMR (CD_3OD) spectra of [(CpCO-Leu-Gly-Gly-OH)Re(CO)$_3$] **4**



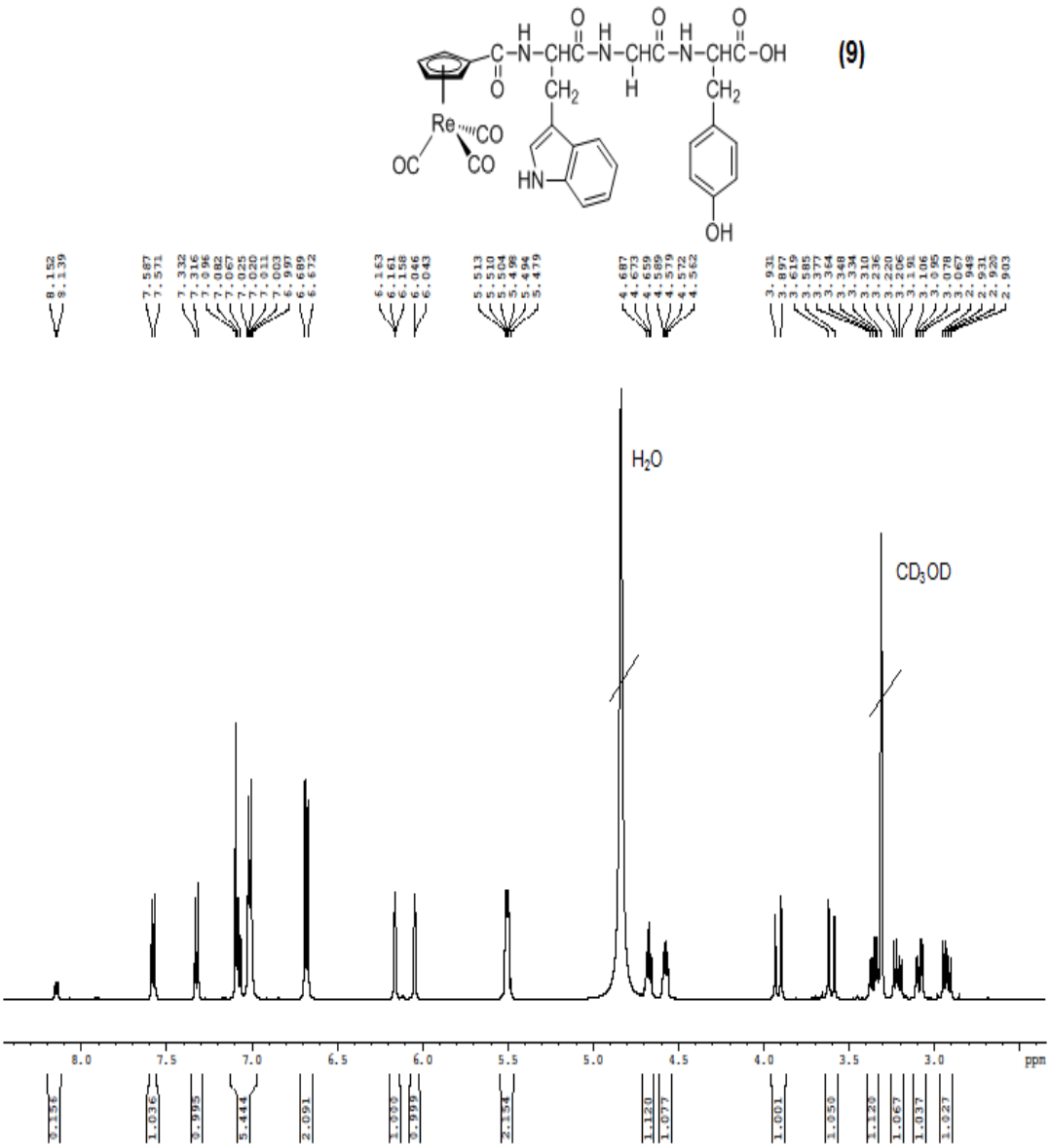
SI 7-^{13}C- ^{1}H Correlation (HSQC) (CD_3OD) spectra of [(CpCO-Leu-Gly-Gly-OH)$Re(CO)_3$] **4**



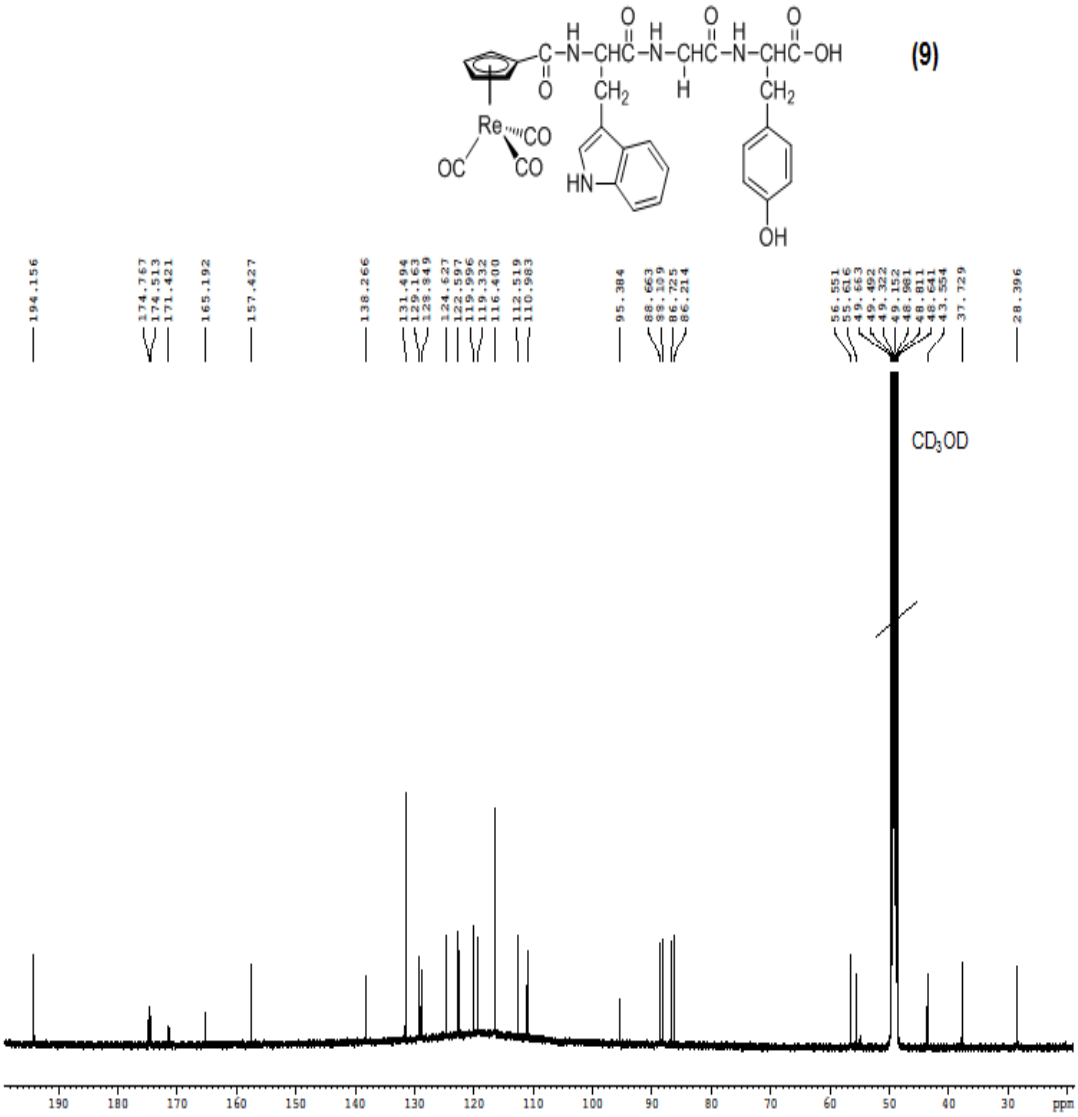
SI 8-^{13}C DEPT (CD_3OD) spectra of [(CpCO-Leu-Gly-Gly-OH)$Re(CO)_3$] **4**



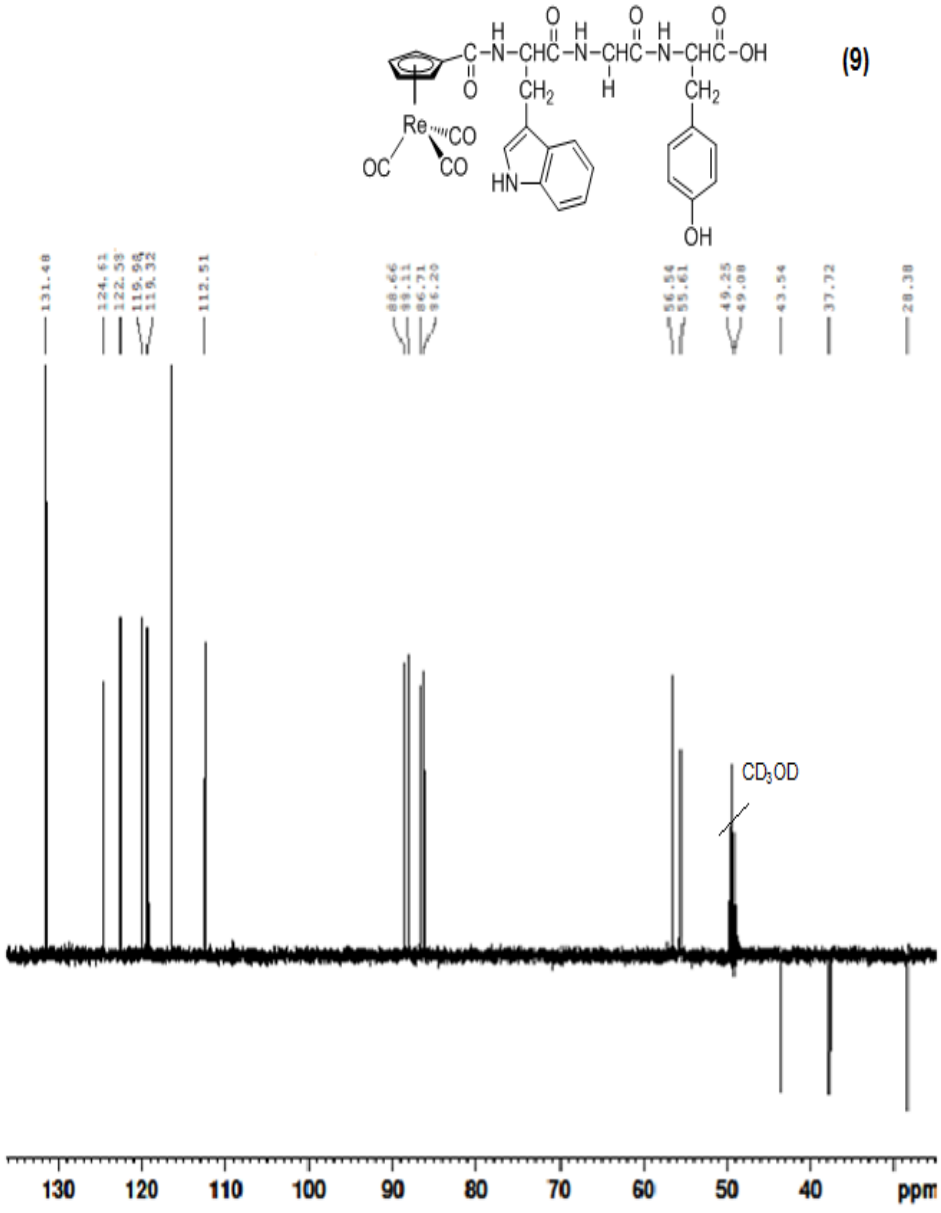
SI 9-^{1}H NMR (CD_3OD) spectra of [(CpCO-Trp-Gly-Tyr-OH)Re(CO)$_3$] **9**



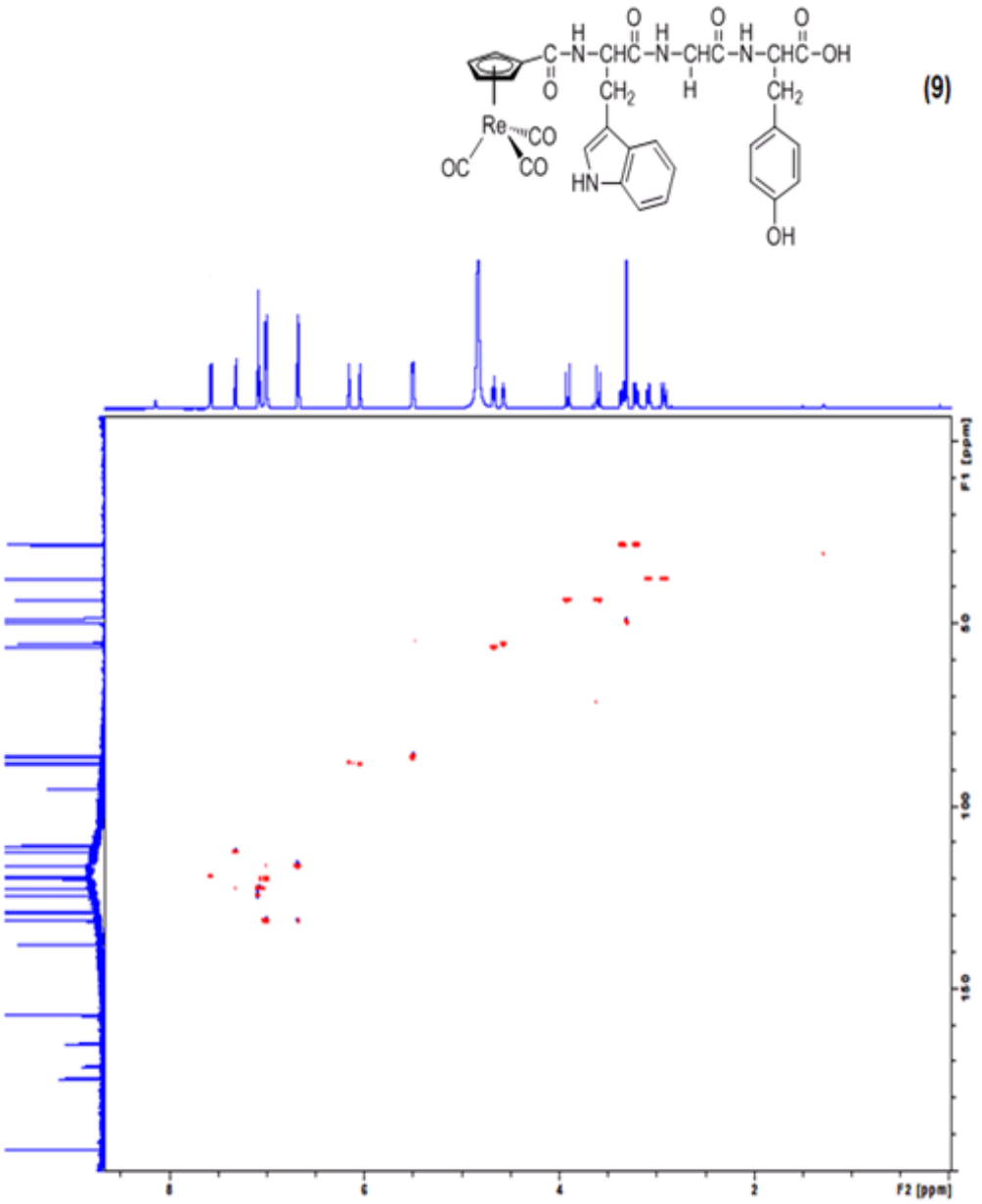
SI 10-^{13}C NMR (CD_3OD) spectra of [(CpCO-Trp-Gly-Tyr-OH)Re(CO)$_3$] **9**



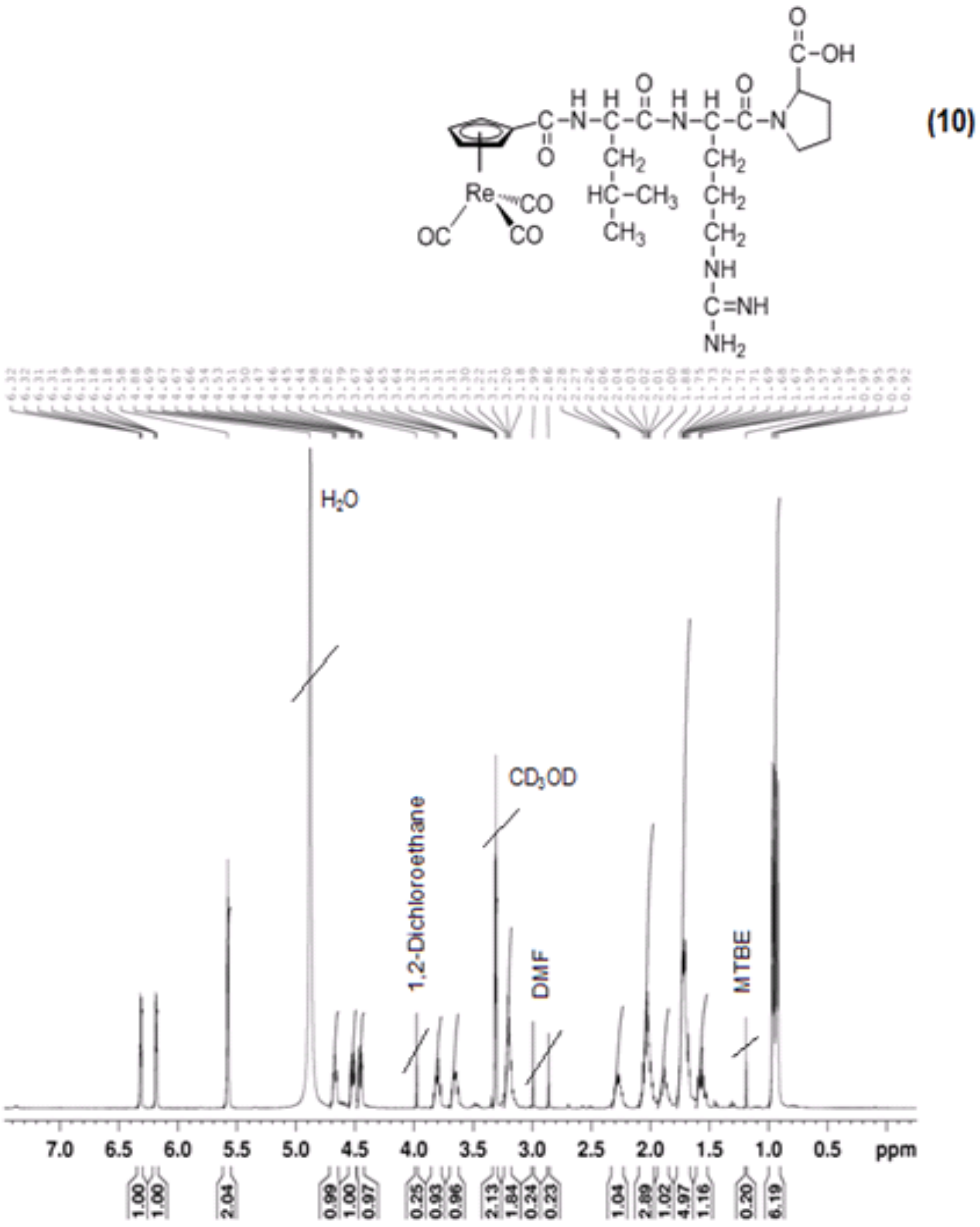
SI 11-DEPT^{13}C NMR (CD_3OD) spectra of [(CpCO-Trp-Gly-Tyr-OH)$Re(CO)_3$] **9**



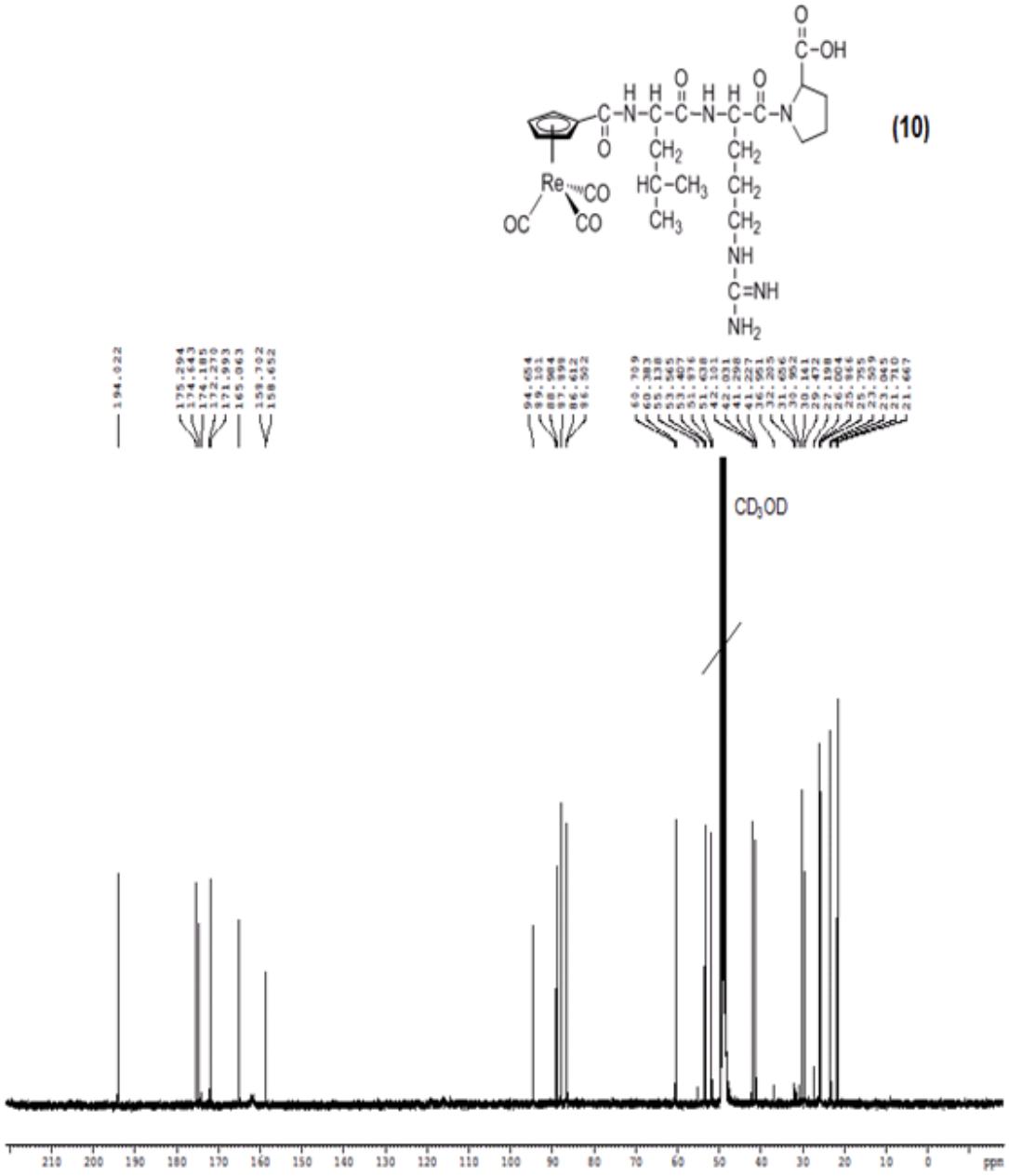
SI 12-^{13}C- ^{1}H Correlation (HSQC) (CD_3OD) spectra of [(CpCO-Trp-Gly-Tyr-OH)$Re(CO)_3$] **9**



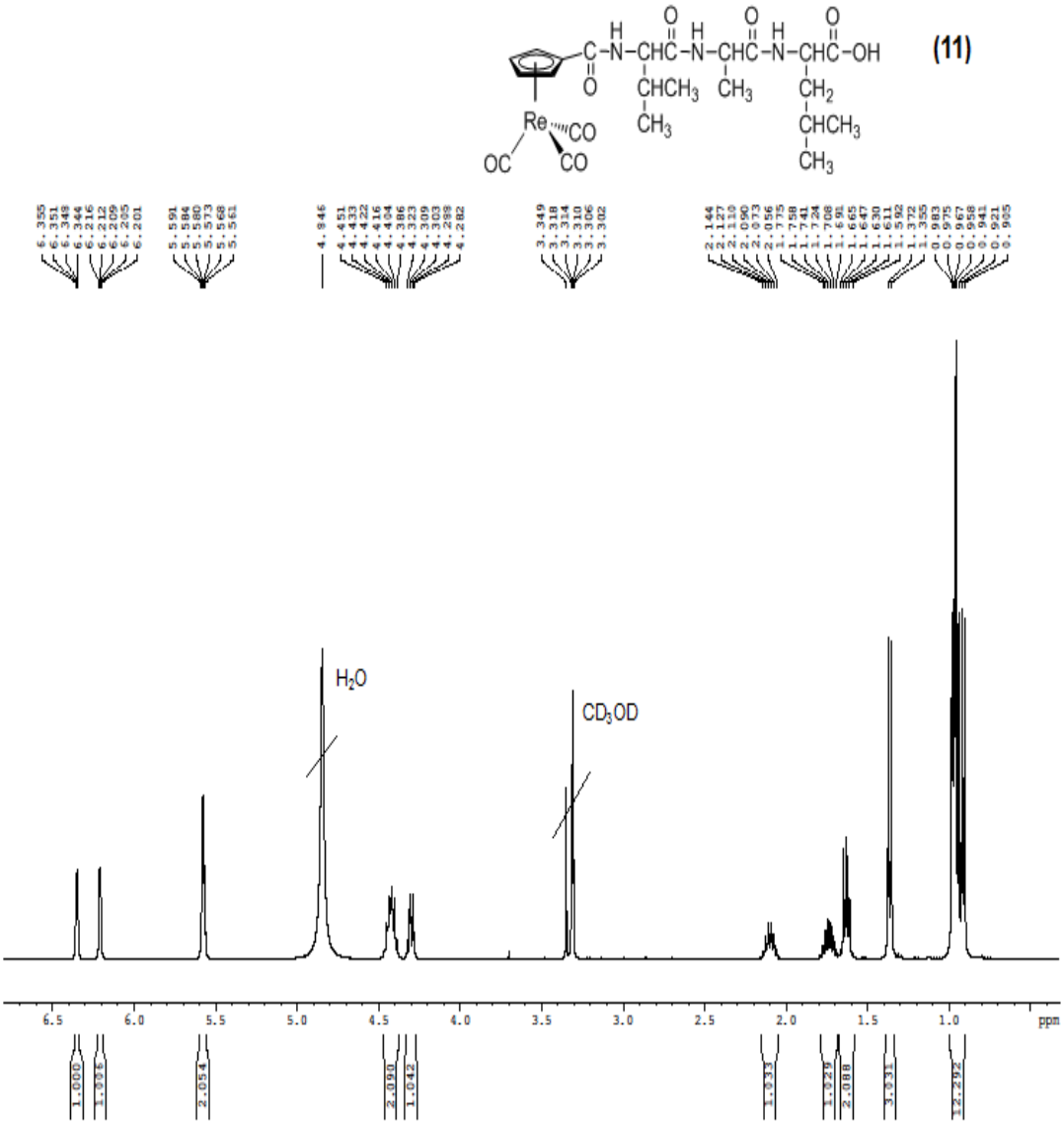
SI 13-^{1}H NMR (CD_3OD) spectra of [(CpCO-Leu-Arg-Pro-OH)$Re(CO)_3$] **10**



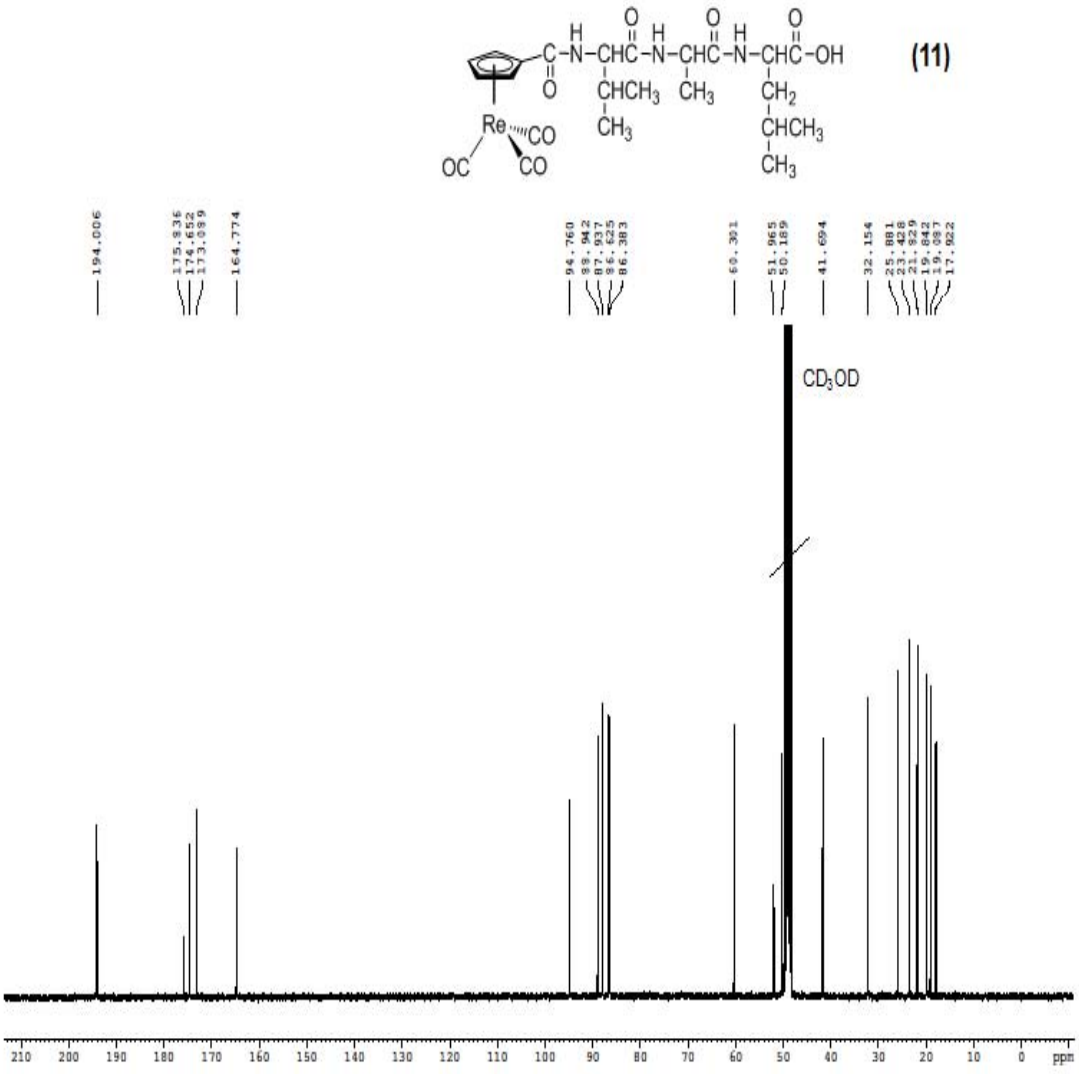
SI 14-^{13}C NMR (CD_3OD) spectra of [(CpCO-Leu-Arg-Pro-OH)Re(CO)$_3$] **10**



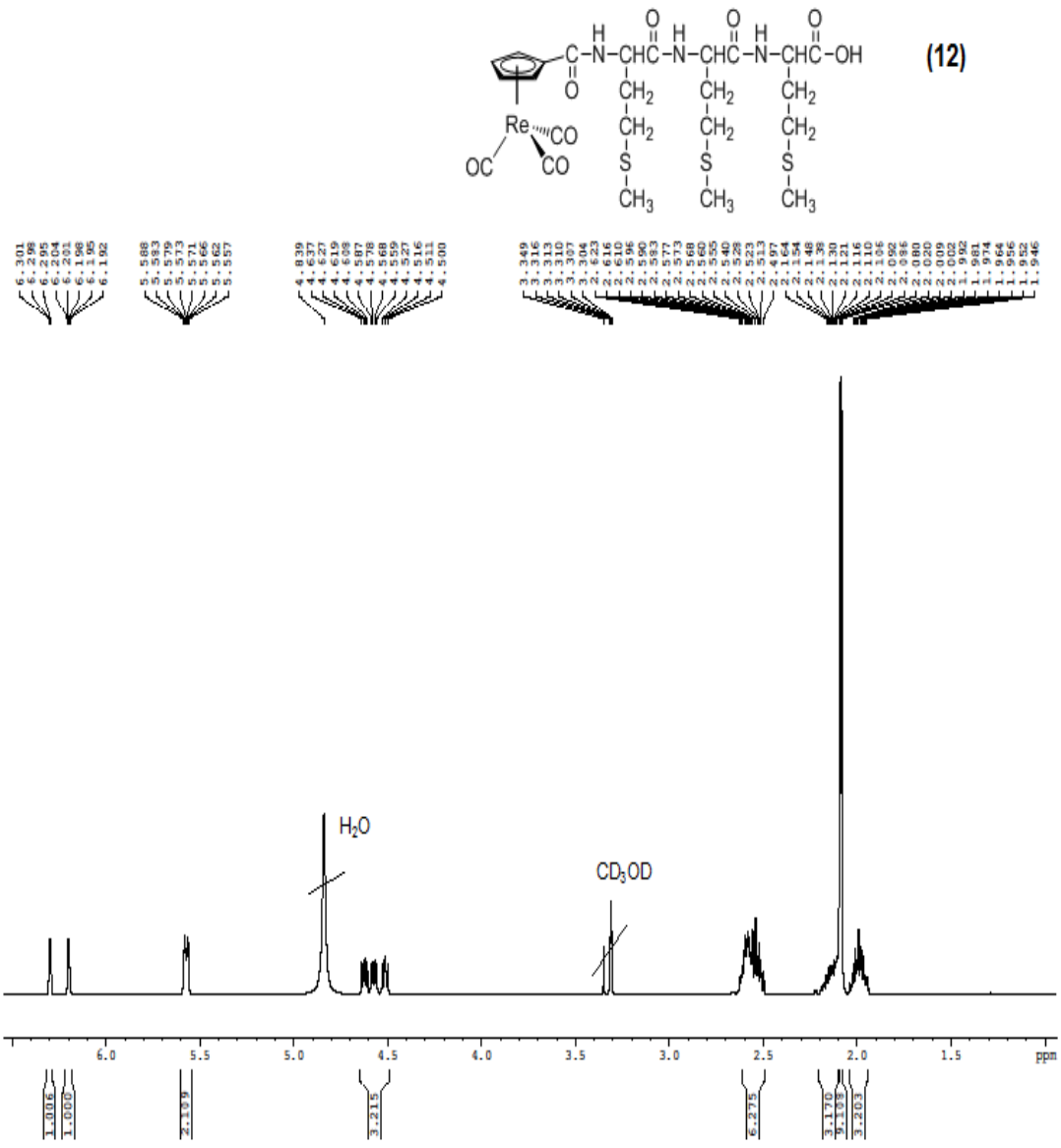
SI 15-^{1}H NMR (CD_3OD) spectra of [(CpCO-Val-Ala-Leu-OH)Re(CO)$_3$] **11**



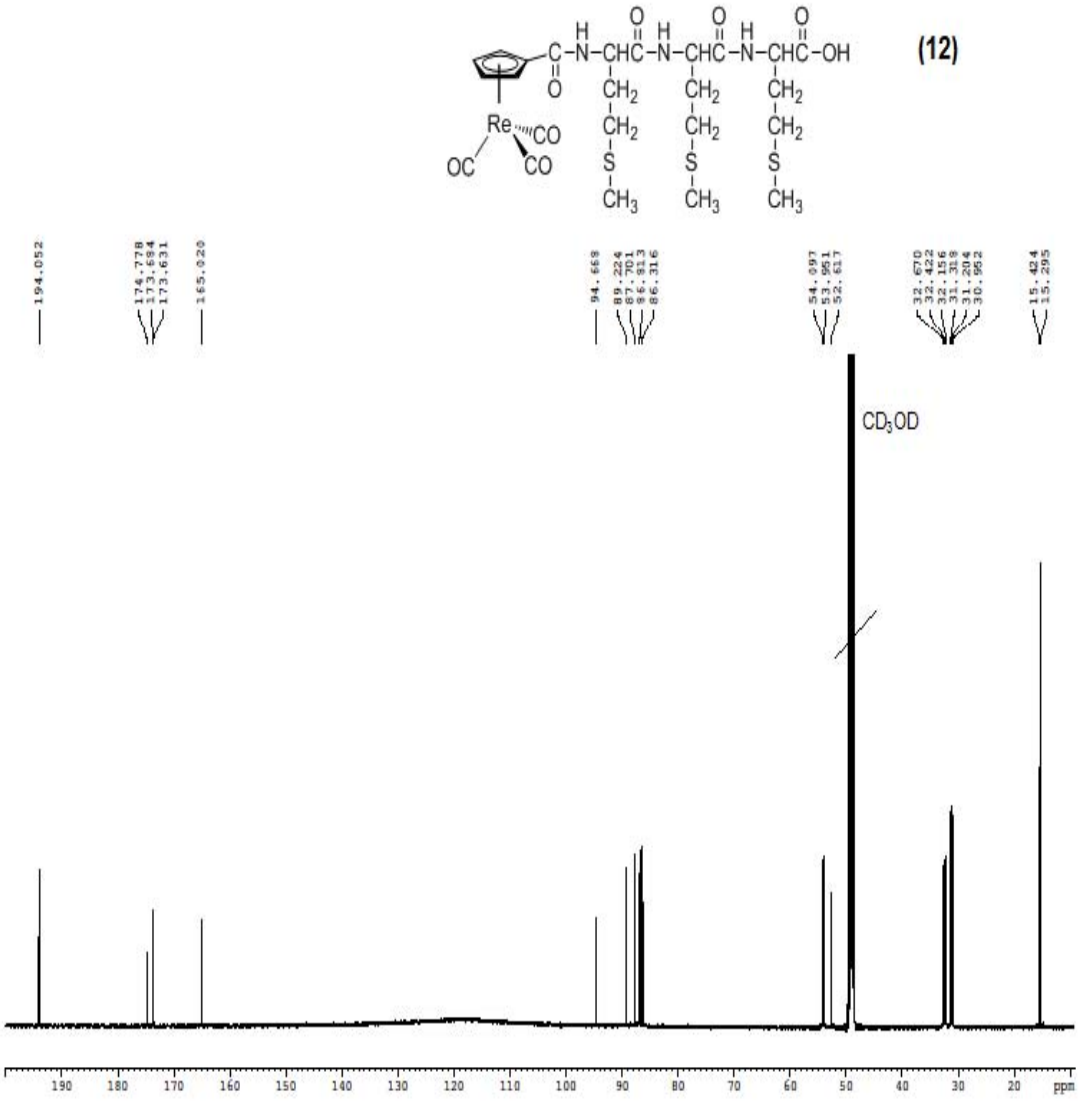
SI 16-^{13}C NMR (CD_3OD) spectra of [(CpCO-Val-Ala-Leu-OH)Re(CO)$_3$] **11**



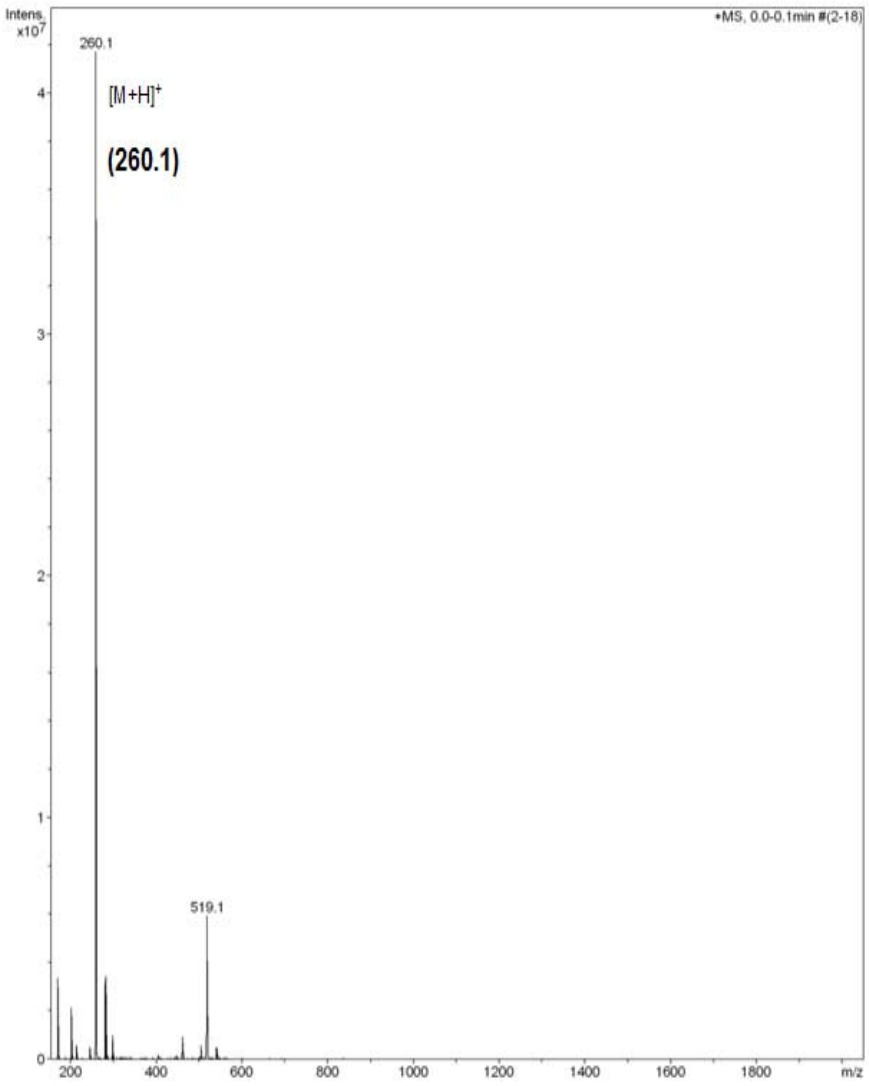
SI 17-^{1}H NMR (CD_3OD) spectra of [(CpCO-Met-Met-Met-OH)Re(CO)$_3$] **12**



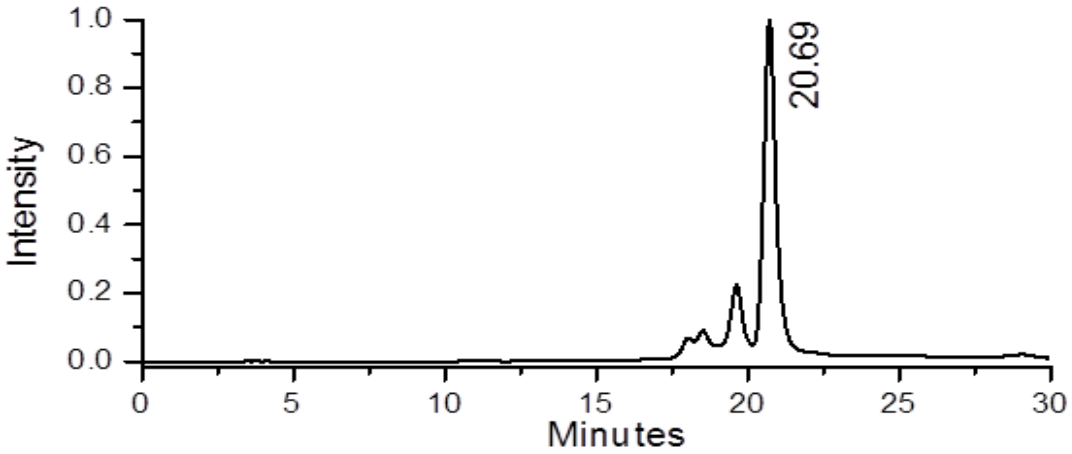
SI 18-^{13}C NMR (CD_3OD) spectra of [(CpCO-Met-Met-Met-OH)Re(CO)$_3$] **12**



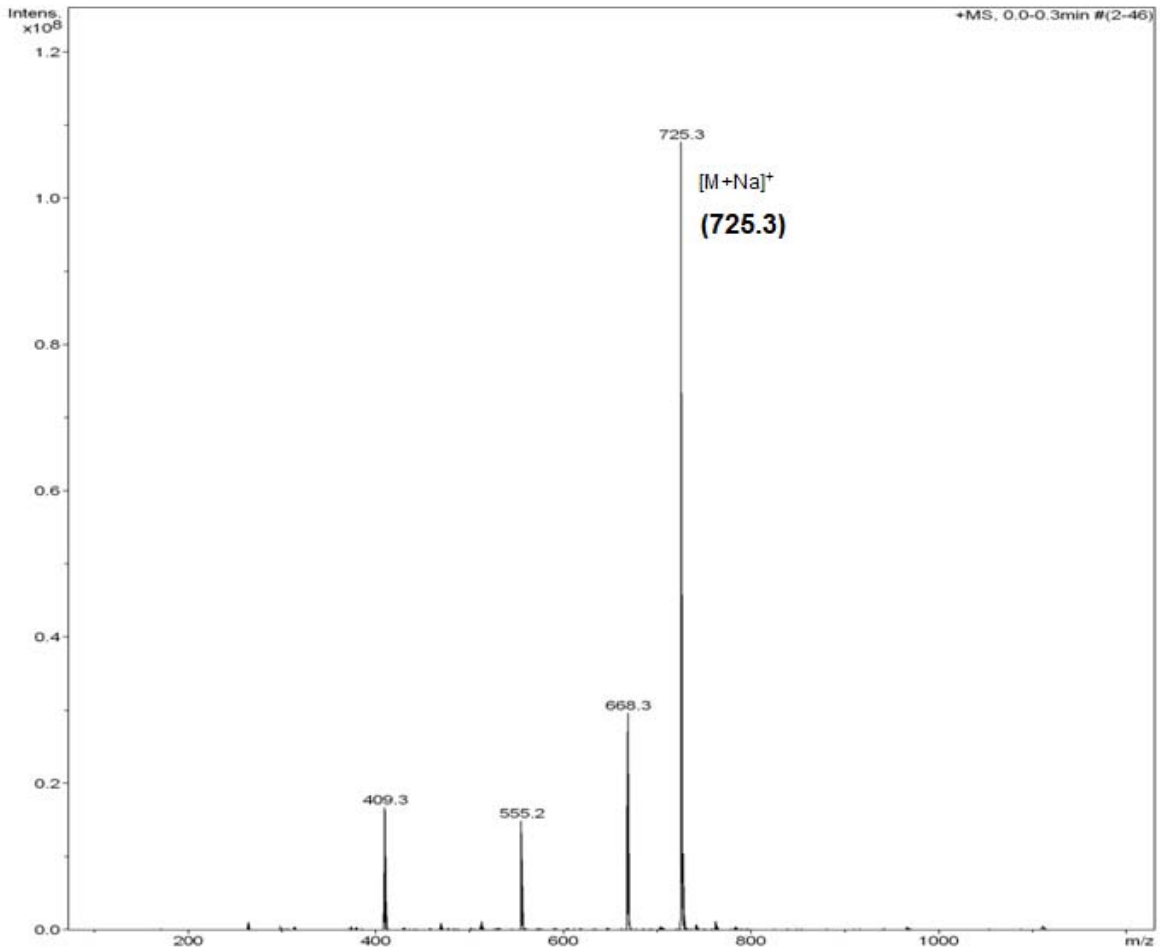
SI 19-MS(ESI) of compound **1**



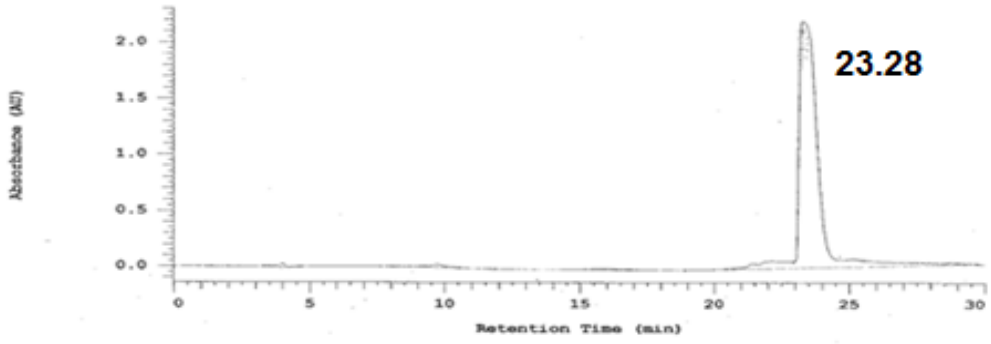
SI 20-HPLC trace (UV) of compound **2**



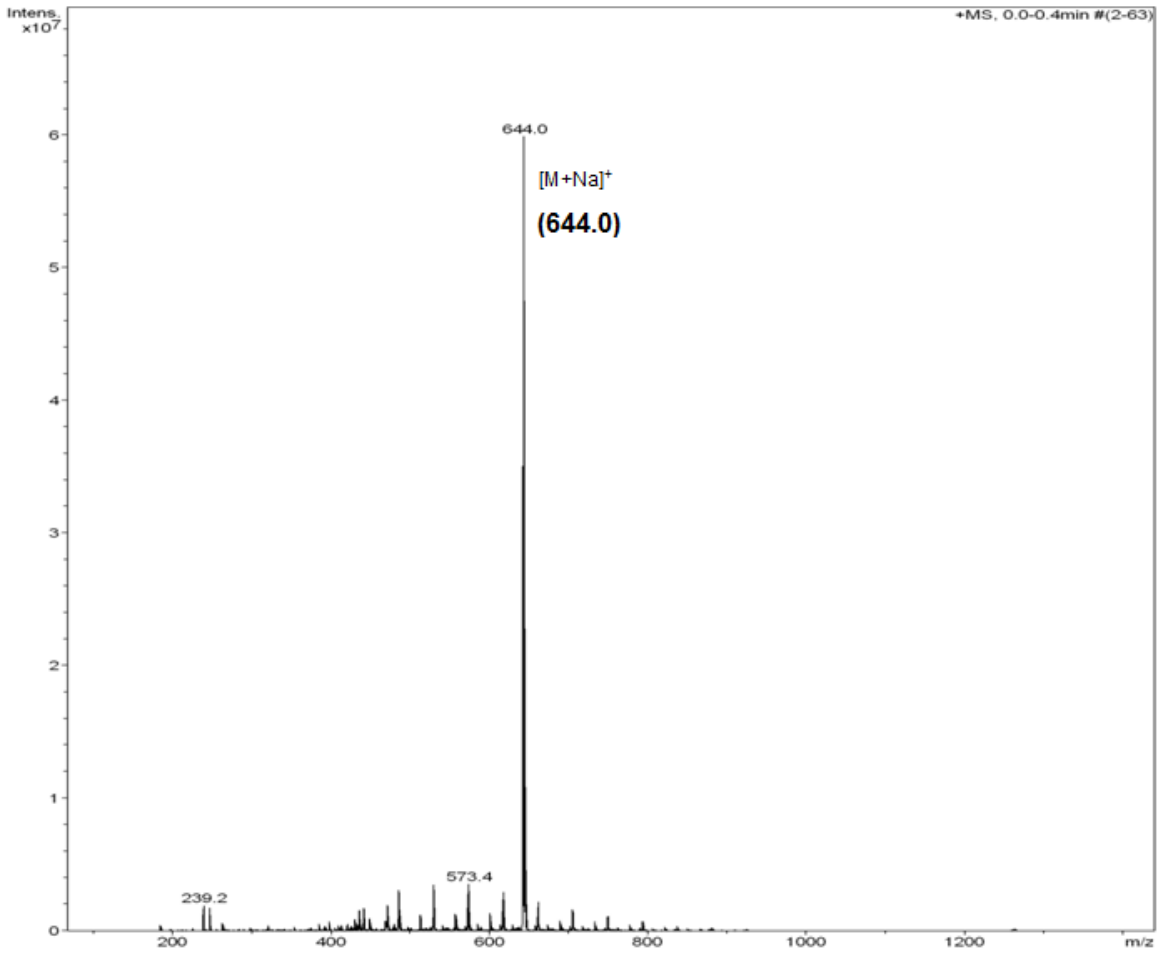
SI 21-MS(ESI) of compound **2**



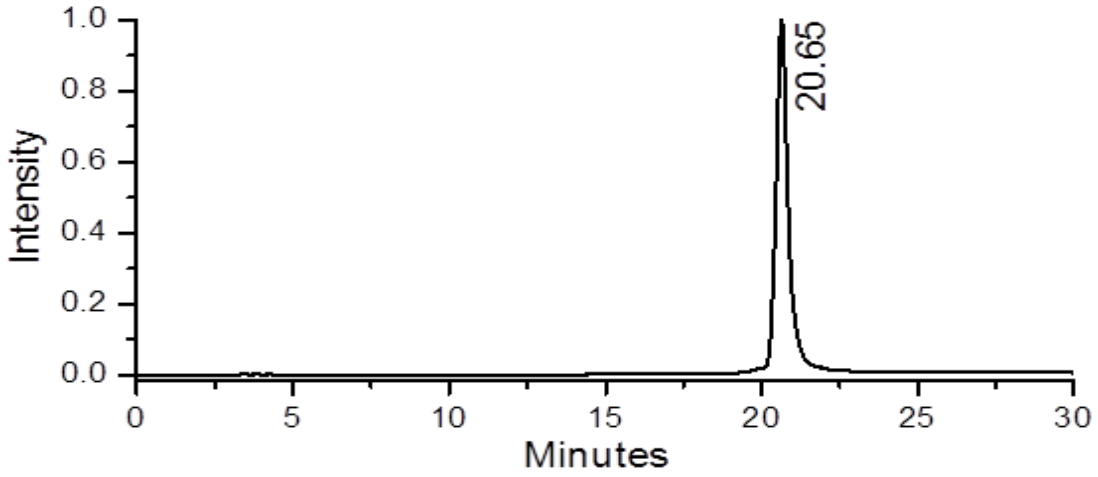
SI 22-HPLC trace (UV) of compound **3**



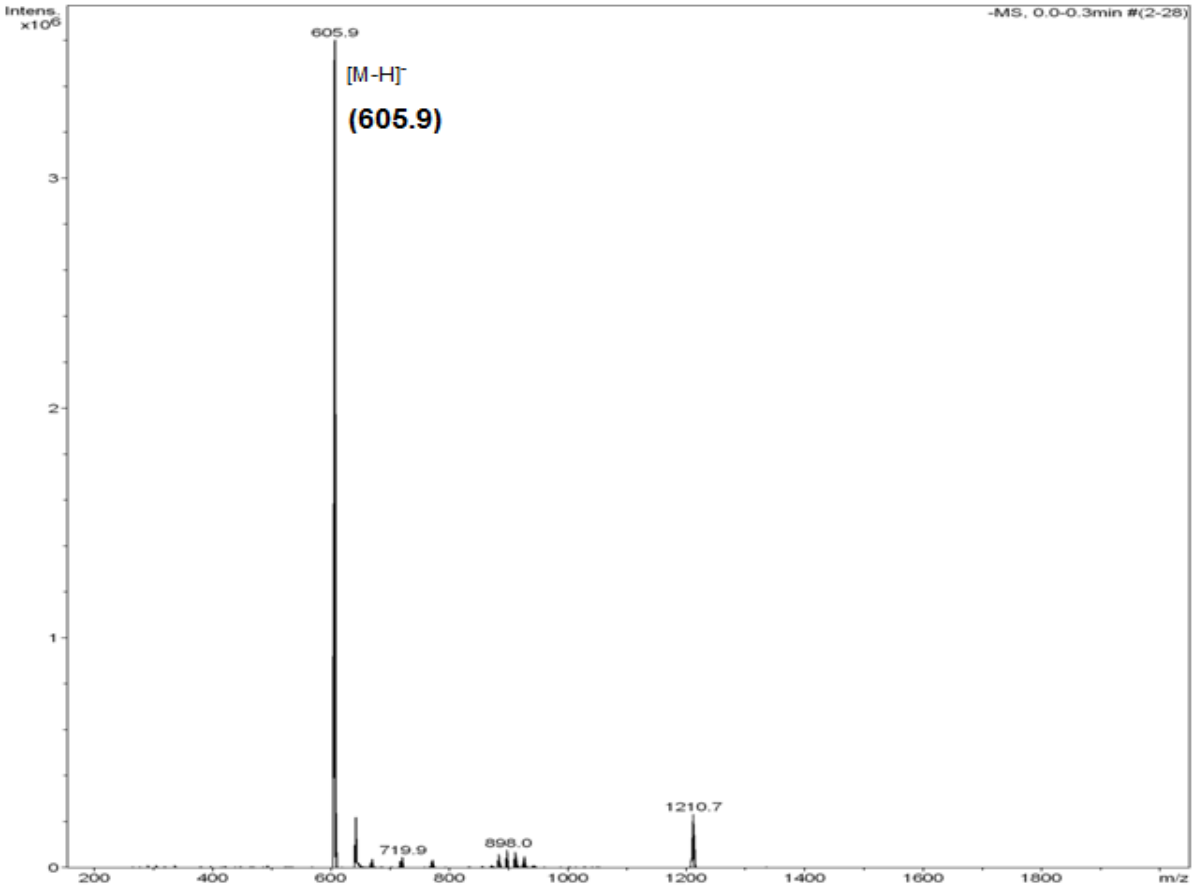
SI 23-MS(ESI) of compound **3**



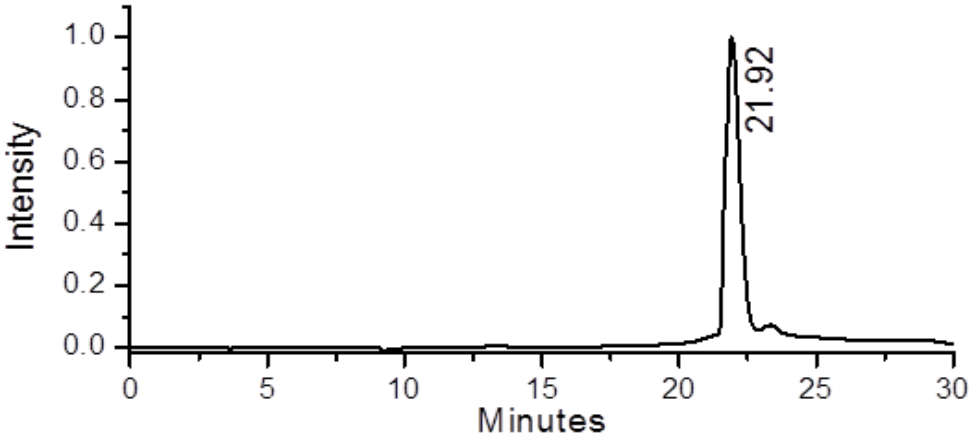
SI 24-HPLC trace (UV) of compound **4**



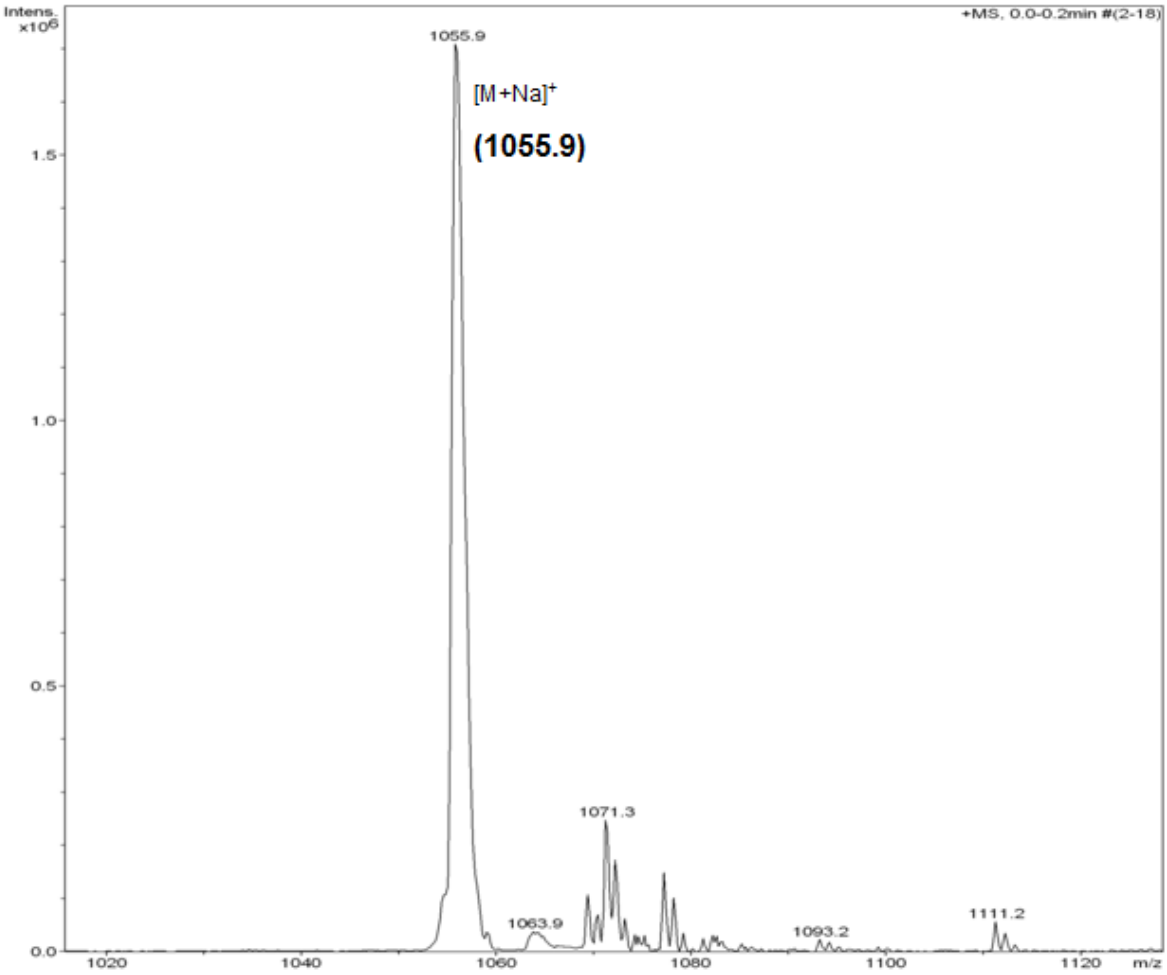
SI 25-MS(ESI) of compound **4**



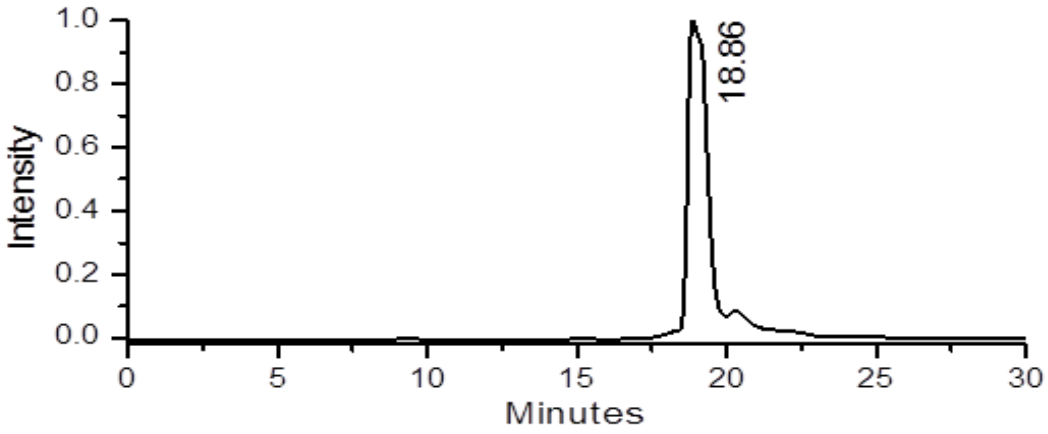
SI 26-HPLC trace (UV) of compound **5**



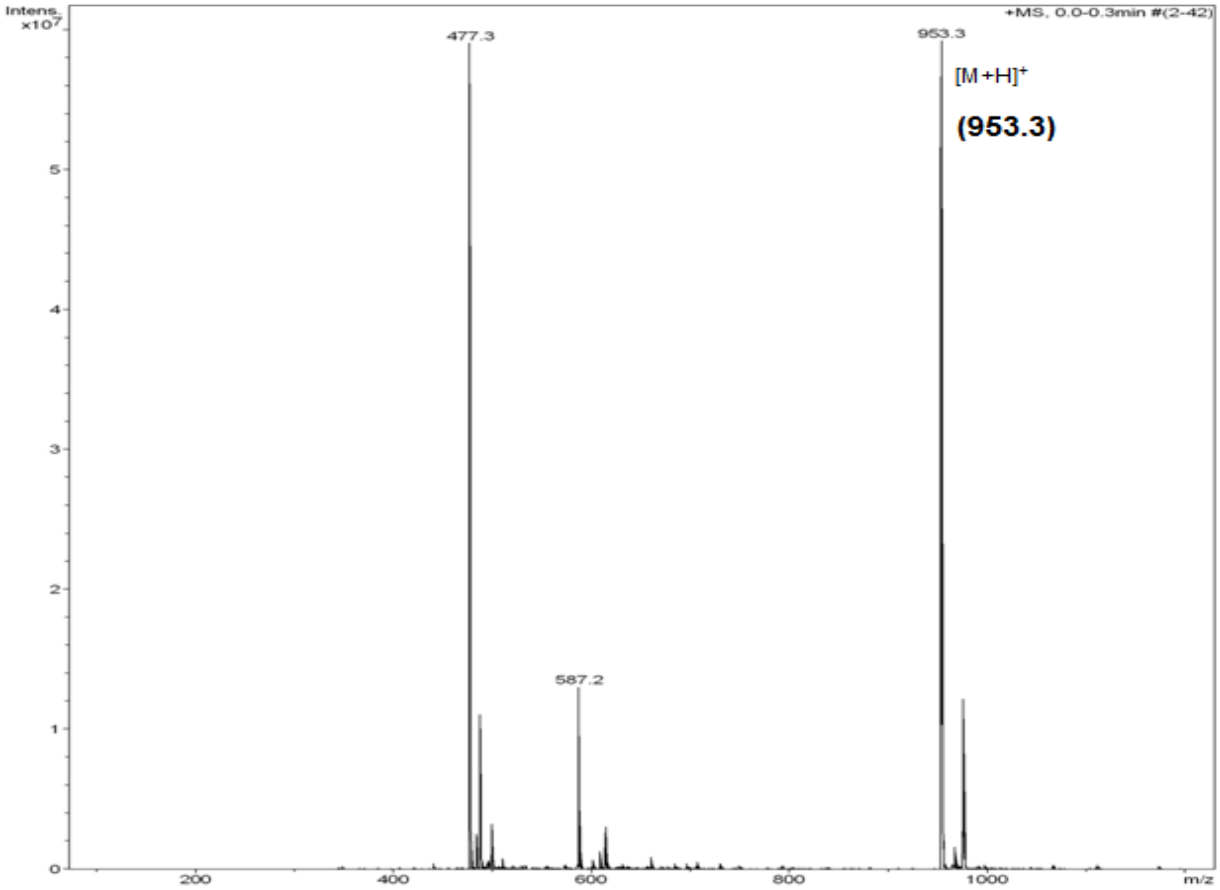
SI 27-MS(ESI) of compound **5**



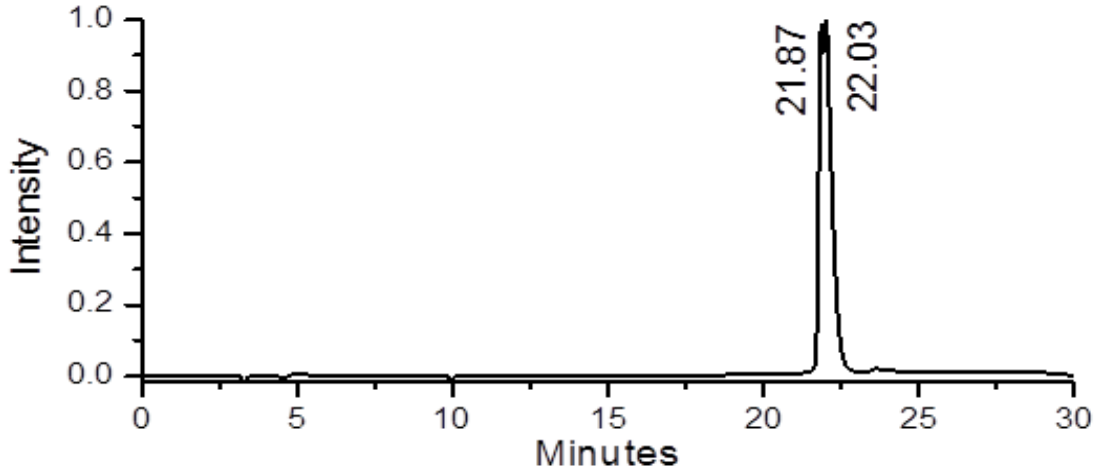
SI 28-HPLC trace (UV) of compound **6**



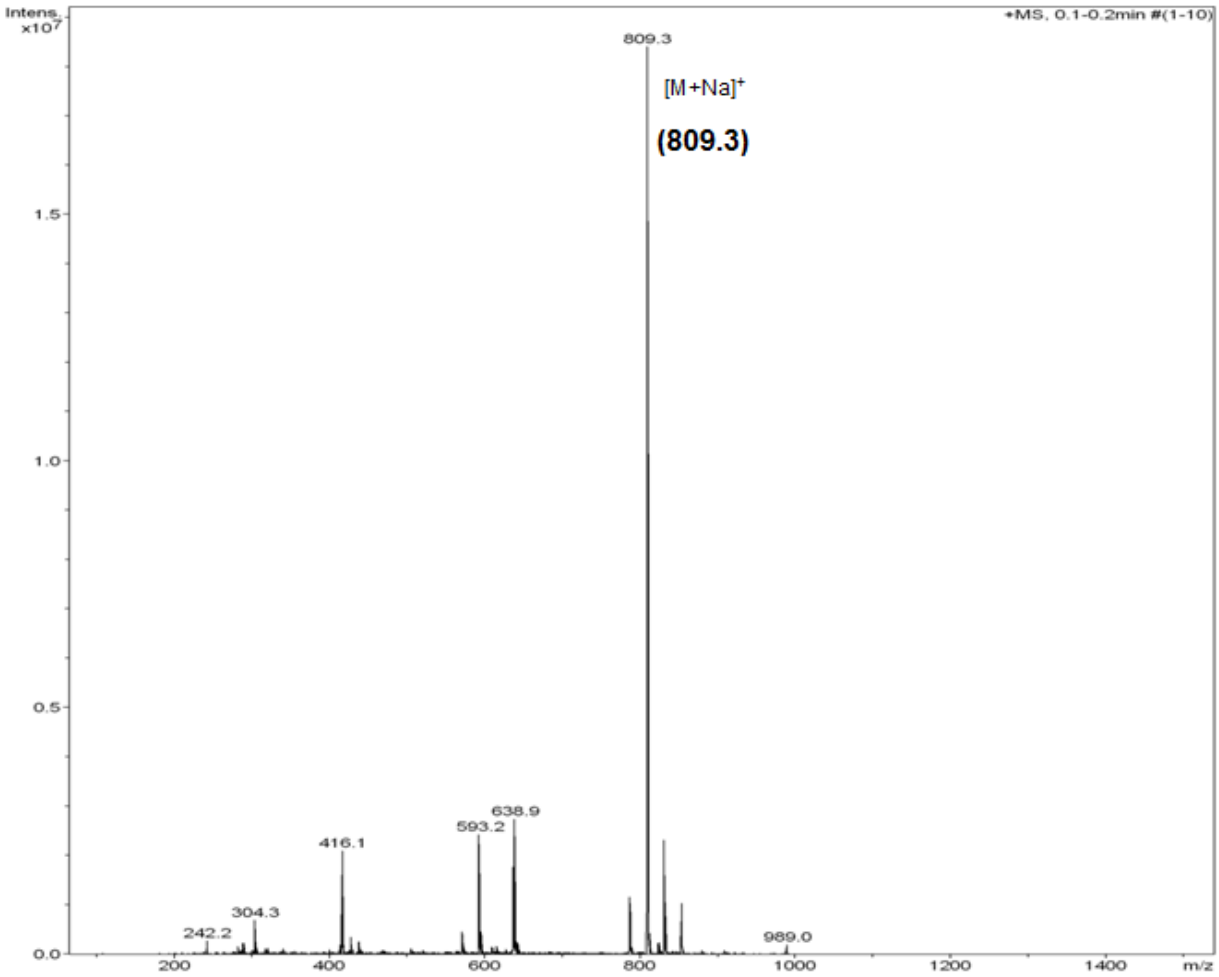
SI 29-MS(ESI) of compound **6**



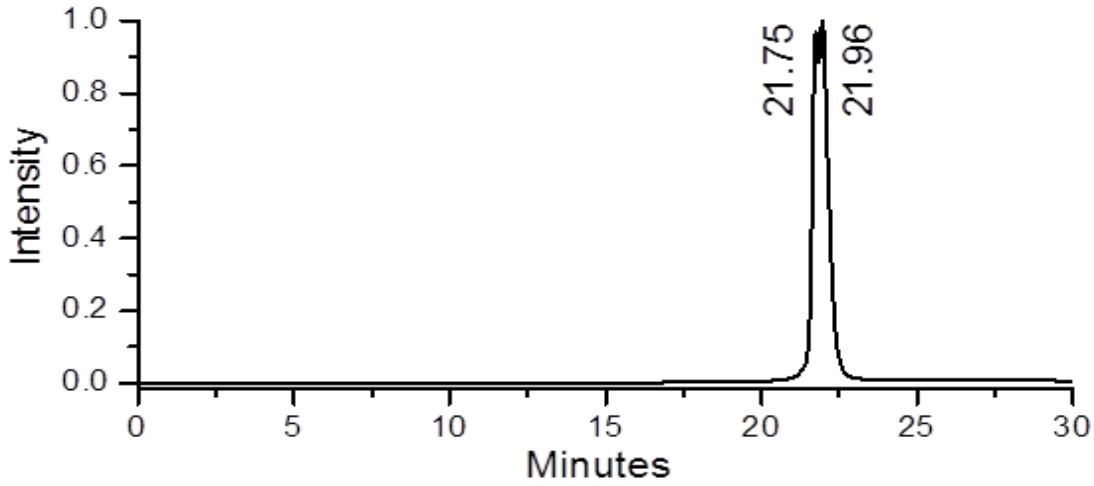
SI 30-HPLC trace (UV) of compound **7**



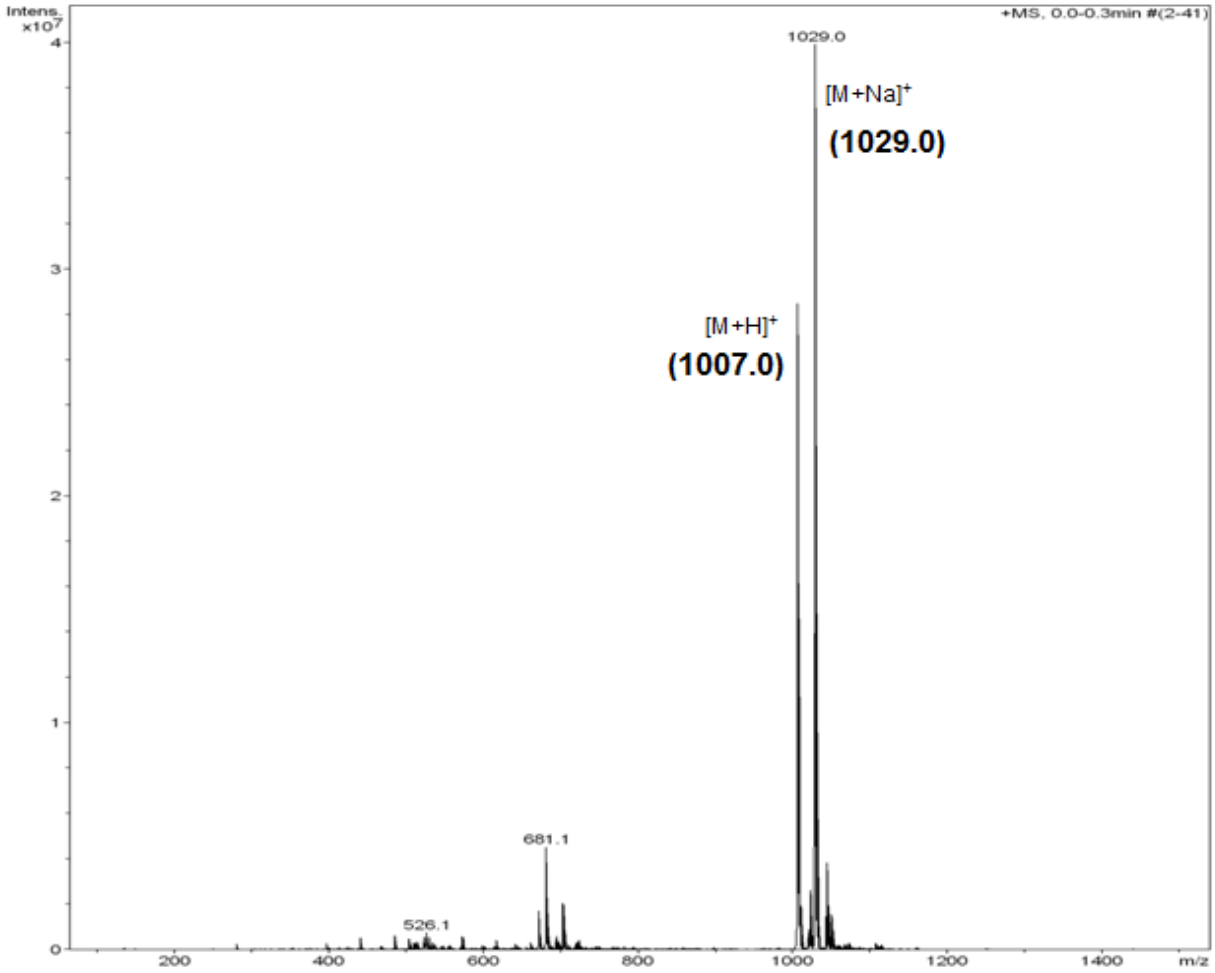
SI 31-MS(ESI) of compound **7**



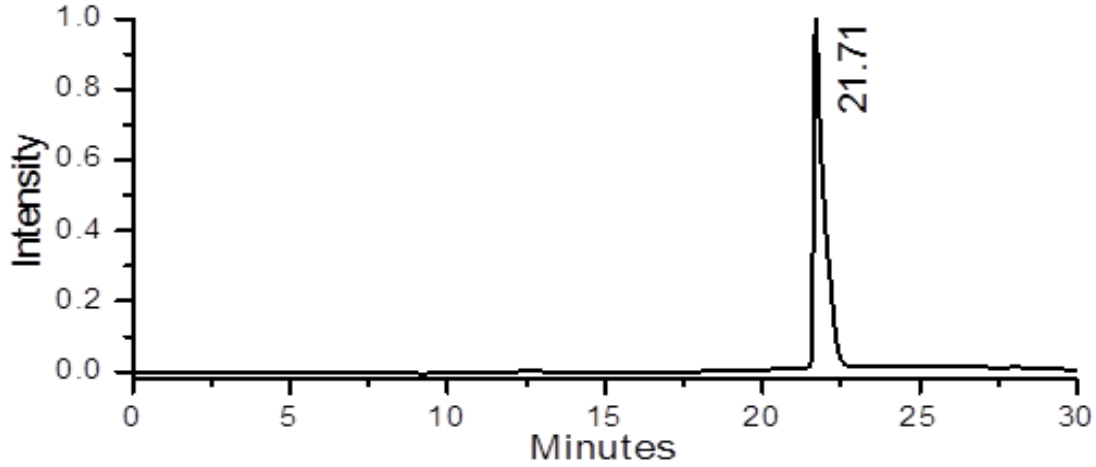
SI 32-HPLC trace (UV) of compound **8**



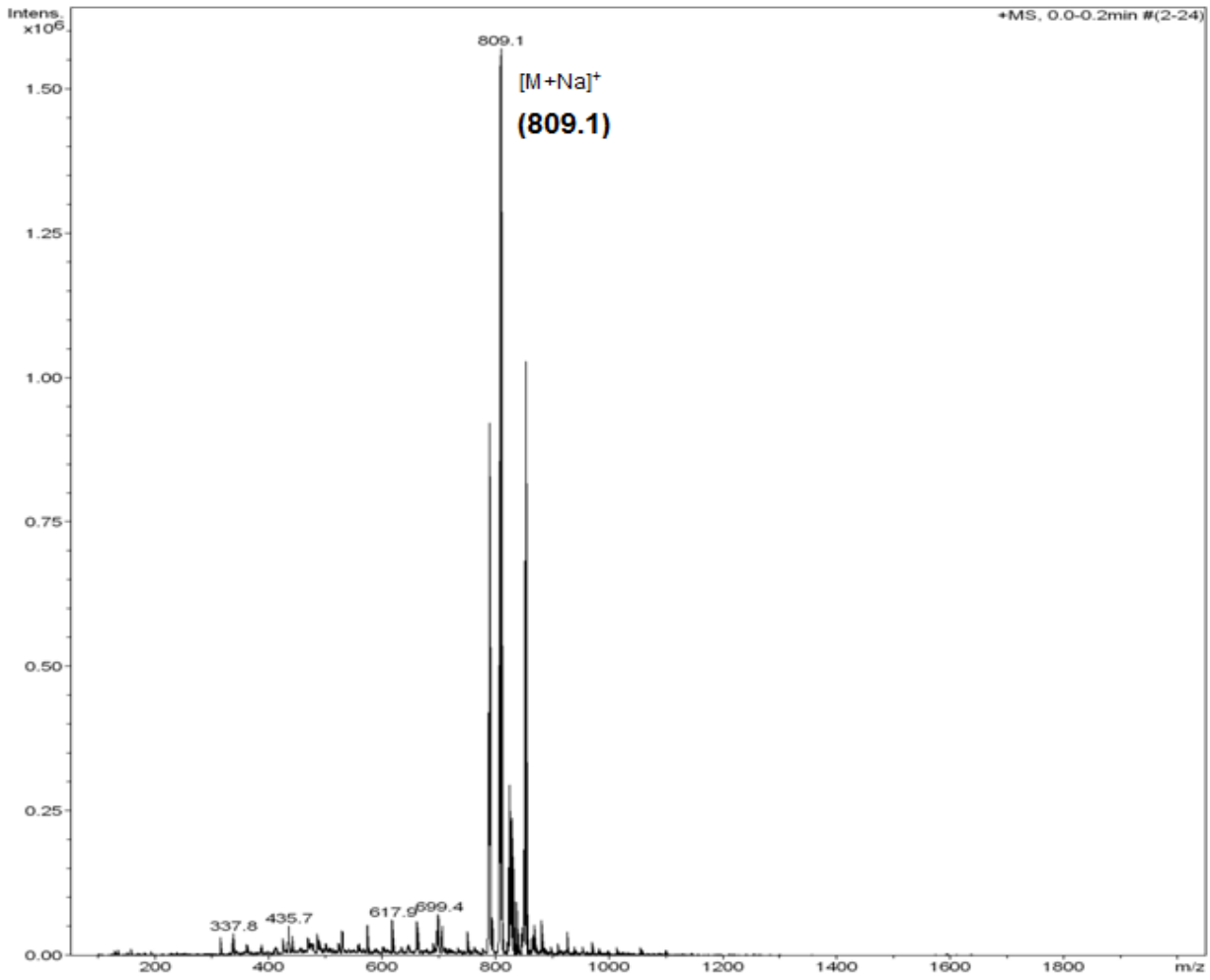
SI 33-MS(ESI) of compound **8**



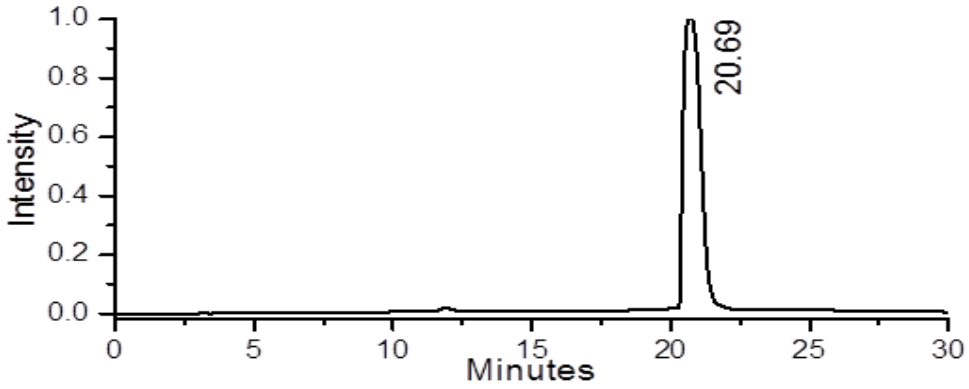
SI 34-HPLC trace (UV) of compound **9**



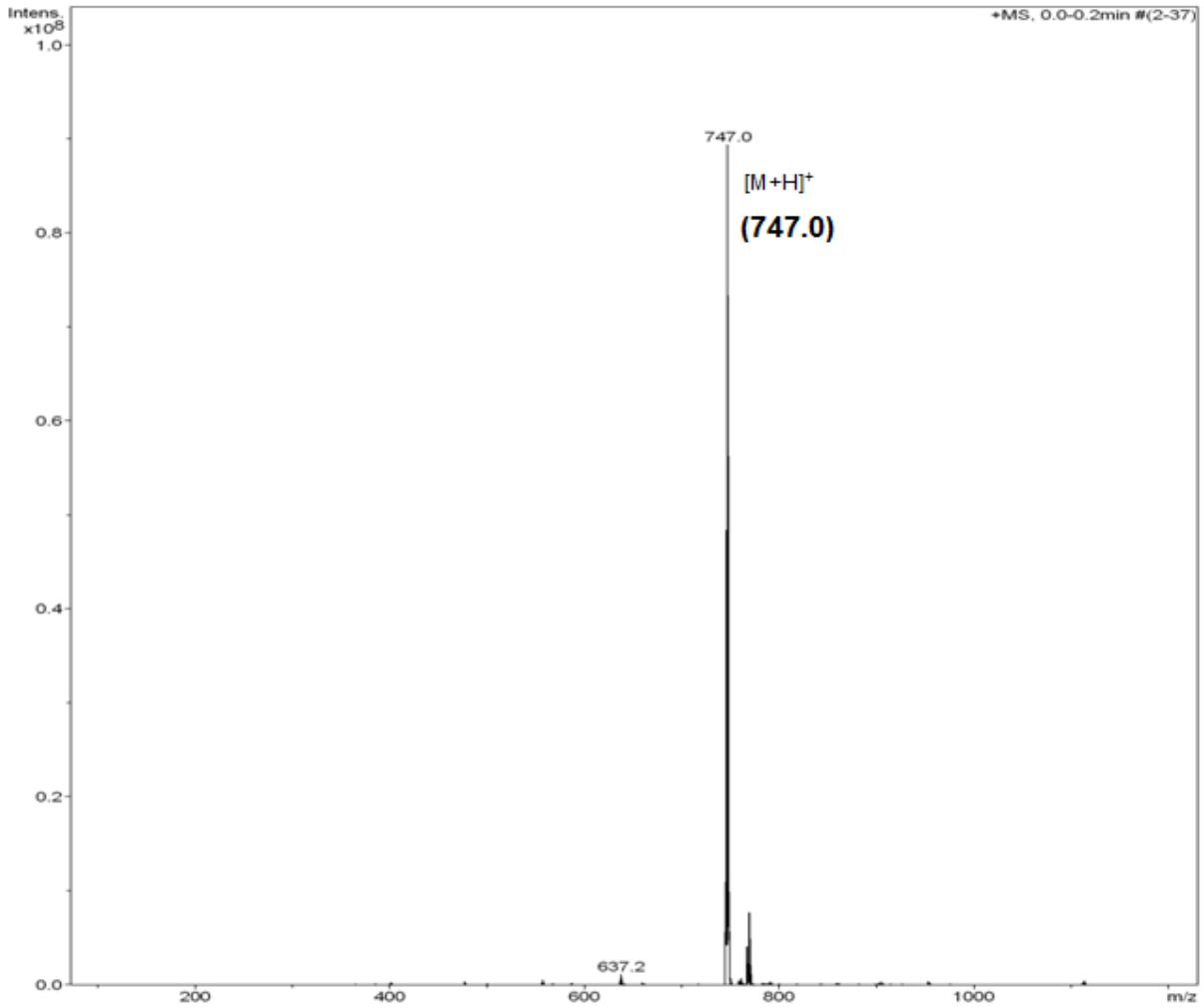
SI 35-MS(ESI) of compound **9**



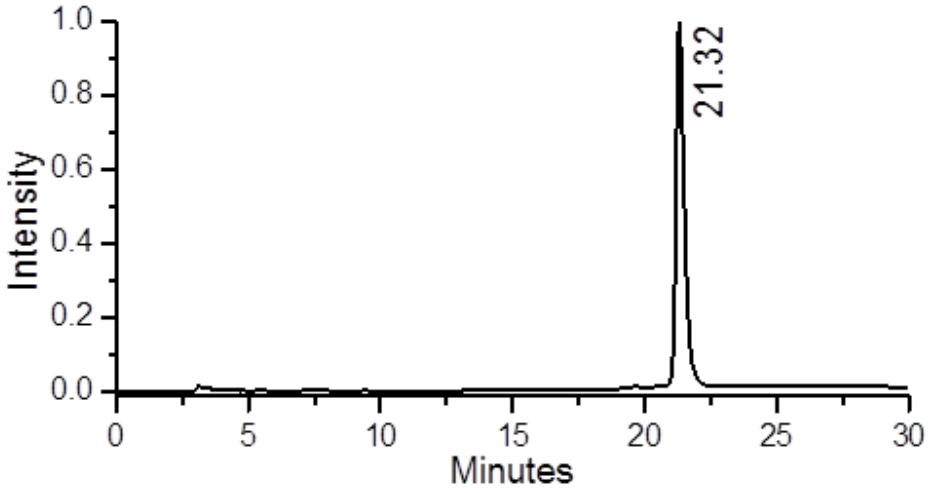
SI 36-HPLC trace (UV) of compound **10**



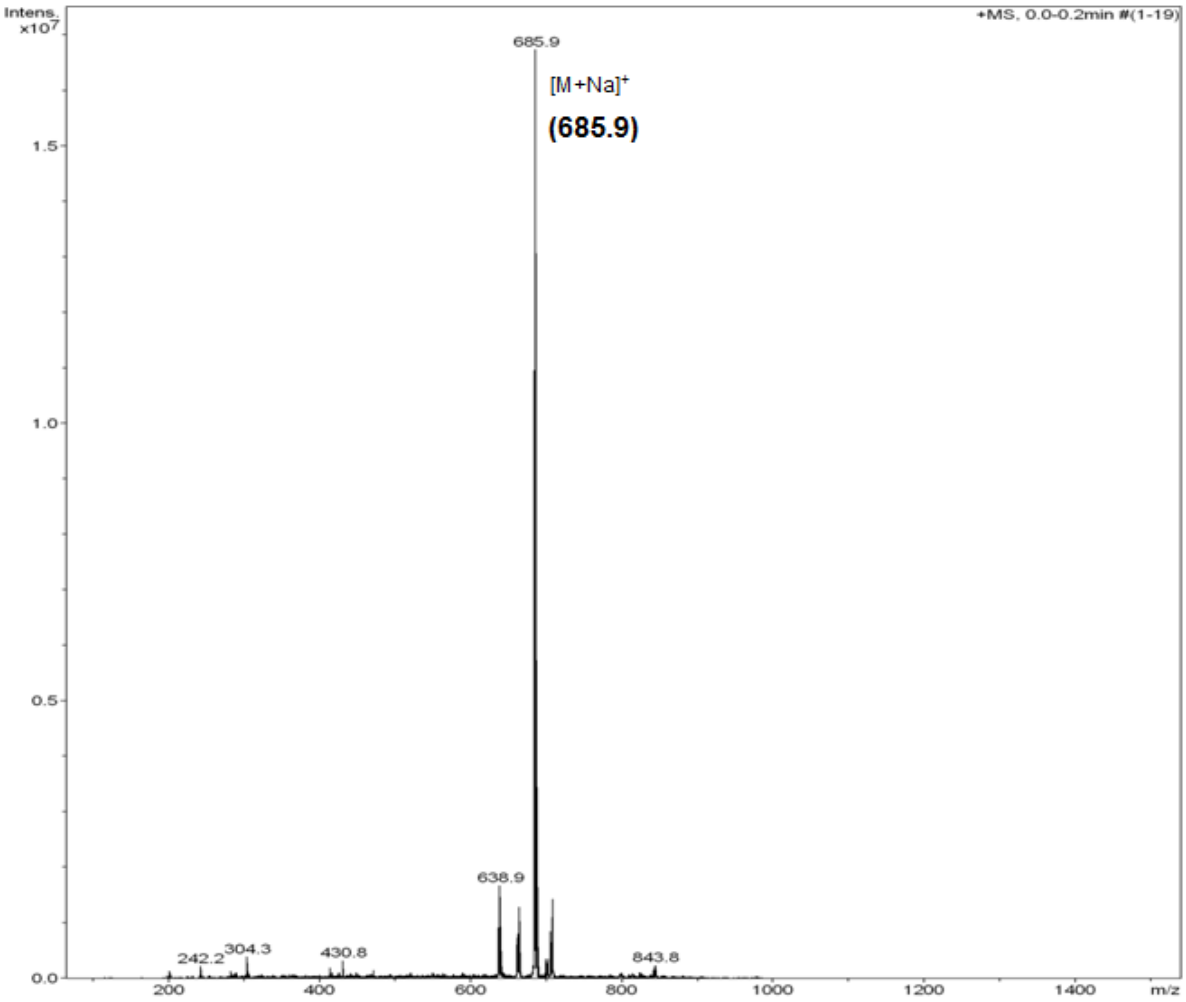
SI 37-MS(ESI) of compound **10**



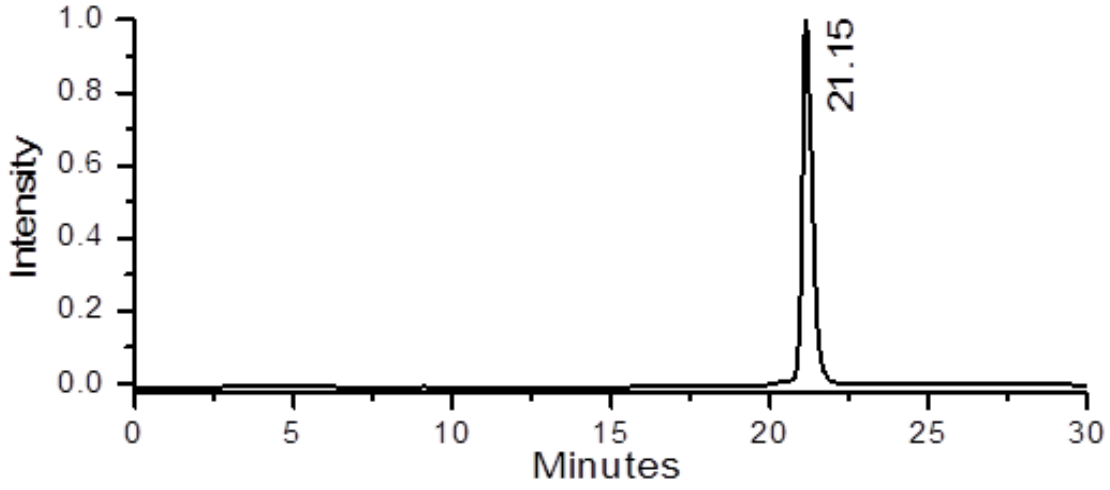
SI 38-HPLC trace (UV) of compound **11**



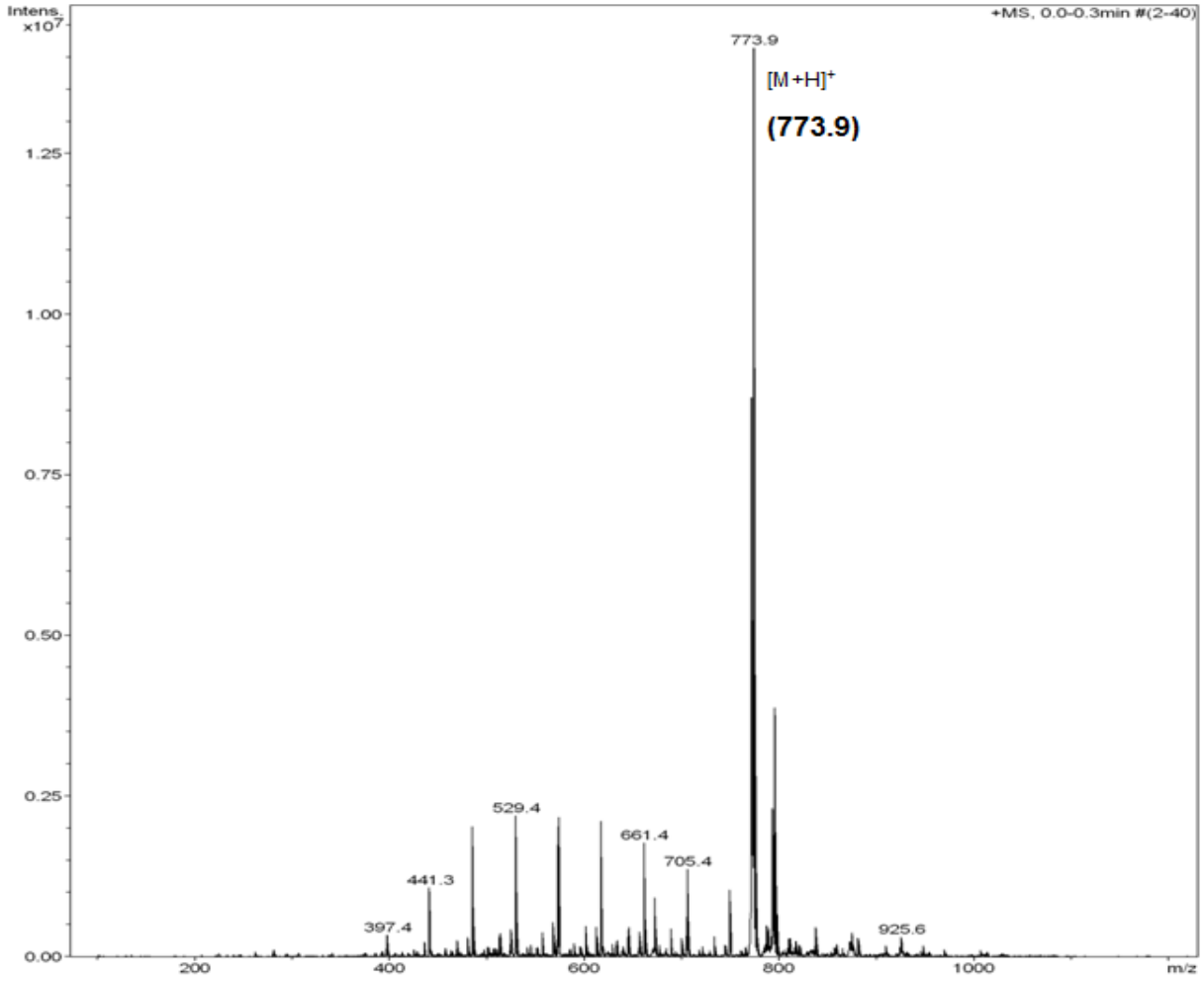
SI 39-MS(ESI) of compound **11**



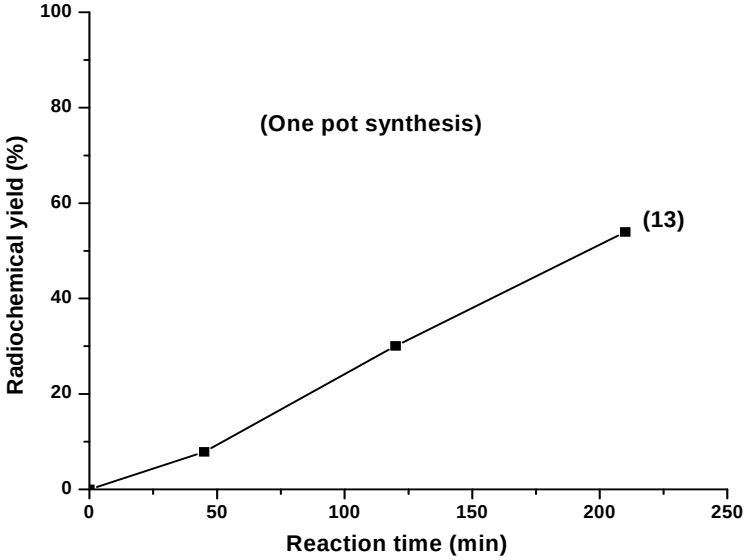
SI 40-HPLC trace (UV) of compound **12**



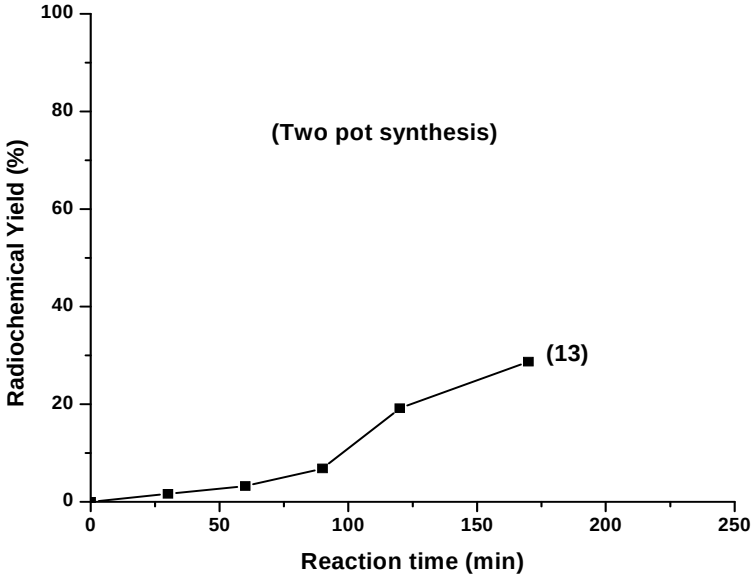
SI 41-MS(ESI) of compound **12**



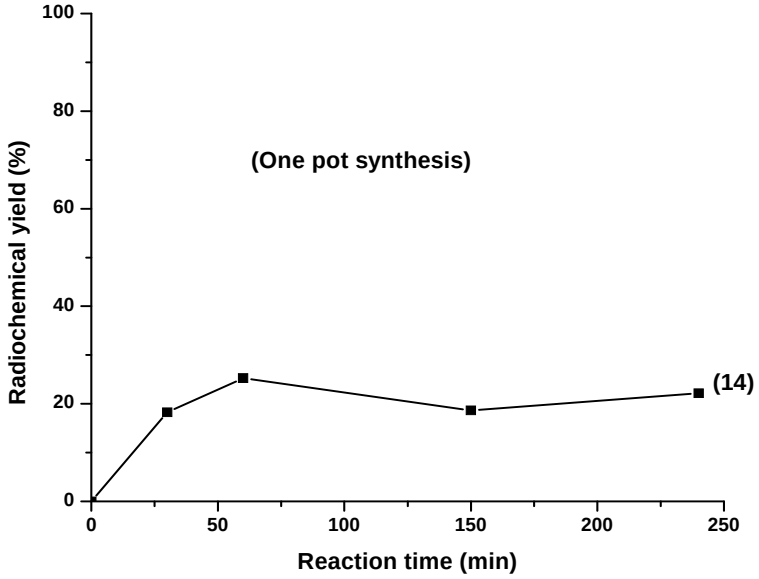
SI 42-Variation of radiochemical yield (%) of ^{99m}Tc-complex **13** with time by one pot method from ligand **2** (5 mg) at 90 ^{0}C



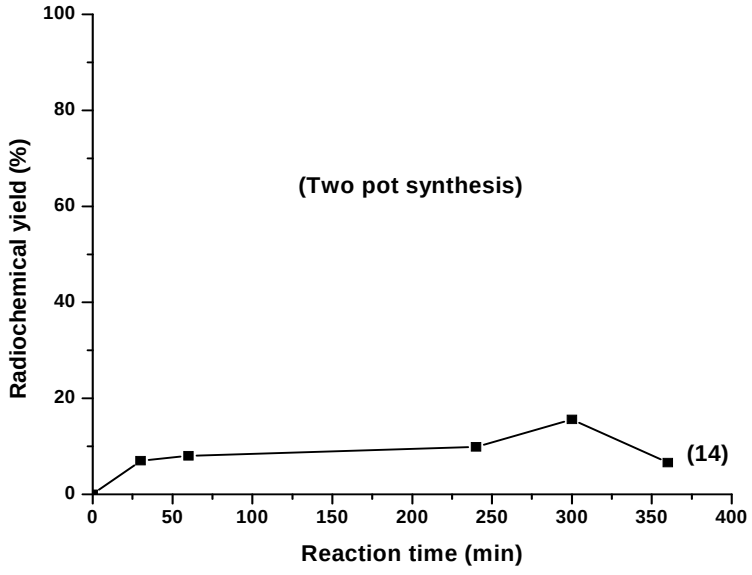
SI 43-Variation of radiochemical yield (%) of ^{99m}Tc-complex **13** with time by two pot method from ligand **2** (5 mg) at 90 ^{0}C



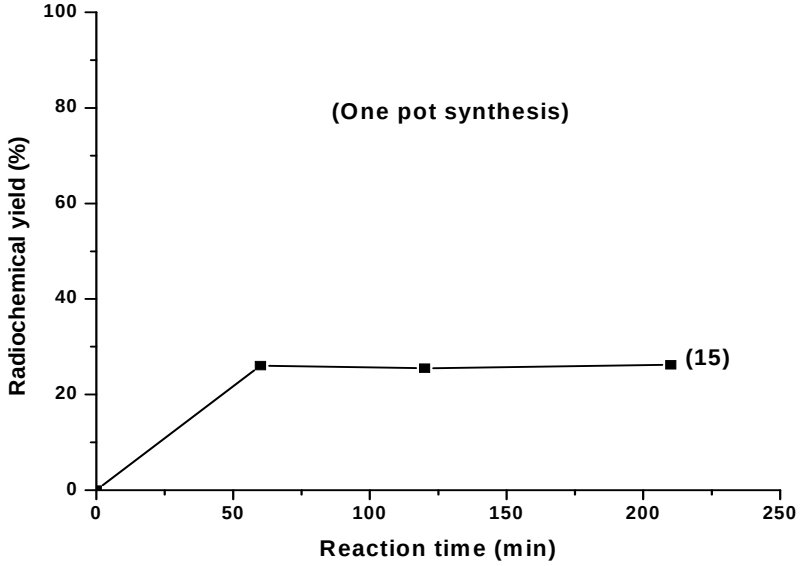
SI 44 -Variation of radiochemical yield (%) of ^{99m}Tc-complex **14** with time by one pot method from ligand **5** (2 mg) at 90 ^{0}C



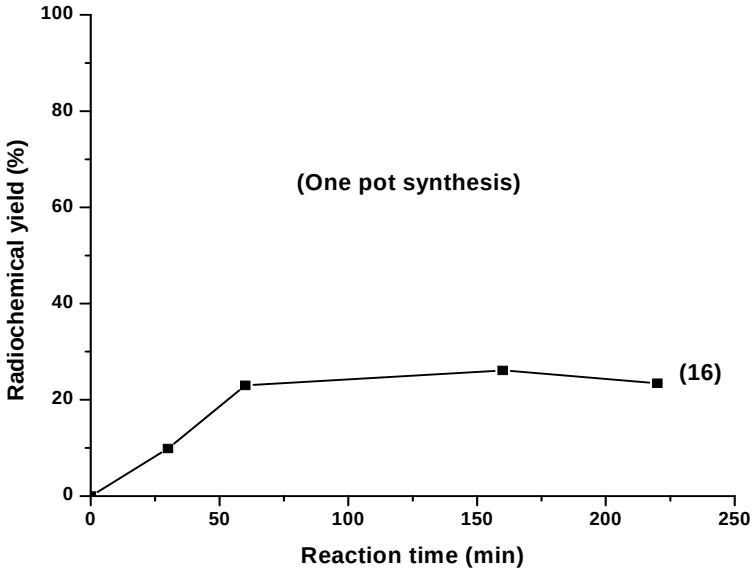
SI 45-Variation of radiochemical yield (%) of ^{99m}Tc-complex **14** with time by two pot method from ligand **5** (5.7 mg) at 90 ^{0}C



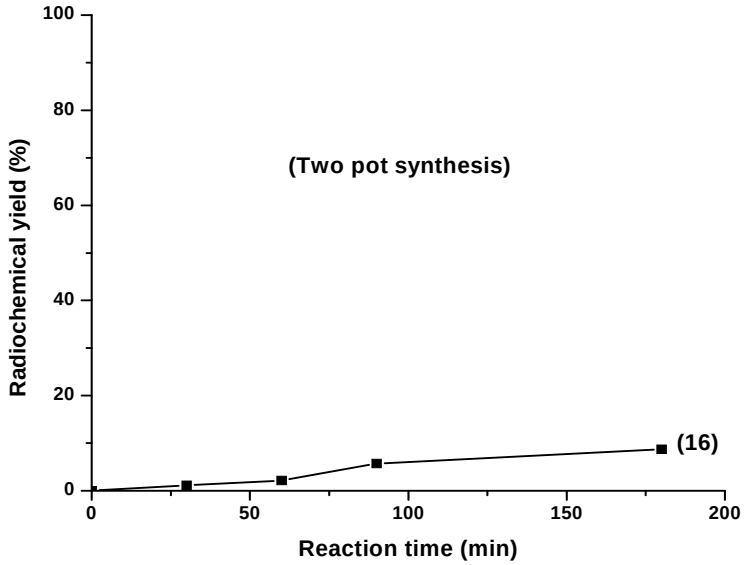
SI 46-Variation of radiochemical yield (%) of ^{99m}Tc-complex **15** with time by one pot method from ligand **6** (2 mg) at 90 ^{0}C



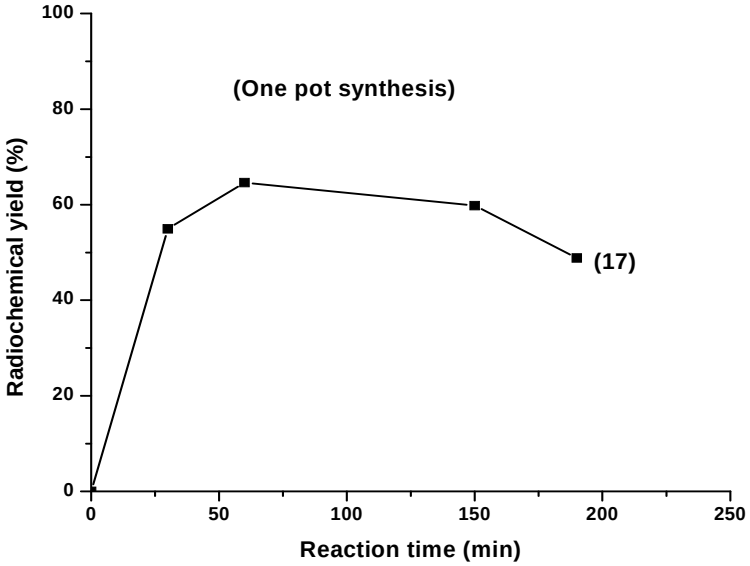
SI 47-Variation of radiochemical yield (%) of ^{99m}Tc-complex **16** with time by one pot method from ligand **7** (2 mg) at 90 ^{0}C



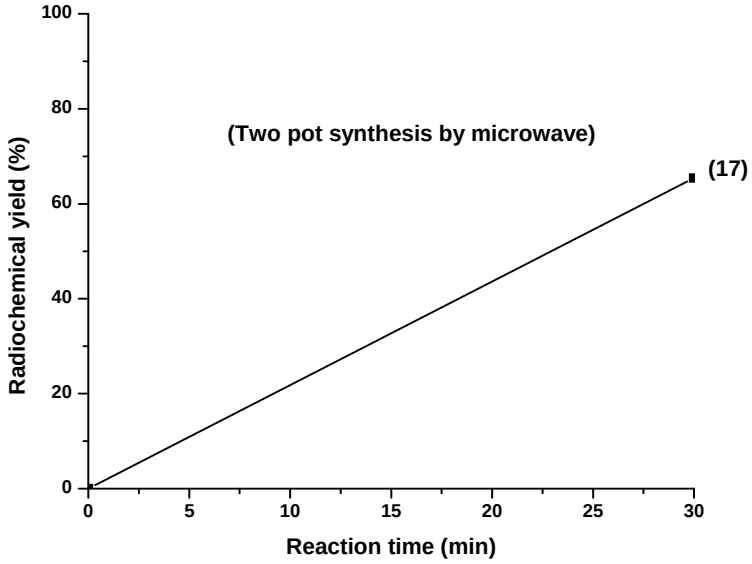
SI 48-Variation of radiochemical yield (%) of ^{99m}Tc-complex **16** with time by two pot method from ligand **7** (5.3 mg) at 90 ^{0}C



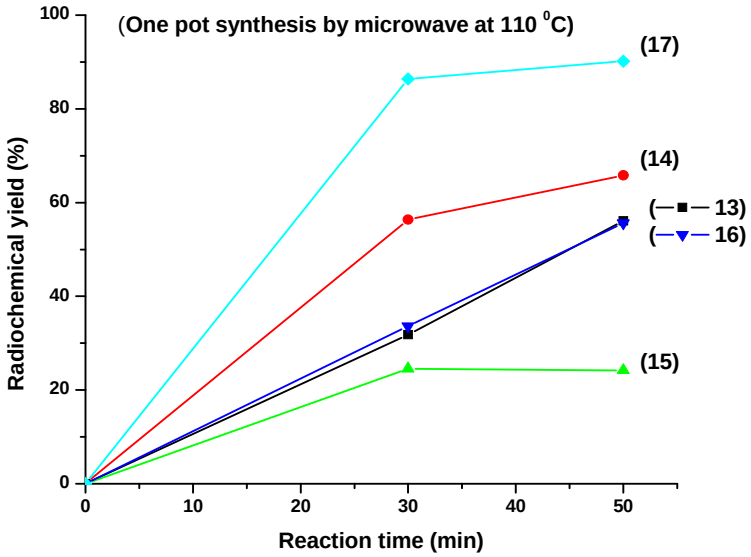
SI 49-Variation of radiochemical yield (%) of ^{99m}Tc-complex **17** with time by one pot method from ligand **8** (2 mg) at 90 ^{0}C



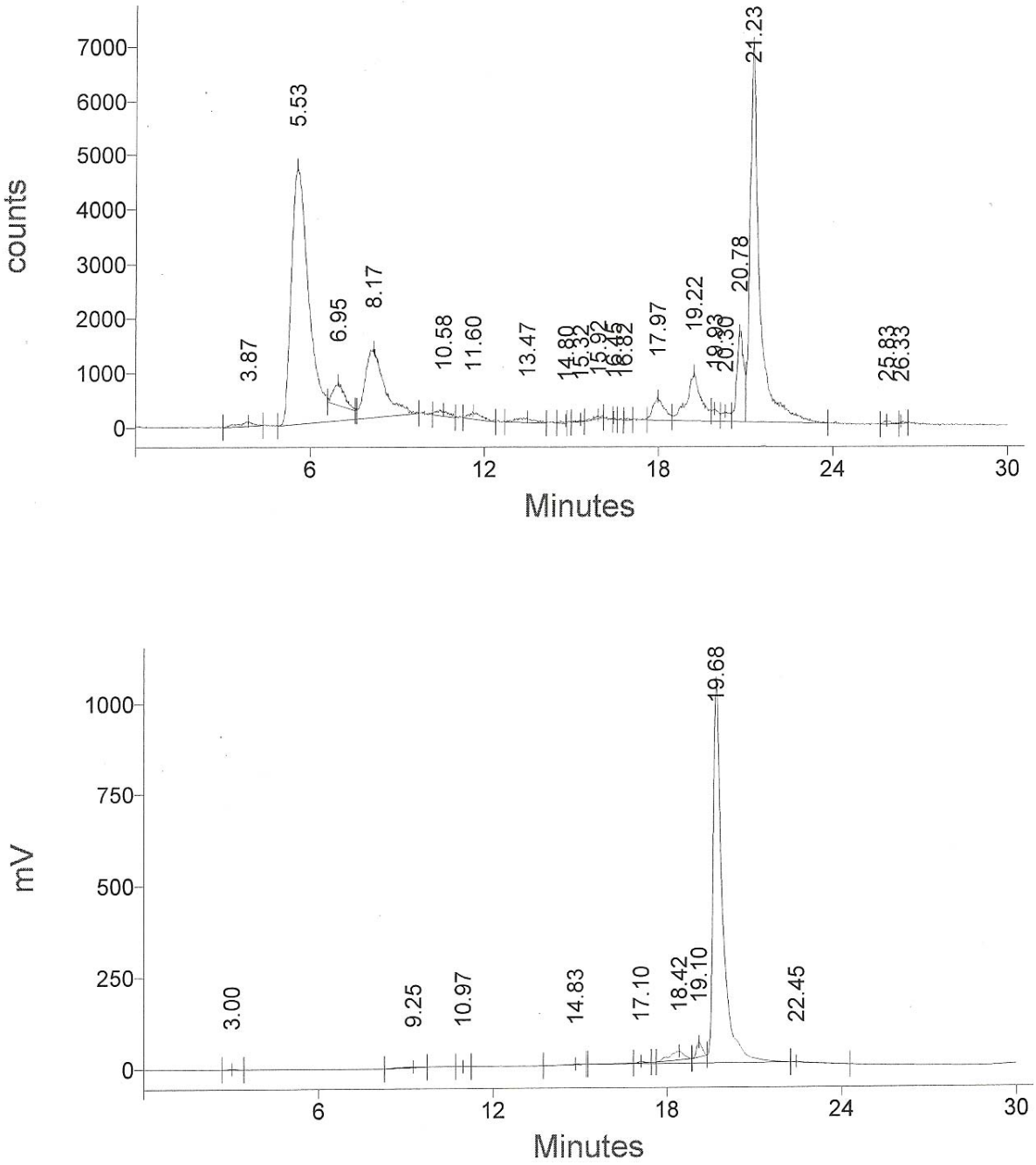
SI 50-Variation of radiochemical yield (%) of ^{99m}Tc-complex **17** with time by two pot method from ligand **8** (5.8 mg) under microwave at 110 ^{0}C



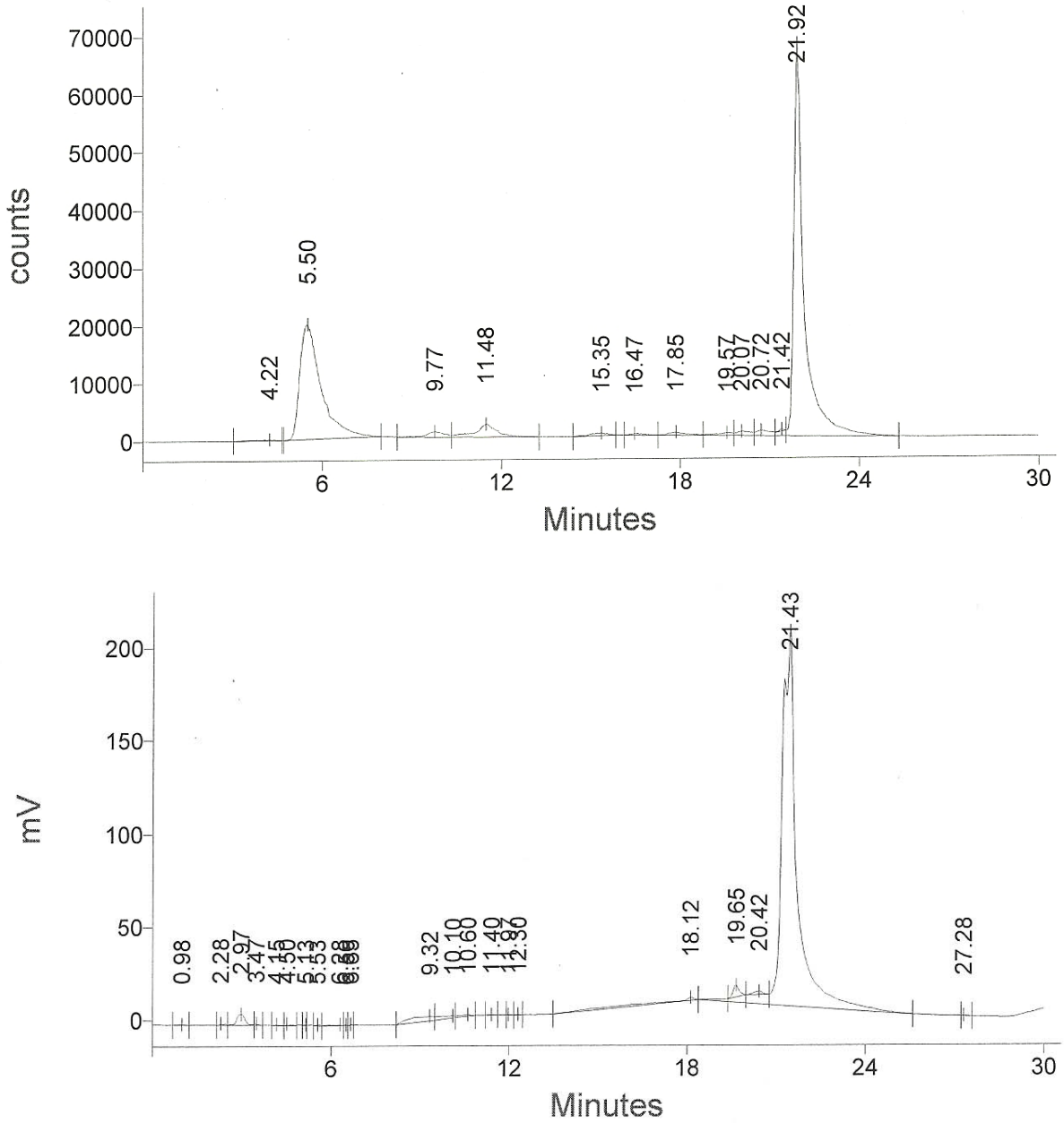
SI 51-Variation of radiochemical yield of ^{99m}Tc-complexes **13-17** with time by one pot method from ligand **2, 5-7** (0.6 mg), **8** (1.5 mg) under microwave at 110 ^{0}C



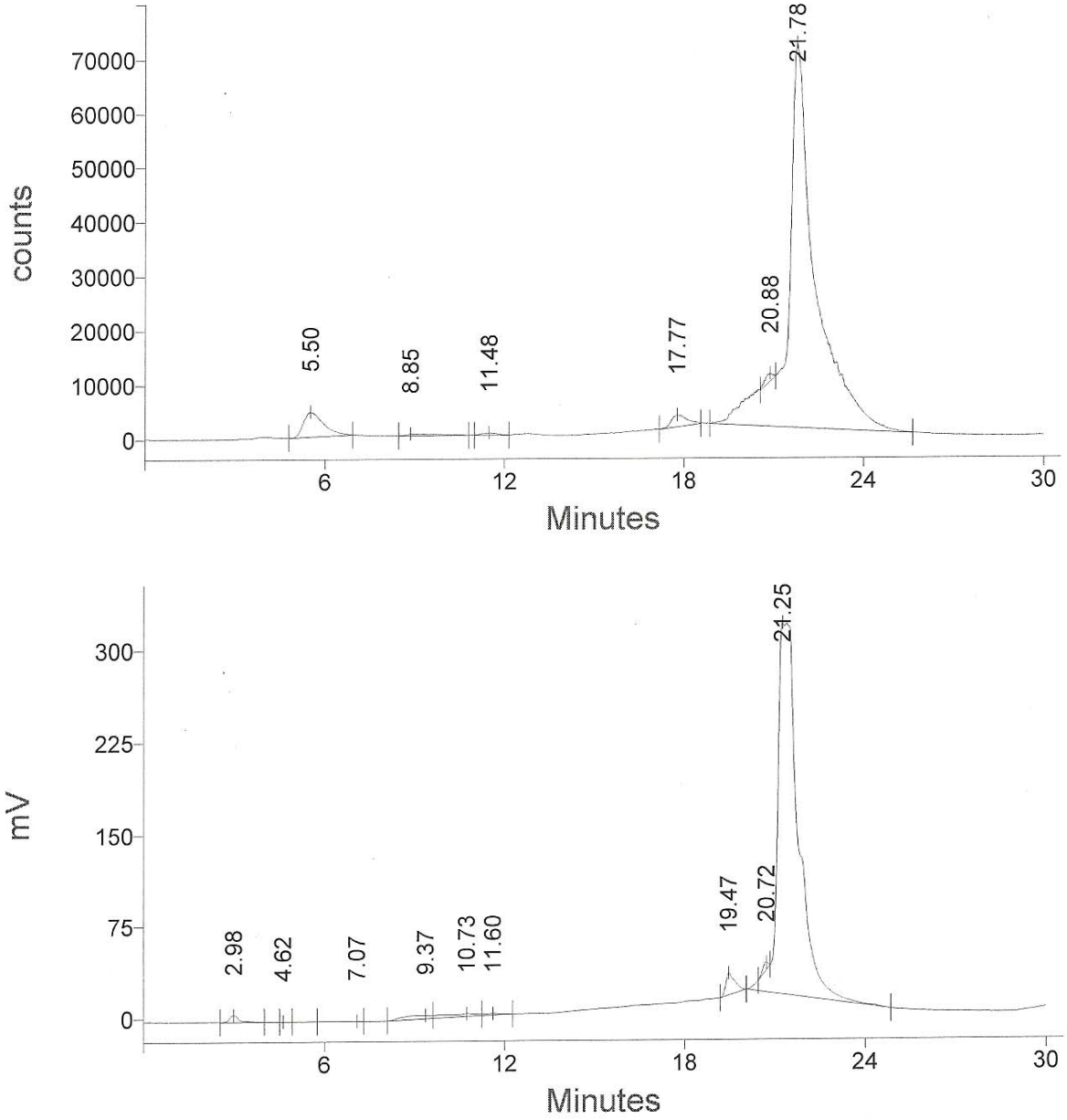
SI 52 -HPLC traces of crude labeling solutions with dipeptide **2** yielding ^{99m}Tc compound **13** (γ-trace top and UV trace bottom)



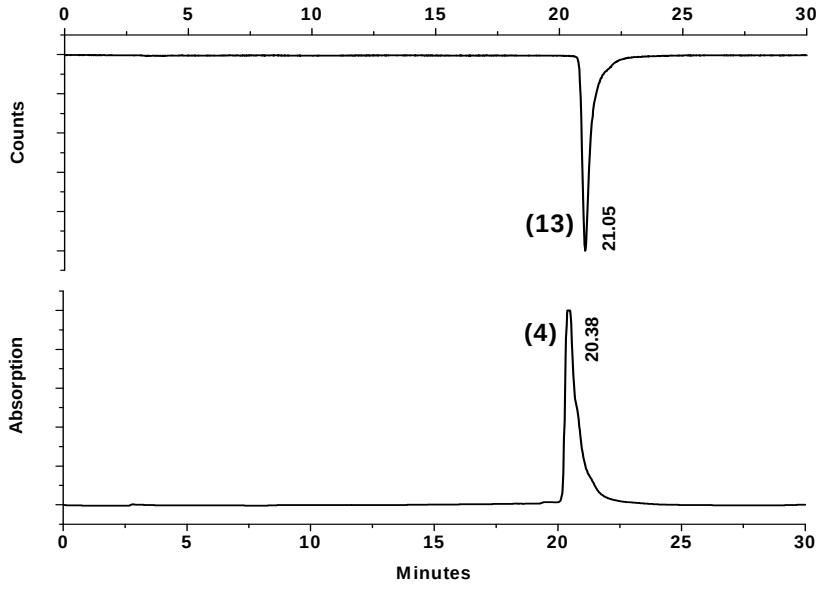
SI 53-HPLC traces of crude labeling solutions with dipeptide **7** yielding ^{99m}Tc compound **16** (γ-trace top and UV trace bottom)



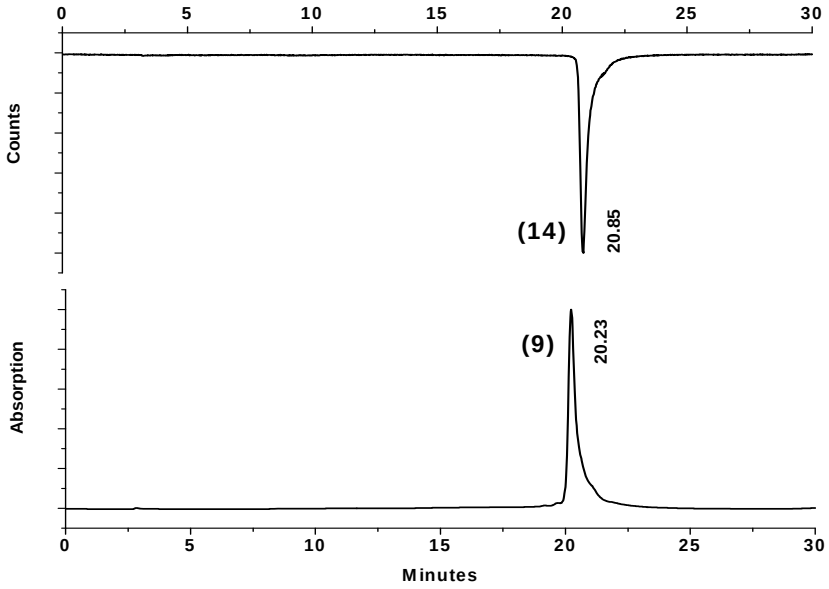
SI 54-HPLC traces of crude labeling solutions with dipeptide **8** yielding ^{99m}Tc compound **17** (γ-trace top and UV trace bottom)



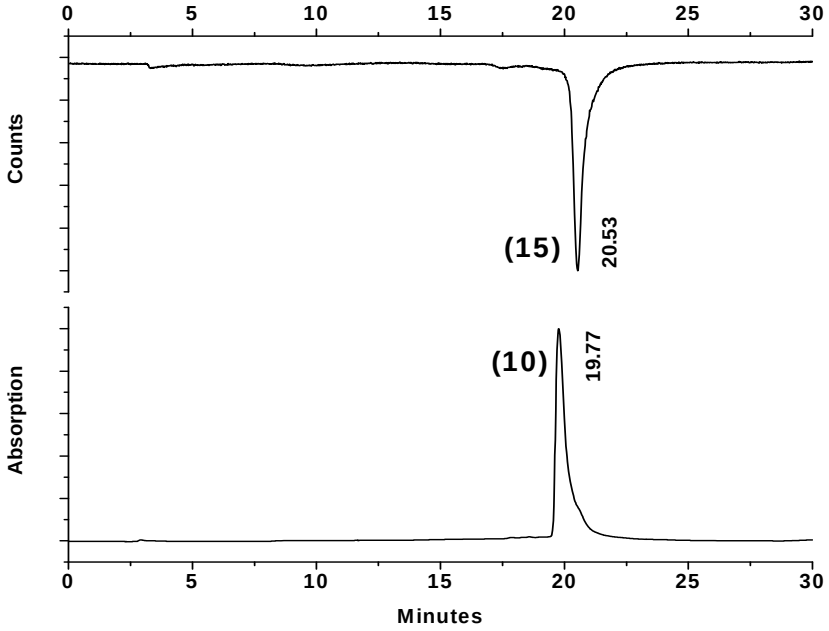
SI 55-HPLC coinjection traces of Re-complex **4** and the corresponding ^{99m}Tc-complex **13**



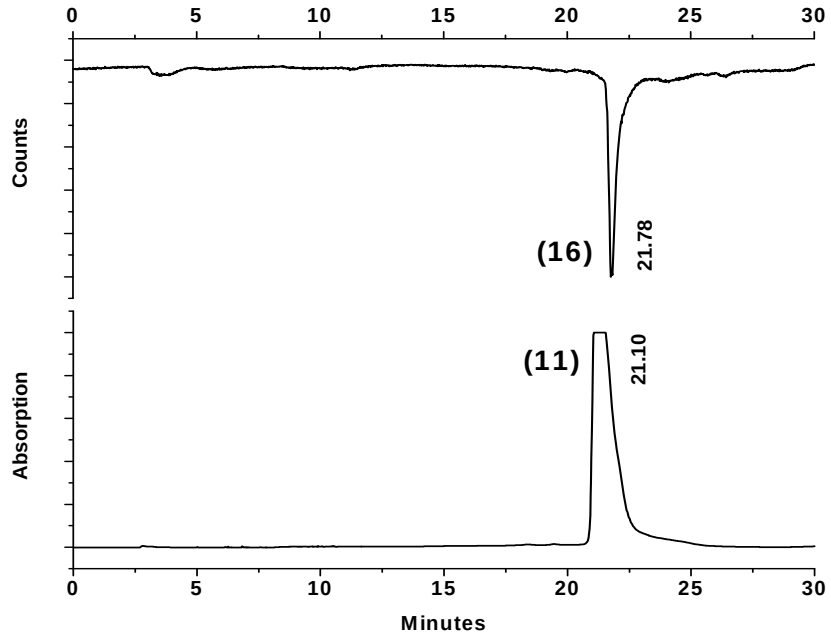
SI 56-HPLC coinjection traces of Re-complex **9** and the corresponding ^{99m}Tc-complex **14**



SI 57-HPLC coinjection traces of Re-complex **10** and the corresponding ^{99m}Tc-complex **15**



SI 58-HPLC coinjection traces of Re-complex **11** and the corresponding ^{99m}Tc-complex **16**



SI 59-HPLC coinjection traces of Re-complex **12** and the corresponding ^{99m}Tc-complex **17**