

Supplementary data

Synthesis and in vitro Properties of Trimethylamine- and Phosphonate-substituted Carboranylporphyrins for Application in BNCT

Michael W. Easson, Frank R. Fronczek, Timothy Jensen and M. Graça H. Vicente

Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803, USA

Table of Contents

HRMS (ESI).....	2
Combined fluorescence emission spectra.....	8
Dark cytotoxicity.....	9
Calculated intracellular boron levels at 24 h.....	9

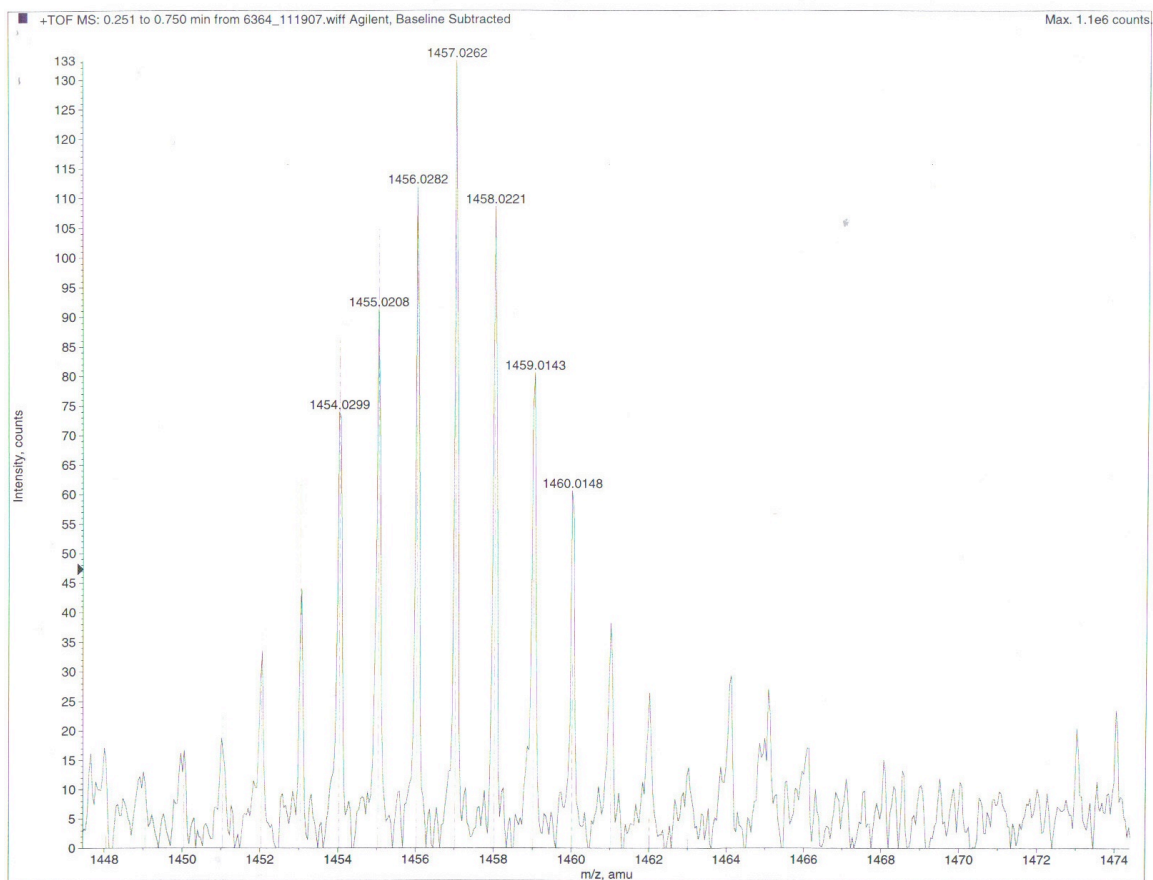


Figure 1. HRMS (ESI) for porphyrin **5d**; observed (solid line), calculated (dot line).

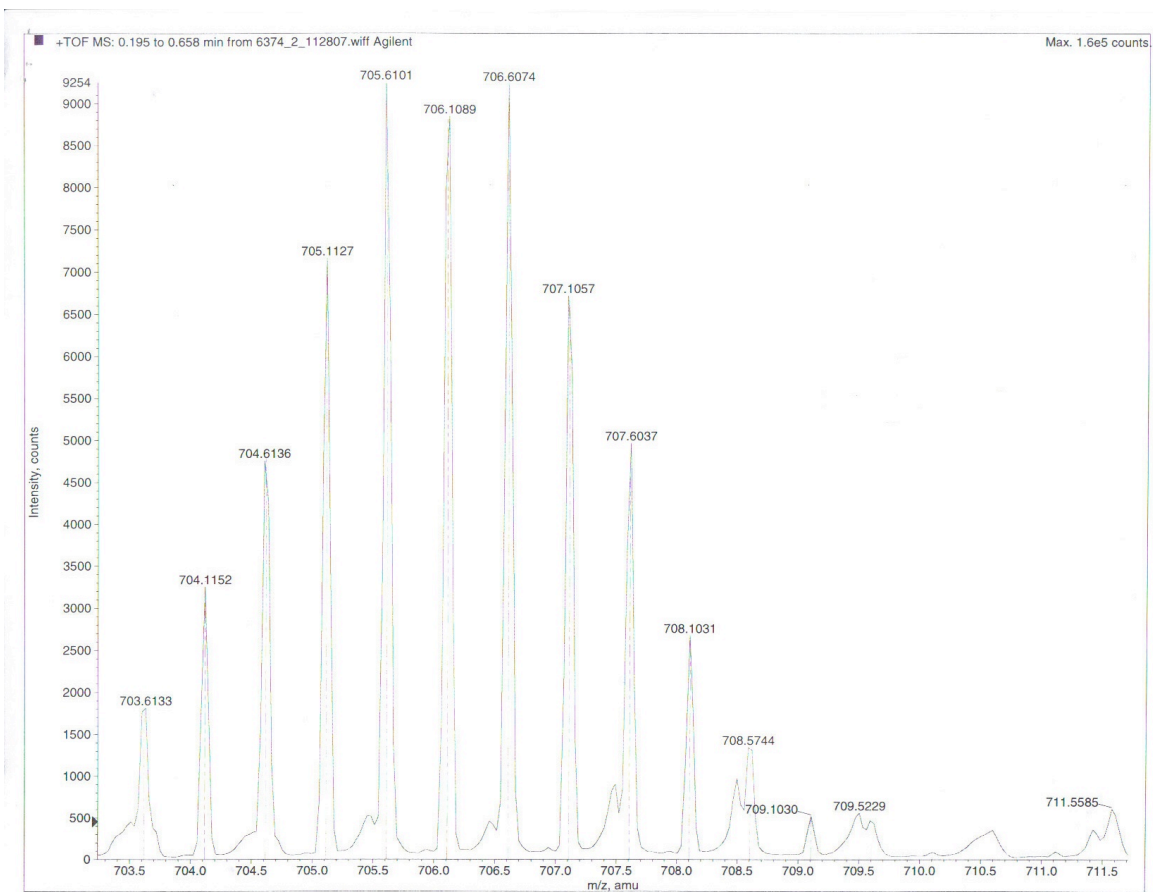


Figure 2. HRMS (ESI) for porphyrin **6c**; observed (solid line), calculated (dot line).

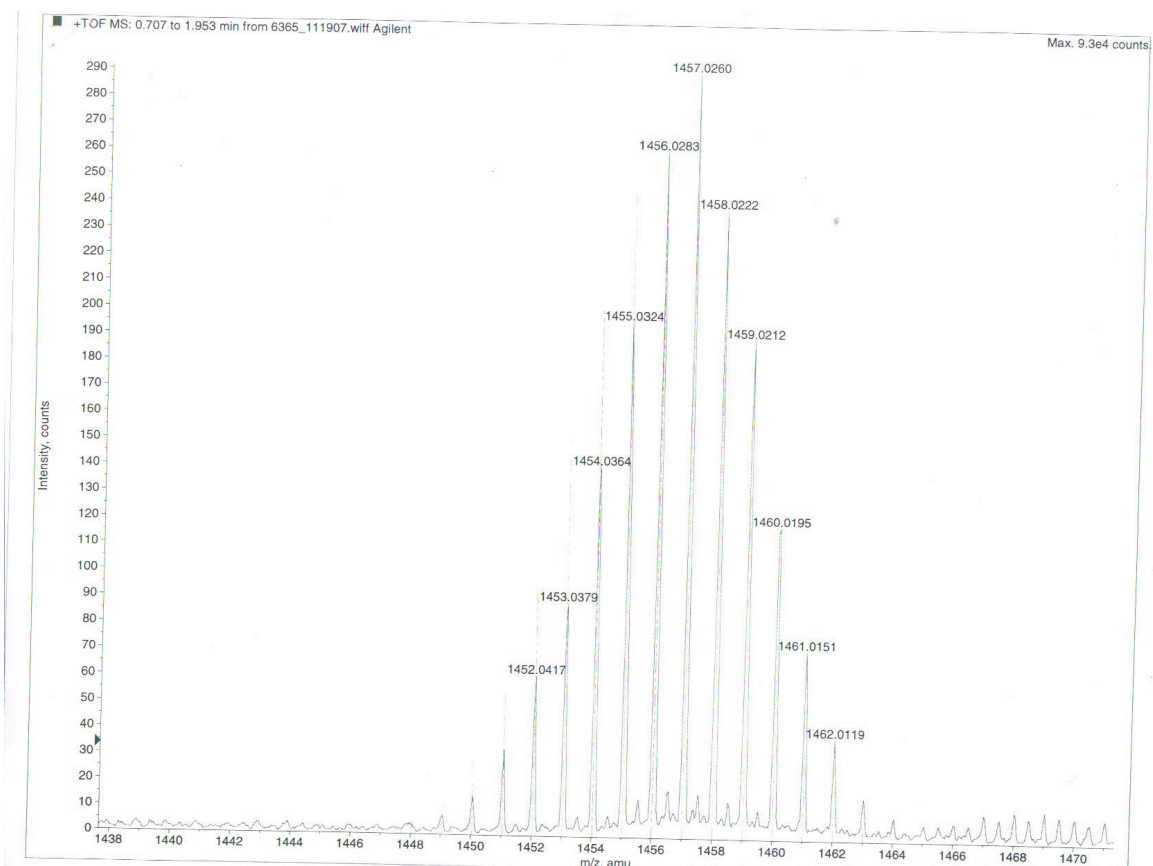


Figure 3. HRMS (ESI) for porphyrin **6d**; observed (solid line), calculated (dot line).

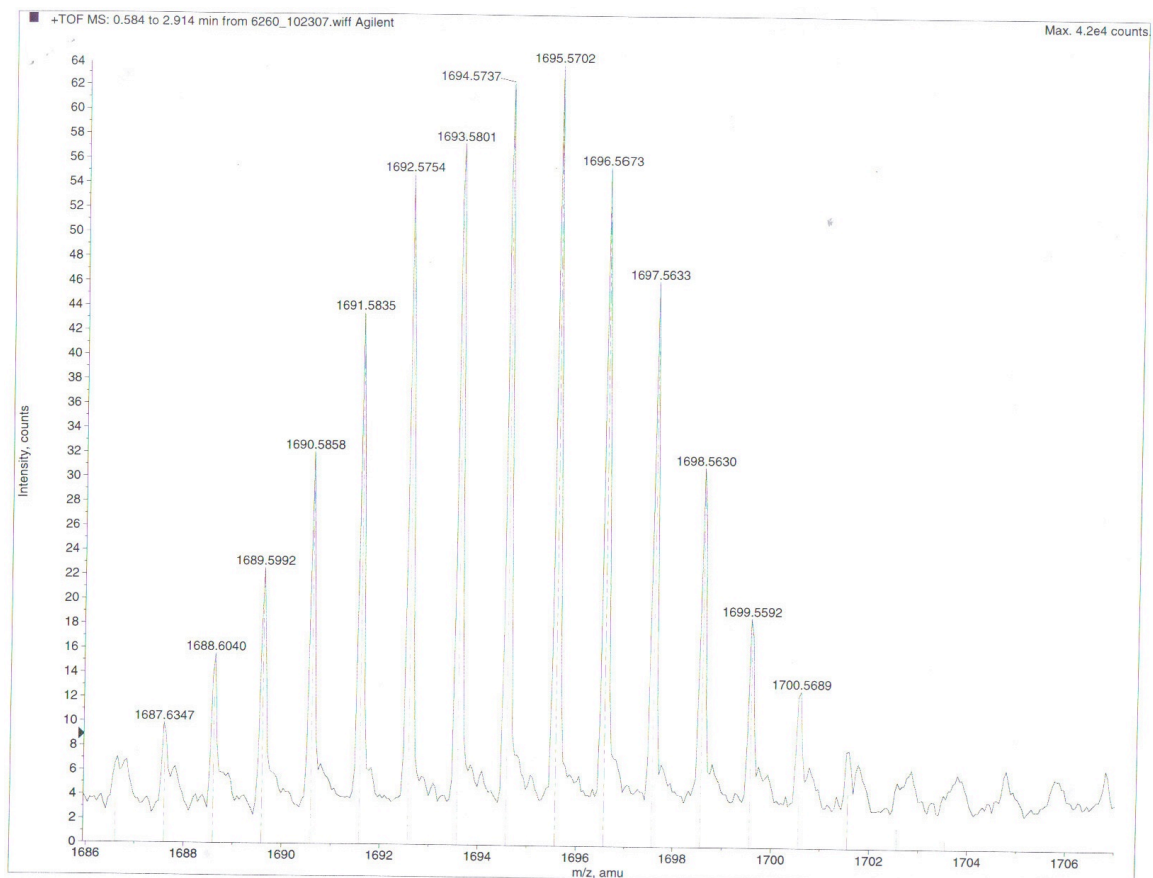


Figure 4. HRMS (ESI) for porphyrin **7c**; observed (solid line), calculated (dot line).

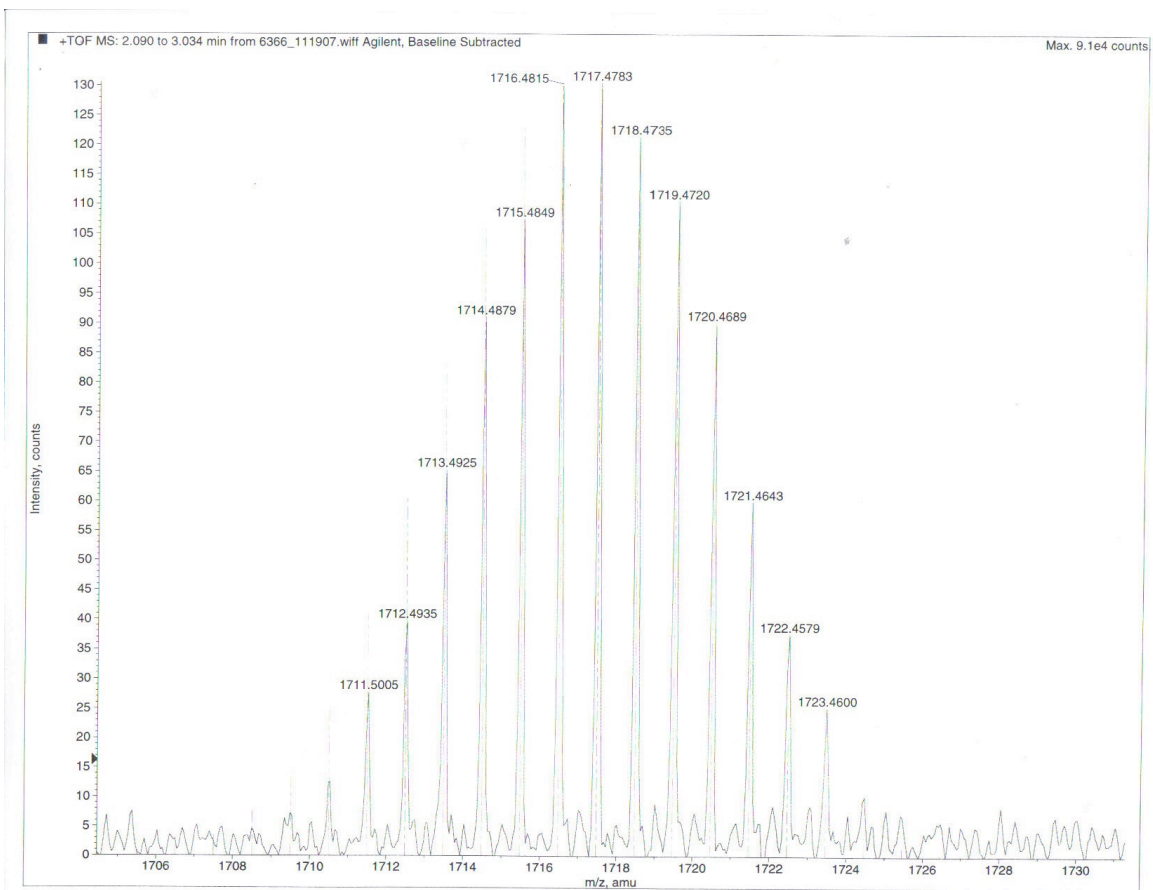


Figure 5. HRMS (ESI) for porphyrin **7d**; observed (solid line), calculated (dot line).

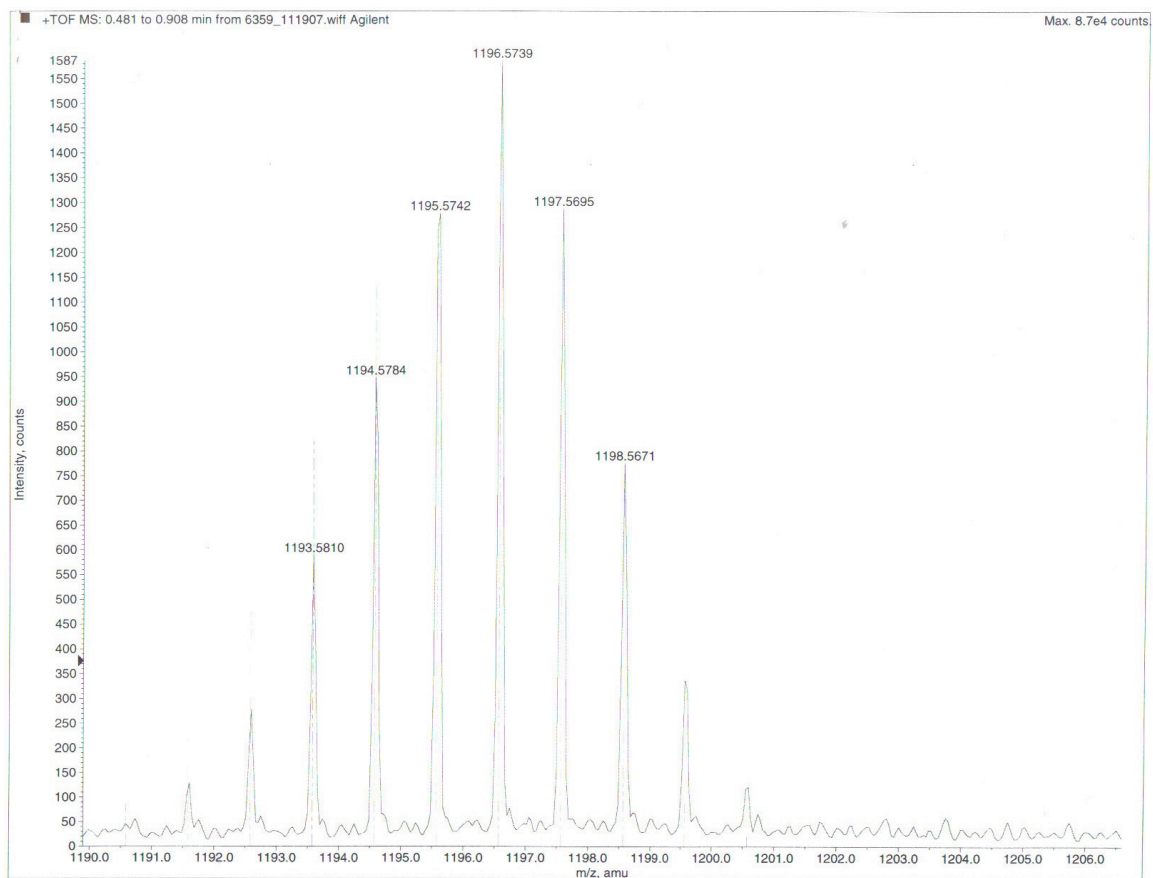


Figure 6. HRMS (ESI) for porphyrin **8d**; observed (solid line), calculated (dot line).

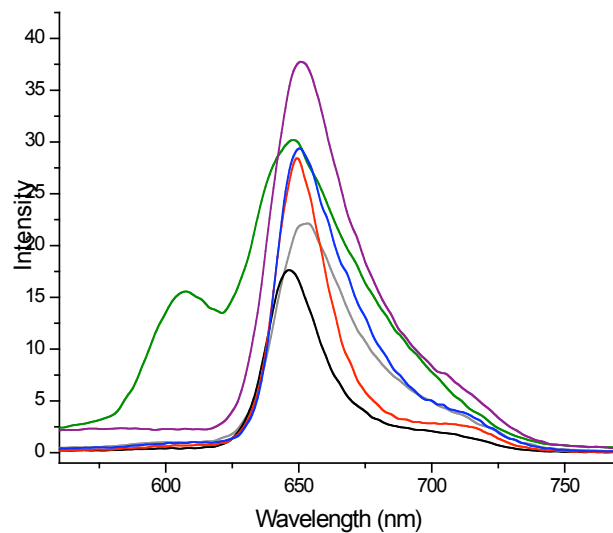


Figure 7. Fluorescence emission of porphyrins **5d** (gray), **6c** (purple), **6d** (black), **7c** (blue), **7d** (red), and **8d** (green) at 1×10^{-6} M in freshly prepared HEPES buffer (20 mM, pH 7.4) containing 1% DMSO. Excitation at 420 nm.

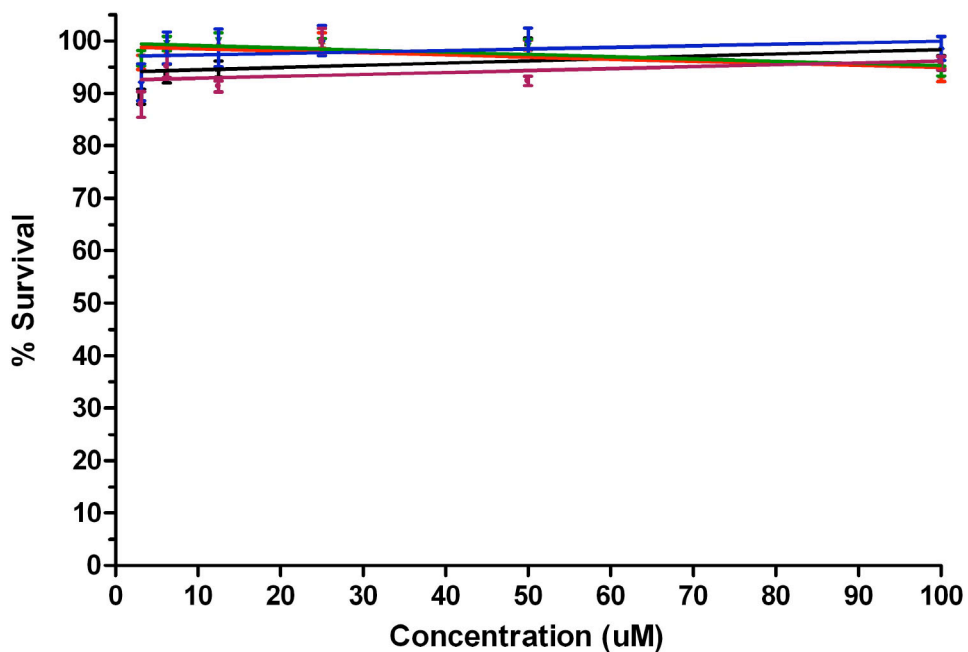


Figure 8. Dark cytotoxicity of porphyrins **6c** (purple), **6d** (black), **7c** (blue), **7d** (red) and **8d** (green) toward HEP2 cells using the Cell Titer Blue assay.

Table 1. Calculated $\mu\text{g B/g}$ for each porphyrin after 24 h uptake by T98G cells

Porphyrin	$\mu\text{g at 24 h}$	% B by weight	$\mu\text{g B/g}$
6c	0.025 ± 0.002	26	147.4 ± 15.1
6d	0.018 ± 0.002	30	111.8 ± 5.2
7c	0.010 ± 0.004	36	92.6 ± 16.2
7d	0.025 ± 0.003	38	220.0 ± 35.0
8d	0.027 ± 0.001	18	108.8 ± 10.3