

Supporting Information

Comparative Positron-Emission Tomography (PET) Imaging and Phototherapeutic Potential of ¹²⁴I- Labeled Methyl- 3-(1'-iodobenzyloxyethyl) pyropheophorbide-a vs. the Corresponding Glucose- and Galactose-Conjugates

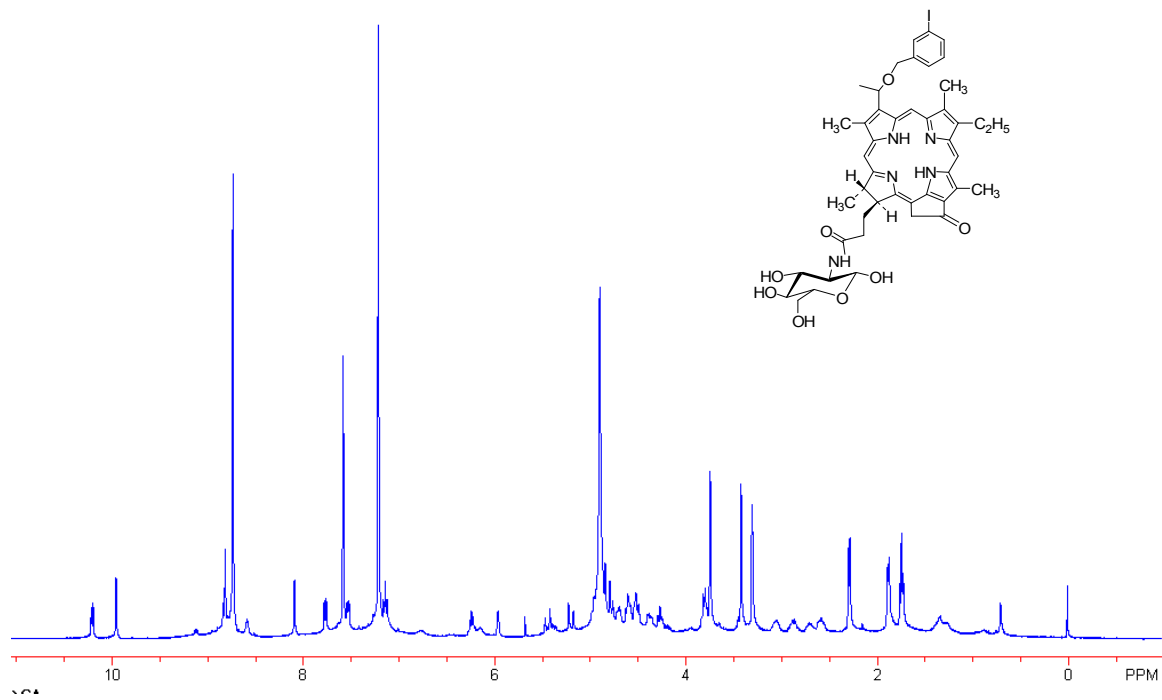
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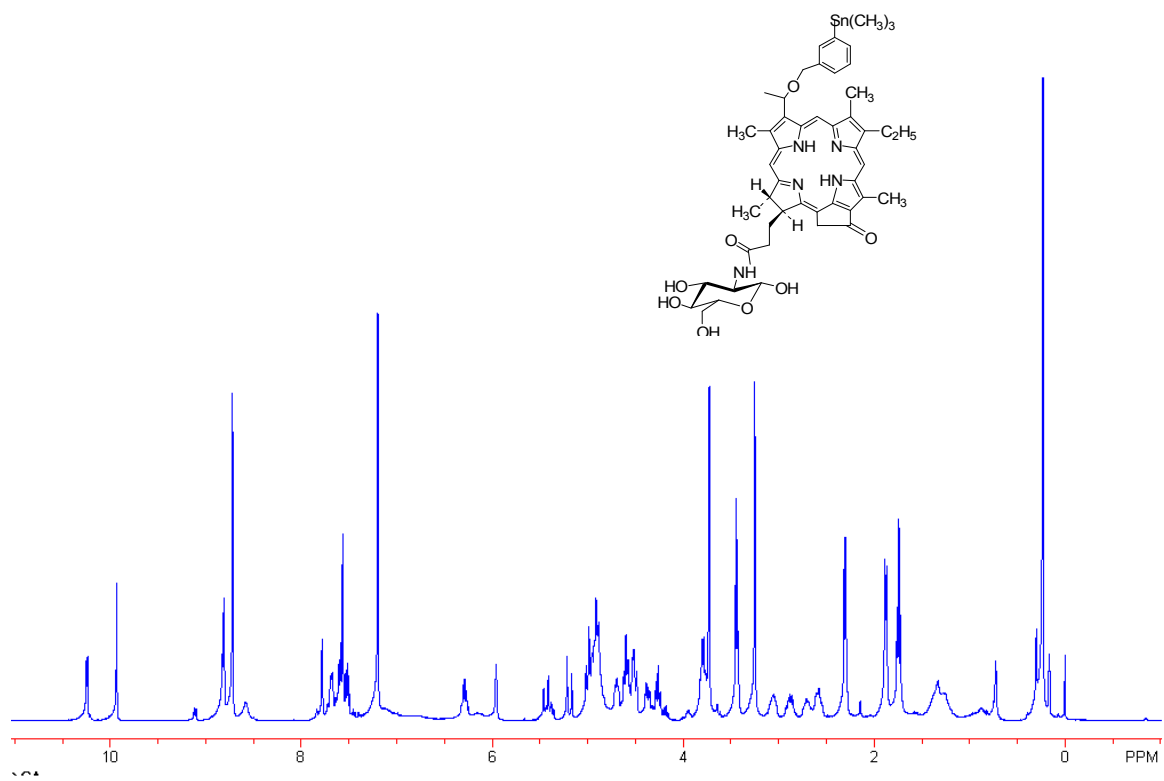
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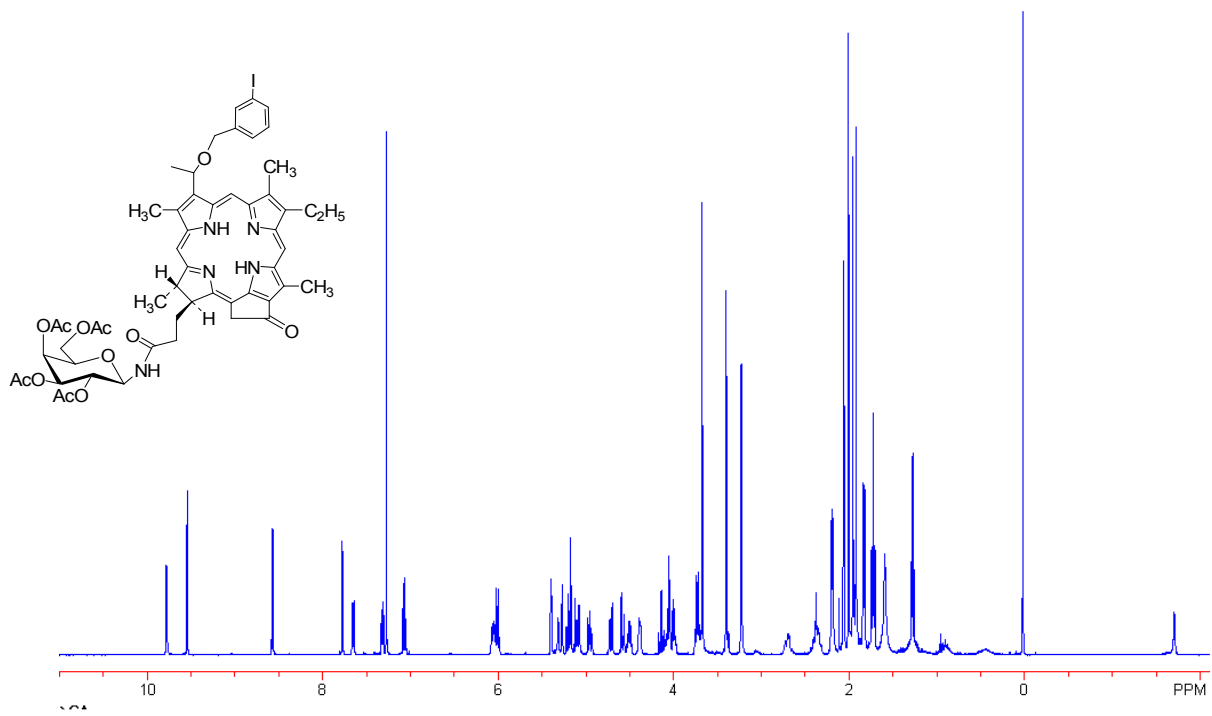
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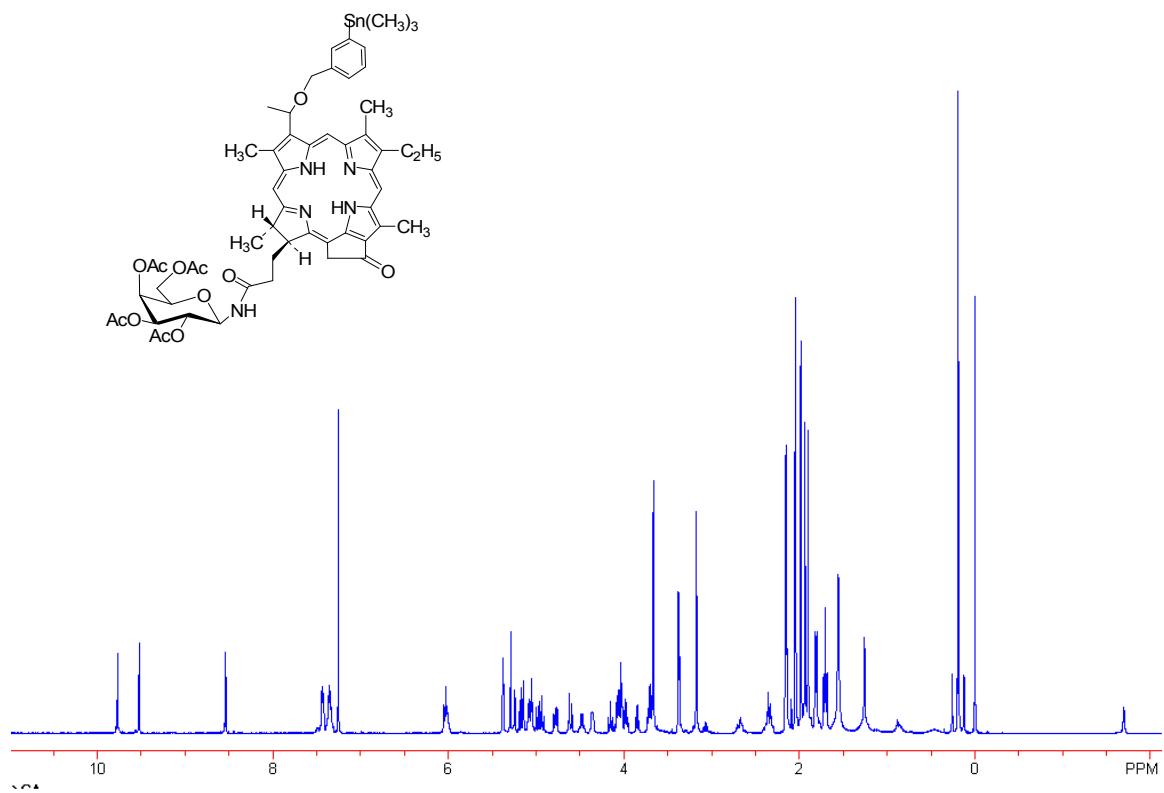
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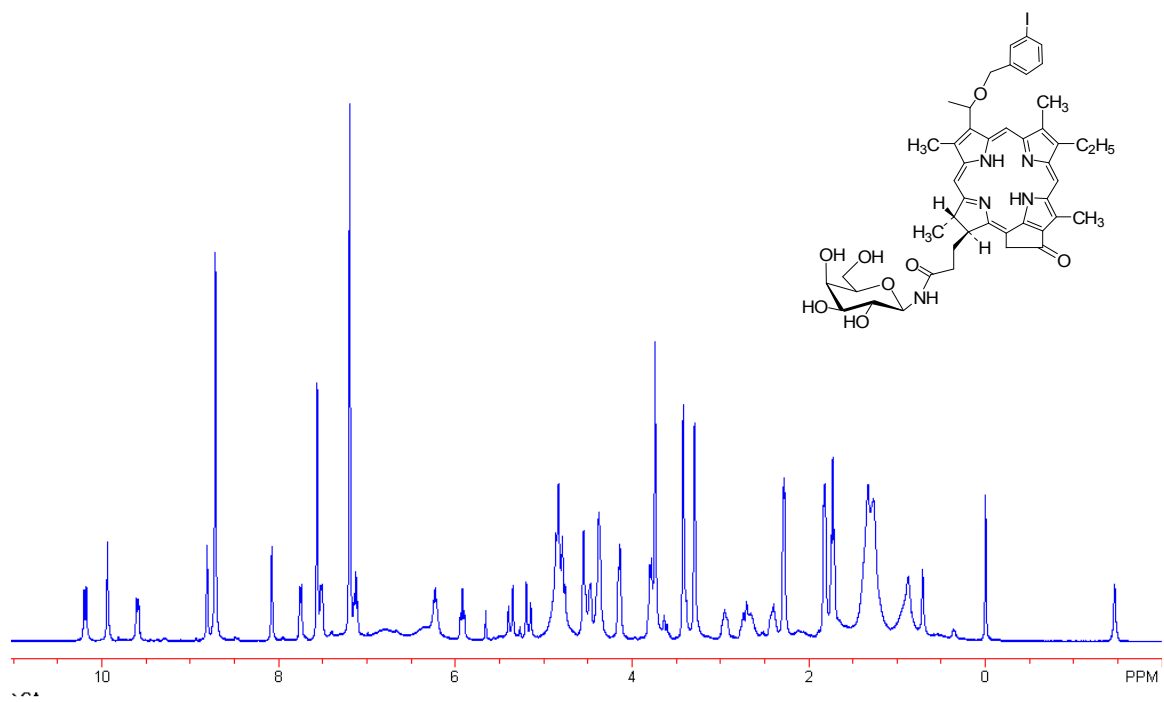
S1	Title page
S2	NMR spectrum of compound 1
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S4	NMR spectrum of compound 2
S5	H NMR spectrum of compound 9 (trimethyltin analog of 2)
S6	H NMR spectrum of compound 6
S7	H NMR spectrum of compound 10 (trimethyltin analog of 6)
S8	H NMR spectrum of compound 3
S9	H NMR spectrum of compound 12 (trimethyltin analog of 3)
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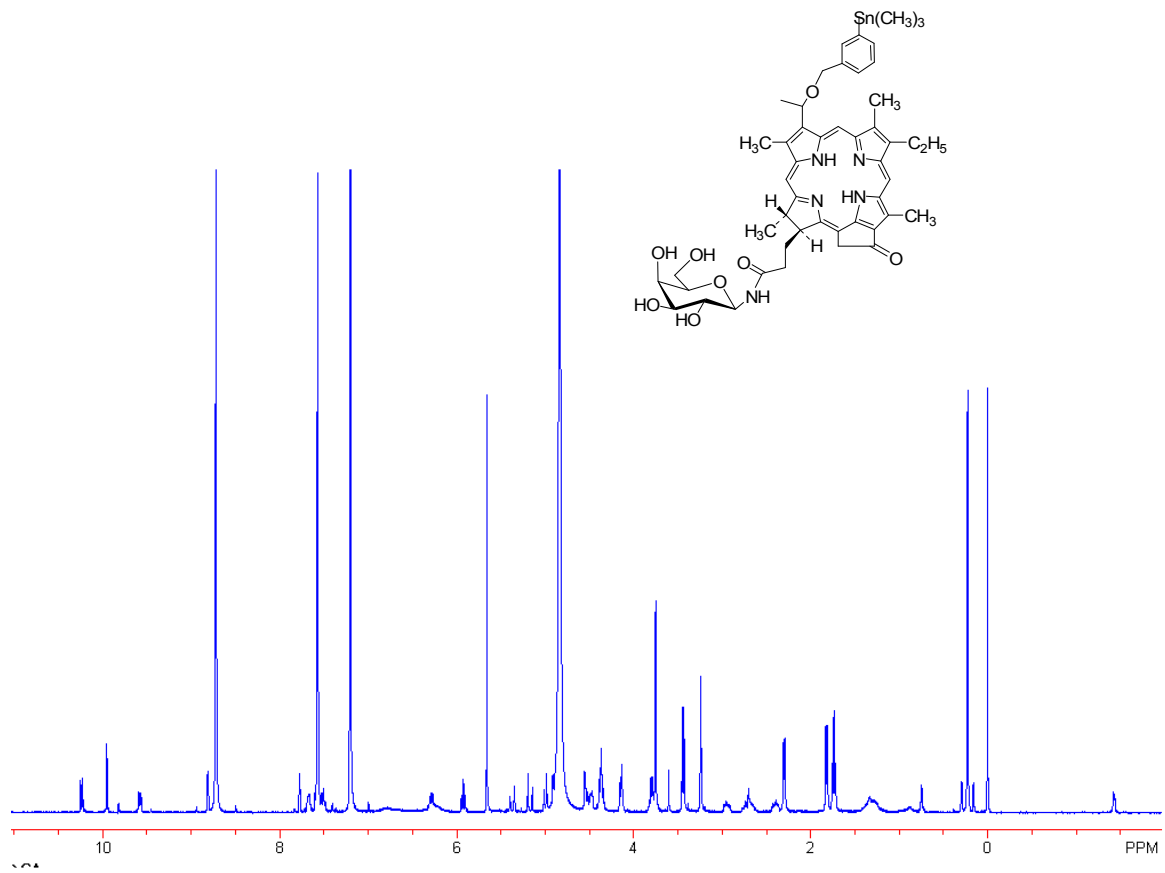












Analytical Details

Compound No.	Mol. Formula	HRMS	HPLC Analysis	Does the analysis agree to the desired product
1	C ₄₁ H ₄₃ N ₄ O ₄ I	Analysis calcd: C, 62.91; H, 5.54; N, 7.16, I, 16.21 Found: C, 62.60; H, 5.59; N, 7.13, I, 16.45.	RT: 20.97 min Purity: 96%	Yes NMR: See the Expt. Section
2	C ₄₆ H ₅₂ N ₅ O ₈ I	Calcd: 929.2862 Found (M+1): 930.2854	RT: 8.17 min Purity: >96%	Yes NMR: See the Expt. Section
3	C ₄₆ H ₅₂ N ₅ O ₈ I	Calcd: 929.2862 Found (M+1): 930.2806	RT: 8.02 min Purity: >96%	Yes NMR: See the Expt. Section
4	C ₄₀ H ₄₁ N ₄ O ₄ I	Calcd: 768.2174 Found (M+1): 769.2207	Intermediate	Yes NMR: See the Expt. Section
5	C ₄₄ H ₄₄ N ₅ O ₆ I	Calcd: 865.2328 Found (M+1): 866.2312	Intermediate	Yes NMR: See the Expt. Section
6	C ₅₄ H ₆₀ N ₅ O ₁₂ I	Calcd: 1097.3284 Found (M+1): 1098.3277	Intermediate	Yes NMR: See the Expt. Section
7	C ₄₃ H ₅₀ N ₄ O ₄ Sn	Calcd: 806.2853 Found (M+1): 807.2848	Intermediate	Yes NMR: See the Expt. Section
8	C ₄₇ H ₅₃ N ₅ O ₆ Sn	Calcd: 903.3017 Found (M+1): 904.3009	Intermediate	Yes NMR: See the Expt. Section
9	C ₄₉ H ₆₁ N ₅ O ₈ Sn	Calcd: 967.3541 Found (M+1): 968.3534	Intermediate RT: 10.51 min Purity: >96%	Yes NMR: See the Expt. Section
10	C ₅₇ H ₆₉ N ₅ O ₁₂ Sn	Calcd: 1135.3964 Found (M+1): 1136.3786	Intermediate	Yes NMR: See the Expt. Section
11	C ₄₉ H ₆₁ N ₅ O ₈ Sn	Calcd: 967.3541 Found (M+1): 968.3542	Intermediate RT: 9.88 min Purity: >96%	Yes NMR: See the Expt. Section
12	C ₄₅ H ₅₂ N ₄ O ₄ Sn	Analysis calcd: C, 64.99; H, 6.30; N, 6.74 Found: C, 64.56; H, 6.66; N, 6.59.	Intermediate RT: 27.88 min Purity: >96%	Yes NMR: See the Expt. Section