

Supporting Information

Photodynamic Inactivation of Microorganisms Using Semi-Synthetic Chlorophyll a Derivatives as Photosensitizers

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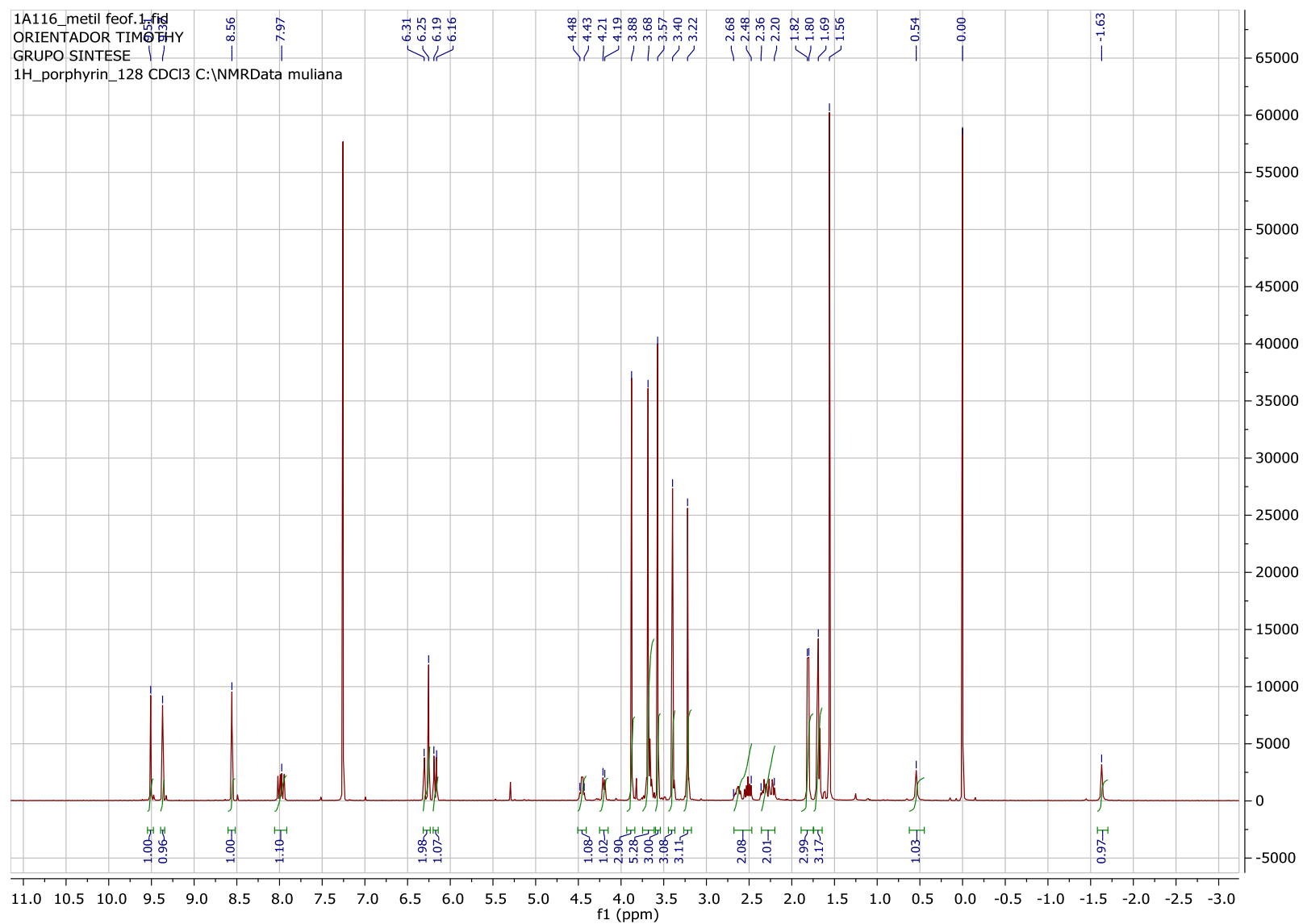


Figure S1: ^1H -NMR (CDCl_3) spectrum of methyl pheophorbide-*a* (**1**)

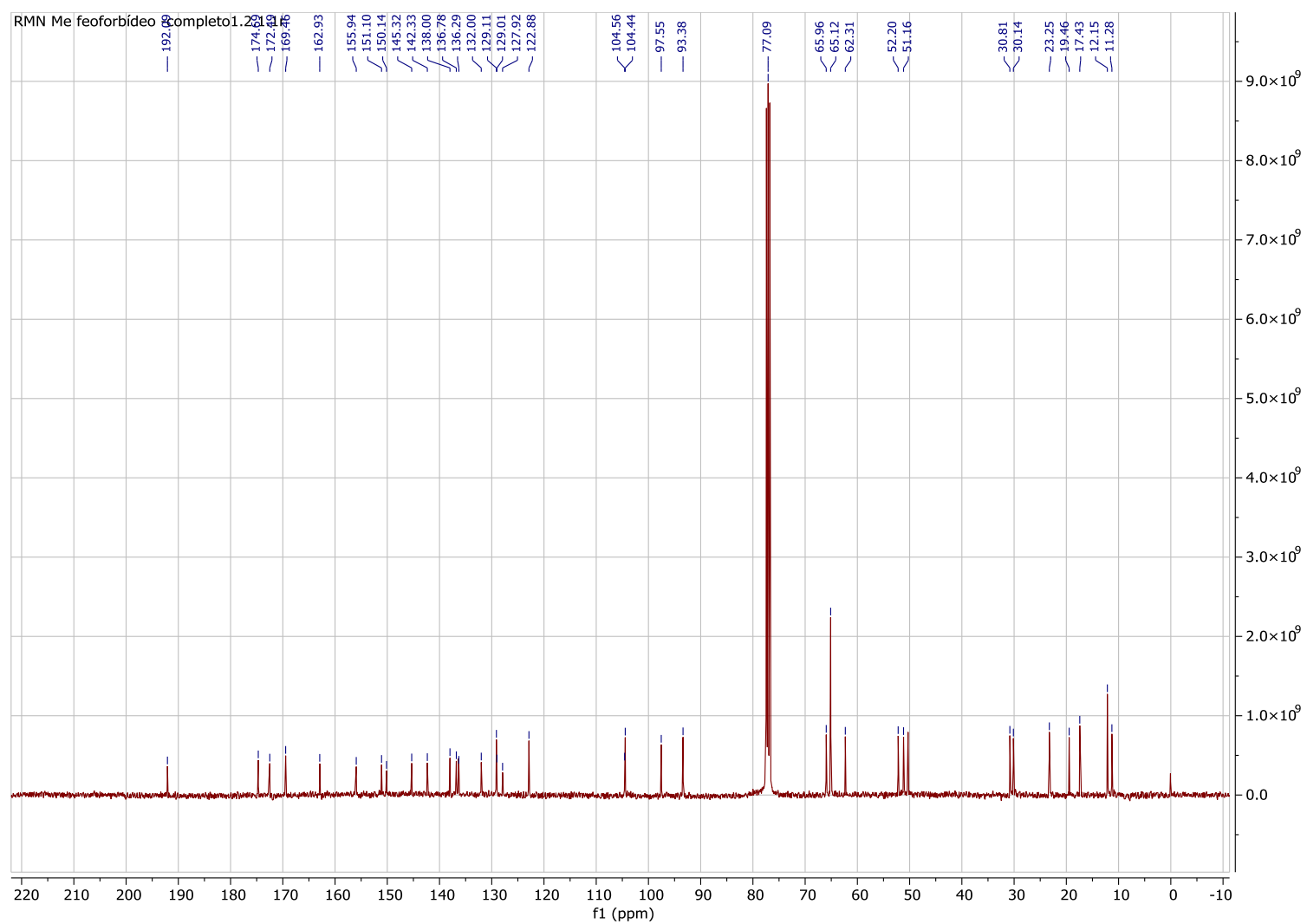


Figure S2: ^{13}C -NMR (CDCl_3) spectrum of methyl pheophorbide-*a* (**1**)

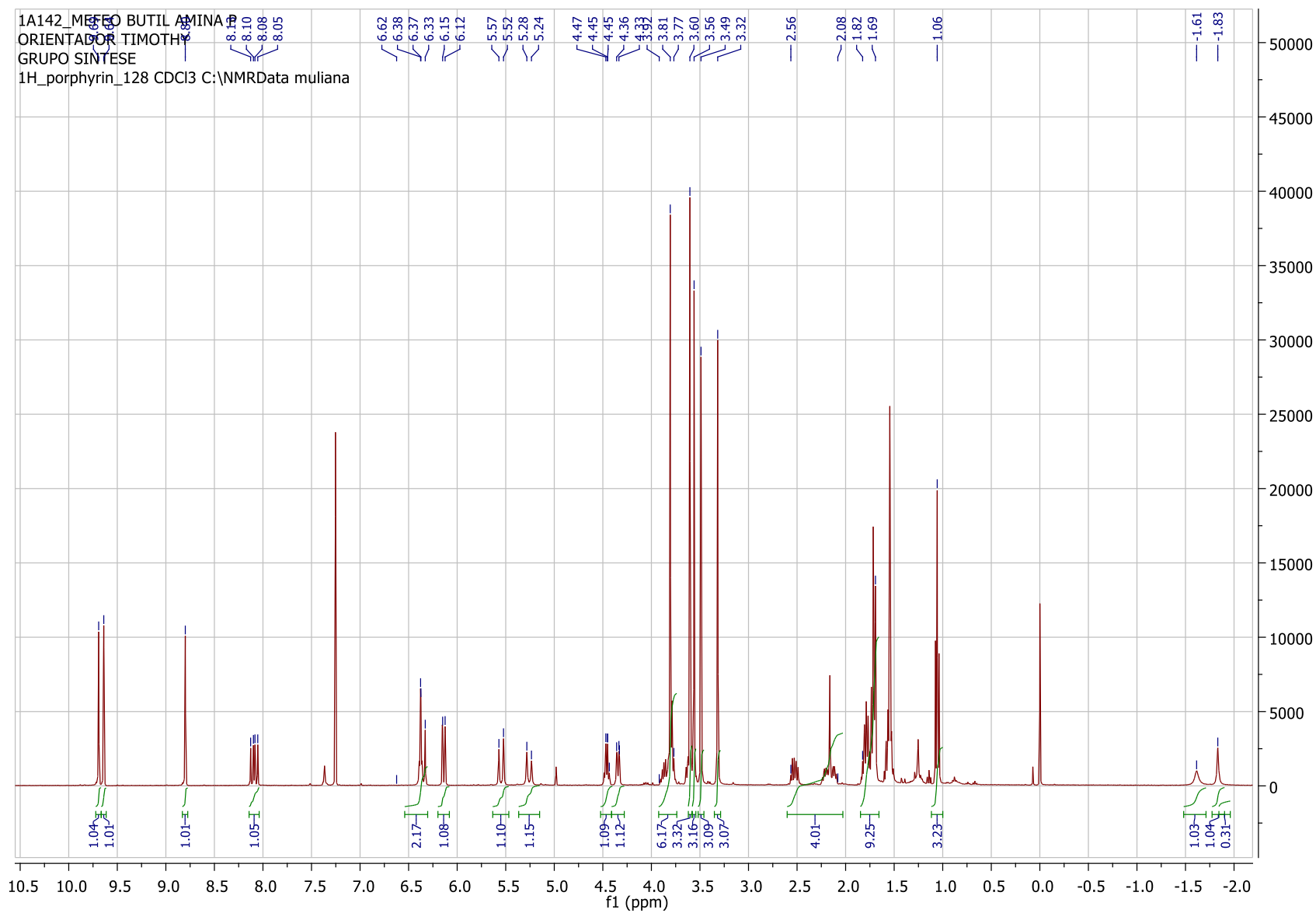


Figure S3: ^1H -NMR (CDCl_3) spectrum of 13-(Butylcarbamoyl)chlorin *e*6 15,17-dimethyl ester (**2**)

mefeobutil+_150303151426 #4 RT: 0.14 AV: 1 NL: 8.88E7
T: FTMS + p ESI Full ms [500.00-1000.00]

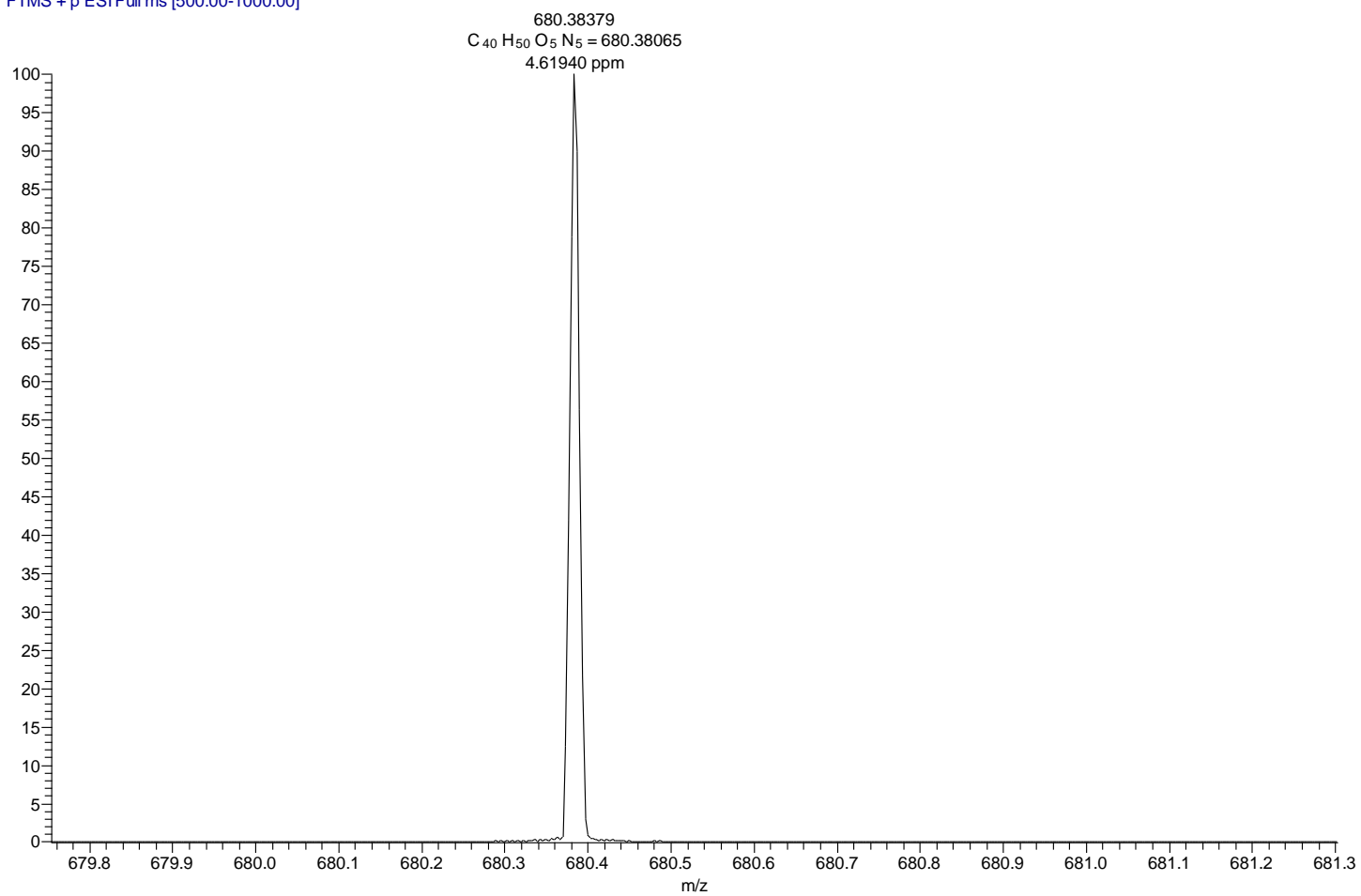


Figure S4: HRMS (ESI) of 13-(Butylcarbamoyl)chlorin *e*6 15,17-dimethyl ester (**2**)

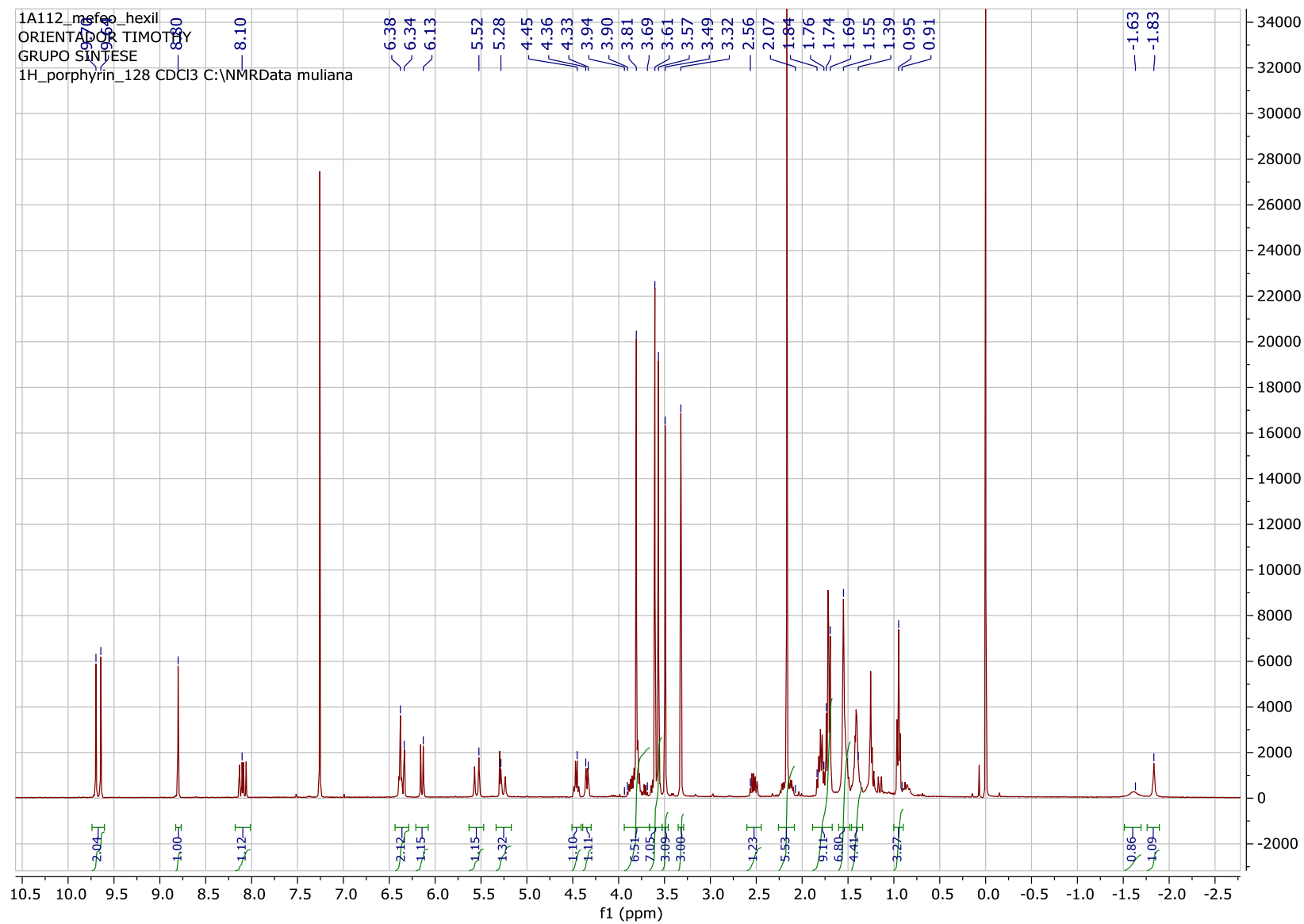


Figure S5: ^1H -NMR (CDCl_3) spectrum of 13-(Hexylcarbamoyl)chlorin e6 15,17-dimethyl ester (**3**)

mefeohehil+_150303153159 #1 RT: 0.01 AV: 1 NL: 7.55E7
T: FTMS +p ESI Full ms [500.00-1000.00]

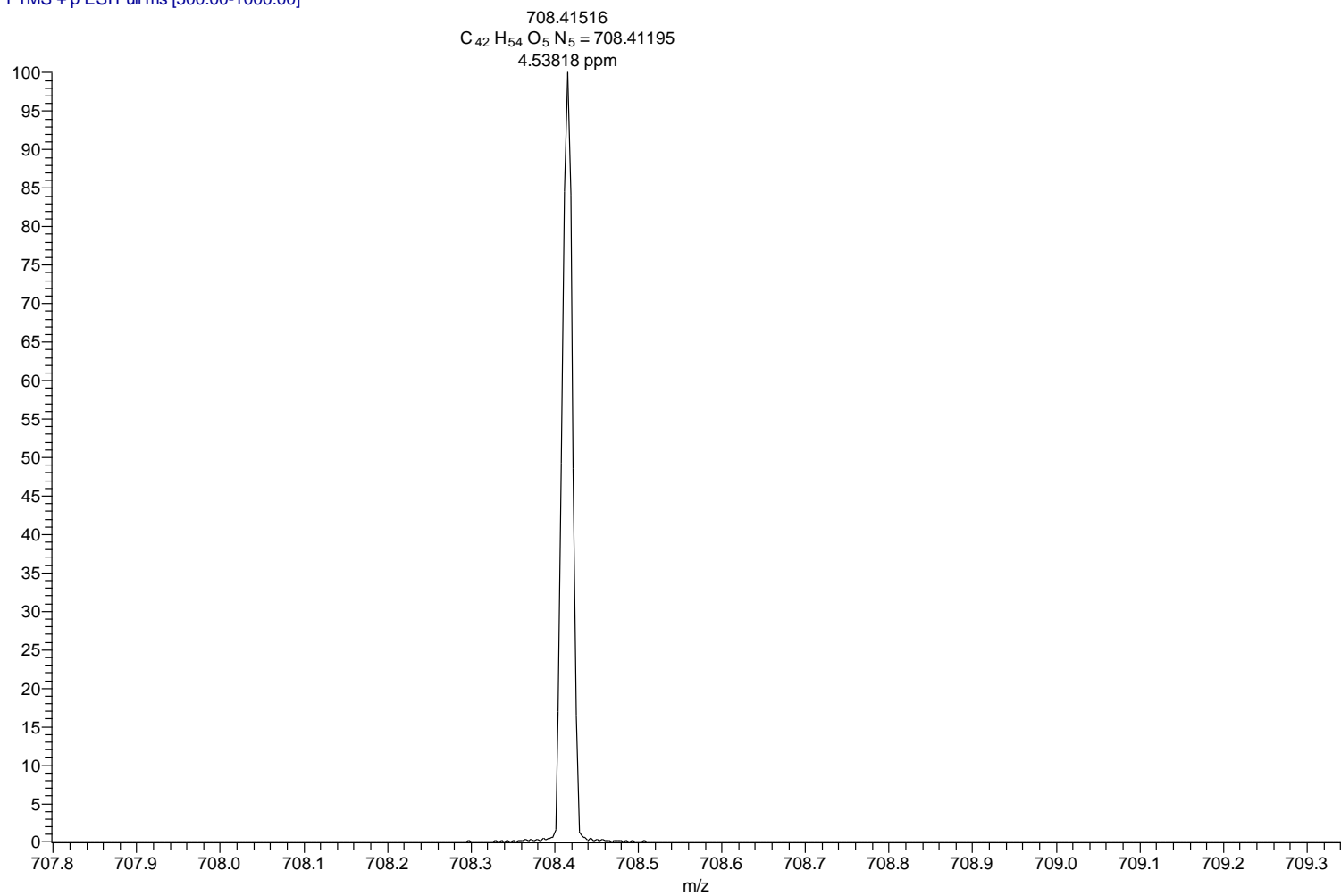


Figure S6: HRMS (ESI) of 13-(Hexylcarbamoyl)chlorin *e*6 15,17-dimethyl ester (**3**)

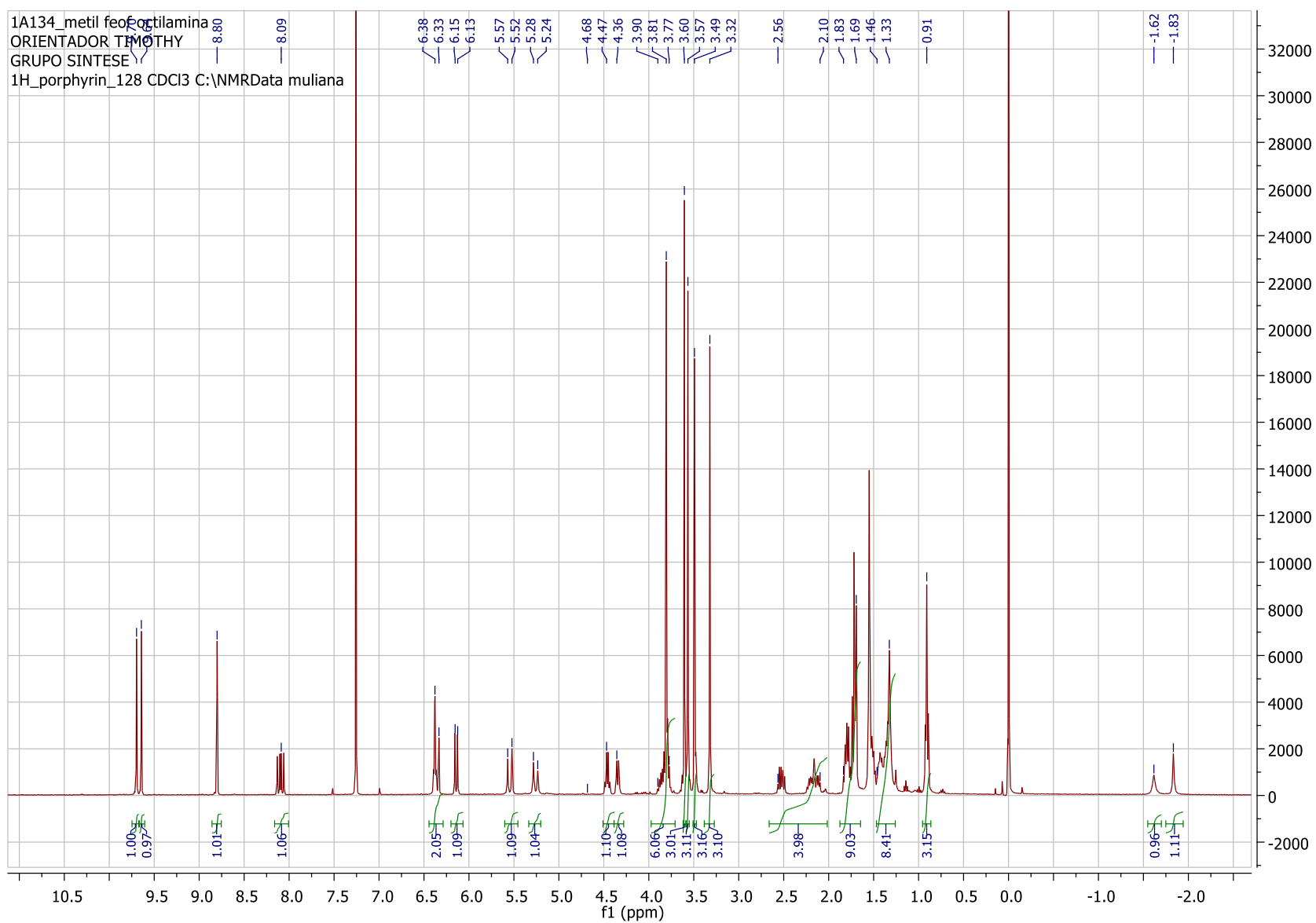


Figure S7: ^1H -NMR (CDCl_3) spectrum of 13-(Octylcarbamoyl)chlorin *e6* 15,17-dimethyl ester (**4**)

mefeoctil+_150303155145 #4 RT: 0.14 AV: 1 NL: 3.09E7
T: FTMS + p ESI Full ms [700.00-800.00]

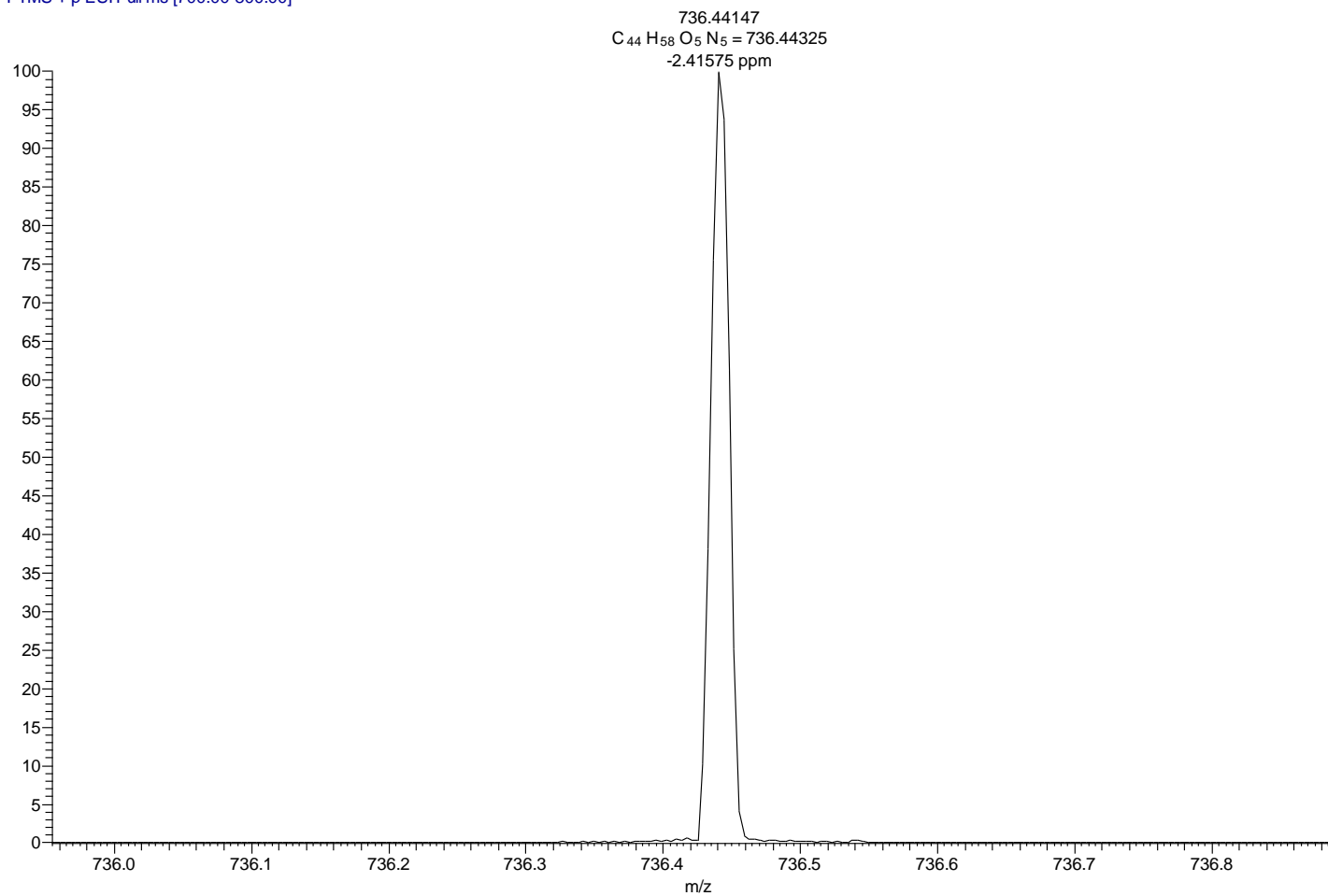


Figure S8: HRMS (ESI) of 13-(Octylcarbamoyl)chlorin *e*6 15,17-dimethyl ester (**4**)

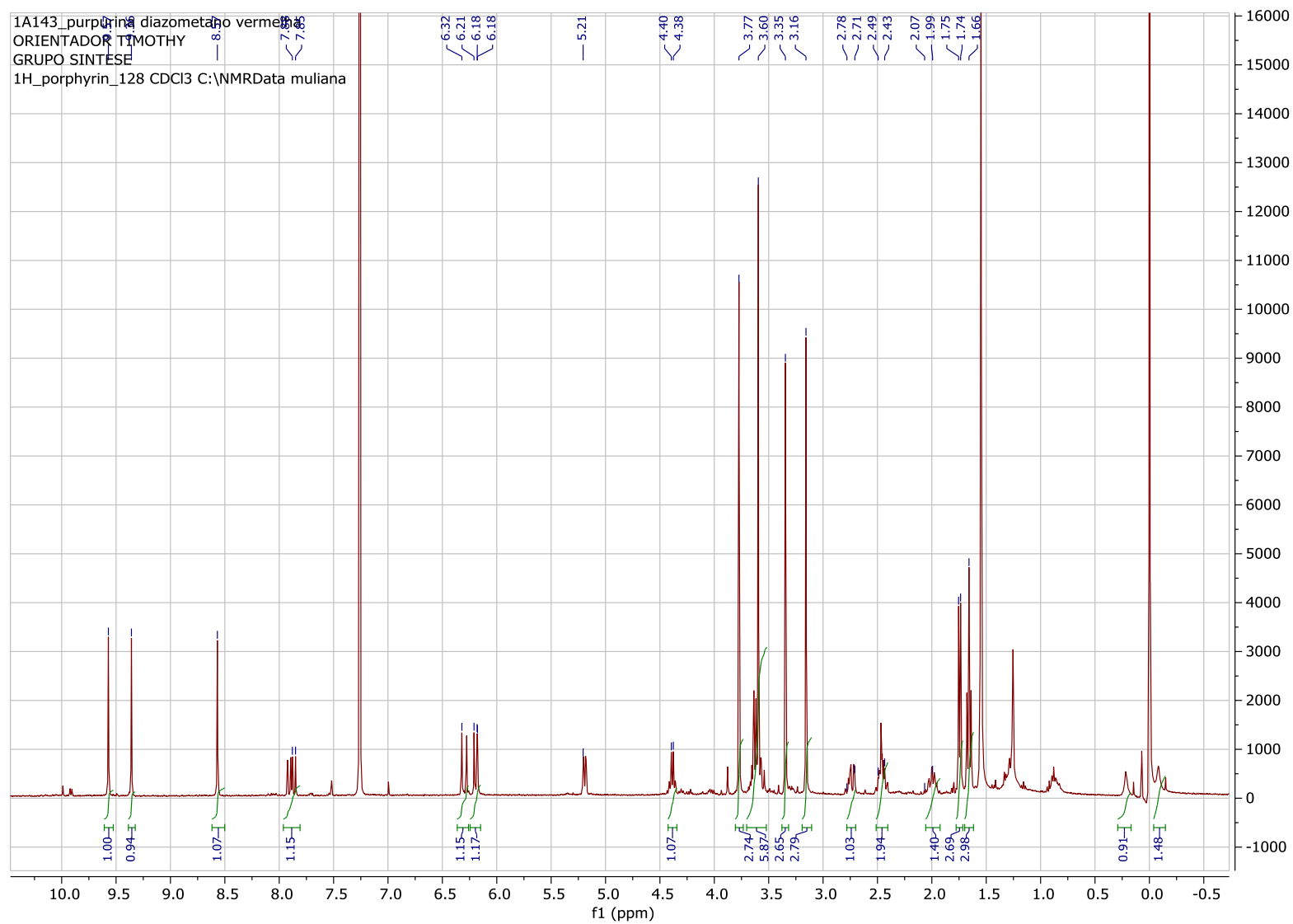


Figure S9: ^1H -NMR (CDCl_3) spectrum of Purpurin-18 Methyl Ester (**5**)

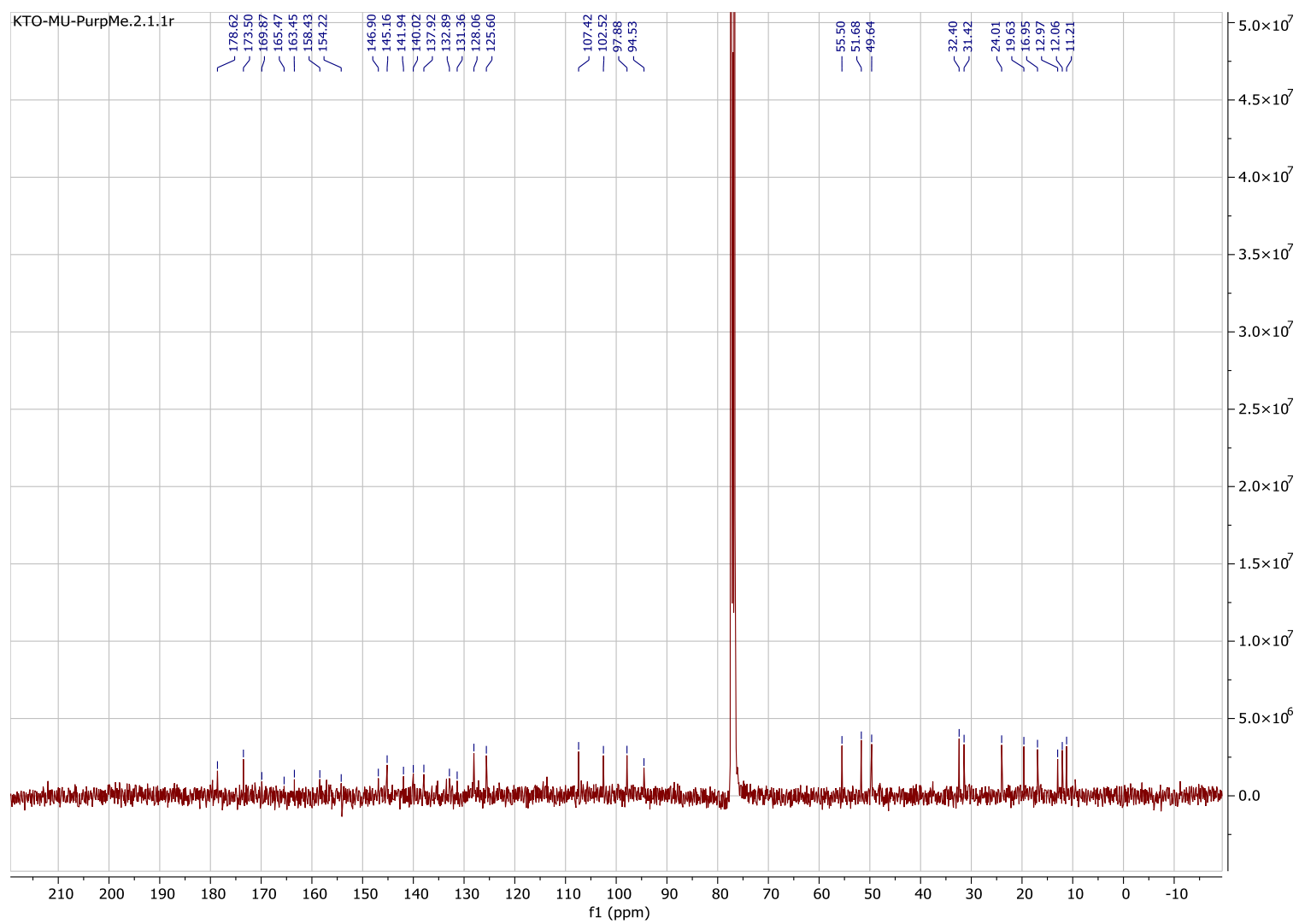


Figure S10: ^{13}C -NMR (CDCl_3) spectrum of Purpurin-18 Methyl Ester (**5**)

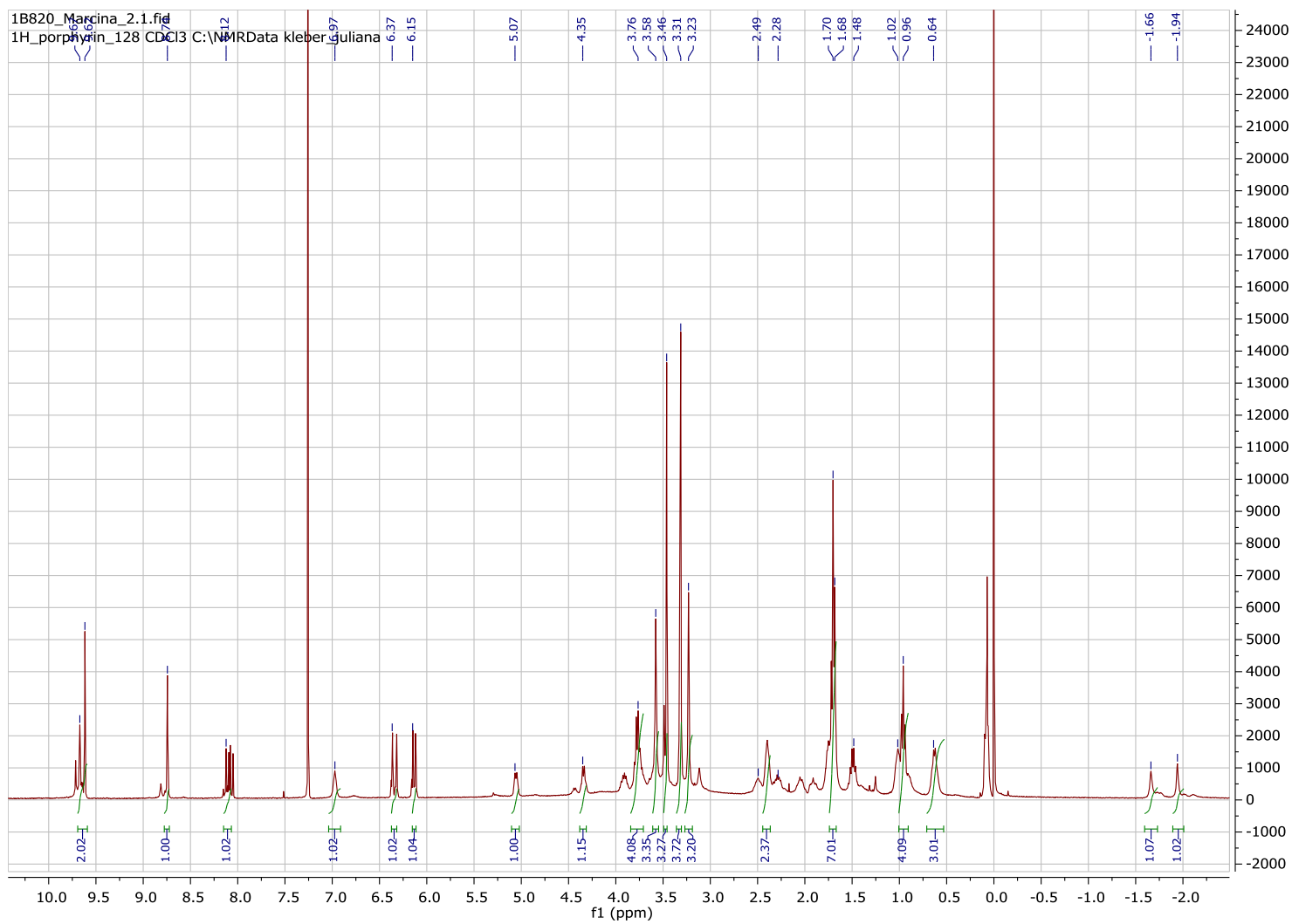


Figure S11: ^1H -NMR (CDCl_3) spectrum of Chlorin-p, 6-N-Butylamide-7-methyl Ester (**6**)

pupurinabutil(+)_150303150500 #1 RT: 0.01 AV: 1 NL: 8.46E7
T: FTMS + p ESI Full ms [600.00-700.00]

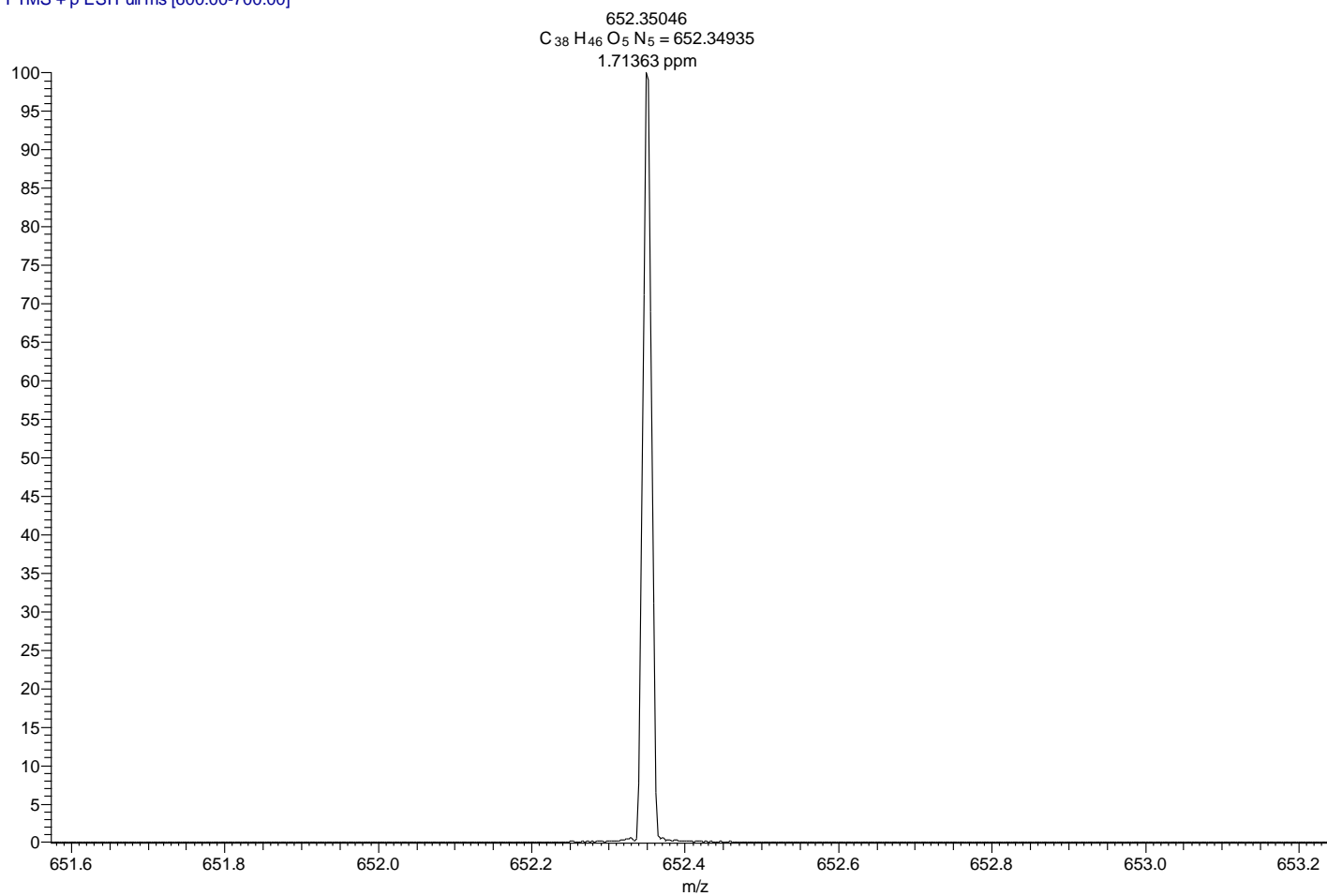
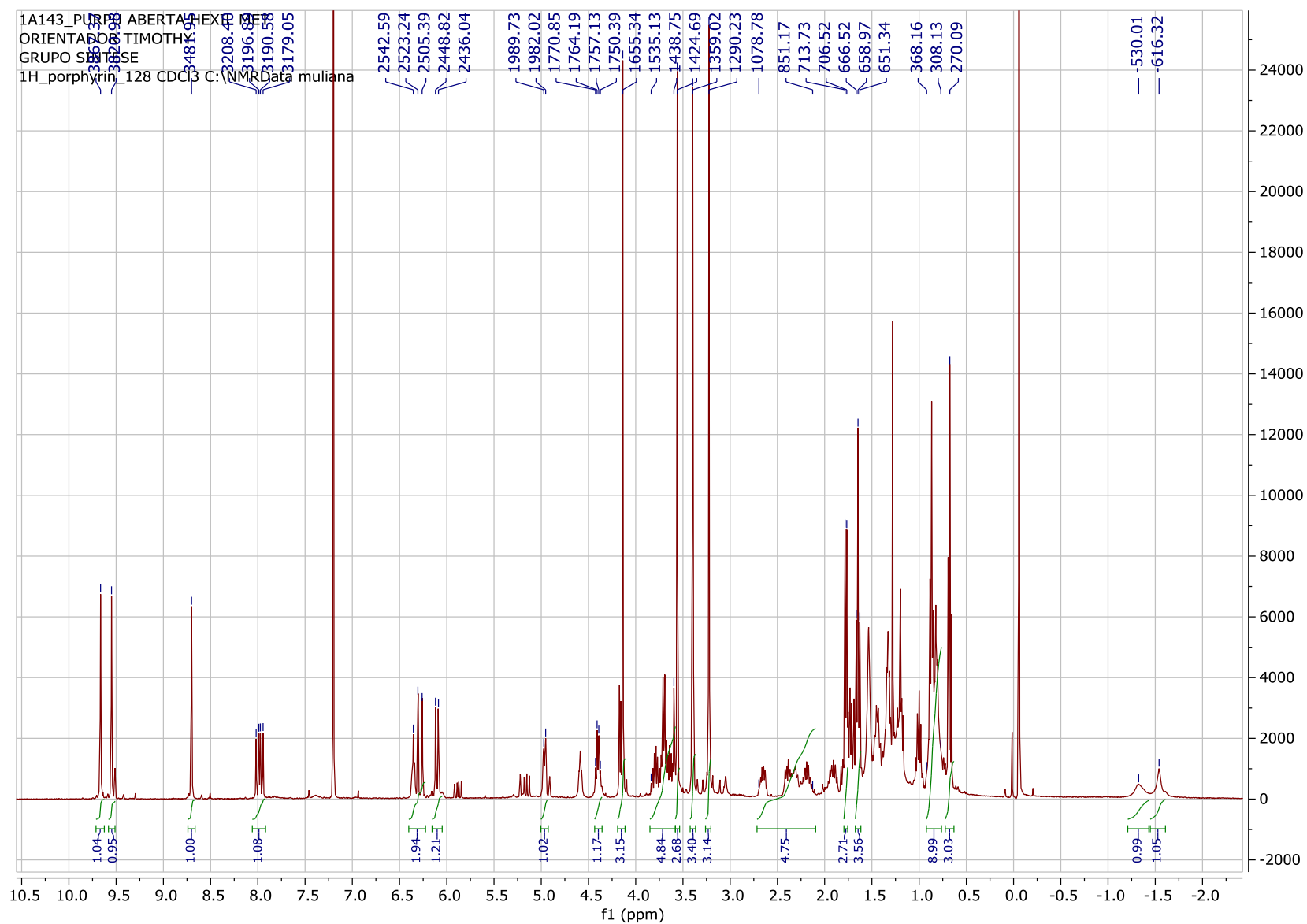


Figure S12: HRMS (ESI) of Chlorin-p, 6-N-Butylamide-7-methyl Ester (**6**)



purpurina hexil(+)_150110103539 #1 RT: 0.01 AV: 1 NL: 7.18E6
T: FTMS + p ESI Full ms [650.00-750.00]

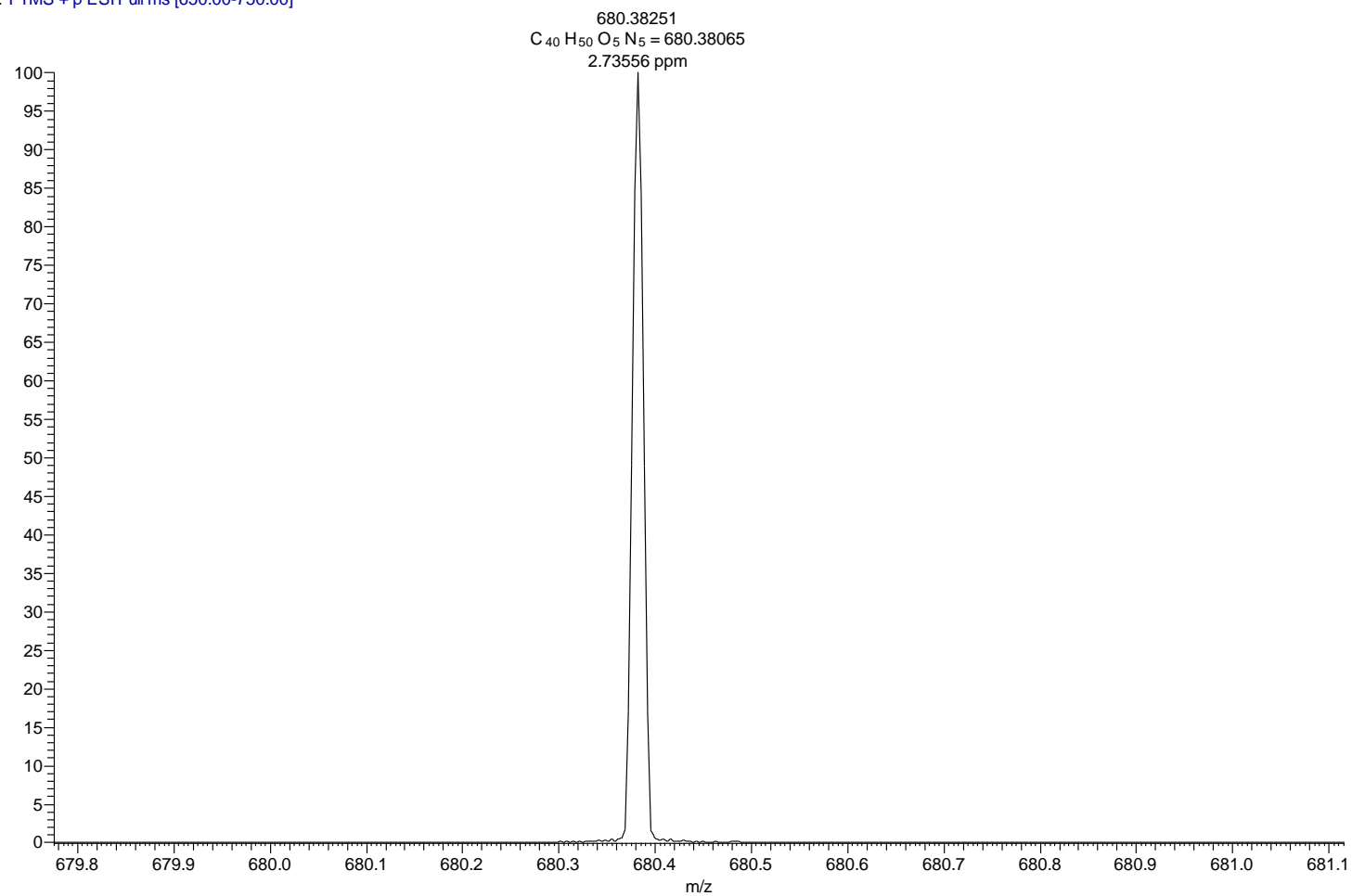


Figure S14: HRMS (ESI) of Chlorin-p, 6-N-hexylamide-7-methyl Ester (**7**)

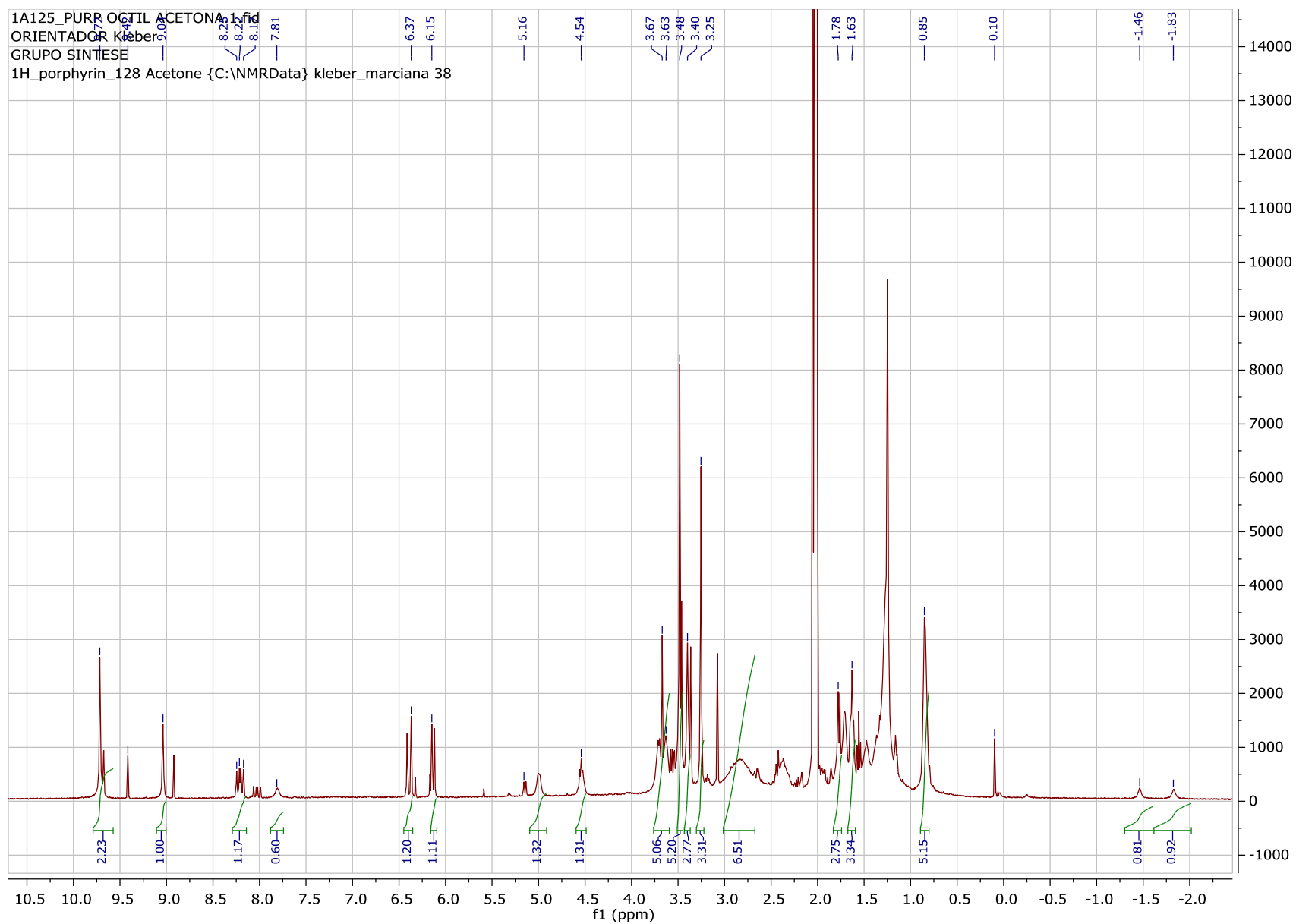


Figure S15: ^1H -NMR (CDCl_3) spectrum of Chlorin-p, 6-N-octylamide-7-methyl Ester (**8**)

purpurina octil(+)_150110103539 #1 RT: 0.01 AV: 1 NL: 2.03E7
T: FTMS + p ESI Full ms [650.00-750.00]

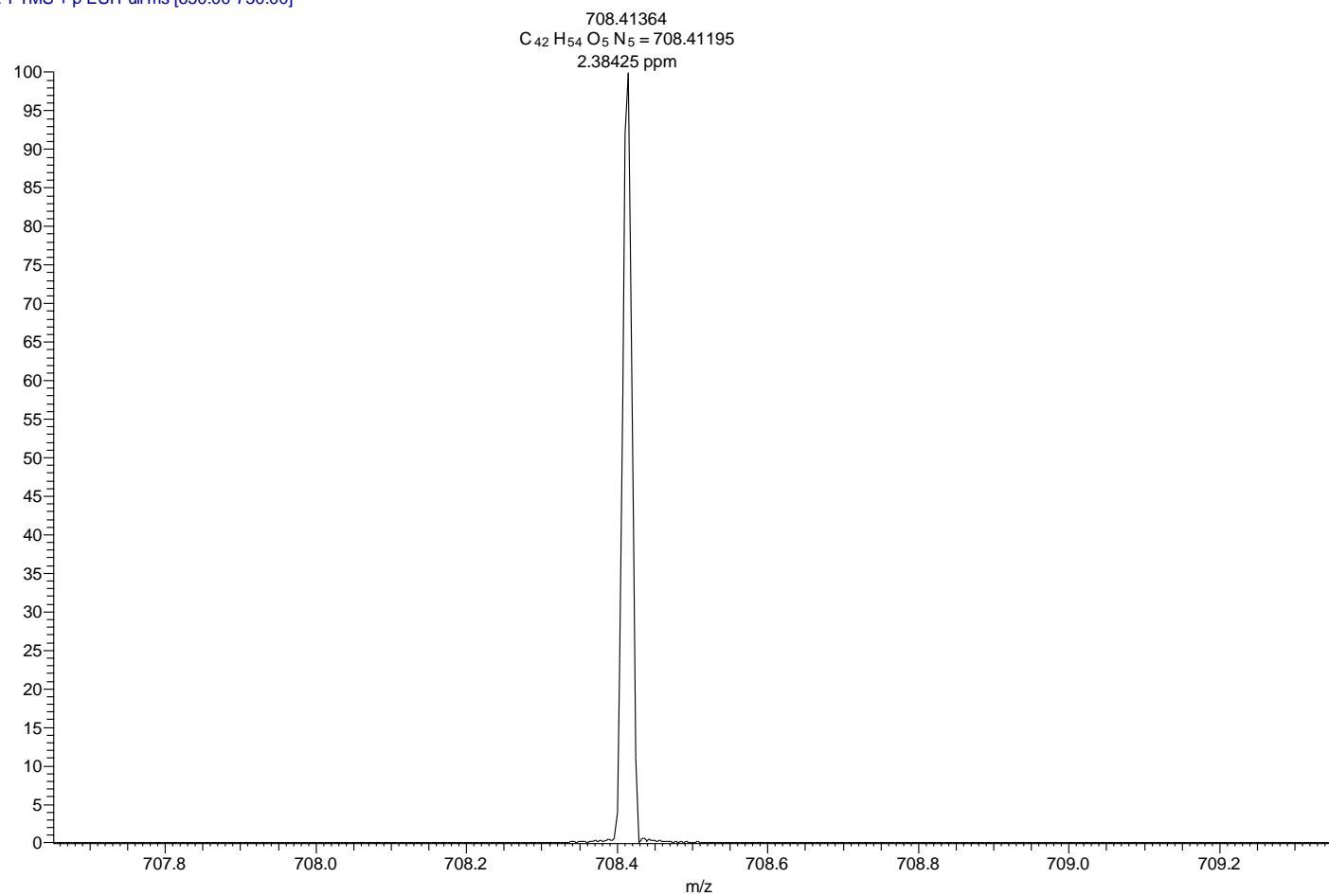


Figure S16: HRMS (ESI) of Chlorin-p, 6-N-octylamide-7-methyl Ester (**8**)



Figure S17: Homemade engineered Biotable model for PDI studies (660 nm).

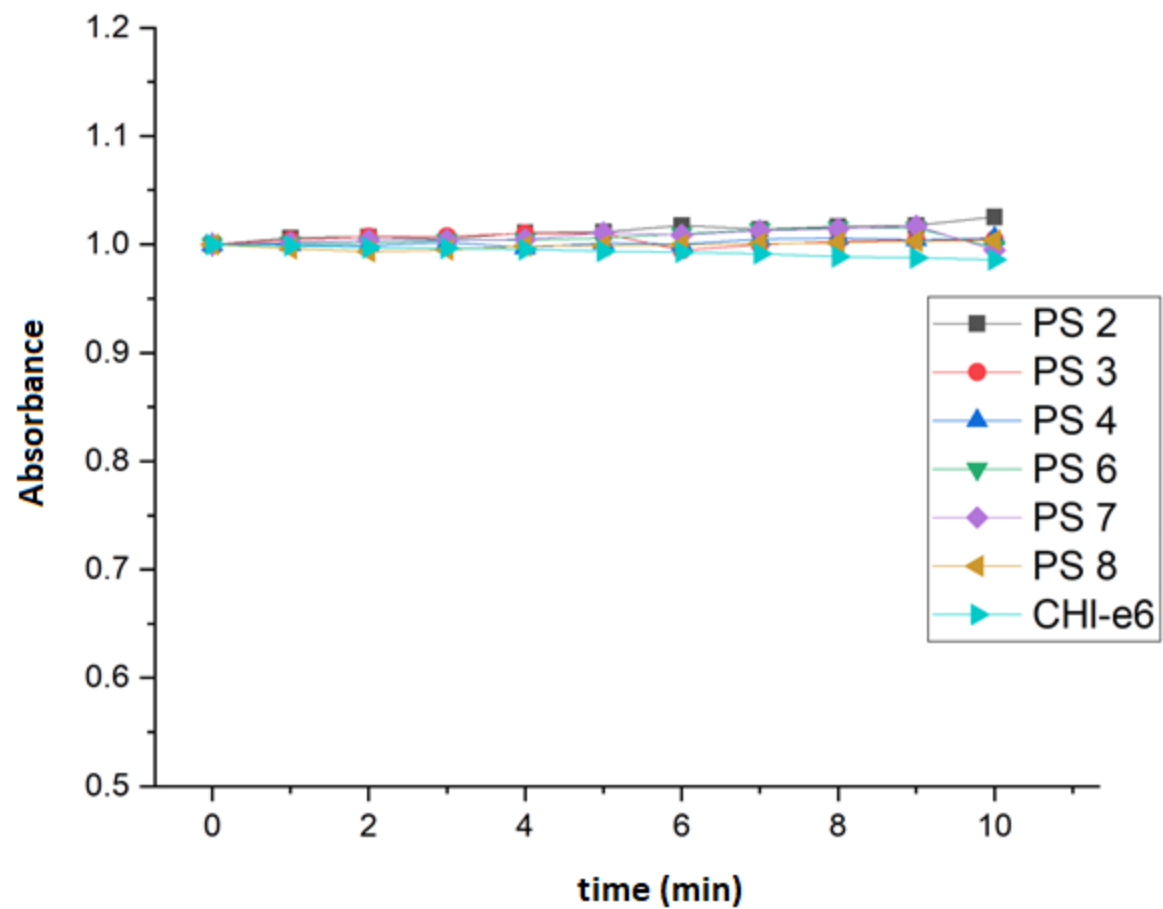


Figure S18: Photodegradation experiment at 660 nm at 63.7 mWcm⁻² using ethyl acetate as solvent.

Table S1: Wavelengths data and Quantum yield of Singlet Oxygen $^1\text{O}_2$ data of the literature for some of the compounds.

PS	Our work (UV-Vis)	Literature data (UV-Vis) and Literature data Quantum yield of singlet oxygen $^1\text{O}_2$
Methyl pheophorbide-a (1)	λ_{max} (CH_2Cl_2) (nm): 666, 609, 534, 505, 409.	λ_{max} (CH_2Cl_2) 668 (44 600), 610 (8 620), 538 (9 710), 506 (10 800), 412 (106 000) ¹ Quantum yield of singlet oxygen $^1\text{O}_2$ 0.44 (in benzene); 0.47 (in 1-octanol) ²
13-(Butylcarbamoyl)-chlorin e6 15,17-dimethyl ester (2)	λ_{max} (CH_2Cl_2) (nm): 662, 607, 528, 498, 399.	λ_{max} , nm (CHCl_3) 664, 608, 558, 529, 501 402. ³
13-(Hexylcarbamoyl)chlorin e6 15,17-dimethyl ester (3)	λ_{max} (CH_2Cl_2) (nm): 663, 605, 527, 497, 398.	λ , nm (CHCl_3): 664, 609, 558, 528, 501, 402. ³
13-(Octylcarbamoyl)chlorin e6 15,17-dimethyl ester (4)	λ_{max} (CH_2Cl_2) (nm): 663, 609, 527, 497, 399.	UV-vis (CHCl_3): λ , nm (log ϵ) 664, 607, 558, 530, 502, 402. ³
Purpurin-18 Methyl Ester (5)	λ_{max} (CH_2Cl_2) (nm): 699, 642, 546, 508, 478, 410.	λ_{max} (nm) (CHCl_3): ($\epsilon \cdot 10^{-3}$): 360 (22.9); 413 (44.6); 481 (1.9); 510 (3.9); 548 (10.9); 646 (4.7); 701 (23.2) ⁴ Quantum yield of singlet oxygen $^1\text{O}_2$ 0.55 (in ethanol); 0.73 (in toluene); 0.80 (in pyridine) ⁵
Chlorin-p, 6-N-Butylamide-7-methyl Ester (6)	λ_{max} (CH_2Cl_2) (nm): 662, 606, 526, 498, 398.	$\lambda_{\text{max}}/\text{nm}$ 664 (ϵ 4.56 x 10 ⁴), 608 (1.08 x 10 ⁴), 532(1.13 x 10 ⁴), 500(1.90 x 10 ⁴) and 404(1.37 x 10 ⁵) ⁶

Chlorin-p, 6-N-hexylamide-7-methyl Ester (7)	λ_{max} (CH ₂ Cl ₂) (nm): 666, 608, 528, 497, 398.	λ_{max} THF/CH ₂ Cl ₂ (1:4) (nm): 666 (1.78 x 10 ⁴), 612 (1.85 x 10 ³), 528 (1.73 x 10 ³), 498 (4.92 x 10 ³), 402 (5.11 x 10 ⁴) ⁷
Chlorin-p, 6-N-octylamide-7-methyl Ester (8)	λ_{max} (CH ₂ Cl ₂) (nm): 663, 605, 528, 499, 399.	Don't have this data

Reference:

¹ Ma, L.; Dolphin, D.; Nucleophilic reaction of 1,8- diazabicyclo[5.4.0]undec-7-ene and 1,5- diazabicyclo[4.3.0]non-5-ene with methyl pheophorbide a. Unexpected products. *Tetrahedron*, **1996**, 52 (3), 849-860. [https://doi.org/10.1016/0040-4020\(95\)00944-2](https://doi.org/10.1016/0040-4020(95)00944-2).

² Kustov, A. V.; Belykh, D. V.; Startseva, O. M.; Kruchin, S. O.; Venediktov, E. A.; Berezin, D. B. *Pharm Anal Acta*. **2016**, 7(5), 1-5. <https://doi.org/10.4172/2153-2435.1000480>.

³ Belykh, D. V.; Tarabukina, I. S.; Gruzdev, I. V.; Kodess, M. I.; Kutchin, A. V. Aminomethylation of chlorophyll a derivatives using bis(N,N-dimethylamino)methane. *Porphyrins Phthalocyanines* **2009**, 13, 949–956. <https://doi.org/10.1142/S1088424609001133>.

⁴ Drohat, N.; Barriere, M.; Granet, R.; Sol, V.; Krausz, P. High yield preparation of purpurin-18 from *Spirulina maxima*. *Dyes Pigm.* **2011**, 88 (1), 125-127, <https://doi.org/10.1016/j.dyepig.2010.05.006>.

⁵ Redmond, R. W.; Gamlin, J. N. A Compilation of Singlet Oxygen Yields from Biologically Relevant Molecules. *Photochem. Photobiol.* **1999**, 70 (4), 391- 475. <https://doi.org/10.1111/j.1751-1097.1999.tb08240.x>

⁶ Lee, S. J. H.; Jagerovic, N.; Smith, K. M. Use of the Chlorophyll derivative, Purpurin-18, for Syntheses of Sensitizers for use in Photodynamic Therapy. *Journal of the Chemical Society-Perkin Transactions 1*. **1993**, (19), 2369-2377. <https://doi.org/10.1039/p19930002369>

⁷ Journal of Medicinal Chemistry (2001), 44(10), 1540-1559. <https://scifinder-n-cas.ez350.periodicos.capes.gov.br/searchDetail/reaction/62fbd8f0fd474116c001ae34/reactionDetails> CAS Method Number 3-366-CAS-9701836