

Supplementary data

The effect of conjugation with octaarginine, a cell-penetrating peptide on antifungal activity of imidazoacridinone derivative

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1. The synthesis of C-1296, C-1305, C-1311, C-1410 and Compound 1

1.1. The synthesis of triazoloacridinone derivatives

The 8-substituted 5-[(aminoalkyl)amino]-6H-v- triazolo [4,5,l-de]-acridin-6-ones (C-1305, C-1296 and C-1410) presented in Scheme I were prepared according to the previously reported procedure [Cholody, W.M., Martelli, S., Konopa, J., 8-Substituted 5[(aminoalkyl-amino-6H-[1,2,3]-triazolo[4,5,l-de]acridin-6-ones as potential antineoplastic agents. Synthesis and biological activity. J. Med. Chem., 1990, 33, 2852-2856, doi:10.1021/jm00172a028]. The required starting materials 1-chloro-4-nitro-9(10H)-acridinones (**I**) was prepared on the basis of the method published earlier [Capps D. B., Dunbar J., Kesten S. R., Shillis J., Werbel L. M., 2-(Aminoalkyl)-5-nitropyrazolo[3,4,5-kl]-acridines, a New Class of Anticancer Agents, J. Med. Chem., 1992, 35, 4770-4778]. The studied derivatives of 5-amino-6H-v-triazolo[4,5,l-de]acridin-6-one were prepared by the condensation of triazoloacridinones (**III**) with suitable aliphatic amines in DMSO or DMA. The compounds were obtained as hydrochlorides.

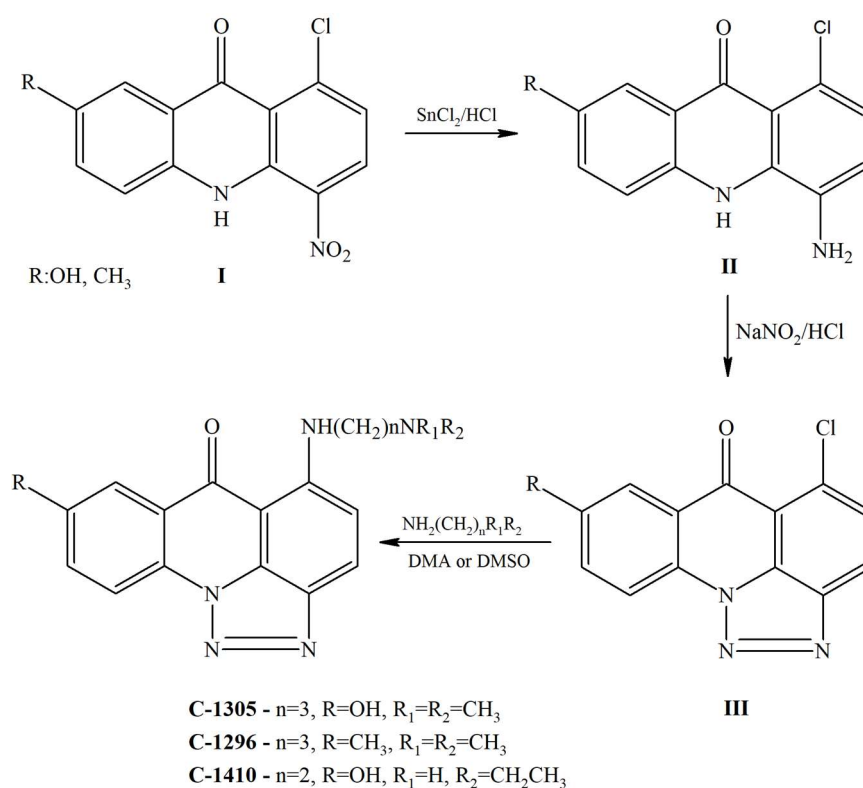
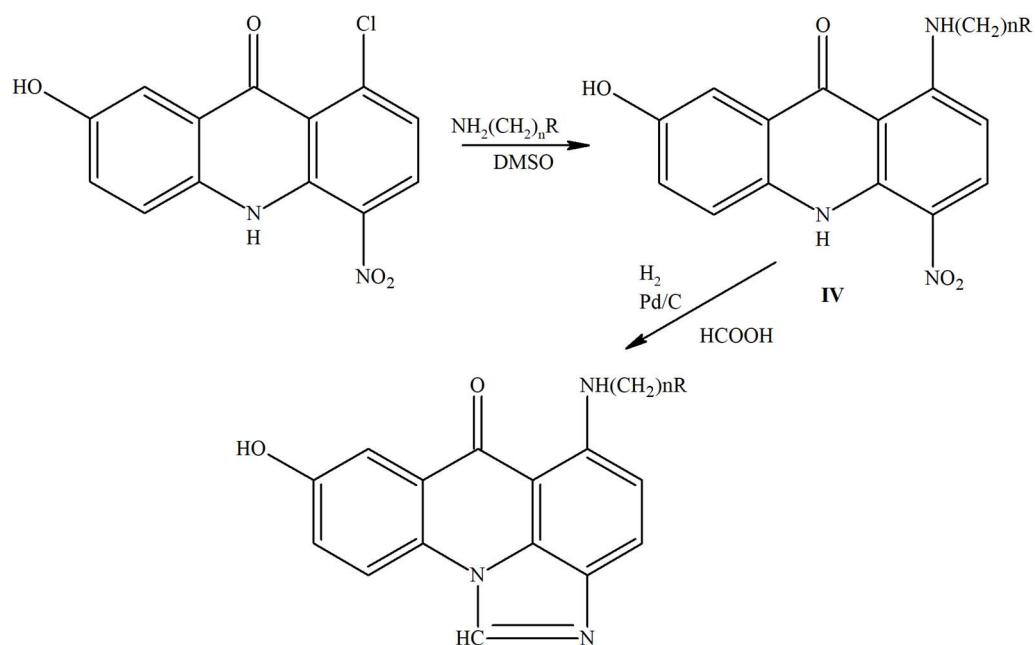


Figure S1. Strategy of the synthesis of compounds C-1305, C-1296 and C-1410.

1.2. The synthesis of imidazoacridinone derivatives

Compounds **C-1311** and **Compound 1** were synthesized starting from 1-chloro-7-hydroxy-4-nitro-9(10H)-acridinone, through the substitution of aliphatic amines, reduction and cyclization of the resulting derivatives. This method of synthesis was described previously [Chołody W.M., Martelli S., Pardziej-Lukowicz J. Konopa J., 5-[(Aminoalkyl)amino]imidazo[4,5,1-de]acridin-6-ones as a novel class of antineoplastic agents. Synthesis and biological activity, J. Med. Chem., 1990, 33, 49-52, doi:10.1021/jm00163a009; Konieczny M.T., Konopa J.K., Acridone derivatives and preparation of 8-hydroxy-imidazoacridinone derivatives, 1998, GB 2317888]. The strategy of **C-1311** and **Compound 1** synthesis is presented on Figure S2.



C-1311: $n=2$, $\text{R}=\text{N}(\text{CH}_2\text{CH}_3)_2$

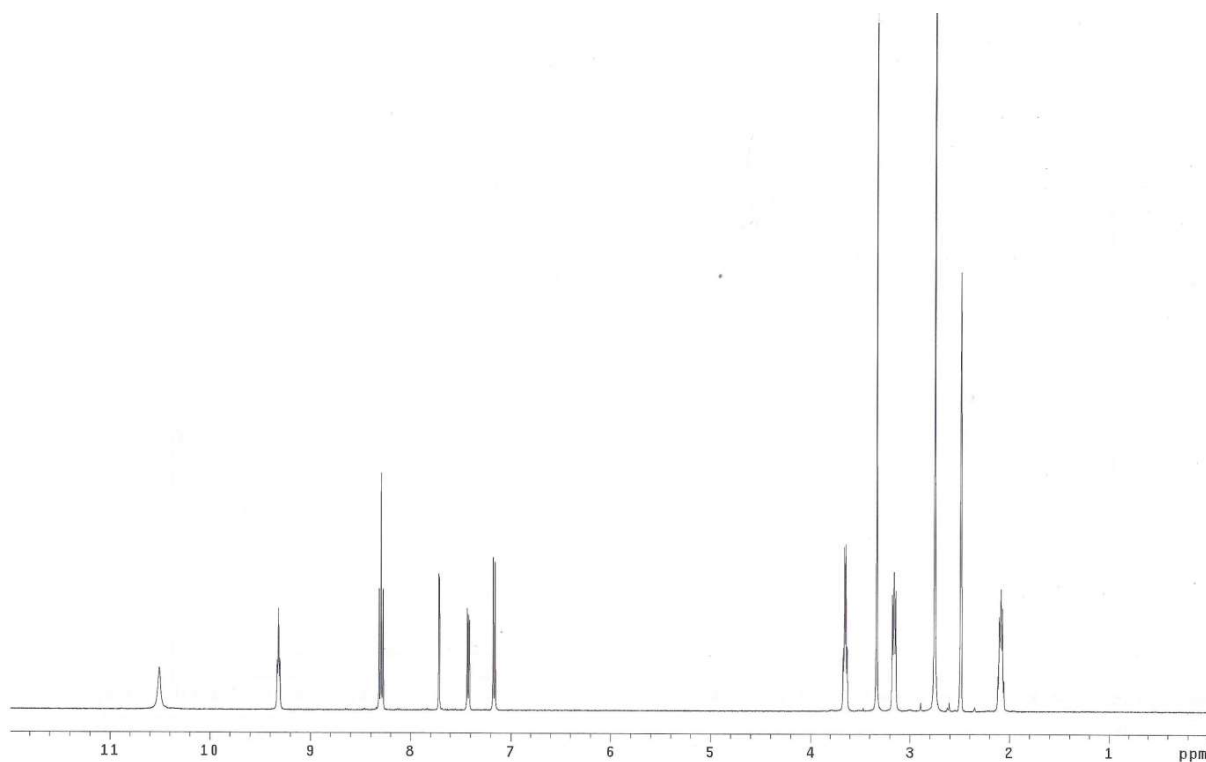
Compound 1: $n=2$, $\text{R}=\text{NH}_2$

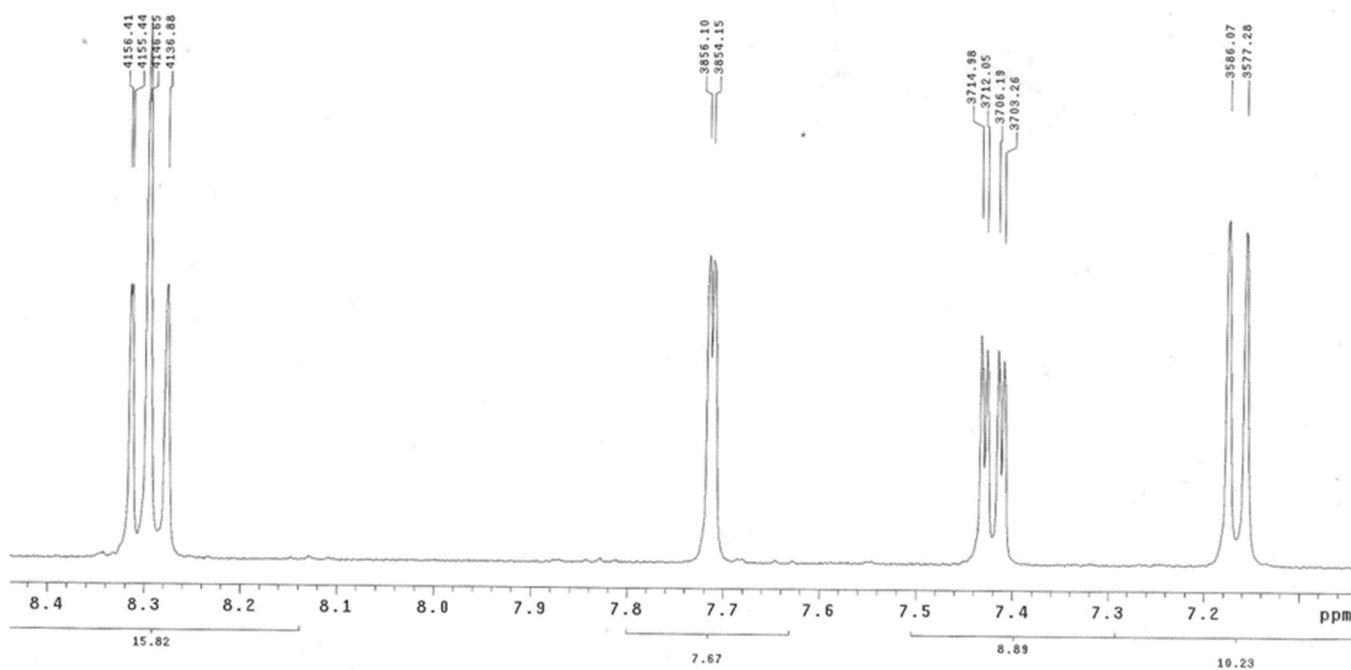
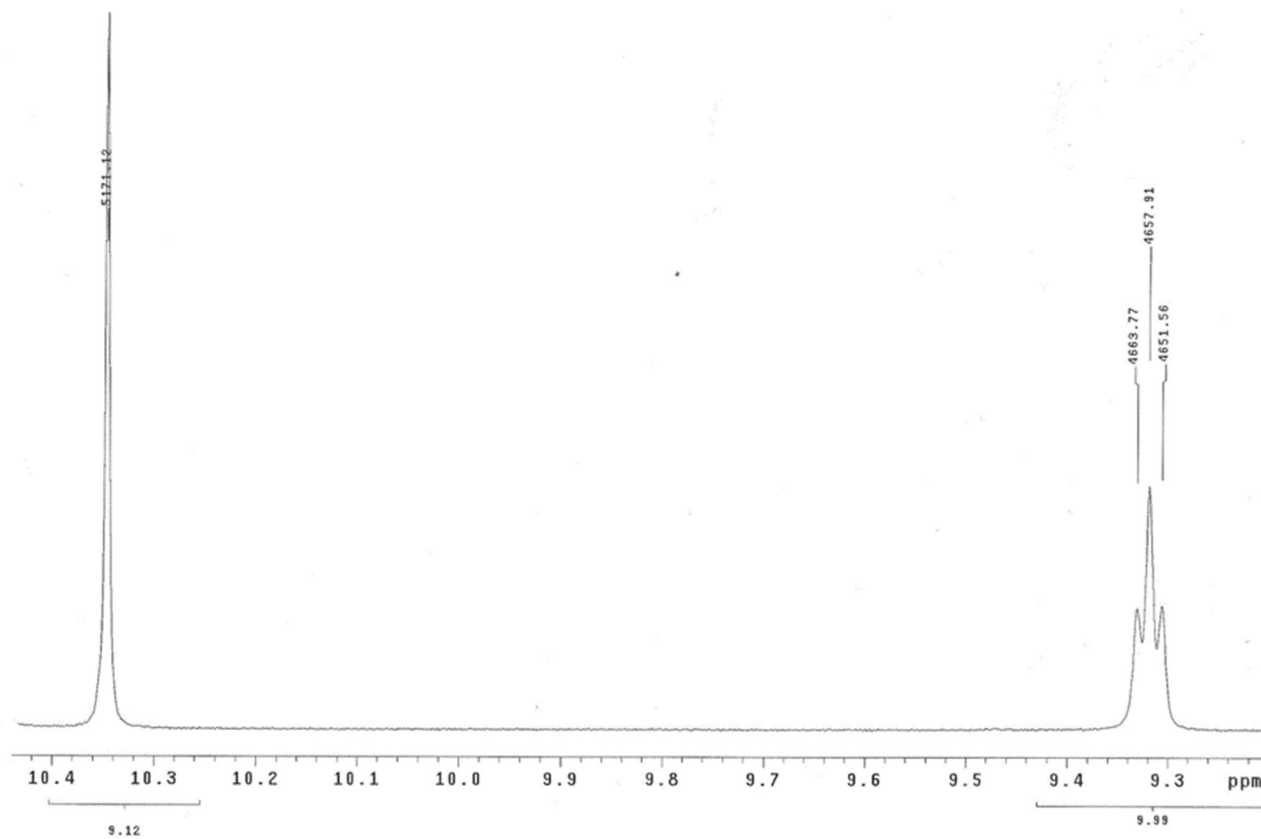
Figure S2. The strategy of C-1305 and Compound 1 synthesis.

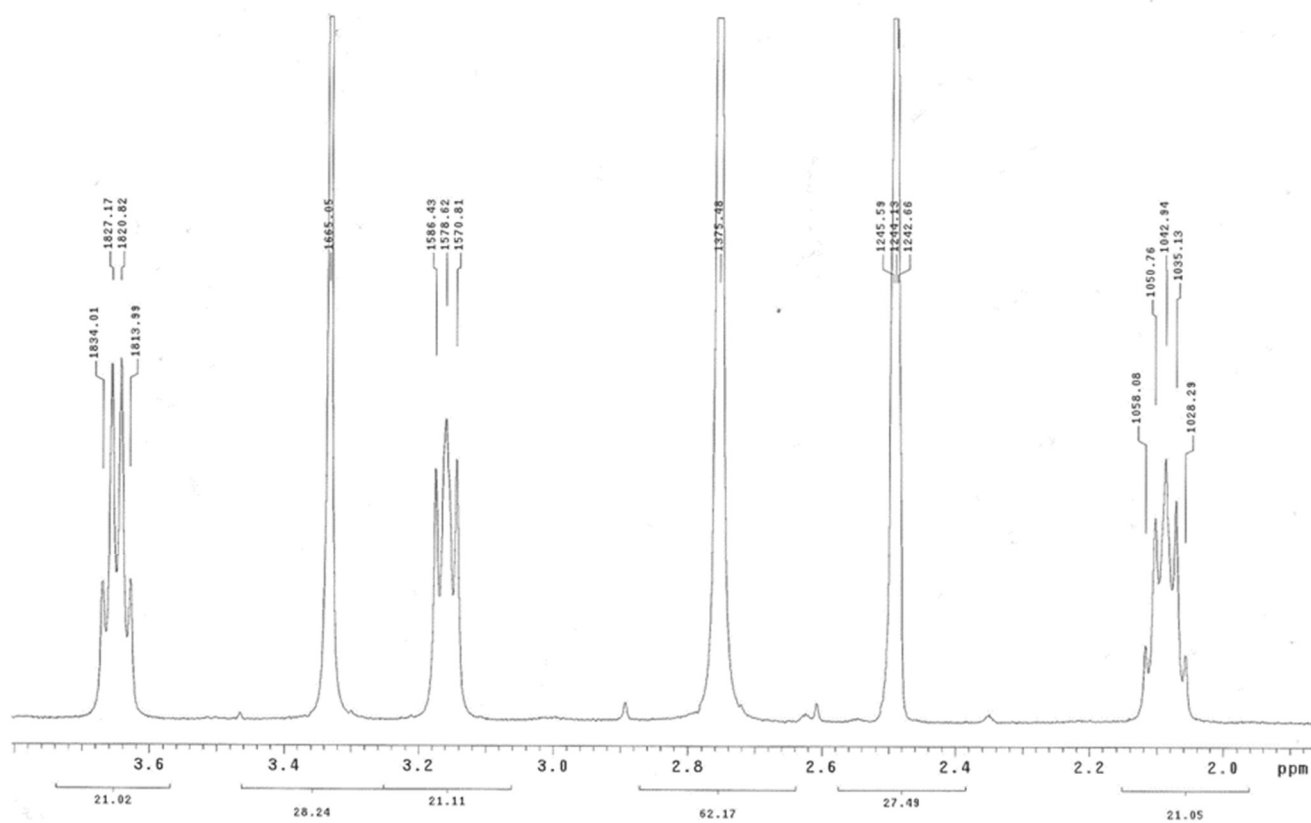
1.3. ^1H NMR, ^{13}C NMR and ESI-MS Spectra for imidazo and triazoloacridinone derivatives

C-1305 analysis

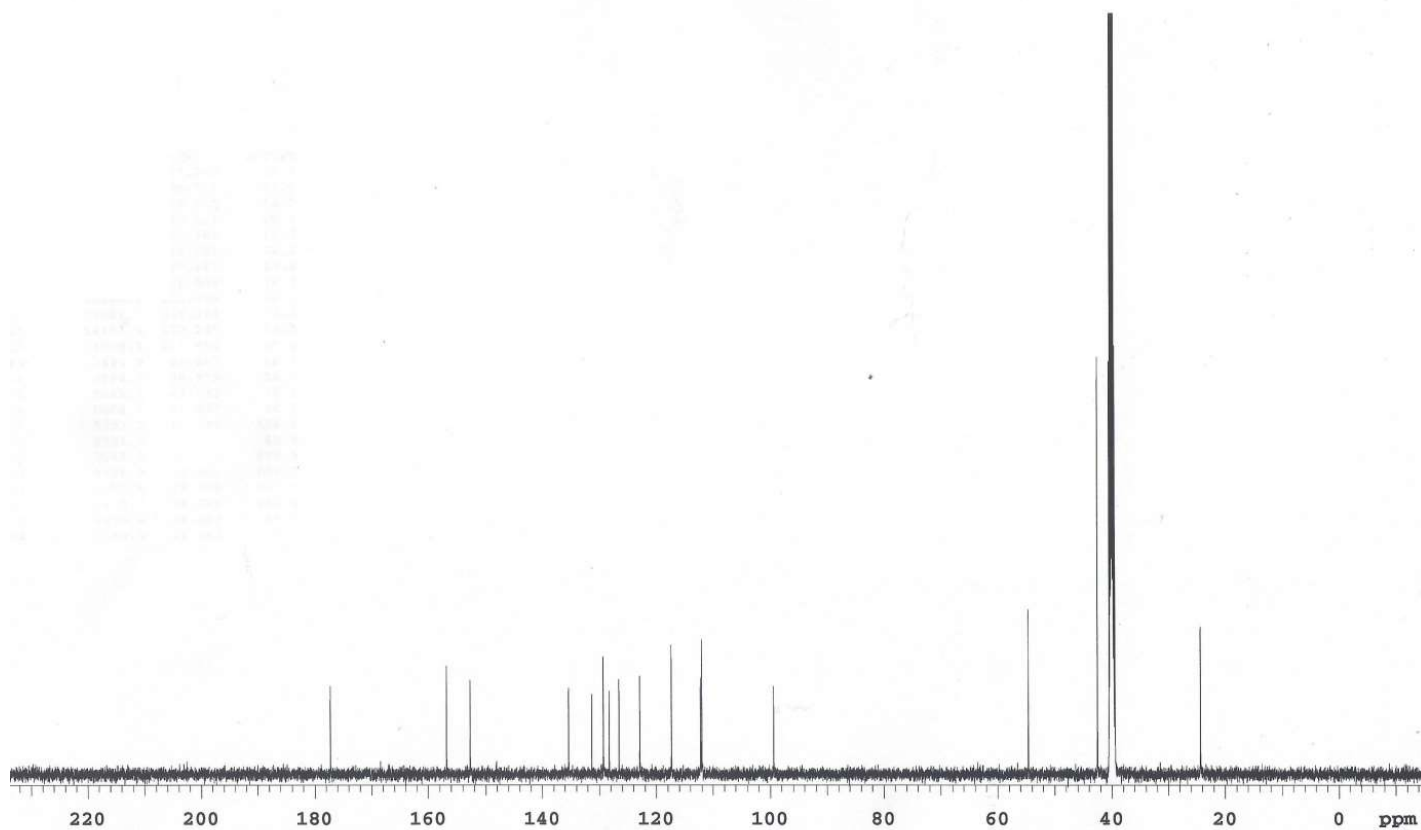
^1H NMR



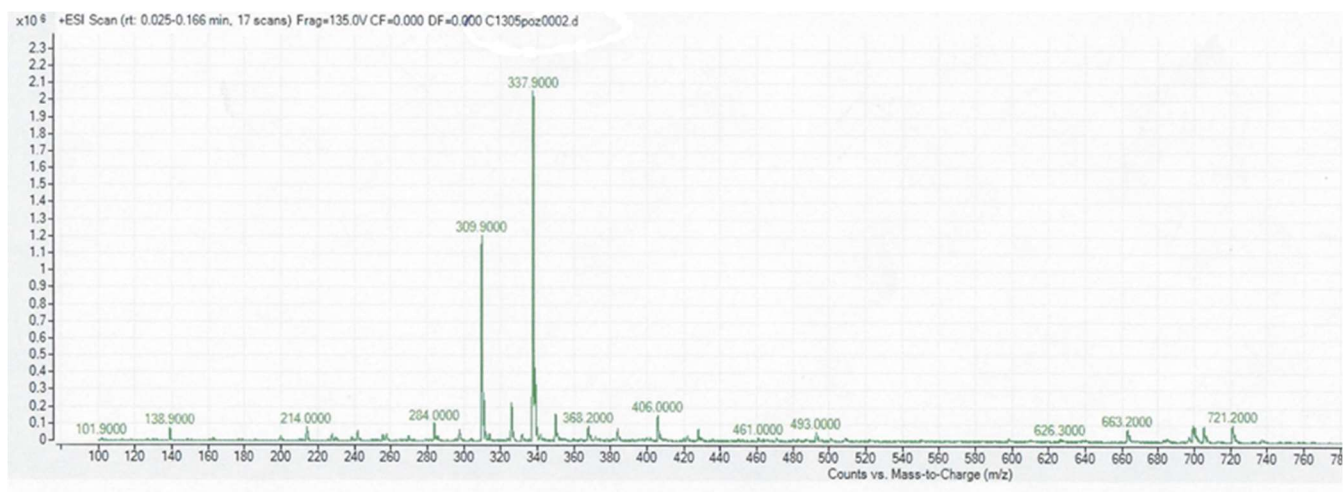




^{13}C NMR

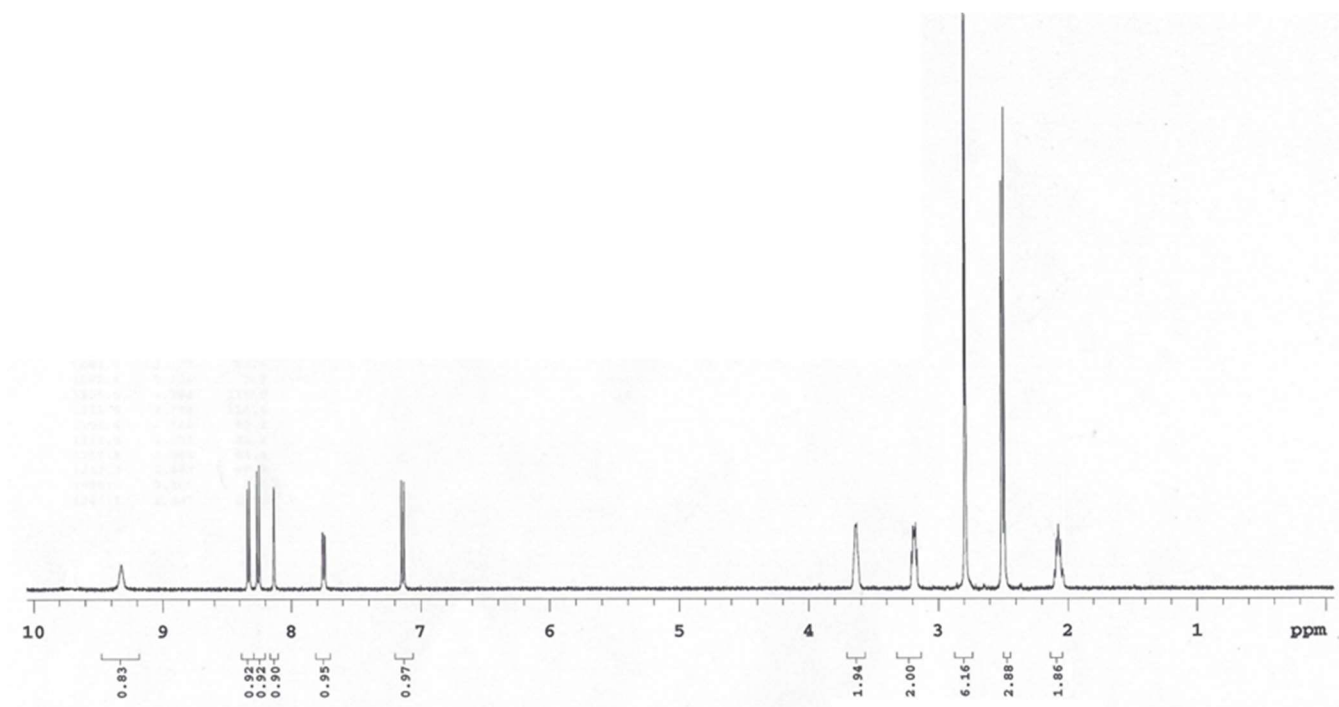


ESI-MS Spectra

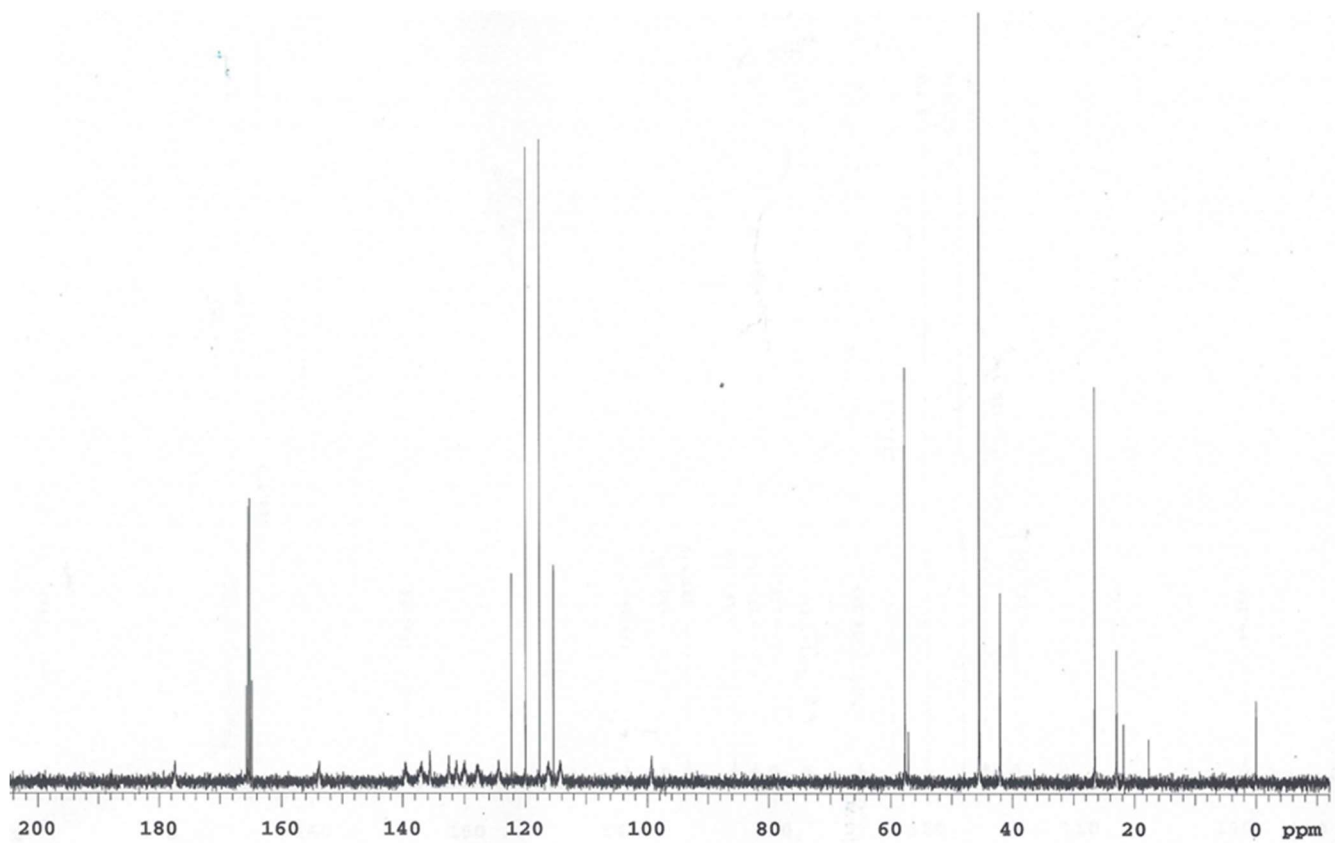


C-1296 analysis

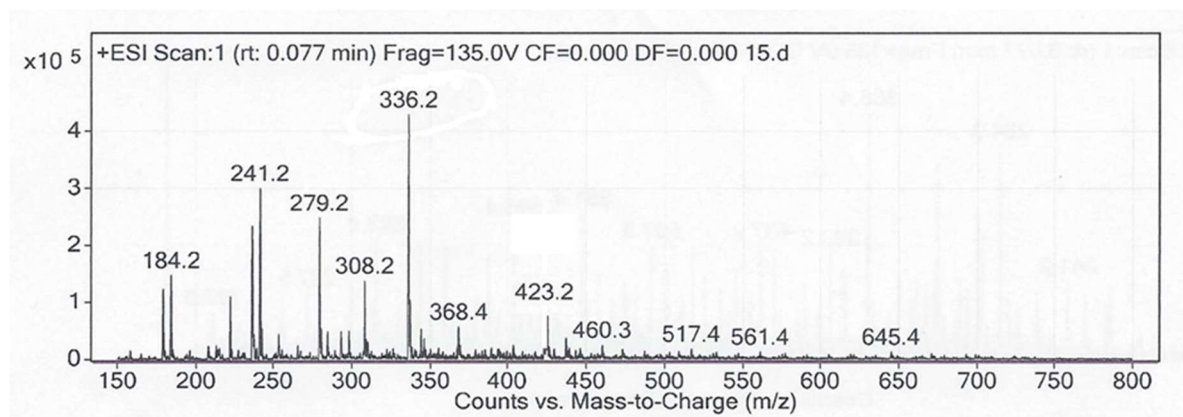
¹H NMR



¹³C NMR

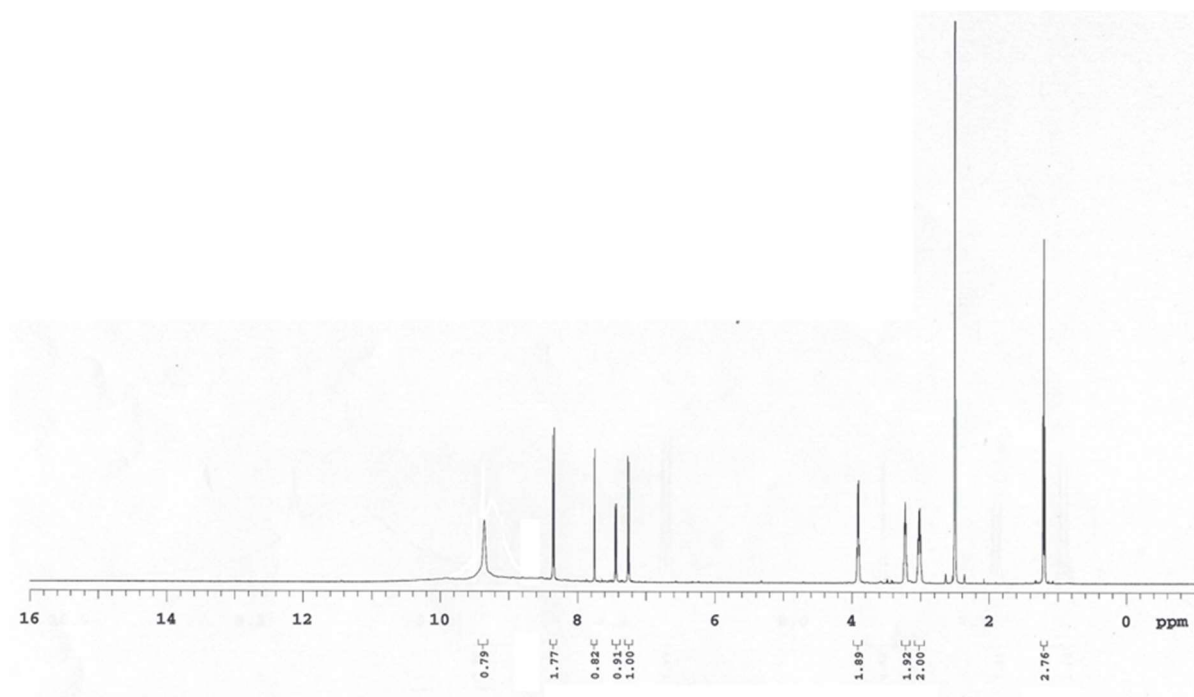


ESI-MS Spectra

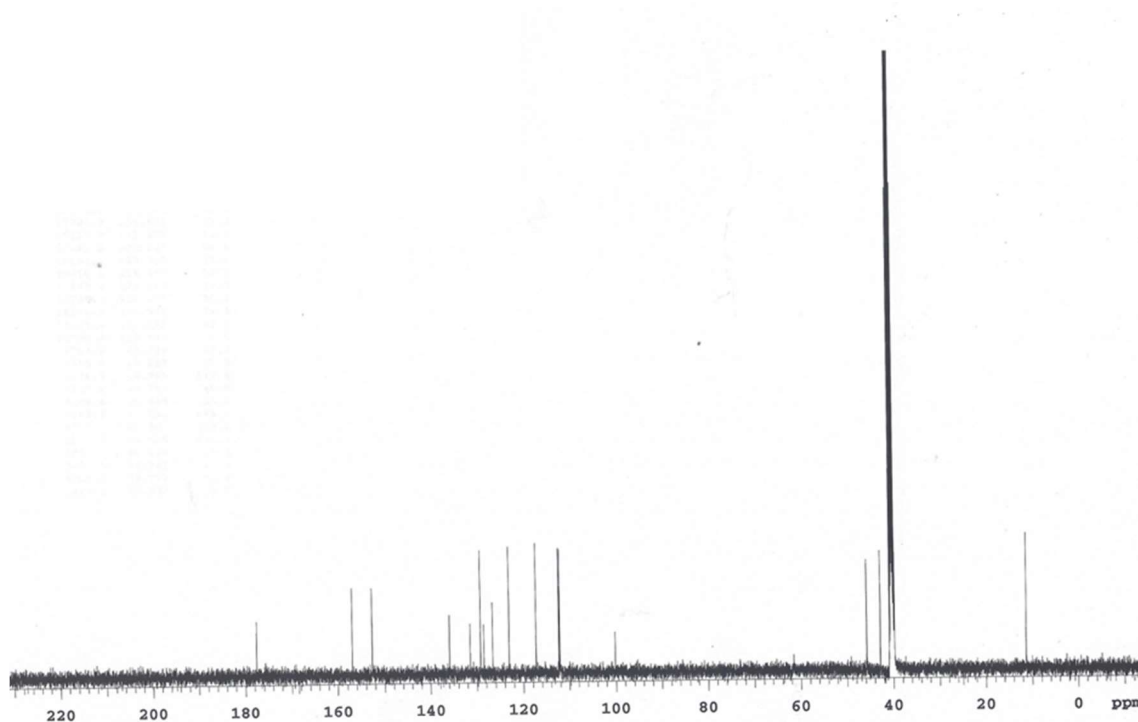


C-1410 analysis

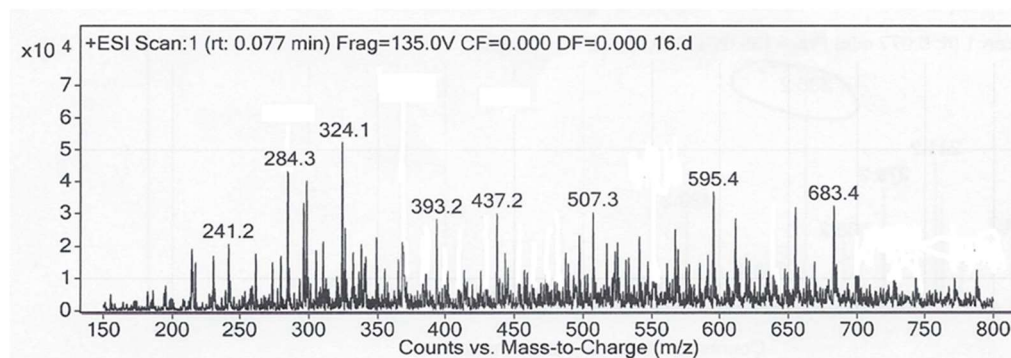
¹H NMR



^{13}C NMR

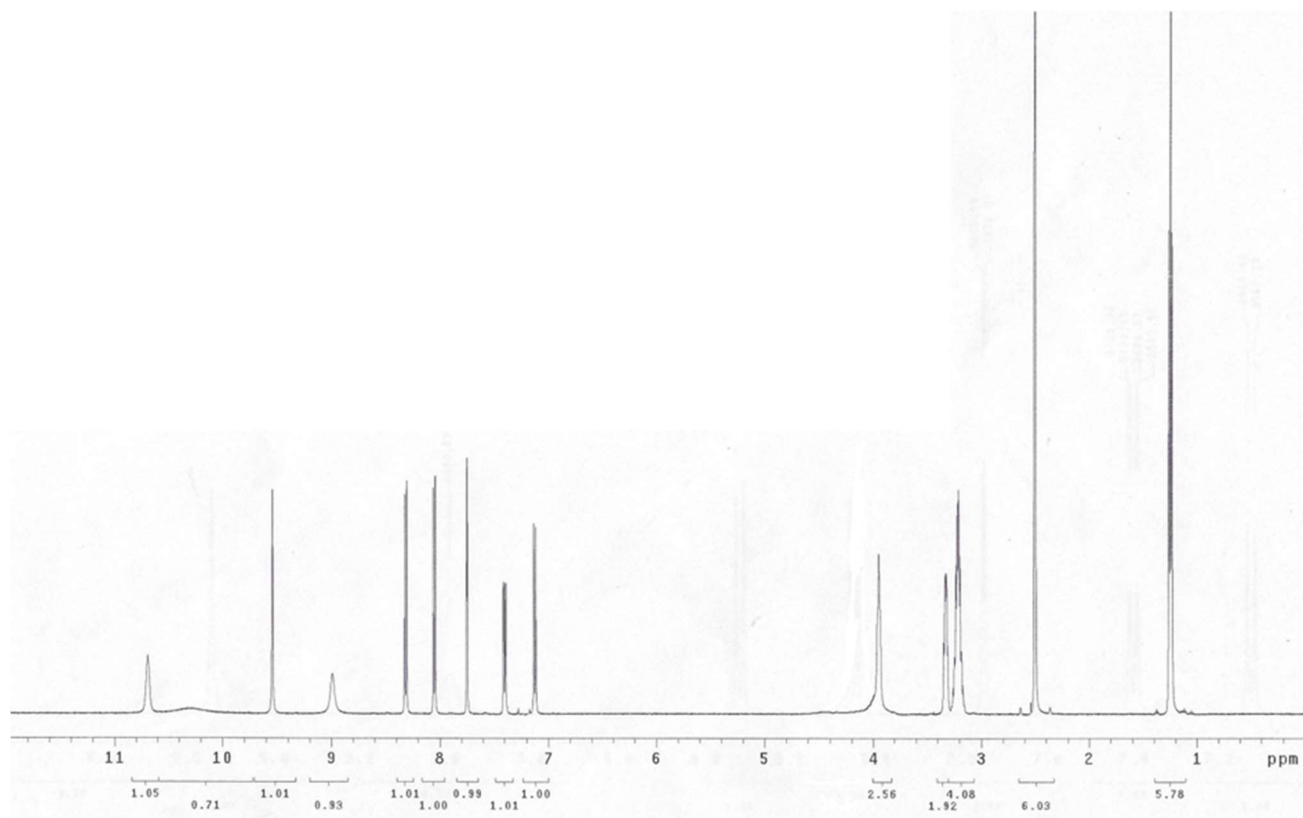


ESI-MS Spectra

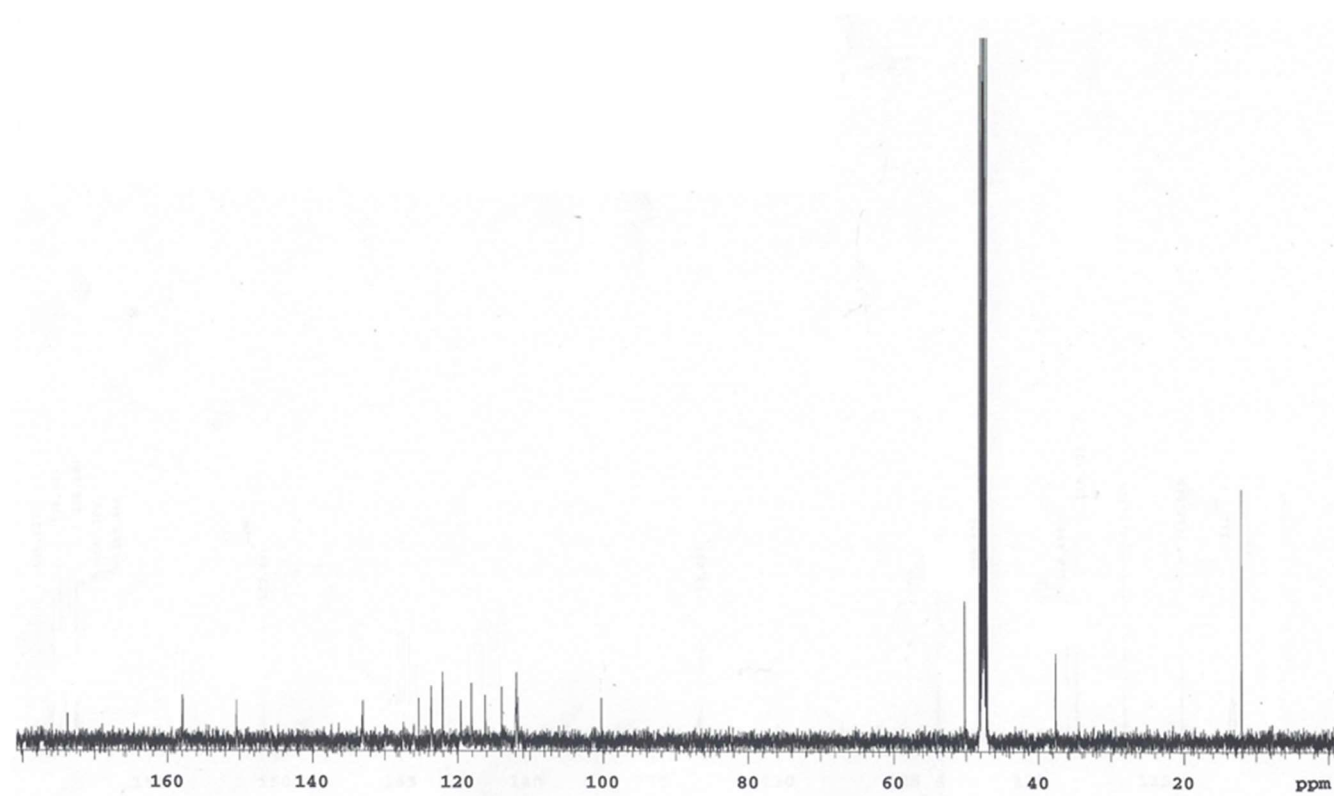


C-1311 analysis

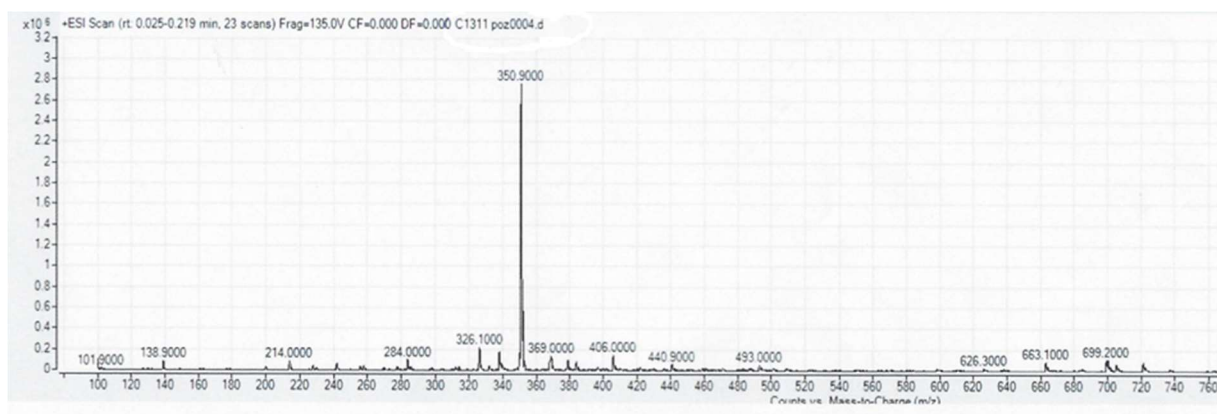
^1H NMR



^{13}C NMR

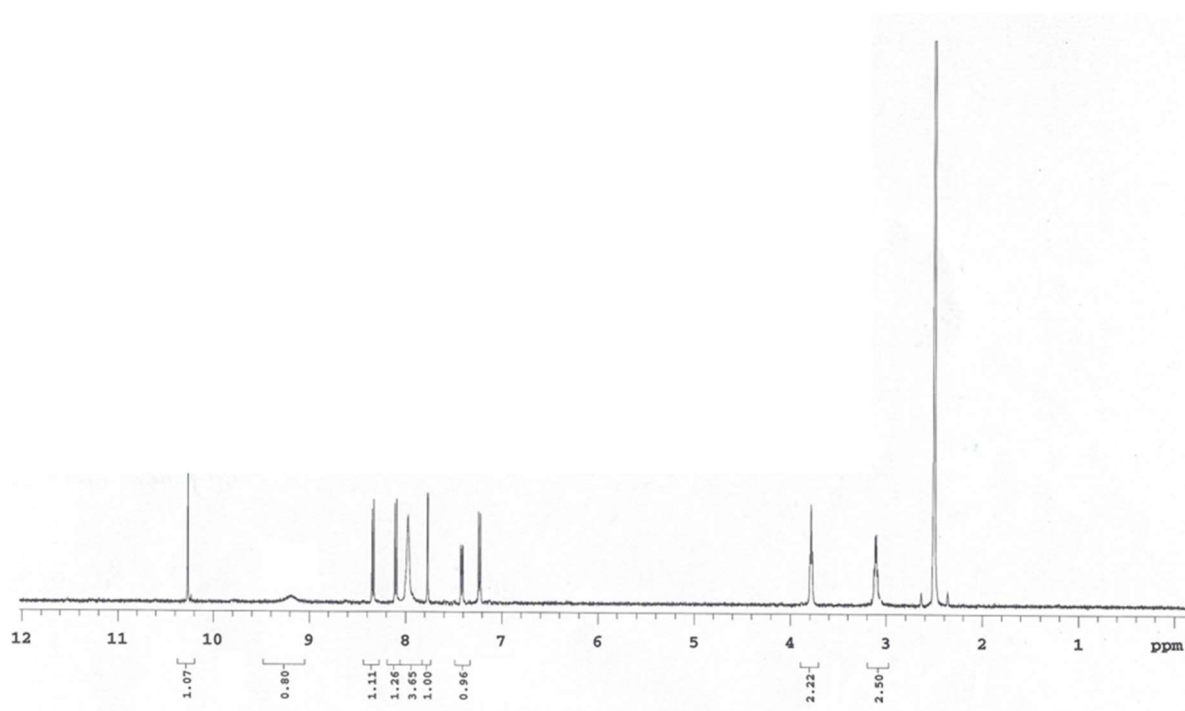


ESI-MS Spectra

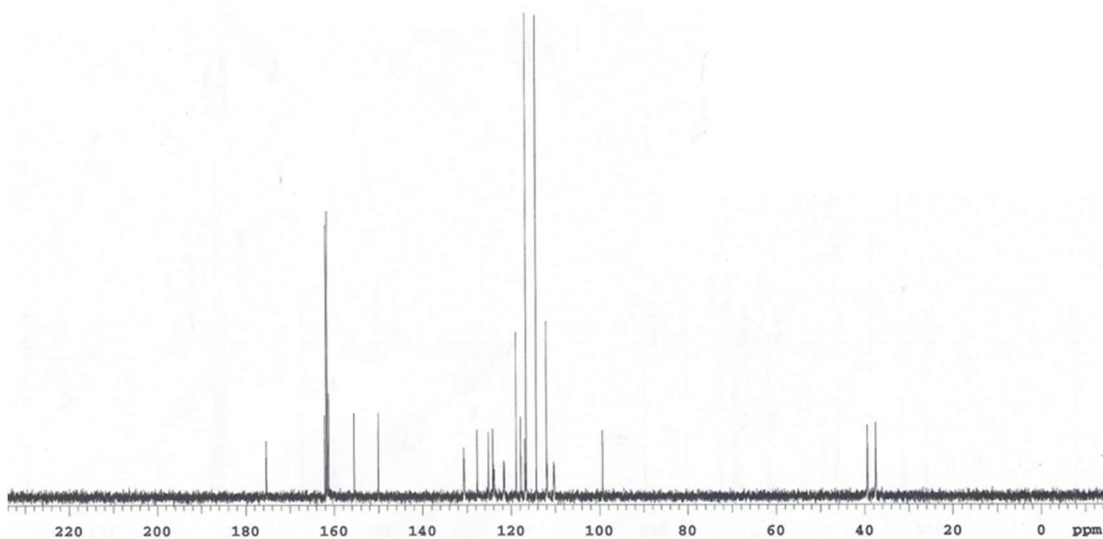


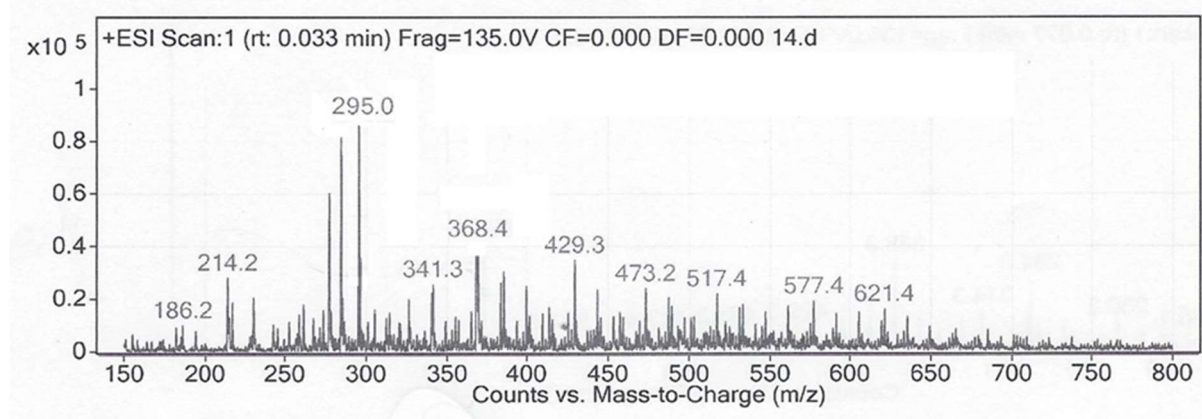
Compound 1 analysis

^1H NMR



^{13}C NMR





2. Compound 1-R8 synthesis and chemical analysis

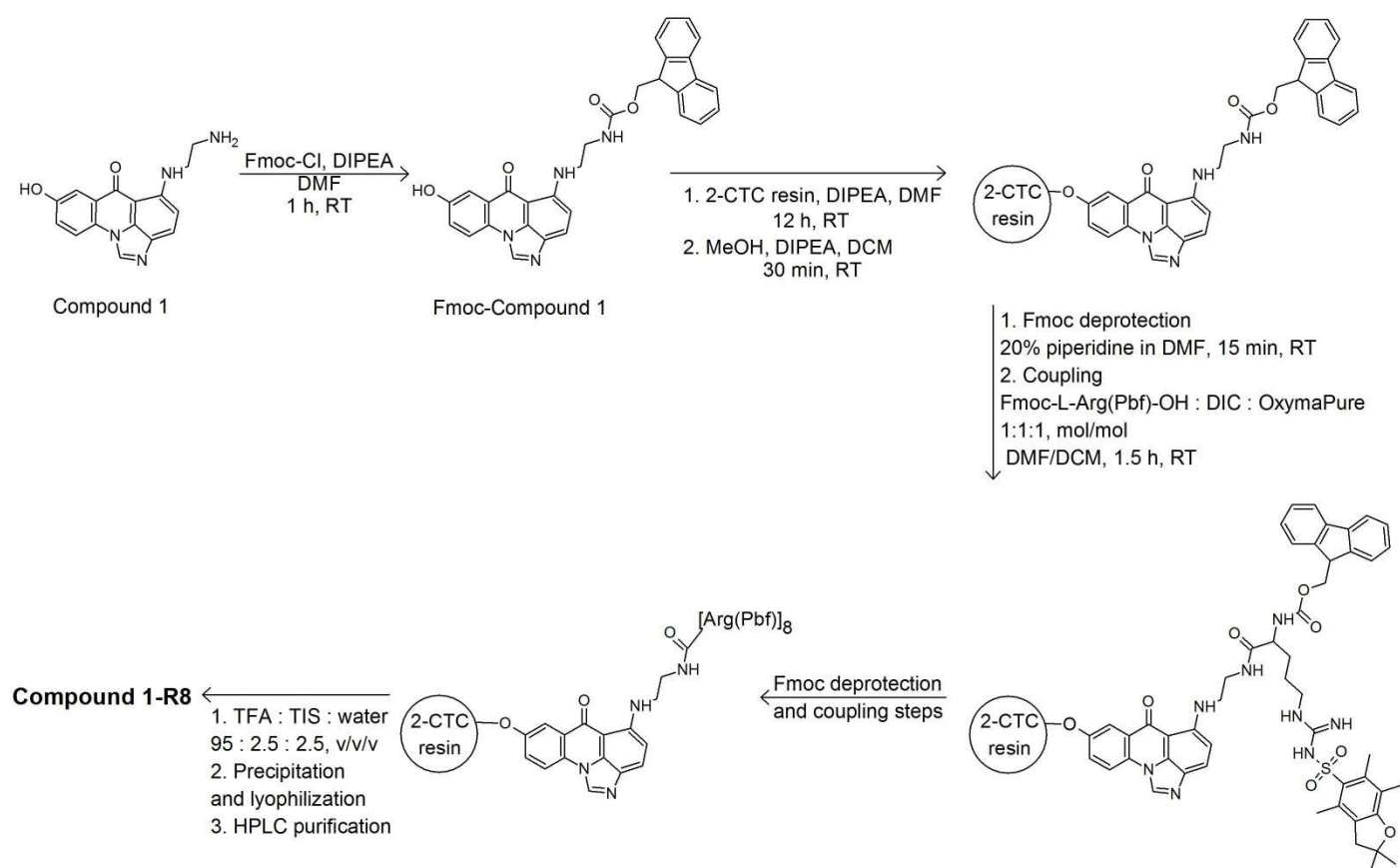
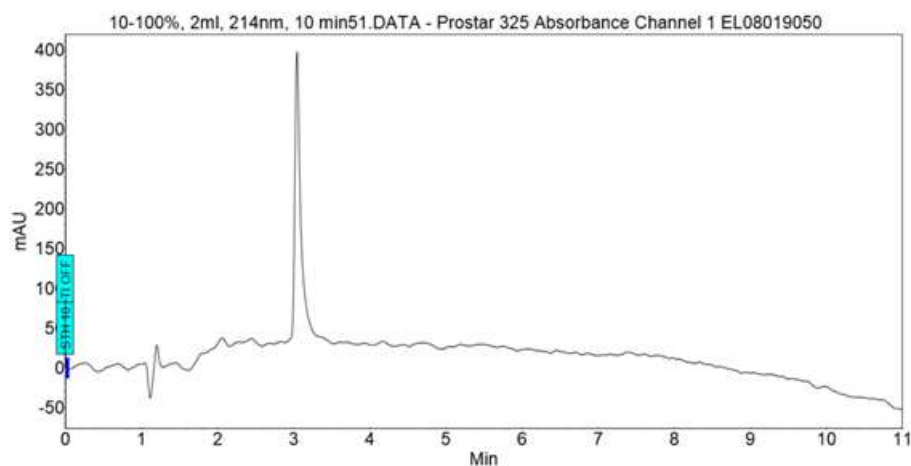


Figure S3. Scheme of Compound 1-R8 synthesis

Table S1. MS data for Compound 1-R8. Average mass: 1543.79 Da; monoisotopic mass: 1542.92 Da. Calc. mass for $(M + 2H/2)^+ = 772.47$ Da, $(M + 3H/3)^+ = 515.31$ Da and $(M+4H/4)^+ = 386.74$ Da.

z	m/z calc.	m/z exp.
1	1543.93	-
2	772.47	772.43
3	515.31	515.69



3. Compound 1-R ¹H NMR and COSY

