

Article

A “Pincer” Type of Acridine–Triazole Fluorescent Dye for Iodine Detection by Both ‘Naked-Eye’ Colorimetric and Fluorometric Modes

Mei Yu ^{1,2}, Lu Jiang ^{1,2}, Lan Mou ^{1,2}, Xi Zeng ^{1,2}, Ruixiao Wang ¹, Tao Peng ¹, Fuyong Wu ^{1,*} and Tianzhu Shi ^{1,*}

¹ Department of Brewing Engineering, Moutai Institute, Renhuai 564500, China; yumei@mtxy.edu.cn (M.Y.); jianglu@mtxy.edu.cn (L.J.); moulan@mtxy.edu.cn (L.M.); zengxi@mtxy.edu.cn (X.Z.); wangruixiao@mtxy.edu.cn (R.W.); edifcztony@126.com (T.P.)

² Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guiyang 550025, China

* Correspondence: wufuyong@mtxy.edu.cn (F.W.); shitianzhu@mtxy.edu.cn (T.S.); Tel.: +86-13423675949 (F.W.); +86-18586420308 (T.S.)

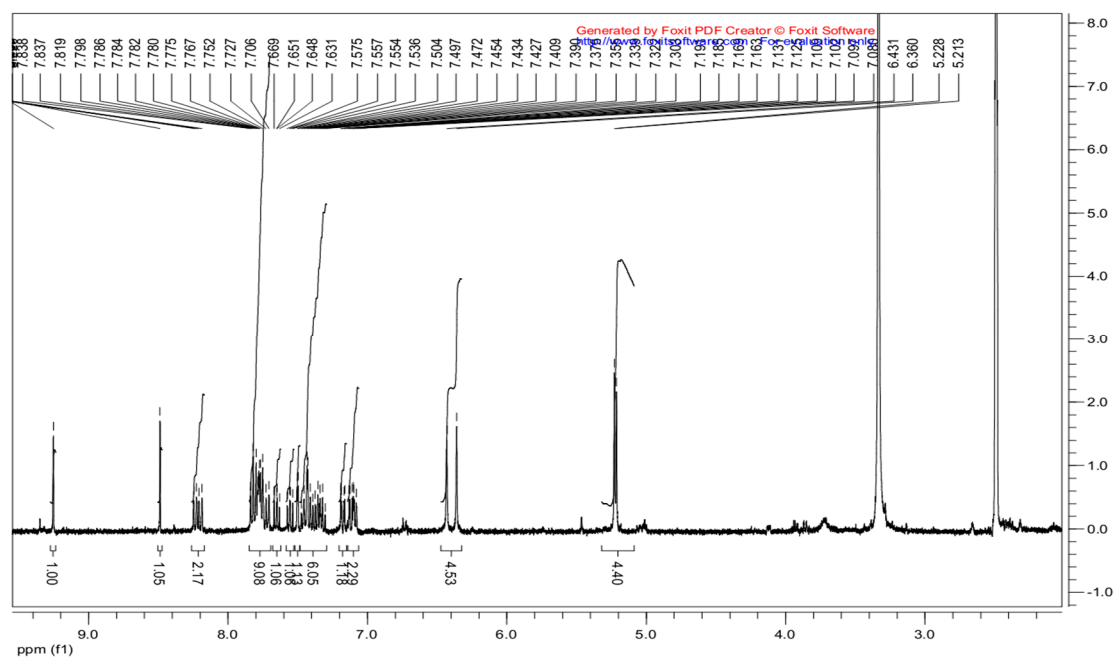


Figure S1 The ^1H NMR spectrum of Probe 1

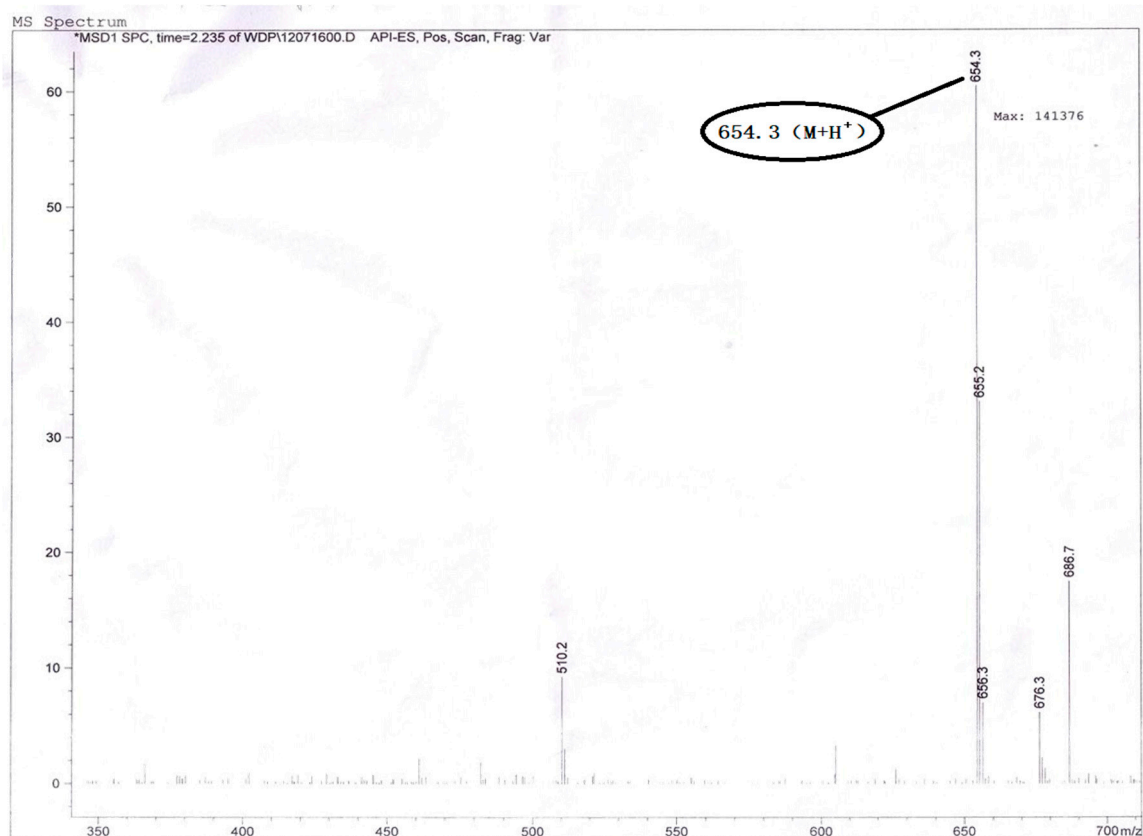


Figure S2 ESI-MS of Probe 1

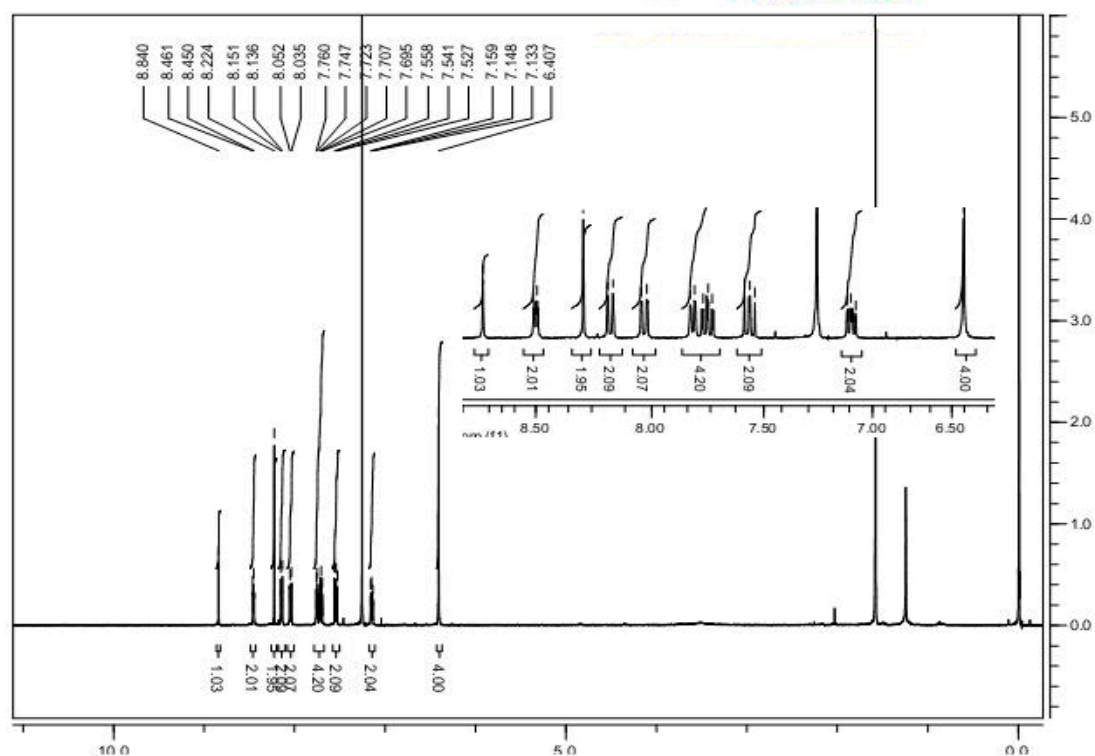


Figure S3 The ^1H NMR spectrum of Probe 2

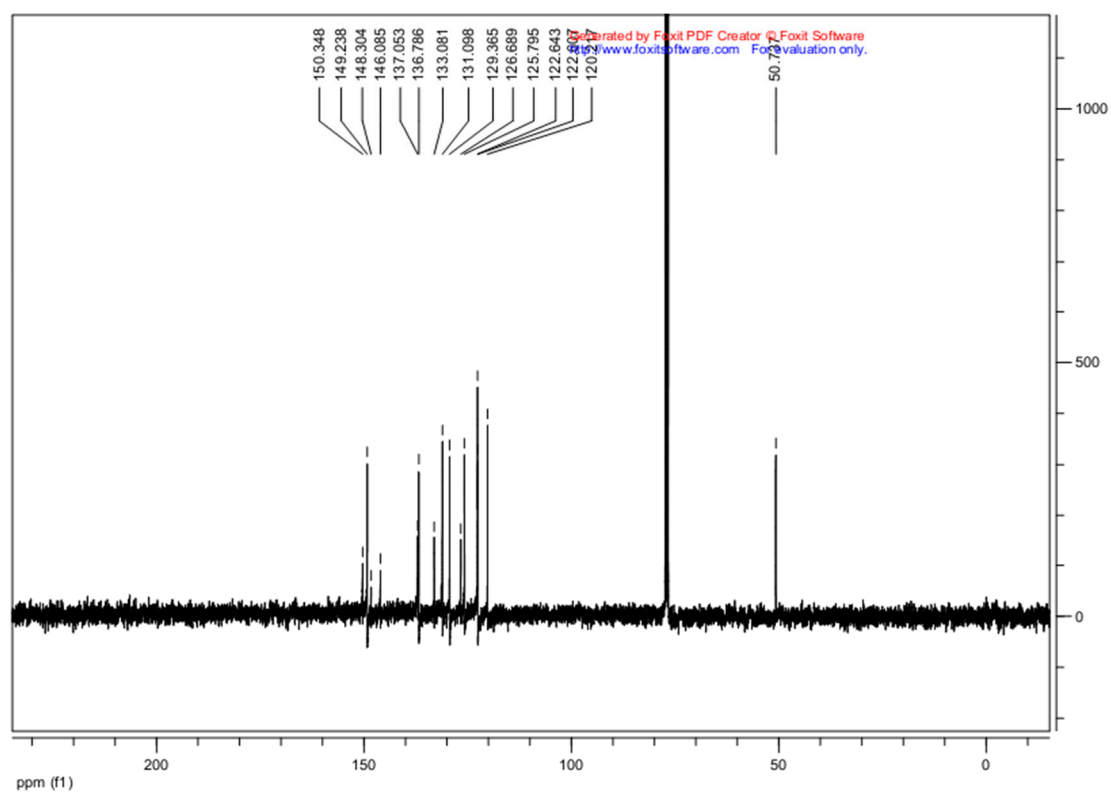


Figure S4 The ^{13}C NMR spectrum of Probe 2

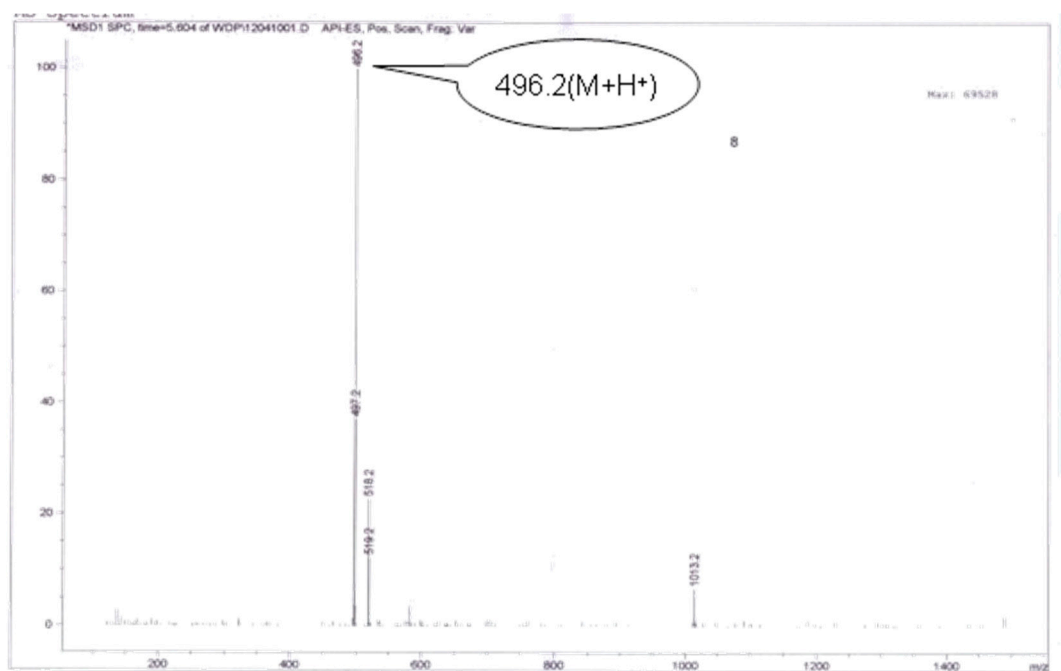


Figure S5 ESI-MS of Probe 2

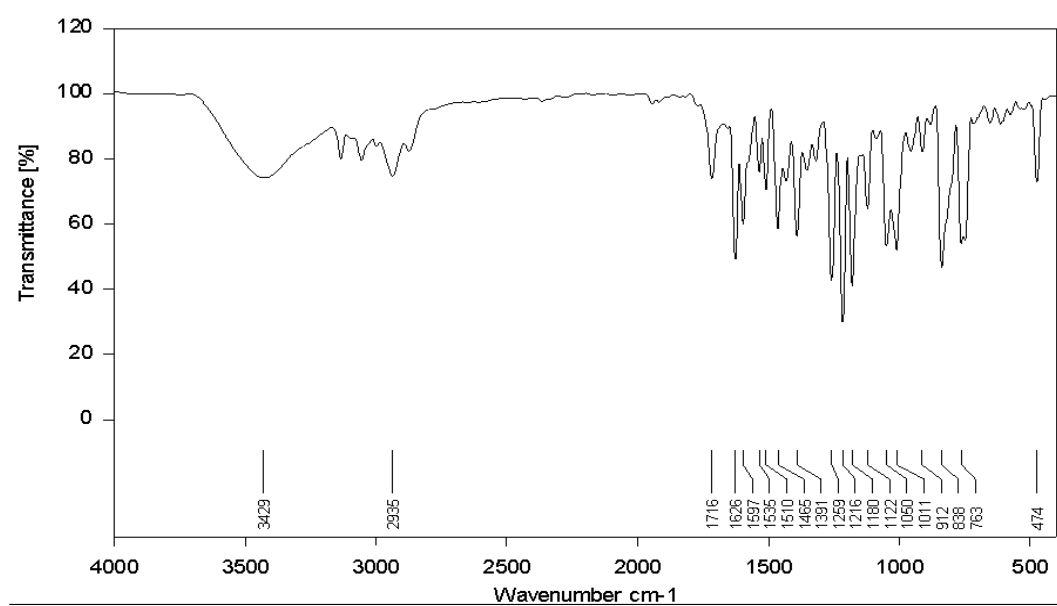
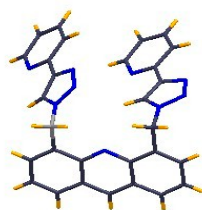


Figure S6 IR of Probe 1

Probe 2



CCDC number	903268
Empirical formula	C ₂₉ H ₂₁ N ₉
Formula weight	495.55
Temperture, K	293(2)
Crystal system	Triclinic
Space group	P-1
a (Å)	9.9302(10)
b (Å)	10.1923(8)
c (Å)	13.3068(10)
α, °	77.319(3)
β, °	79.609(3)
γ, °	64.984(3)
V, Å ³	1184.84(18)
ρ, g cm ⁻³	1.389
Z	2
R(int)	0.0513
R(sigma)	0.0601
μ, mm ⁻¹	0.088
S	1.058
Data integrity	0.974
θ range, (°)	1.58 ≤ θ ≤ 26.00
F(000)	516
Reflection collection	13396
Independent reflection	4551
R, wR [<i>I</i> > 2σ (<i>I</i>)]	0.0606, 0.1671
R, wR (all data)	0.1043, 0.2101
Final R indexes	$w=1/[\sigma^2 (F_o^2)+(0.151$ $2P)^2+0.0000P]$ $P = [F_o^2 + 2 F_c^2] / 3$

Figure S7 crystal data of Probe 2

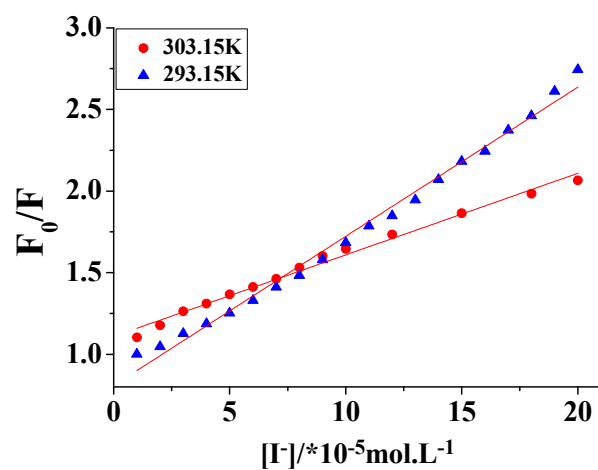


Figure S8 Stern-Volmer plot for probe in the presence of iodide.

$$Y=0.8090+0.0914X(293.15\text{K})$$

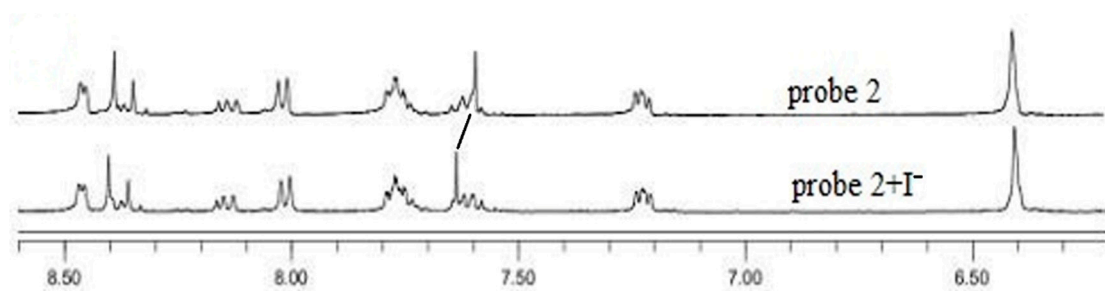


Figure S9 The changes of partial ^1H NMR of probe 2 upon with I^-