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A New Alkaloid from the Root of *Isatis indigotica* Fort

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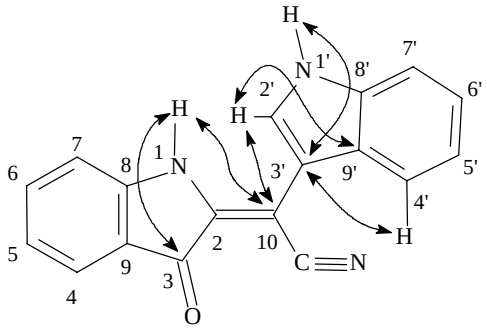
Abstract: A *E*-2-[(3'-indole)cyanomethylene]-3-indolinone was isolated from the root of *Isatis indigotica* Fort. The structure elucidation and ^{1}H, ^{13}C NMR assignments were achieved by spectroscopic method.

Keywords: *Isatis indigotica* Fort., *E*-2-[(3'-indole)cyanomethylene]-3-indolinone.

Isatis indigotica Fort., a most popular Chinese traditional medicine, is usually used to clear heat and detoxicate. We report here the isolation of *E*-2-[(3'-indole)cyanomethylene]-3-indolinone **1** (**Scheme**) from the butanol-soluble fraction of *I. indigotica.*, and structural elucidation of this new alkaloid.

Scheme The HMBC correlation of compound **1**



The 80% EtOH extract of *I. indigotica* was partioned with petroleum ether, chloroform, ethyl acetate and n-butanol, respectively. The *n*-BuOH fraction was further fractionated by silica gel column chromatography to afford cmpound **l**. Compound **1** was isolated as purple needle crystals, mp 213-215°, UV λ_{max} (MeOH) nm: 505, 274, EI-MS *m/z*: 285[M^+], HR-MS: 285.0905, suggested molecular formula to be $C_{18}H_{11}N_3O$ (calculated 285.0902). Its IR spectrum showed the presence of nitrile (2216 cm^{-1}) and a carbonyl group (1685 cm^{-1}). The ^{1}H-NMR spectrum of **1** indicated the presence of two NH groups (δ 12.01, δ 10.13) and nine other protons. The signals at δ 7.95 (1H, d, J = 7.2 Hz), 7.21 (1H, t, J = 7.2, 7.5 Hz), 7.28 (1H, t, J = 7.5, 6.9 Hz), 7.52 (1H, d, J = 6.9 Hz)

and 7.14 (1H, d, J = 8.0 Hz), 7.55 (1H, t, J = 8.0, 7.4Hz), 7.03 (1H, t, J = 7.0, 7.5 Hz), 7.65 (1H, d, J = 7.5 Hz) indicated that there were two ortho-benzene moieties, while the signal at δ 7.93 gave the evidence of another double bond.

The ^{13}C-NMR spectrum gave eighteen carbon signals. The DEPT spectrum revealed nine tertiary carbons and nine quaternary carbons. It was indicated that there were a carbonyl (δ 183.4), two benzenes, two double bonds, and a nitrile (δ 117.7)[1]. The COLOC spectrum showed that the signal of δ_C183.4 (C-3) was correlated with the signal at δ_H10.13 (H-1), δ_C106.0 (C-3') with δ_H7.95 (H-4') and 12.01 (H-1'). The NOESY spectrum gave the correlation between signal of δ_H10.13 (H-1) and 7.14 (H-7). Above data mentioned suggested the presence of an indole moiety and a 3-indolinone moiety[2]. ^{1}H- and ^{13}C-NMR spectra data of **1** are listed in **Table 1**.

Table 1 ^{1}H- and ^{13}C-NMR spectra data of **1** (DMSO-d_6)

H	δ ppm	J_{Hz}	C	δ ppm
1	10.13(s)		2	139.8s
4	7.65 (d)	7.2	3	183.3s
5	7.03 (t)	7.2, 7.5	4	124.4d
6	7.55 (t)	7.5, 6.9	5	120.9d
7	7.14 (d)	6.9	6	136.7d
1'	12.01 (s)		7	112.6d
2'	7.93 (s)		8	120.2s
4'	7.95(d)	7.5	9	151.9s
5'	7.21(t)	7.5, 7.4	10	86.0s
6'	7.28(t)	7.4, 8.0	2'	128.5d
7'	7.52(d)	8.0	3'	106.0s
			4'	119.4d
			5'	120.4d
			6'	122.5d
			7'	112.3d
			8'	136.4s
			9'	125.0s
			CN	117.7s

The signal at δ 86.0 (tertiary carbon) observed in ^{13}C-NMR spectrum suggested that this carbon connected with nitrile moiety. The correlation between signal of δ 10.13 (H-1) and δ 7.93 (H-2') observed in NOESY spectrum indicated that **1** must be in *E* configuration. **1** was then assigned as *E*-2-[(3'-indole) cyanomethylene]-3-indolinone.

Acknowledgments

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