

SUPPLEMENTARY MATERIAL

Sesbagrandidflorain A and B: isolation of two new 2-arylbenzofurans from the stem bark of *Sesbania grandiflora*

Noviany, Arief Nurhidayat, Sutopo Hadi, Tati Suhartati, Muhammad Aziz, Neny Purwitasari, and Iman Subasman

Abstract: Native to tropical Asia, *Sesbania grandiflora* (L.) Pers is a member of the Fabaceae family of flowering plants. All parts of *S. grandiflora* are used in traditional medicine for the treatment of hepatitis, parasites, and different kinds of infections as well as inflammation of skin and mucous membranes. Several phytochemical investigations also have been conducted on extracts of the leaves, seeds, and roots of *S. grandiflora* to provide scientific validation of its properties. However, to date, no study has determined the phytochemical constituents of the stem bark of *S. grandiflora*. This study aimed to isolate and purify the secondary metabolites from the stem bark of *S. grandiflora*. The stem bark of *S. grandiflora* was air-dried, powdered, extracted exhaustively with *n*-hexane, EtOAc, and 90% aqueous MeOH sequentially. The EtOAc extract was separated and fractionated by using silica-gel VLC and CC techniques using appropriate solvents. In this study, we successfully isolated two new 2-arylbenzofurans, sesbagrandidflorain A and B, from the EtOAc extract of *S. grandiflora* stem bark. In addition, we determined the structures and phytochemical constituents of these compounds using one- and two-dimensional nuclear magnetic resonance, ultraviolet and infrared spectroscopy, and electrospray ionization time-of-flight mass spectrometry. The heteronuclear multiple bond correlations of each compound were modeled. The finding expands the understanding of the natural constituents of the Fabaceae and, in particular, the *Papilionoideae* genera.

Table S1. ^1H and ^{13}C nuclear magnetic resonance data for Compounds **1** and **2**.

Ring	No atom C	1^a		2^a	
		δ_{H} (ppm); J (Hz) ^b	δ_{C} (ppm)	δ_{H} (ppm); J (Hz) ^b	δ_{C} (ppm)
A	4	7.55 (<i>d</i> , J = 8.4)	133.75	7.53 (<i>d</i> , J = 8.4)	133.52
	5	6.67 (<i>dd</i> , J = 8.4 & 2.2)	109	6.61 (<i>dd</i> , J = 8.4 & 2.2)	109.17
	6	-	160	-	157.85
	7	6.71 (<i>d</i> , J = 2.2)	100.56	6.64 (<i>d</i> , J = 2.2)	104.2
	8	-	162.91	-	162.51
	9	-	109.34	-	108.25
	MeO-C HO	3.88 (<i>s</i>)	56.17	- 9.42 (<i>s</i>)	- -
B	1'	-	107.79	-	107.89
	2'	-	157.36	-	157.34
	3'	-	152.79	-	152.79
	4'	6.34 (<i>d</i> , J = 2.2)	98.89	6.34 (<i>d</i> , J = 2.2)	98.84
	5'	-	161.96	-	161.89
	6'	6.68 (<i>d</i> , J = 2.2)	88.5	6.67 (<i>d</i> , J = 2.2)	88.5
C	2	-	164.44	-	164.68
	3	-	119.18	-	118.71
	MeO-C HO	3.83 (<i>s</i>) 10.21 (<i>s</i>)	56.11	3.83 (<i>s</i>) 9.23 (<i>s</i>) & 10.26 (<i>s</i>)	56.1
	CHO	9.82 (<i>s</i>)	191.1	9.97 (<i>s</i>)	191.29

^a ^1H NMR (500 MHz) and ^{13}C NMR (125 MHz) measured in Acetone- d_6 .^b Multiplicity of signals is given in parentheses: *s*, singlet; *d*, doublet; *dd*, doubledoublet; coupling constants (apparent splittings) are reported as numerical values in Hz.

Figure S1. The heteronuclear multiple bond correlations of Compound **1**.

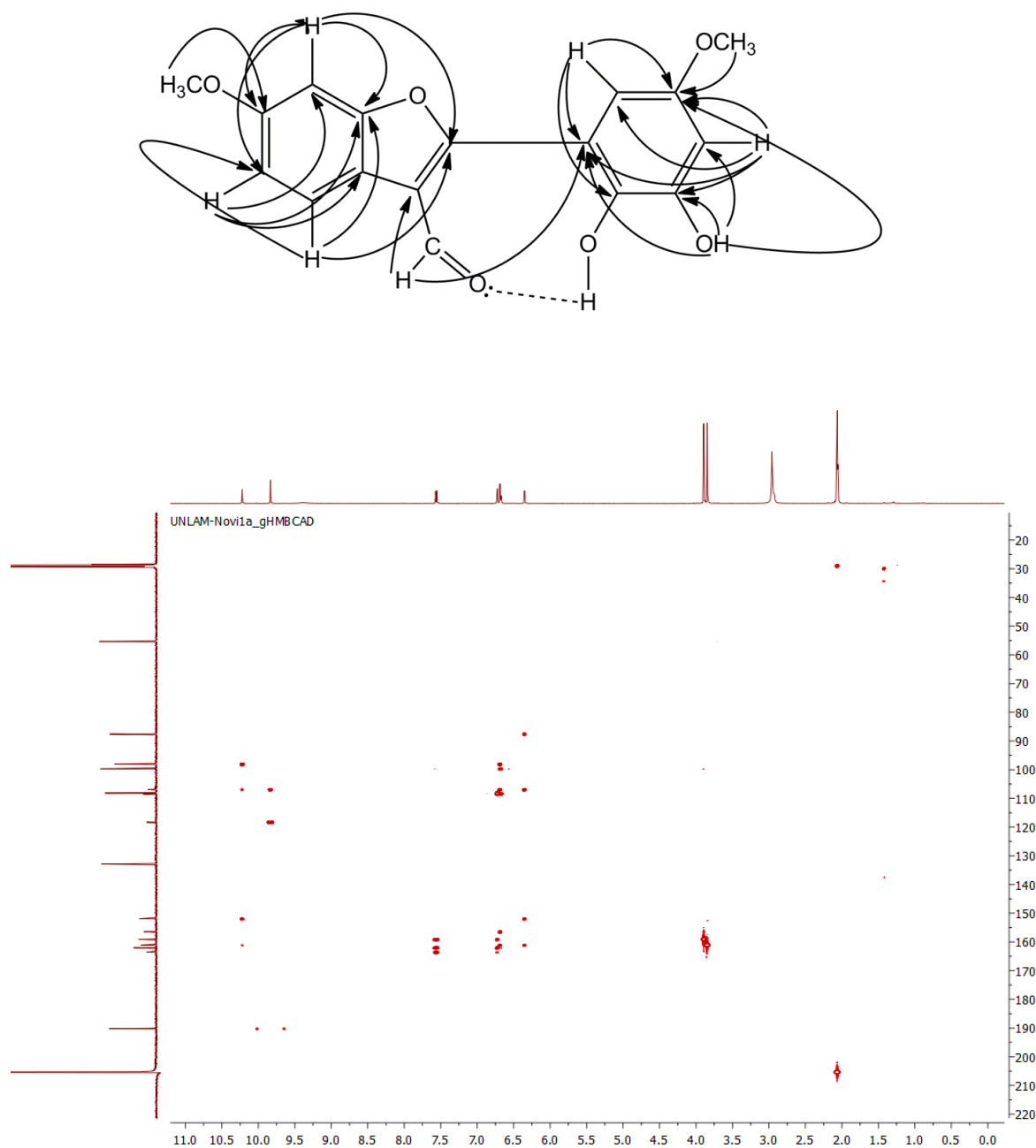


Figure S2. The nuclear Overhauser enhancement interactions of Compound **1**.

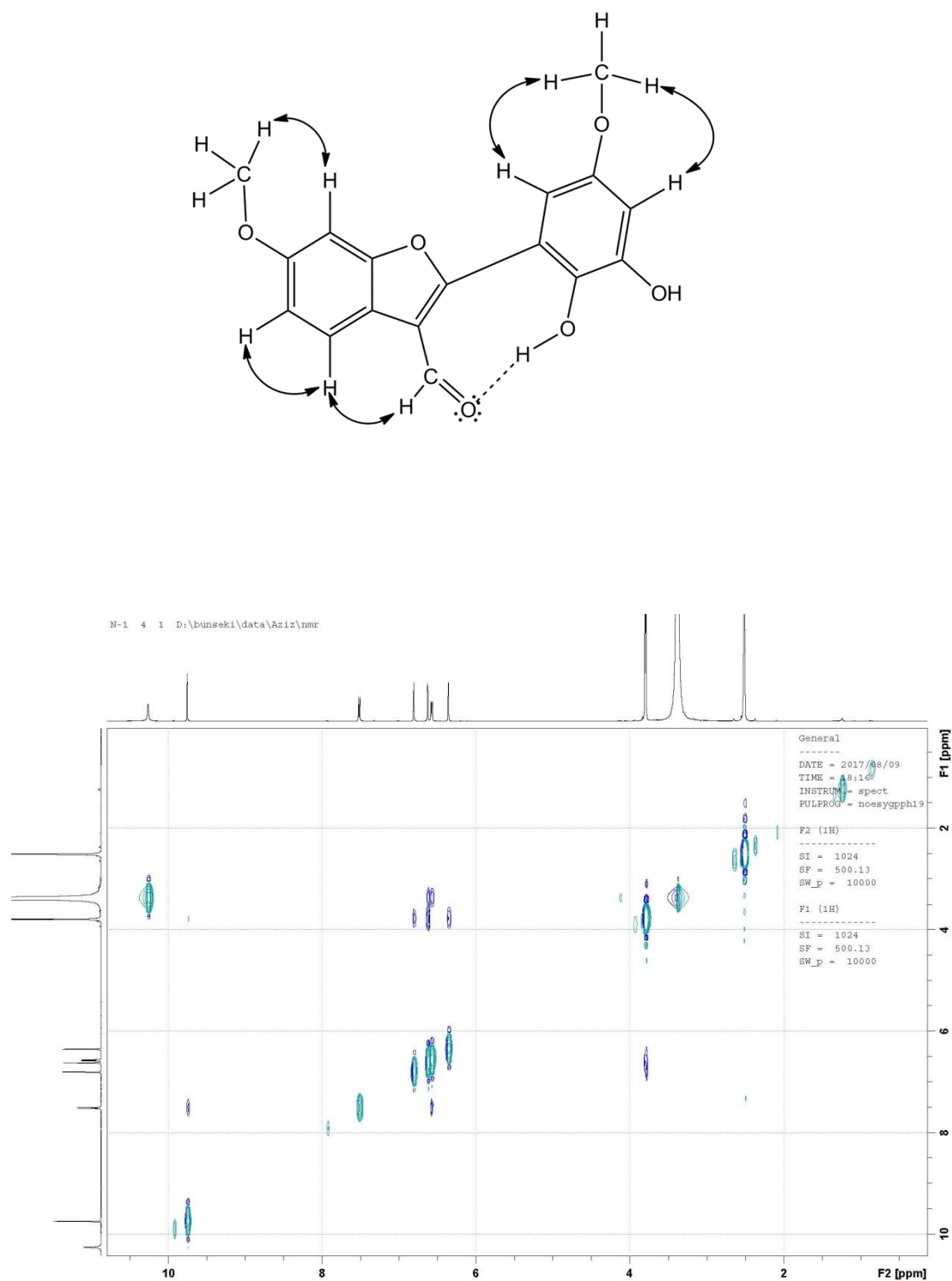


Figure S3. The heteronuclear multiple bond correlations of Compound **2**

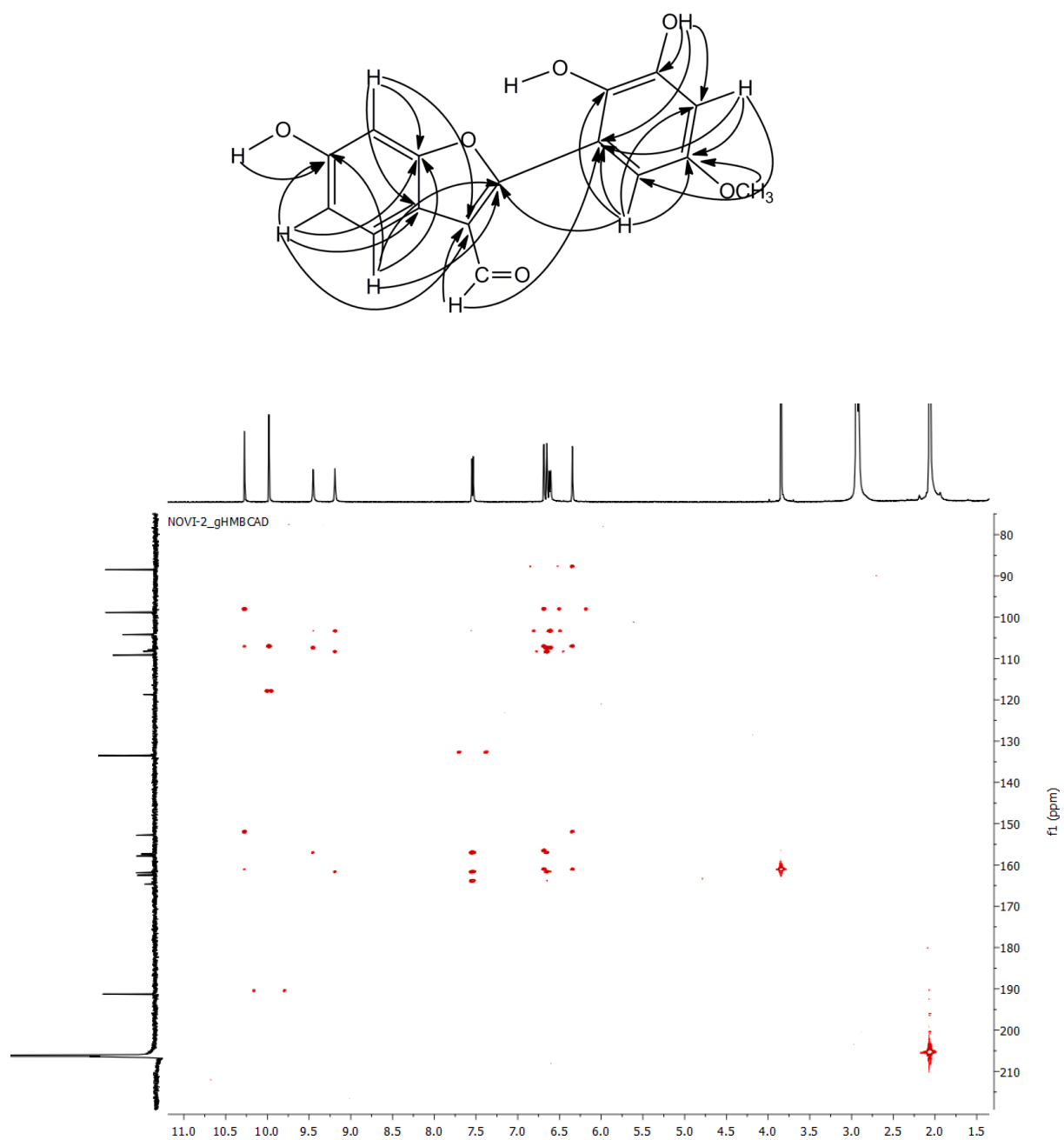


Figure S4. The nuclear Overhauser enhancement interactions of Compound 2.

