

Supporting Information for

Cellular stress upregulates indole signaling metabolites in *E. coli*.

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Supplementary figures.

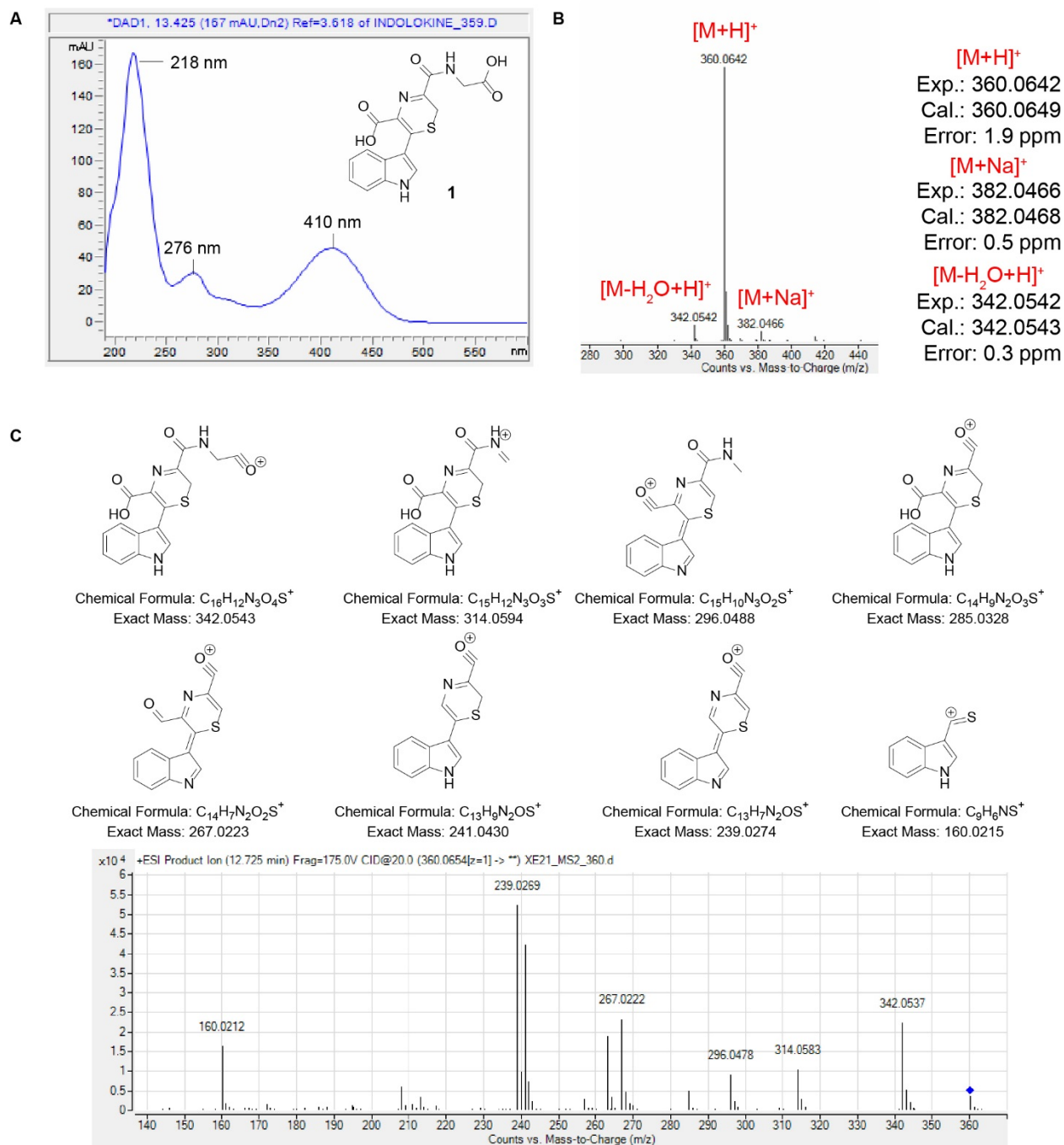


Figure S1. UV-Vis, HR-MS, and tandem MS data of 1 (related to Figure 1). **A**, The UV-Vis spectrum of **1** showed the maximum absorptions at 218, 276, and 407 nm. **B**, The HR-ESI-QTOF-MS data of **1** supported its structural assignment with <2 ppm error for [M+H]⁺, [M+Na]⁺, and [M-H₂O+H]⁺ ion peaks. **C**, Fragment ion structures (top) and tandem MS spectrum of **1** (bottom) are shown.

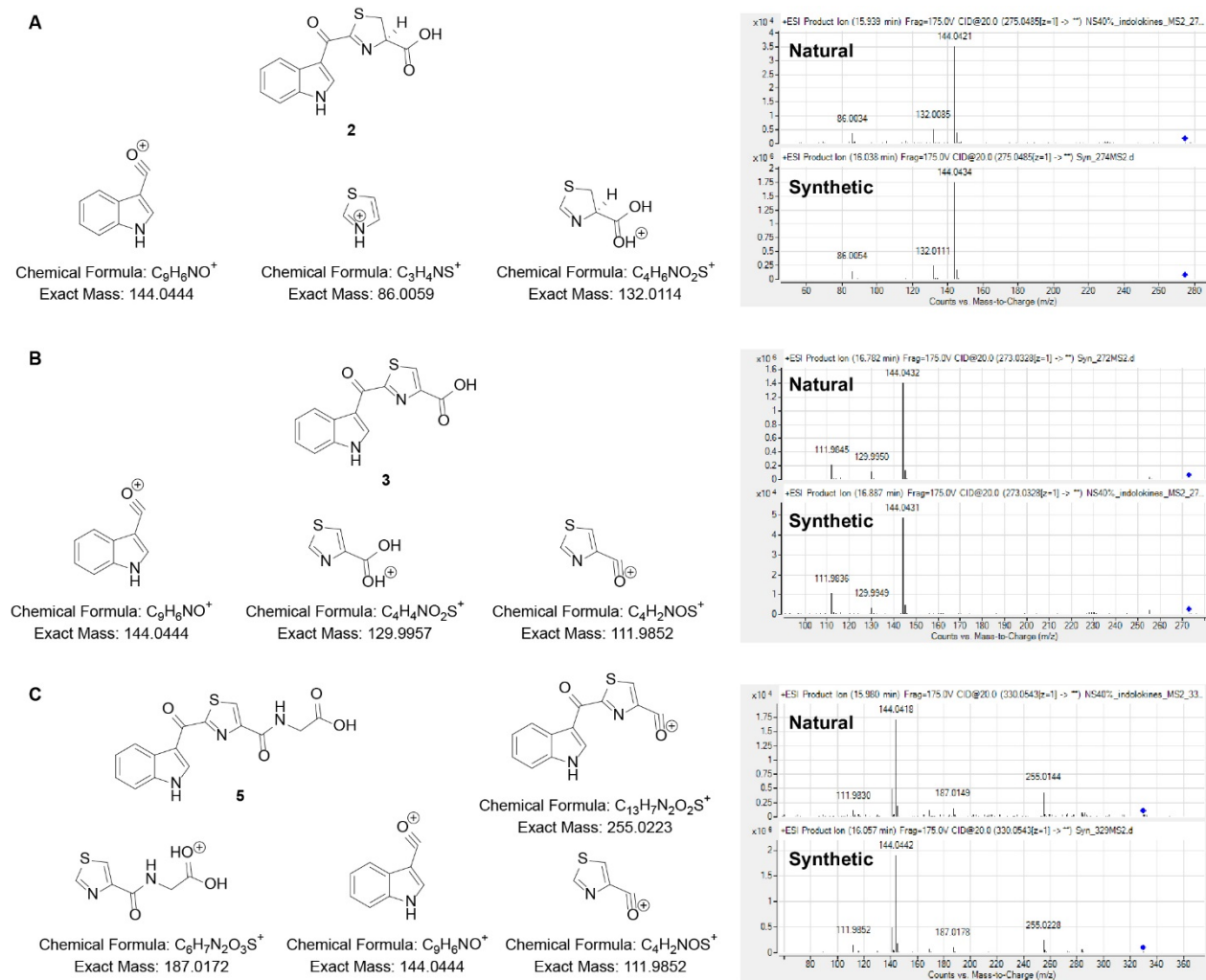


Figure S2. Structural identification of bacterial indolokines 2 (A), 3 (B), and 5 (C) by comparing their tandem MS spectra to those of synthetic compounds (related to Figure 1). Structure of the parent molecule and its fragment ions (left), and tandem MS spectra of natural and synthetic indolokines (right) are shown.

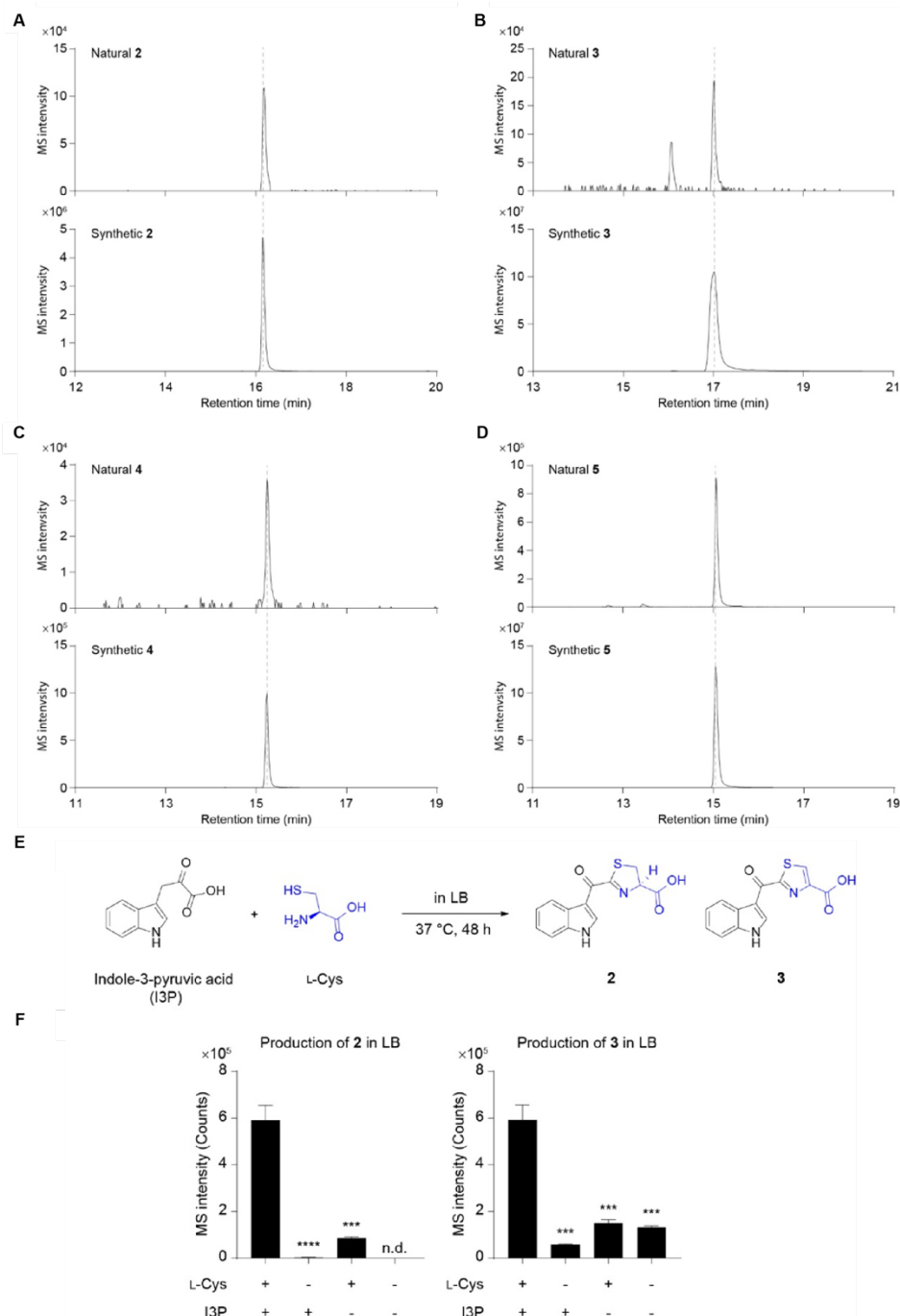


Figure S3. Structural identification of bacterial indolokines 2-5 by comparing their retention times to those of synthetic compounds and biomimetic synthesis of 2 and 3 in LB medium (related to Figure 1 and Figure 3). EICs of natural (top) and synthetic (bottom) indolokines 2-5 (A-D, respectively). E, Scheme of metabolites 2 and 3 and their formation by non-enzymatic reactions. F, Metabolites 2 and 3 were produced when both L-Cys and I3P were present in the LB

medium. Because of diverse components in LB, small amounts of **2** and **3** were observed when either L-Cys or I3P were not added under these conditions. $n = 3$ biological replicates. Data are mean \pm s.d. *** $P < 0.001$, **** $P < 0.0001$. n.d., not detected. Two-tailed t-test.

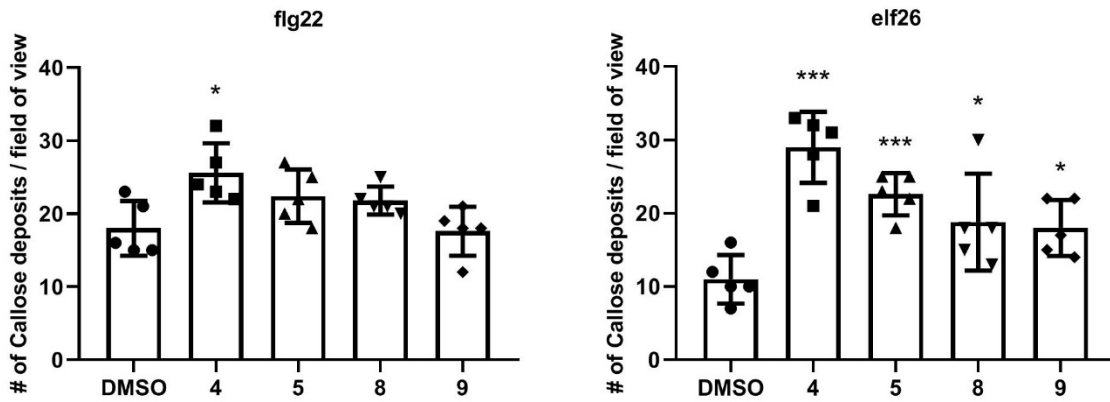


Figure S4. Quantification of callose deposition of *Arabidopsis* seedlings (related to Figure 4). Seedlings were elicited with flg22 (left) or elf26 (right) supplemented indolokine A2 (4), A3 (5), B2 (8) and B3 (9). $n = 5$ biological replicates. Data are mean \pm s.d. * $P < 0.05$, *** $P < 0.001$. Two-tailed t-test.

Table S1. ^1H and ^{13}C NMR data of **1** and **5** isolated from *X. bovienii* (related to Figure 1).

pos.	1 ^a		5 ^b	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
	[ppm, mult. (<i>J</i> in Hz)]		[ppm, mult.]	
1	7.79, d (2.8)	131.9	9.32, s	139.7
2		111.3		113.8
3		124.7		127.9
4	7.40, d (8.0)	119.9	8.37, m	122.8
5	7.12, brt (7.5)	120.4	7.27, m	123.6
6	7.18, brt (7.5)	122.3	7.28, m	124.6
7	7.46, d (8.1)	112.4	7.52, m	112.9
8		137.1		137.9
9		135.7		178.4
10		130.2		171.6
11		164.1	8.49, s	129.9
12	3.62, s	23.5		151.6
13		137.0		163.3
14		162.5	4.19, s	41.8
15	3.97, d (6.1)	41.2		172.9
16		171.0		
1-NH	11.89, brs			
14-NH	9.09, t (6.1)			

^aMeasured in DMSO-*d*₆

^bMeasured in methanol-*d*₄

