Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

Syusuke Egoshi[1], Yousuke Takaoka[1], Hiroaki Saito[2], Yuuki Nukadzuka[1], Kengo Hayashi[1], Yasuhiro Ishimaru[1], Hiroyuki Yamakoshi[3], Kosuke Dodo[3], Mikiko Sodeoka[3], and Minoru Ueda[1*]

1. Department of Chemistry, Tohoku University, 6-3 Aramaki-Aza-Aoba, Aoba-ku, Sendai 980-8578, Japan.
2. Institute of Science and Engineering, Kanazawa University, Kakuma, Kanazawa, Ishikawa, Japan.
3. Synthetic Organic Chemistry Laboratory, RIKEN, Saitama 351-0198, Japan.

Table of Contents:

Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

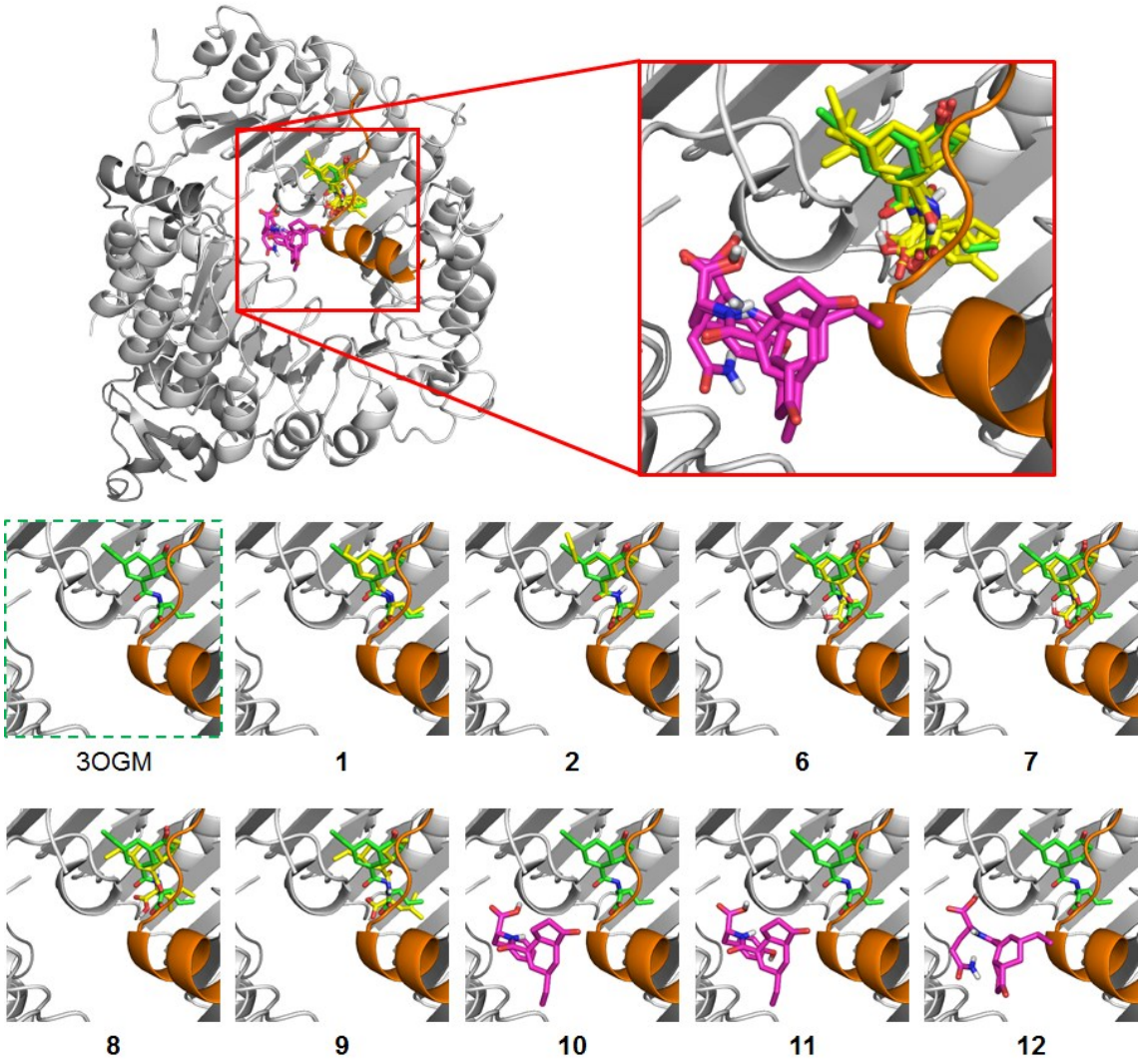
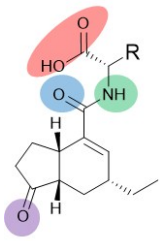


Figure. S1 Docking Study of CFA-AAs on COI1-JAZ1 complex protein *in silico*.

Structure of COR in 3OGM is green. Structure of COR, JAIle, CFA-L-Ala, CFA-L-Val, CFA-L-Ile and CFA-L-Leu are yellow. Structure of CFA-L-Phe, CFA-L-Tyr and CFA-L-Gln are purple. Yellow compounds entry in COI1-COR-JAZ binding pocket but purples cannot.

Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

Table S1 The hydrogen bonds network obtained in the docking study between CFA-AAs (**6-12**) and COI1-JAZ1 co-receptor.



ligand	binding free energy (kcal/mol)	distance from functional groups (Å)							
		COI1							JAZ1
		R85	R348	E350	Y386	R409	Y444	R496	A204
1	-11.1 ± 0.1	2.6	2.9, 3.0, 3.4	3.1	3.0, 3.2	3.4	3.2	2.9	2.8
2	-10.3 ± 0.1	2.4	2.9, 3.0, 3.2	—	—	2.6	3.5	3.3	3.1
6	-9.8 ± 0.1	3.0, 3.0, 3.5	2.9, 3.0	—	2.8	3.1, 3.3	3.3	3.0	3.1
7	-9.8 ± 0.1	2.9, 3.2	3.0, 3.4	—	2.7	2.9, 3.2	3.3	2.9	3.1
8	-9.7 ± 0.1	2.8, 3.2	3.3	—	2.7	3.0, 3.4	3.3	2.9	3.1
9	-9.7 ± 0.1	3.0, 3.3	2.8, 3.5	—	3.3	3.0, 3.2	—	3.0	2.8
10	-8.2 ± 0.1	—	—	—	—	—	—	—	—
11	-8.2 ± 0.1	—	—	—	—	—	—	—	—
12	-7.1 ± 0.1	—	—	—	—	—	—	—	—

Docking simulation of **1**, **2** and CFA-AAs (**6-12**) were calculated by AutoDock Vina 1.1.2 software. This table shows binding free energy and distance within 3.5 Å between the amino acids in binding pocket of COI1-JAZ1 and ligands, oxygen of amide is colored in blue, amide nitrogen in green, oxygen atoms of carboxyl acid in red, oxygen atom of ketone in purple.

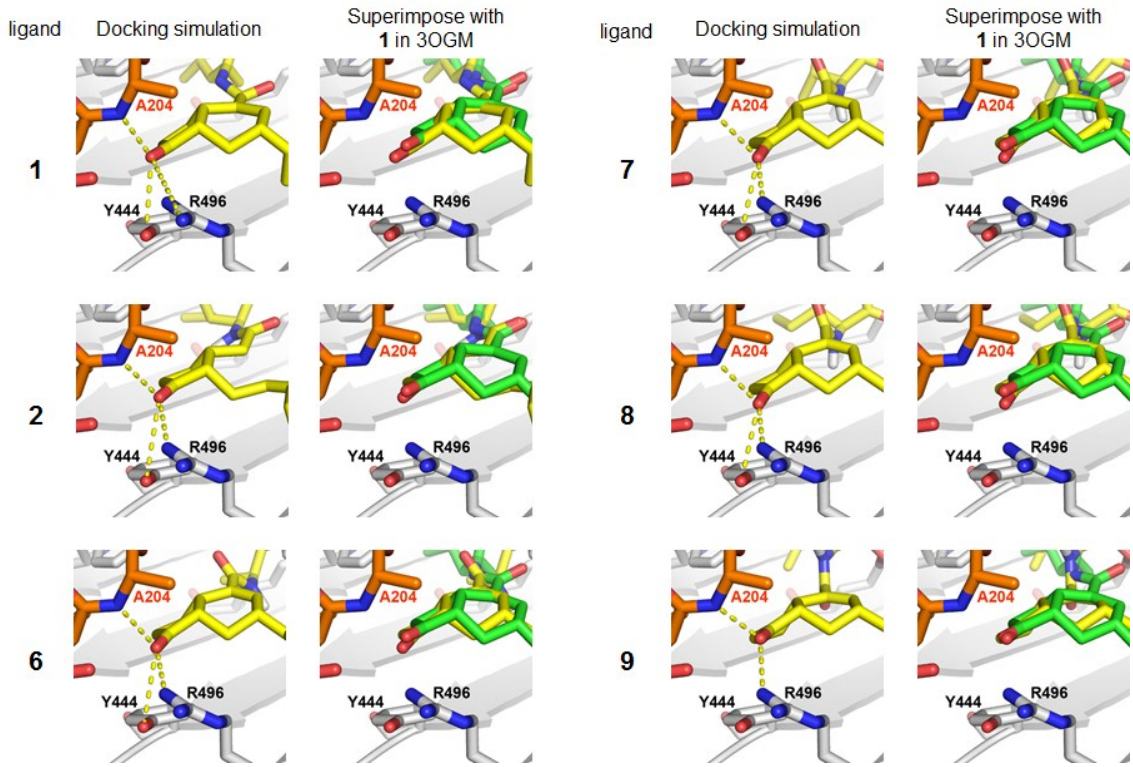


Figure. S2 Docking Study of CFA-AAs on COI1-JAZ1 complex protein *in silico*.

Structure of COR in 3OGM is green. Structure of COR, JAIle, CFA-L-Ala, CFA-L-Val, CFA-L-Ile and CFA-L-Leu are yellow. In docking simulations (left), yellow line represents the distance within 3.5 Å from ketone carbonyl: Y444 (COI1), R496 (COI1) and A204 (JAZ1).

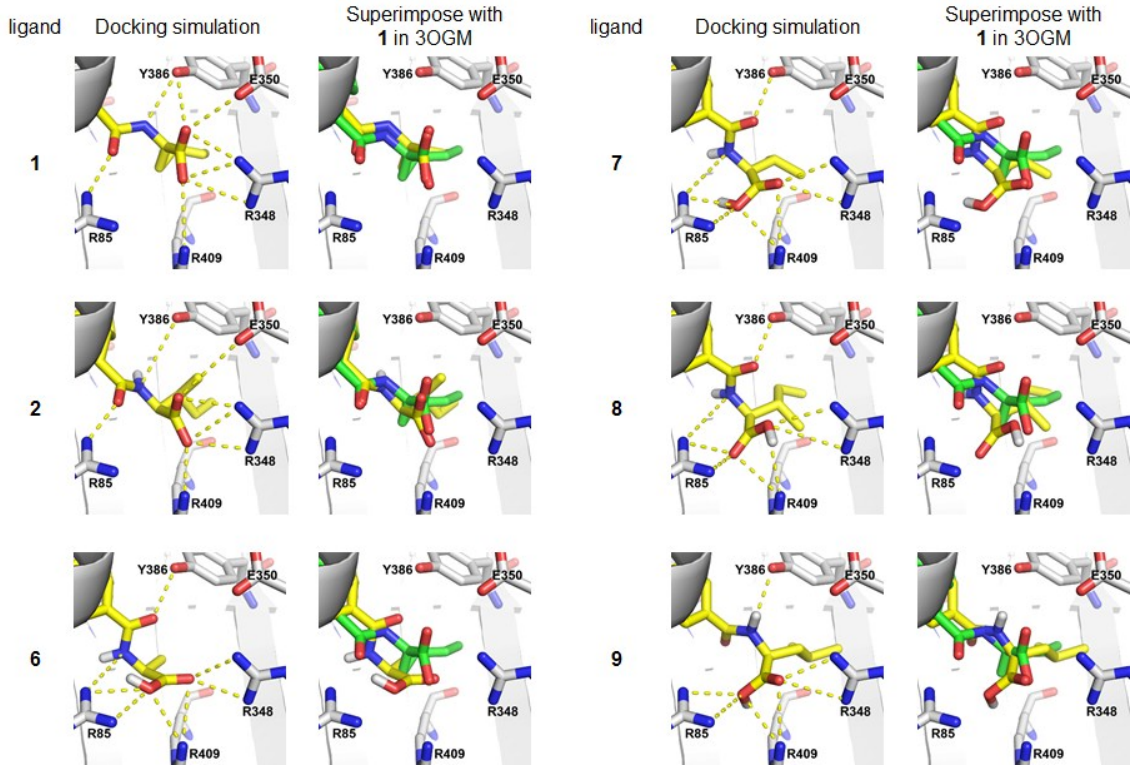


Figure. S3 Docking Study of CFA-AAs on COI1-JAZ1 complex protein *in silico*.

Structure of COR in 3OGM is green. Structure of COR, JAIle, CFA-L-Ala, CFA-L-Val, CFA-L-Ile and CFA-L-Leu are yellow. In docking simulations (left), yellow line represents the distance within 3.5 Å from the amino acids of COI1, such as R85, R348, E350, Y386 and R409, and amide carbonyl , amide nitrogen and oxygen atoms of carboxyl acid of ligands.

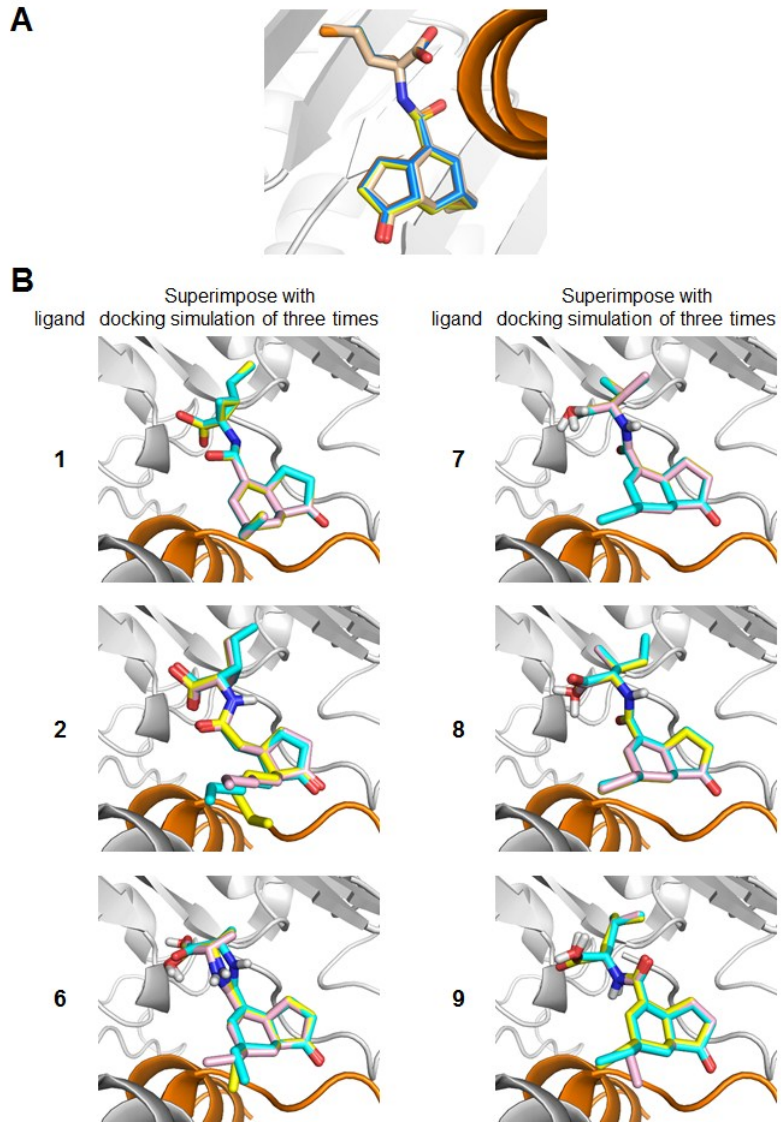


Figure. S4 Docking Study of CFA-AAs on COI1-JAZ1 complex protein *in silico*.

A: Superimposed structures of the docking study in each grid size of COR (1) on COI1-JAZ1 complex protein *in silico*, showing the reproducibility of these results. Structure of COR (**1**) calculated in 20×20×20 grid points (x, y, and z axes) is showed as blue, 30×30×30 grid points is yellow, 40×40×40 grid points is tint, and 50×50×50 grid points is orange stick models.

B: Superimposed structures of each three trial of the docking study of CFA-AAs on COI1-JAZ1 complex protein *in silico*, showing the reproducibility of these results. First calculated structure of COR (**1**), JAIle (**2**), CFA-L-Ala (**6**), CFA-L-Val (**7**), CFA-L-Ile (**8**) and CFA-L-Leu (**9**) are showed as yellow, second are cyan, and third are pink stick models.

Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

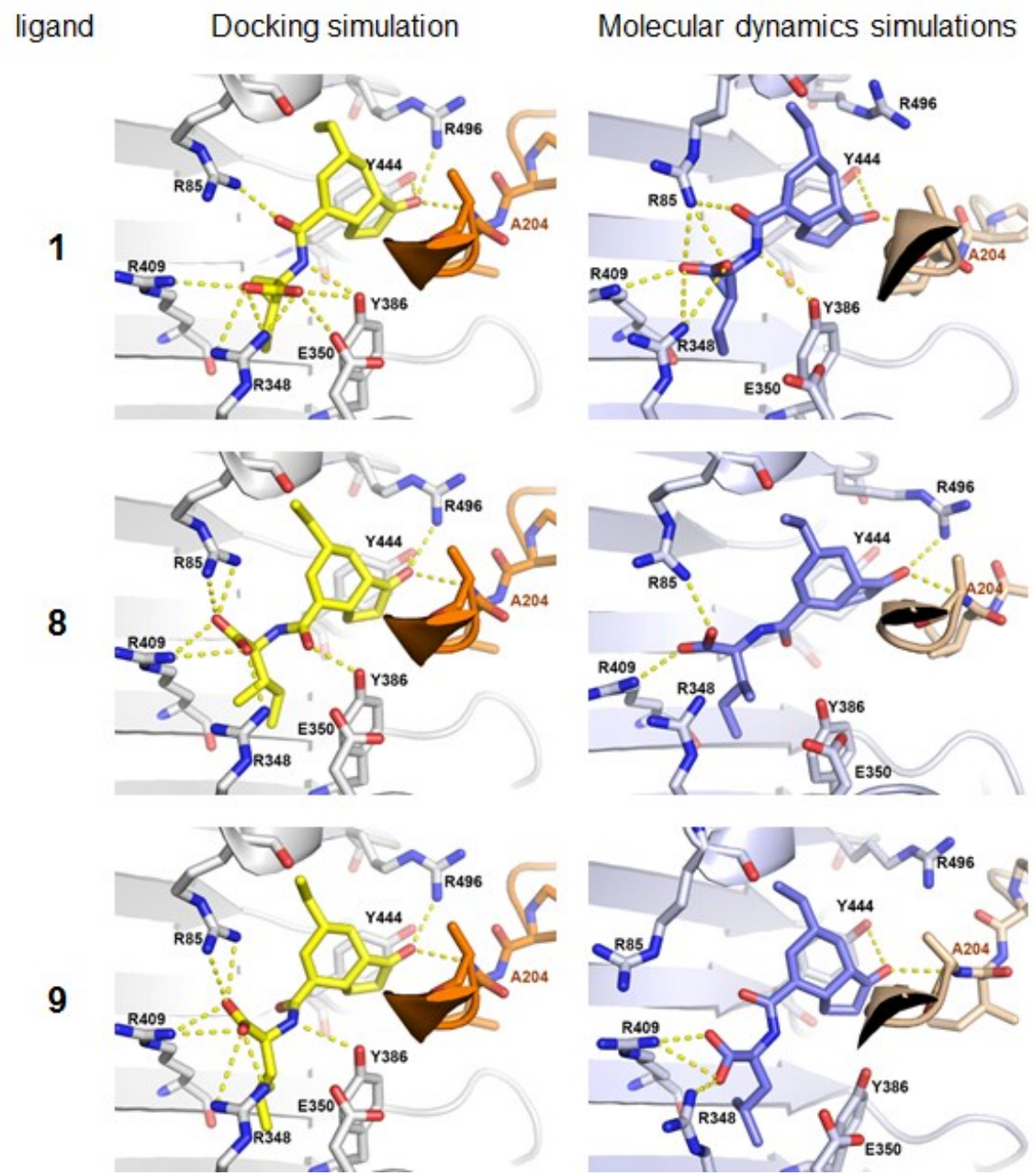
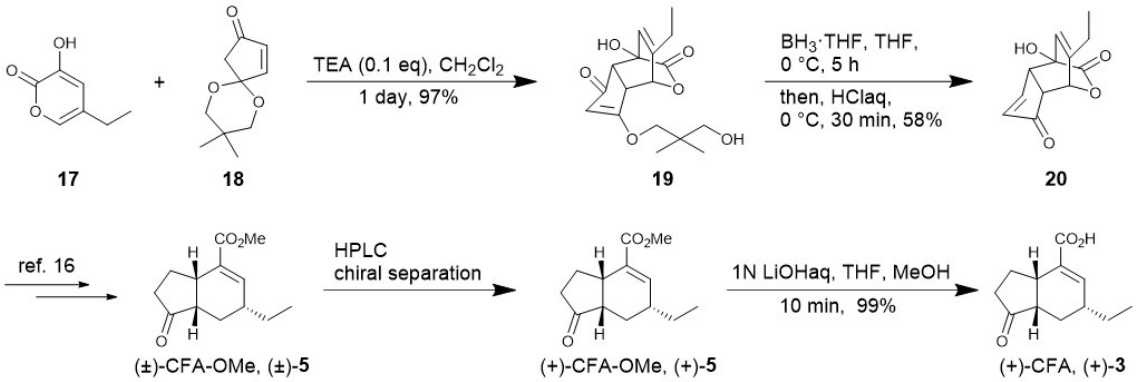
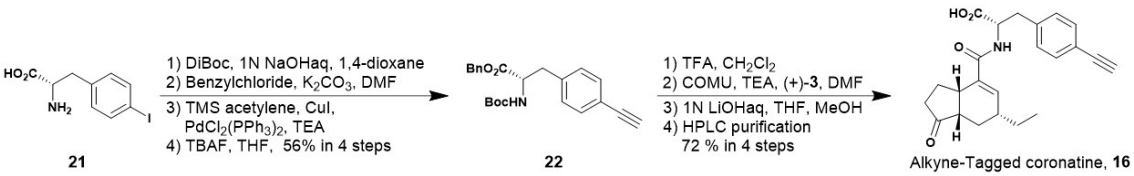


Figure. S5 Molecular dynamics (MD) simulations of the COI1-JAZ1 with COR, CFA-Ile and CFA-Leu.

In docking simulations (left) and in MD simulations (right), yellow line represents the distance within 3.5 Å from the amino acids of COI1 or JAZ1, such as R85, R348, E350, Y386, R409, Y444, R496 and A204 (JAZ1)., and ketone carbonyl, amide carbonyl , amide nitrogen or oxygen atoms of carboxyl acid of ligands.



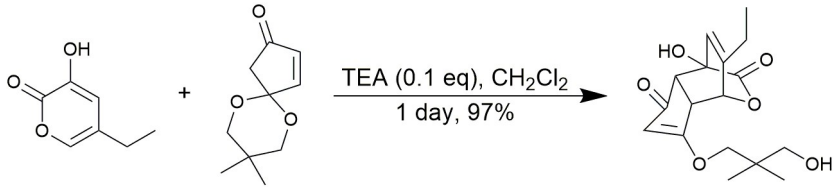
Scheme S1 Synthesis of (+)-coronafacic acid (+)-**3**



Scheme. S2 Synthesis of Alkyne-Tagged coronatine (**16**)

Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

Materials and Methods

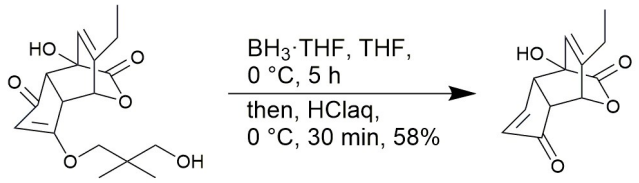


17 **18** **19**

(3a*R*,4*S*,7*S*,7a*S*)-5-ethyl-7-hydroxy-3-(3-hydroxy-2,2-dimethylpropoxy)-3a,4,7,7a-tetrahydro-1*H*-4,7-(epoxymethano)indene-1,8-dione (**19**)

To a solution of 5-ethyl-3-hydroxypyrone [*cas*. 1187021-54-0] **17** (1.40 g, 10.0 mmol) in CH_2Cl_2 (150 mL) was added cyclopentene [*cas*. 129822-78-2] **18** (2.17 g, 11.1 mmol) and TEA (10.9 mg, 1.07 mmol) at 0 °C under argon atmosphere. The reaction mixture was stirred for 2 days. After evaporation, the residue was purified by silica gel column chromatography (*n*-hexane/EtOAc = 5/1). Each solution was concentrated by evaporation gave **19** (3.14mg, 9.73 mmol, 97%) as a white solid.

^{1}H-NMR (400 MHz, $CDCl_3$) δ_H; 6.07 (q. J = 2.0 Hz, 1H), 5.39 (d, J = 0.8 Hz, 1H), 5.02 (t. J = 2.0 Hz, 1H), 4.09 (s, 1H), 3.88 (dd. J = 20.8, 9.6 Hz, 2H), 3.50 (dd. J = 5.2, 3.2 Hz, 2H), 3.23 (ddd. J = 7.6, 1.6, 0.8 Hz, 1H), 2.81 (d. J = 7.6 Hz, 1H), 2.29 (qd. J = 7.2, 2.0 Hz, 2H), 1.98 (d. J = 5.2 Hz, 1H), 1.11 (t. J = 7.2, 3H), 1.03 (s, 3H), 1.02 (s, 3H); ^{13}C-NMR (100MHz, $CDCl_3$) δ_c: 201.7, 186.4, 172.4, 145.1, 128.0, 107.6, 77.8, 76.9, 76.1, 68.0, 50.5, 47.7, 36.6, 24.7, 21.3, 21.3, 11.0; IR (film) cm^{-1}: 3346, 2964, 2927, 2877, 1769, 1680, 1589, 1473, 1387, 1345, 1299, 1256, 1230, 1187, 1048, 1005, 961; HRMS (ESI, positive) *m/z* $[M+Na]^+$ calcd. for $C_{17}H_{22}O_6Na$: 345.1314, found: 345.1302.



19 **20**

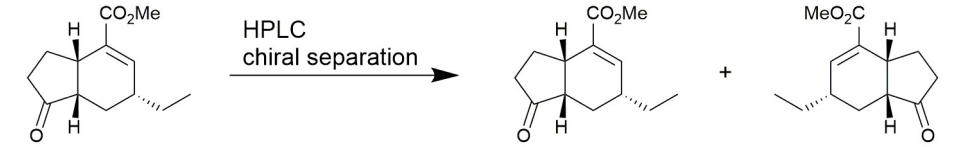
(3a*R*,4*S*,7*R*,7a*S*)-5-ethyl-7-hydroxy-3a,4,7,7a-tetrahydro-3*H*-4,7-(epoxymethano)indene-3,8-dione (**20**)

To a solution of **19** (219.2 g, 0.659 mmol) in THF (16 mL) was added BH_3·THF solution (1M in THF, 1.2 mL) at 0 °C under argon atmosphere. The reaction mixture was stirred for 3 h, and then BH_3·THF solution (1M in THF, 1.2 mL) was added again. The reaction mixture was stirred for 3 h, and then 6M HClaq (3.5 mL) was added. After the reaction mixture was stirred for 30 min, the reaction mixture was quenched with H_2O. The mixture was extracted with EtOAc (3 × 50 mL) and brine (50 mL) washed. The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by silica gel column chromatography ($CHCl_3$/MeOH = 100/1). Each solution was concentrated by evaporation gave **20** (86.2 mg, 0.392 mmol, 58%) as a colorless crystalline solid.

Compound data in Ref 16 [*cas.* 1260503-15-8]

Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

HPLC chiral separation of CFA methyl ester



(±)-CFA-OMe, (±)-**5** (+)-CFA-OMe, (+)-**5** (-)-CFA-OMe, (-)-**5**

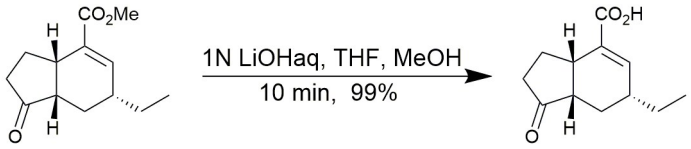
Synthesized racemic Coronafacic methyl ester (*rac.* CFA-Me [*cas.* 73961-72-5]) was chiral separation by HPLC on silica gel column (CHIRALPAK IA, 20 × 250 mm, DAICEL co., ltd.) with a solution (n-Hex : EtOH = 47 : 3) at 5 mL/min for 5 times recycled to give (-)-CFA-Me ((-)-**5**) (Rt = 235-242 min) and (+)-CFA-Me ((+)-**5**) (Rt = 246-255 min). Each solution was concentrated by evaporation gave (-)-**5** as a colorless crystalline solid and (+)-**5** as a colorless crystalline solid.

(+)-CFA-OMe, (+)-**5**

^{1}H-NMR (400MHz, $CDCl_3$) δ_H; 6.92 (s, 1H), 3.77 (s, 3H), 3.08 (dt. *J* = 11.2, 7.2 Hz, 1H), 2.56 (dt. *J* = 12.4, 8.0 Hz, 1H), 2.45-2.15 (m, 4H), 1.86 (dt. *J* = 13.2, 4.8 Hz, 1H), 1.63-1.35 (m, 3H), 1.08 (td. *J* = 13.2, 11.2 Hz, 1H), 0.98 (t. J = 7.2 Hz, 3H); ^{13}C-NMR (100MHz, $CDCl_3$) δ_c: 220.4, 167.3, 144.2, 131.3, 51.7, 46.7, 38.2, 37.7, 36.2, 28.2, 27.8, 25.8, 11.2; IR (film) cm^{-1}: 2957, 2877, 2858, 1742, 1712, 1641, 1464, 1436, 1259, 1145, 1098, 1069, 752; HRMS (ESI, positive) *m/z* $[M+Na]^+$ calcd. for $C_{13}H_{18}O_3Na$: 245.1154, found: 245.1149; $[\alpha]_D^{24}$ +122° (*c* 0.20, $CHCl_3$).

(-)-CFA-OMe, (-)-**5**

^{1}H-NMR (400MHz, $CDCl_3$) δ_H; 6.92 (s, 1H), 3.77 (s, 3H), 3.08 (dt. *J* = 11.2, 7.2 Hz, 1H), 2.56 (dt. *J* = 12.4, 8.0 Hz, 1H), 2.45-2.15 (m, 4H), 1.86 (dt. *J* = 13.2, 4.8 Hz, 1H), 1.63-1.35 (m, 3H), 1.08 (td. *J* = 13.2, 11.2 Hz, 1H), 0.98 (t. J = 7.2 Hz, 3H); ^{13}C-NMR (100MHz, $CDCl_3$) δ_c: 220.4, 167.3, 144.2, 131.3, 51.7, 46.7, 38.2, 37.7, 36.2, 28.2, 27.8, 25.8, 11.2; IR (film) cm^{-1}: 2957, 2877, 2858, 1742, 1712, 1641, 1464, 1436, 1259, 1145, 1098, 1069, 752; HRMS (ESI, positive) *m/z* $[M+Na]^+$ calcd. for $C_{13}H_{18}O_3Na$: 245.1154, Found: 245.1150; $[\alpha]_D^{23}$ -122° (*c* 0.26, $CHCl_3$).



(+)-CFA-OMe, (+)-**5** (+)-CFA, (+)-**3**

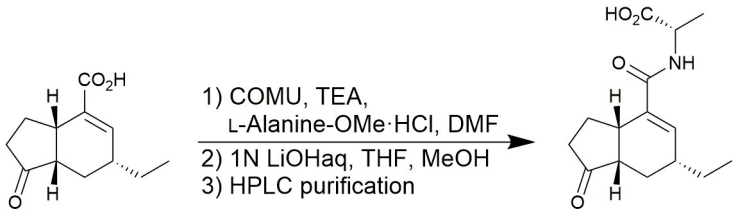
(+)-CFA, (+)-**3** [*cas.* 62251-98-3]

Compound (+)-**5** (5.4 mg, 24.3 μmol) in MeOH (0.2 mL) was added THF (0.1mL) and 1N aqueous LiOH (0.1 mL). After the reaction mixture was stirred for 10 min, the reaction mixture was quenched with 1N aqueous $KHSO_4$ (0.2 mL). The mixture was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by HPLC on silica gel column (COSMOSIL SC_{18}-AR, 20 × 250 mm, Nacalai Tesque co., ltd.) with solution (CH_3CN / aqueous = 30 / 70) in 0.1% HCO_2H at 6.5 mL/min to give (+)-**3** (Rt = 28-31 min), respectively. Each solution was concentrated *in vacuo*., gave (+)-**3** (5.0 mg, 24.0 μmol, 99%) as a colorless crystalline solid.

$[\alpha]_D^{23}$ +120° (*c* 0.25, MeOH)

(-)-**3** [*cas.* 87335-74-8]

$[\alpha]_D^{23}$ -121° (*c* 0.40, MeOH)

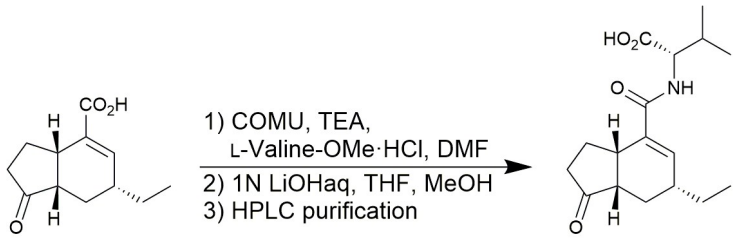


(+)-CFA, (+)-**3** CFA-L-Ala, **6**

CFA-L-Ala (**6**)

To a solution of (+)-CFA (2.1 mg, 10.1 μmol) in DMF (0.25 mL) was added COMU (4.7 mg, 11.0 μmol) and TEA (2.9 mg, 28.7 μmol) at room temperature under argon atmosphere. The reaction mixture was stirred for 10 min, and then L-Alanine methyl ester hydrochloride (1.6 mg, 11.5 μmol) was added. After the reaction mixture was stirred for 2.5 h, the reaction mixture was quenched with saturated aqueous $NaHCO_3$. The mixture was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by silica gel column chromatography (*n*-hexane/EtOAc = 3/1). Each solution was concentrated by evaporation gave mixture compound. To a solution of the residue in MeOH (0.2 mL) was added THF (0.1mL) and 1N aqueous LiOH (0.1 mL). After the reaction mixture was stirred for 10 min, the reaction mixture was quenched with 1N aqueous $KHSO_4$. The mixture was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by HPLC on silica gel column (COSMOSIL SC_{18}-AR, 20 × 250 mm, Nacalai Tesque co., ltd.) with 0.05% HCO_2H solution (MeOH / aqueous = 45 / 55) at 8.0 mL/min to give **6** (Rt = 31-35 min), respectively. Each solution was concentrated by evaporation gave **6** (2.1 mg, 7.52 μmol, 75%) as a colorless crystalline solid.

^{1}H-NMR (400MHz, $CDCl_3$) δ_H; 6.40 (s, 1H), 6.36 (brs, 1H), 4.61 (1H, brs), 3.17 (m, 1H), 2.50-2.24 (m, 4H), 2.15 (m, 1H), 1.90 (dt. *J* = 12.8, 4.4 Hz, 1H), 1.68-1.32 (m, 6H), 1.07 (td. *J* = 12.8, 11.2 Hz, 1H), 0.99 (t. J = 7.6 Hz, 3H); ^{13}C-NMR (100MHz, $CDCl_3$) δ_c: 220.1, 168.6, 137.9, 135.1, 46.4, 38.1, 36.1, 28.0, 27.7, 25.9, 17.8, 11.3; IR (film) cm^{-1}: 3333, 2964, 2931, 2877, 1735, 1655, 1618, 1530, 1458, 1450, 1213, 1152, 753; HR MS (ESI, negative) *m/z* $[M-H]^-$ calcd. for $C_{15}H_{20}NO_4$: 278.1392, found: 278.1395; $[\alpha]_D^{23}$ +77° (*c* 0.10, $CHCl_3$).

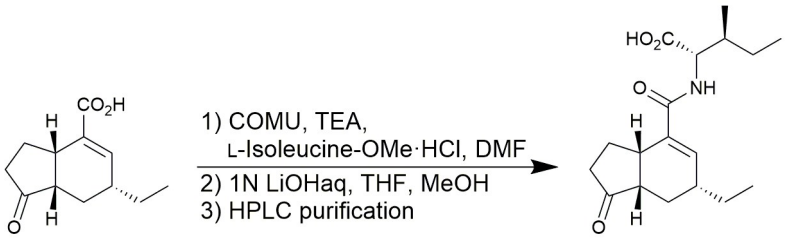


(+)-CFA, (+)-**3** CFA-L-Val, **7**

CFA-L-Val (**7**)

To a solution of (+)-CFA (2.1 mg, 10.1 μmol) in DMF (0.25 mL) was added COMU (4.6 mg, 10.7 μmol) and TEA (2.9 mg, 28.7 μmol) at room temperature under argon atmosphere. The reaction mixture was stirred for 10 min, and then L-Valine methyl ester hydrochloride (1.9 mg, 11.3 μmol) was added. After the reaction mixture was stirred for 2 h, the reaction mixture was quenched with saturated aqueous $NaHCO_3$. The mixture was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by silica gel column chromatography (*n*-hexane/EtOAc = 3/1). Each solution was concentrated by evaporation gave mixture compound. To a solution of the residue in MeOH (0.2 mL) was added THF (0.1mL) and 1N aqueous LiOH (0.1 mL). After the reaction mixture was stirred for 10 min, the reaction mixture was quenched with 1N aqueous $KHSO_4$. The mixture was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by HPLC on silica gel column (COSMOSIL SC_{18}-AR, 20 × 250 mm, Nacalai Tesque co., ltd.) with 0.05% HCO_2H solution (MeOH / aqueous = 50 / 50) at 8.0 mL/min to give **7** (Rt = 40-44 min), respectively. Each solution was concentrated by evaporation gave **7** (1.7 mg, 4.58 μmol, 64%) as a colorless crystalline solid.

^{1}H-NMR (400MHz, $CDCl_3$) δ_H; 6.41 (s, 1H), 6.27 (brs, 1H), 4.58 (brs, 1H), 3.18 (dt. *J* = 9.6, 7.2, 1H), 2.48-2.23 (m, 5H), 2.16 (m, 1H), 1.91 (dt. *J* = 12.8, 4.4 Hz, 1H), 1.63-1.33 (m, 3H), 1.07 (td. *J* = 12.8, 11.2 Hz, 1H), 1.03-0.96 (m, 9H); ^{13}C-NMR (100MHz, $CDCl_3$) δ_c: 220.1, 168.5, 137.6, 135.4, 46.4, 38.1, 37.4, 36.2, 30.1, 28.1, 27.8, 26.0, 19.2, 18.0, 11.3; IR (film) cm^{-1}: 3333, 2965, 2929, 2875, 1735, 1654, 1617, 1522, 1465, 1405, 1306, 1215, 1148, 755; HR MS (ESI, negative) *m/z* $[M-H]^-$ calcd. for $C_{17}H_{24}NO_4$: 306.1705, found: 306.1710. $[\alpha]_D^{23}$ +64° (*c* 0.11, $CHCl_3$).

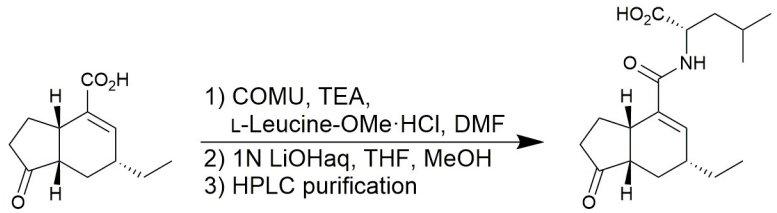


(+)-CFA, (+)-**3** CFA-L-Ile, **8**

CFA-L-Ile (**8**)

To a solution of (+)-CFA (3.1 mg, 14.9 μmol) in DMF (0.25 mL) was added COMU (4.6 mg, 10.7 μmol) and TEA (2.9 mg, 28.7 μmol) at room temperature under argon atmosphere. The reaction mixture was stirred for 10 min, and then L-Isoleucine methyl ester hydrochloride (2.0 mg, 11.0 μmol) was added. After the reaction mixture was stirred for 2.5 h, the reaction mixture was quenched with saturated aqueous $NaHCO_3$. The mixture was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by silica gel column chromatography (*n*-hexane/EtOAc = 3/1). Each solution was concentrated by evaporation gave mixture compound. To a solution of the residue in MeOH (0.2 mL) was added THF (0.1mL) and 1N aqueous LiOH (0.1 mL). After the reaction mixture was stirred for 10 min, the reaction mixture was quenched with 1N aqueous $KHSO_4$. The mixture was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by HPLC on silica gel column (COSMOSIL SC_{18}-AR, 20 × 250 mm, Nacalai Tesque co., ltd.) with 0.05% HCO_2H solution (MeOH / aqueous = 55 / 45) at 8.0 mL/min to give **8** (Rt = 48-53 min), respectively. Each solution was concentrated by evaporation gave **8** (2.1 mg, 6.53 μmol, 65%) as a colorless crystalline solid.

^{1}H-NMR (400MHz, $CDCl_3$) δ_H; 6.40 (s, 1H), 6.30 (brs, 1H), 4.64 (brs, 1H), 3.18 (m, 1H), 2.48-2.24 (m, 4H), 2.16 (m, 1H), 2.01 (m, 1H), 1.89 (dt. *J* = 12.8, 4.4 Hz, 1H), 1.69-1.33 (m, 4H), 1.30-1.21 (m, 1H), 1.07 (td. *J* = 12.8, 11.6 Hz, 1H), 1.00-0.92 (m, 9H); ^{13}C-NMR (100MHz, $CDCl_3$) δ_c: 220.2, 168.7, 137.7, 135.3, 46.4, 41.0, 38.1, 37.4, 36.2, 28.1, 27.7, 25.9, 25.1, 22.9, 21.9, 11.3; IR (film) cm^{-1}: 3345, 2965, 2935, 2877, 1734, 1654, 1622, 1521, 1463, 1405, 1385, 1329, 1217, 1145, 755; HRMS (ESI, negative) *m/z* [M-H]$^-$ calcd. for $C_{18}H_{26}NO_4$: 320.1862, found: 320.1867; $[\alpha]_D^{23}$ +33° (*c* 0.105, $CHCl_3$).

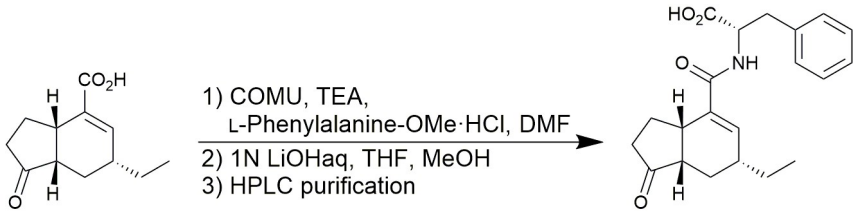


(+)-CFA, (+)-**3** CFA-L-Leu, **9**

CFA-L-Leu (**9**)

To a solution of (+)-CFA (2.1 mg, 10.1 μmol) in DMF (0.25 mL) was added COMU (4.6 mg, 10.7 μmol) and TEA (2.9 mg, 28.7 μmol) at room temperature under argon atmosphere. The reaction mixture was stirred for 10 min, and then L-Leucine methyl ester hydrochloride (2.0 mg, 11.0 μmol) was added. After the reaction mixture was stirred for 2 h, the reaction mixture was quenched with saturated aqueous $NaHCO_3$. The mixture was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by silica gel column chromatography (*n*-hexane/EtOAc = 3/1). Each solution was concentrated by evaporation gave mixture compound. To a solution of the residue in MeOH (0.2 mL) was added THF (0.1mL) and 1N aqueous LiOH (0.1 mL). After the reaction mixture was stirred for 10 min, the reaction mixture was quenched with 1N aqueous $KHSO_4$. The mixture was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by HPLC on silica gel column (COSMOSIL SC_{18}-AR, 20 × 250 mm, Nacalai Tesque co., ltd.) with 0.05% HCO_2H solution (MeOH / aqueous = 55 / 45) at 8.0 mL/min to give **9** (Rt = 49-54 min), respectively. Each solution was concentrated by evaporation gave **9** (2.7 mg, 8.40 μmol, 83%) as a colorless crystalline solid.

^{1}H-NMR (400MHz, $CDCl_3$) δ_H; 6.38 (s, 1H), 6.16 (brs, 1H), 4.64 (brs, 1H), 3.16 (dt. *J* = 9.2, 6.8, 1H), 2.48-2.24 (m, 4H), 2.16 (m, 1H), 1.90 (dt. *J* = 12.8, 4.4 Hz, 1H), 1.82-1.32 (m, 6H), 1.07 (td. *J* = 12.8, 11.2 Hz, 1H), 1.00-0.94 (m, 9H); ^{13}C-NMR (100MHz, $CDCl_3$) δ_c: 220.2, 168.3, 137.6, 135.4, 46.4, 38.1, 37.6, 37.4, 36.2, 28.1, 27.8, 26.0, 25.3, 15.6, 11.6, 11.3; IR (film) cm^{-1}: 3308, 2958, 2936, 2872, 1734, 1653, 1617, 1532, 1465, 1444, 1333, 1270, 1231, 1152, 755; HRMS (ESI, negative) *m/z* $[M-H]^-$ calcd. for $C_{18}H_{26}NO_4$: 320.1862, found: 320.1862; $[\alpha]_D^{23}$ +36° (*c* 0.14, $CHCl_3$).

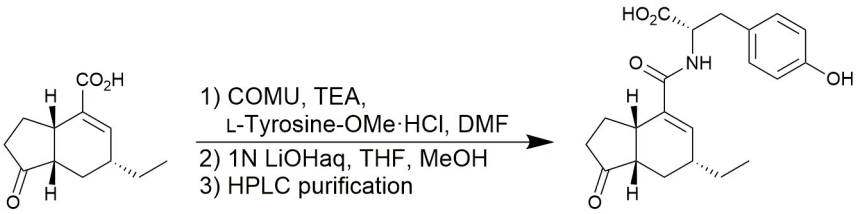


(+)-CFA, (+)-**3** CFA-L-Phe, **10**

CFA-L-Phe (**10**)

To a solution of (+)-CFA (1.5 mg, 7.20 μmol) in DMF (0.22 mL) was added COMU (4.6 mg, 10.7 μmol) and TEA (2.9 mg, 28.7 μmol) at room temperature under argon atmosphere. The reaction mixture was stirred for 10 min, and then L-Phenylalanine methyl ester hydrochloride (2.4 mg, 11.1 μmol) was added. After the reaction mixture was stirred for 1.5 h, the reaction mixture was quenched with saturated aqueous $NaHCO_3$. The mixture was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by silica gel column chromatography (*n*-hexane/EtOAc = 3/1). Each solution was concentrated by evaporation gave mixture compound. To a solution of the residue in MeOH (0.2 mL) was added THF (0.1mL) and 1N aqueous LiOH (0.1 mL). After the reaction mixture was stirred for 10 min, the reaction mixture was quenched with 1N aqueous $KHSO_4$. The mixture was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by HPLC on silica gel column (COSMOSIL SC_{18}-AR, 20 × 250 mm, Nacalai Tesque co., ltd.) with 0.05% HCO_2H solution (MeOH / aqueous = 55 / 45) at 8.0 mL/min to give **10** (Rt = 49-53 min), respectively. Each solution was concentrated by evaporation gave **10** (1.8 mg, 5.06 μmol, 70%) as a colorless crystalline solid.

^{1}H-NMR (400MHz, $CDCl_3$) δ_H; 7.36-7.27 (m, 3H), 7.21 (dd. *J* = 8.0, 1.6 Hz, 2H), 6.21 (s, 1H), 6.09 (brs, 1H), 4.86 (td. *J* = 6.0, 6.0 Hz, 1H), 3.34 (dd. *J* = 6.0, 1.6 Hz, 1H), 3.18 (dd. *J* = 6.0, 1.6 Hz, 1H), 3.07 (dt. *J* = 10.4, 6.8 Hz, 1H), 2.38-2.15 (m, 4H), 2.09 (m, 1H), 1.86 (dt. *J* = 12.8, 4.8 Hz, 1H), 1.54-1.28 (m, 3H), 1.00 (td. *J* = 12.8, 11.2 Hz, 1H), 0.94 (t. *J* = 7.6 Hz, 3H); ^{13}C-NMR (100MHz, $CDCl_3$) δ_c: 219.9, 168.7, 138.4, 135.8, 134.9, 129.4 (2C), 128.8 (2C), 127.4, 46.3, 38.1, 37.4, 36.9, 36.0, 27.9, 27.5, 26.0, 11.2; IR (film) cm^{-1}: 3333, 2959, 2932, 2872, 1739, 1653, 1617, 1521, 1497, 1456, 1269, 1218, 1152, 755; HRMS (ESI, negative) *m/z* $[M-H]^-$ calcd. for $C_{21}H_{24}NO_4$:354.1705, found: 354.1707; $[\alpha]_D^{22}$ +66° (*c* 0.10, $CHCl_3$).

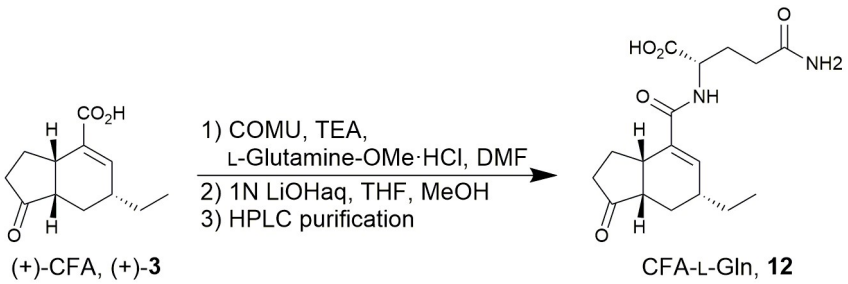


(+)-CFA, (+)-**3** CFA-L-Tyr, **11**

CFA-L-Tyr (**11**)

To a solution of (+)-CFA (1.5 mg, 7.20 μmol) in DMF (0.22 mL) was added COMU (4.7 mg, 11.0 μmol) and TEA (2.9 mg, 28.7 μmol) at room temperature under argon atmosphere. The reaction mixture was stirred for 10 min, and then L-Tyrosine methyl ester hydrochloride (2.6 mg, 11.2 μmol) was added. After the reaction mixture was stirred for 1.5 h, the reaction mixture was quenched with saturated aqueous $NaHCO_3$. The mixture was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by silica gel column chromatography (*n*-hexane/EtOAc = 3/1). Each solution was concentrated by evaporation gave mixture compound. To a solution of the residue in MeOH (0.2 mL) was added THF (0.1mL) and 1N aqueous LiOH (0.1 mL). After the reaction mixture was stirred for 10 min, the reaction mixture was quenched with 1N aqueous $KHSO_4$. The mixture was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by HPLC on silica gel column (COSMOSIL SC_{18}-AR, 20 × 250 mm, Nacalai Tesque co., ltd.) with 0.05% HCO_2H solution (MeOH / aqueous = 55 / 45) at 8.0 mL/min to give **11** (Rt = 49-53 min), respectively. Each solution was concentrated by evaporation gave **11** (1.8 mg, 5.06 μmol, 70%) as a colorless crystalline solid.

^{1}H-NMR (400MHz, CD_3OD) δ_H: 7.05 (d, *J* = 8.4 Hz, 2H), 6.69 (d, *J* = 8.4 Hz, 2H), 6.29 (s, 2H), 4.61 (brs, 1H), 3.19 (dd, *J* = 13.6, 4.4 Hz, 1H), 3.14-2.90 (m, 2H), 2.37-2.21 (m, 2H), 2.17-2.04 (m, 2H), 1.76 (dt, *J* = 13.2, 4.8 Hz, 1H), 1.53-1.34 (m, 3H), 1.07 (dt, *J* = 13.2, 10.8 Hz, 1H), 0.98 (t, *J* = 7.2 Hz, 3H); ^{13}C-NMR (100MHz, CD_3OD) δ_c: 222.9, 172.1, 157.3, 138.7, 138.3, 131.4 (2C), 129.6, 116.1 (2C), 84.0, 47.8, 38.7, 38.6, 37.6, 37.3, 29.1, 28.5, 27.2, 11.6; IR (film) cm^{-1}: 3333, 2964, 2931, 2854, 1733, 1653, 1616, 1516, 1457, 1261, 1226, 1146, 754; HRMS (ESI, negative) *m/z* $[M-H]^-$ calcd. for $C_{21}H_{24}NO_5$: 370.1654, found: 370.1658; $[\alpha]_D^{22}$ +45° (*c* 0.10, MeOH).

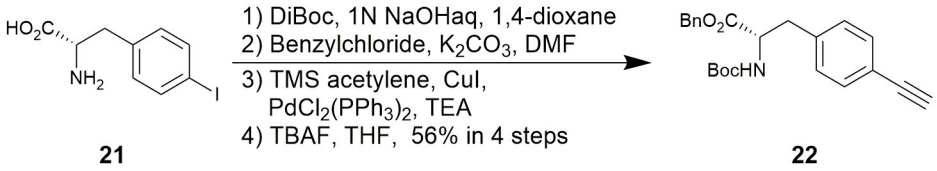


(+)-CFA, (+)-**3** CFA-L-Gln, **12**

CFA-L-Gln (**12**)

To a solution of (+)-CFA (3.1 mg, 14.9 μmol) in DMF (0.3 mL) was added COMU (7.1 mg, 16.6 μmol) and TEA (2.9 mg, 28.7 μmol) at room temperature under argon atmosphere. The reaction mixture was stirred for 10 min, and then L-Glutamine methyl ester (2.5 mg, 17.1 μmol) was added. After the reaction mixture was stirred for 1.0 h, the reaction mixture was quenched with saturated aqueous $NaHCO_3$. The mixture was extracted with EtOAc (3 × 5 mL) and 1N $KHSO_4$aq washed. The organic layer was dried over Na_2SO_4, and filtered. After evaporation, to a solution of the residue in MeOH (0.2 mL) was added THF (0.1mL) and 1N aqueous LiOH (0.1 mL). After the reaction mixture was stirred for 10 min, the reaction mixture was quenched with 1N aqueous $KHSO_4$ (0.11 mL). After freeze dehydration and filtration, the residue was purified by HPLC on silica gel column (COSMOSIL SC_{18}-AR, 20 × 250 mm, Nacalai Tesque co., ltd.) with solution (MeOH / aqueous = 30 / 70) in 0.05% HCO_2H at 8.0 mL/min to give **12** (Rt = 48-52 min), respectively. Each solution was concentrated *in vacuo*., gave **12** formate (3.3 mg, 8.63 μmol, 58%) as a colorless crystalline solid.

^{1}H-NMR (400MHz, CD_3OD) δ_H: 6.52 (s, 1H), 4.59 (brs, 1H), 3.18 (dt. *J* = 10.4, 6.8 Hz, 1H), 2.44-2.28 (m, 6H), 2.26–2.12 (m, 2H), 2.05 (m, 1H) 1.80 (td. *J* = 12.8, 4.8 Hz, 1H), 1.68-1.35 (m, 3H), 1.14 (td, *J* = 12.8, 11.2 Hz, 1H), 1.01 (t, *J* = 7.6 Hz, 3H); ^{13}C-NMR (100MHz, CD_3OD) δ_c: 223.0, 170.5, 138.5, 136.4, 85.0, 47.9, 38.8, 38.7, 37.3, 33.0, 29.1, 29.0, 28.8, 27.1, 11.6 ; IR (film) cm-1; 3417, 2961, 2925, 2853, 1733, 1658, 1616, 1532, 1456, 1404, 1263, 1152, 757; HRMS (ESI, negative) *m/z* $[M-H]^-$ calcd. for $C_{17}H_{23}N_2O_5$: 335.1607, found: 335.1607; $[\alpha]_D^{22}$ +52° (*c* 0.17, MeOH).



21 **22**

Benzyl (*S*)-2-((tert-butoxycarbonyl)amino)-3-(4-ethynylphenyl)propanoate (**22**)

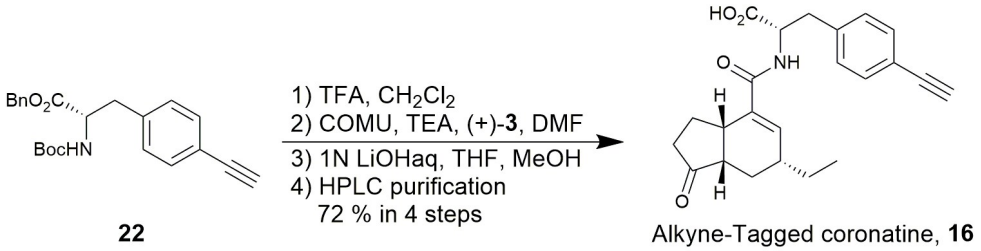
To a solution of 4-iodo-L-Phenylalanine (**21**) [*cas.*: 24250-85-9] in 1,4-dioxane (1.5 mL) was added Di-*tert*-butyl dicarbonate (54.8 μL, 0.238 mmol) and 1 N aqueous NaOH (3 mL) at room temperature nitrogen argon atmosphere. After the reaction mixture was stirred for 1.0 h, the reaction mixture was quenched with 1N aqueous hydrochloride (30mL). The mixture was extracted with EtOAc (3 × 10 mL) and brine washed. The organic layer was dried over Ns_2SO_4, and filtered. After evaporation, the solution of the residue in DMF (5.0 mL) was added the benzylchloride (32 μL, 0.277 mmol) and K_2CO_3 (32.8 mg, 0.237 mmol) at room temperature under nitrogen atmosphere. After the reaction was stirred for 3.0 h, the reaction mixture was quenched with H_2O (40 mL). The mixture was extracted with EtOAc (3 × 25 mL) and brine washed. The organic layer was dried over Na_2SO_4, and filtered.

After evaporation, the solution of the residue in TEA (5.0 mL) was added Bis(triphenylphosphine)palladium(II) dichloride (3.9 mg, 0.495 mmol), copper(I) iodide (2.2 mg, 11.5μmol) and trimethylsilylacetylene (70 μL, 0.495 mmol) at room temperature under nitrogen atmosphere. After the reaction mixture was stirred for 12.0 h, the reaction mixture was quenched with H_2O. The mixture was extracted EtOAc (3 × 25 mL) and brine washed. The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by silica gel column chromatography (tolene/EtOAc = 50/1).

Each solution was concentrated by evaporation gave mixture compound. To a solution of the residue in THF (3.0 mL) was added 1M TBAF in THF solution (0.3 mL) at -78 °C under nitrogen atmosphere. After the reaction mixture was stirred for 2.0 h, the reaction mixture was quenched with H_2O. The mixture was extracted with EtOAc (3 × 5 mL) and brine washed. The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by silica gel column chromatography (*n*-hexane/EtOAc = 7/1). Each solution was concentrated by evaporation gave **22** (53.3 mg, 0.140 mmol, 56%) as a white crystalline solid.

^{1}H-NMR (400MHz, $CDCl_3$) δ_H 7.38-7.32 (m, 5H), 7.28-7.24 (m, 2H), 6.98 (d. J = 7.6, 2H), 5.12 (m, 2H), 4.97 (d, J= 7.2, 1H), 4.62 (dt, J= 7.2, 5.6, 1H), 3.12-3.00 (m, 3H), 1.42 (s, 9H); ^{13}C-NMR (100MHz, $CDCl_3$) δ_C: 171.5, 155.0, 136.9, 135.1, 132.3 (2C), 130.8, 129.4 (2C), 128.7 (2C), 128.6 (2C), 120.8, 83.4, 80.1, 77.3, 67.3, 54.3, 38.2,

28.3(3C); IR (film) cm^{-1}: 3292, 2978, 2933, 2107, 1741, 1712, 1499, 1455, 1366,1250, 1164, 1056, 1020, 825; HRMS (ESI, positive) *m/z* $[M+Na]^+$ calcd. for $C_{23}H_{26}NO_4Na$: 402.1681, found: 402.1707.



22 Alkyne-Tagged coronatine, **16**

Alkyne-Tagged coronatine (**16**)

To a solution of **21** (38.0 mg, 100 μmol) in CH_2Cl_2 (0.75 mL) was added TFA (0.25 mL) at room temperature under argon atmosphere. After the reaction mixture was stirred for 1.0 h, the reaction mixture was quenched with saturated aqueous $NaHCO_3$ (10 mL). The mixture was extracted with EtOAc (3 × 10 mL) and brine washed. The organic layer was dried over Na_2SO_4, and filtered. After evaporation, to a solution of the residue in DMF (0.5 mL) was added CFA (5.0 mg, 24 μmol), COMU (15.8 mg, 39.2 μmol) and TEA (14.5 mg, 143 μmol) at room temperature under argon atmosphere.. After the reaction mixture was stirred for 2.5 h, the mixture was quenched with 1N aqueous hydrochloride (10 mL). The mixture was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by silica gel column chromatography (*n*-hexane/EtOAc = 3/1). Each solution was concentrated by evaporation gave the residue (9.4 mg, 20 μmol, 83%).

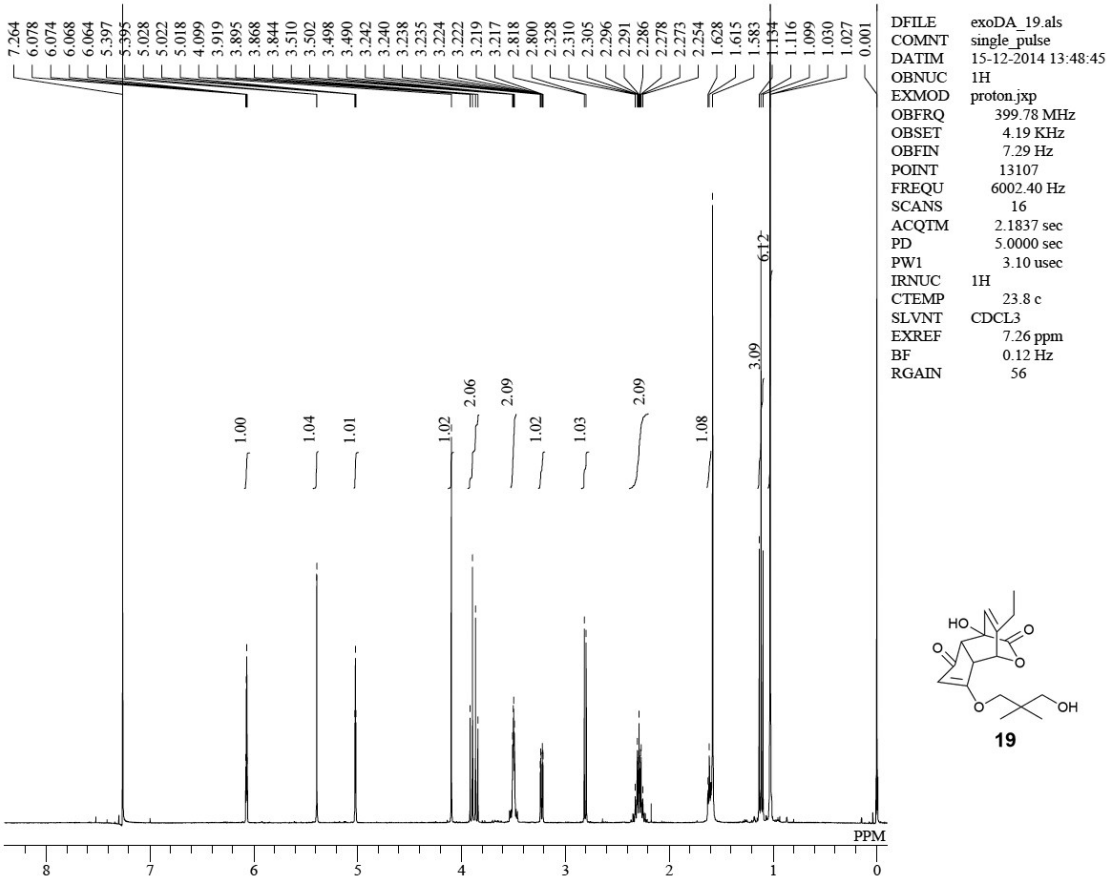
To a solution of the residue (3.7 mg, 7.88 μmol) in MeOH (0.3 mL) was added 1N aqueous LiOH (0.3 mL). After the reaction mixture was stirred for 20 min, the reaction mixture was quenched with 1N aqueous hydrochloride. The mixture was extracted with EtOAc (3 × 5 mL). The organic layer was dried over Na_2SO_4, and filtered. After evaporation, the residue was purified by HPLC on silica gel column (COSMOSIL SC_{18}-AR, 10 × 250 mm, Nacalai Tesque co., ltd.) with 0.05% TFA solution (CH_3CN / aqueous = 55 / 45) at 3.0 mL/min to give **16** (Rt = 62-65 min), respectively. Each solution was concentrated by evaporation gave **16** (2.6 mg, 6.85 μmol, 87%) as a colorless crystalline solid.

^{1}H-NMR (400MHz, CD_3OD) δ_H: 7.38 (d, J = 7.6 Hz, 2H), 7.24 (d, J = 7.6 Hz, 2H), 6.28 (s, 1H), 4.70 (dd, J = 10.0, 4.4 Hz, 1H), 3.42 (s, 1H), 3.22-3.02 (m, 3H), 2.36-2.21 (m, 3H), 2.16-2.05 (m, 2H), 1.76 (dt, J = 12.8, 5.2 Hz, 1H), 1.54-1.33 (m, 3H), 1.08 (dt, J = 12.8, 11.2 Hz, 1H), 0.98 (t, J = 7.2 Hz, 3H); ^{13}C-NMR (100MHz, CD_3OD) δ_c: 222.8, 174.6, 1671.1, 139.9, 138.5, 136.3, 133.1 (2C), 130.4 (2C), 122.3, 84.1, 78.6, 54.9, 47.7, 38.7, 38.5, 37.8, 37.2, 29.0, 28.5, 27.1, 11.6; IR (film) cm^{-1}: 3292, 2962, 2932, 2875, 2017, 1735, 1655, 1614, 1509, 1444, 1404, 1214, 1148, 1068, 827; HRMS (ESI, negative) *m/z* [M-H]$^-$ calcd. for $C_{23}H_{24}NO_4$: 378.1705, found: 378.1705; $[\alpha]_D^{23}$ +85° (*c*

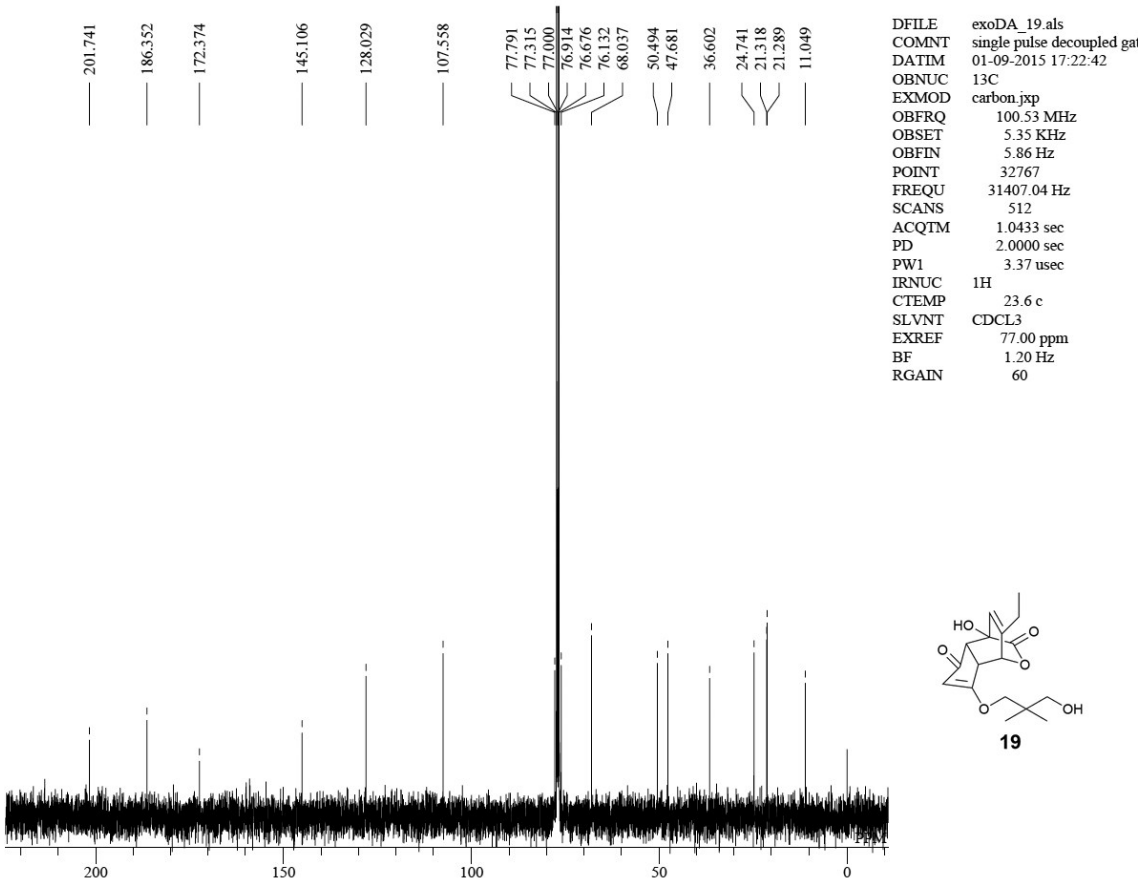
0.10, $CHCl_3$);

Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

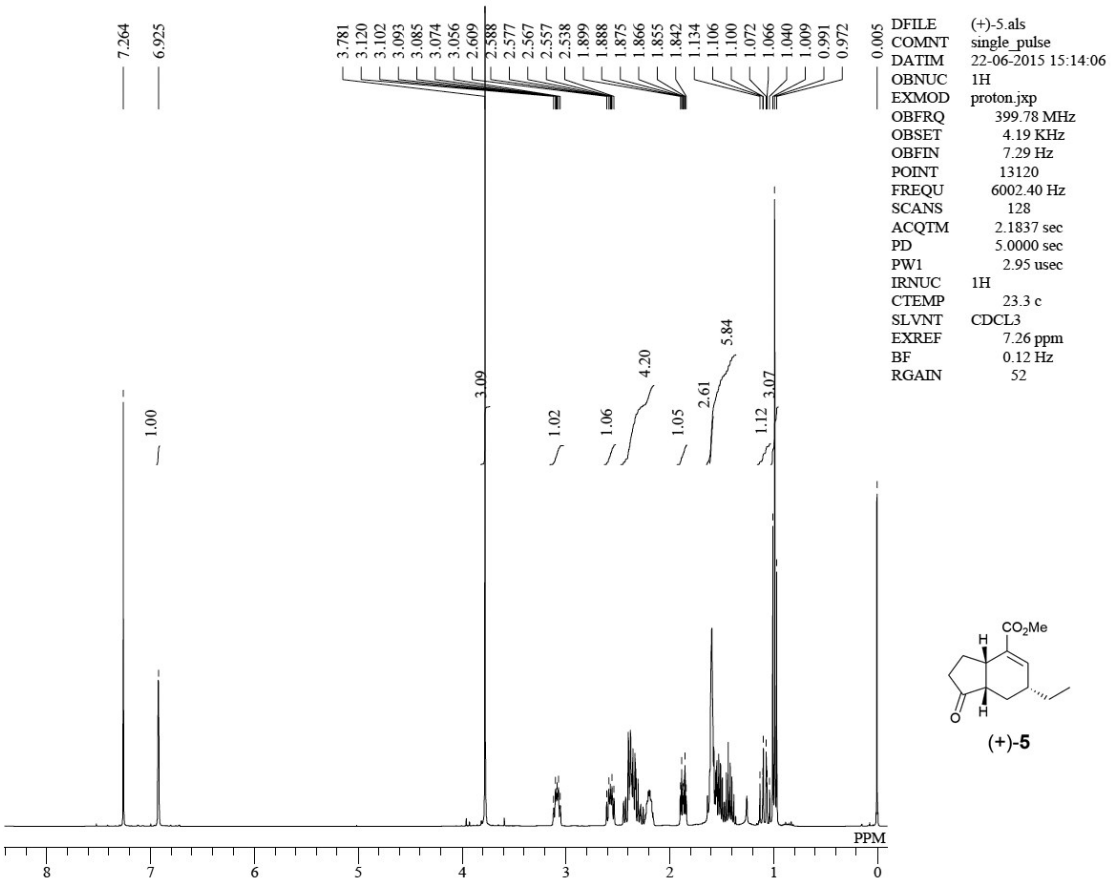
^{1}H and ^{13}C NMR Spectra



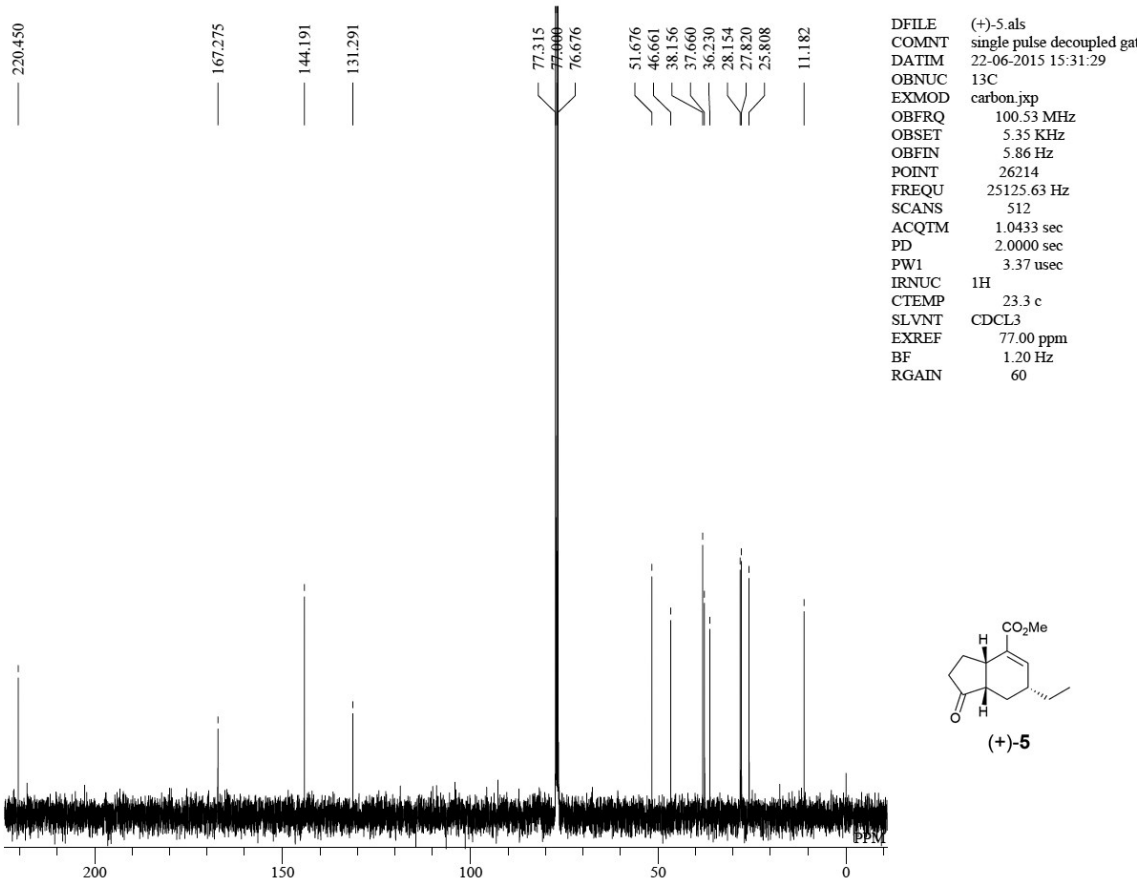
Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.



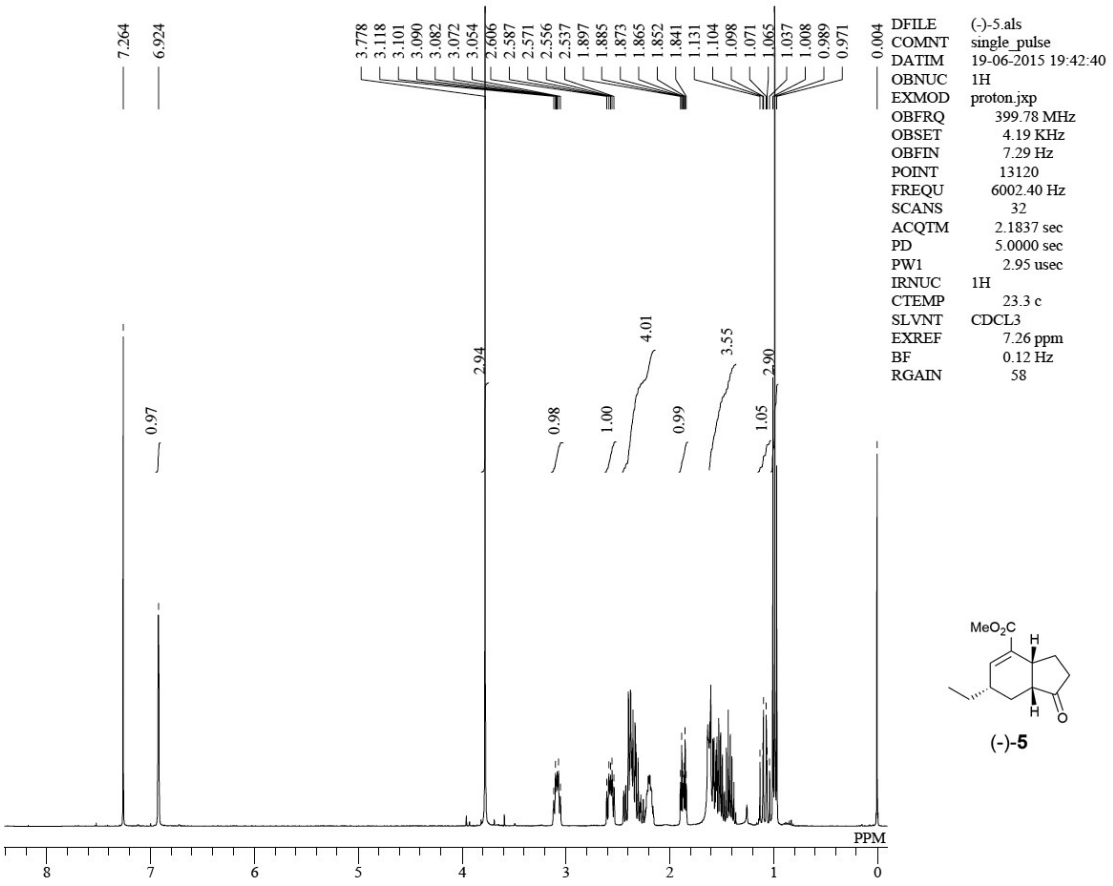
Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.



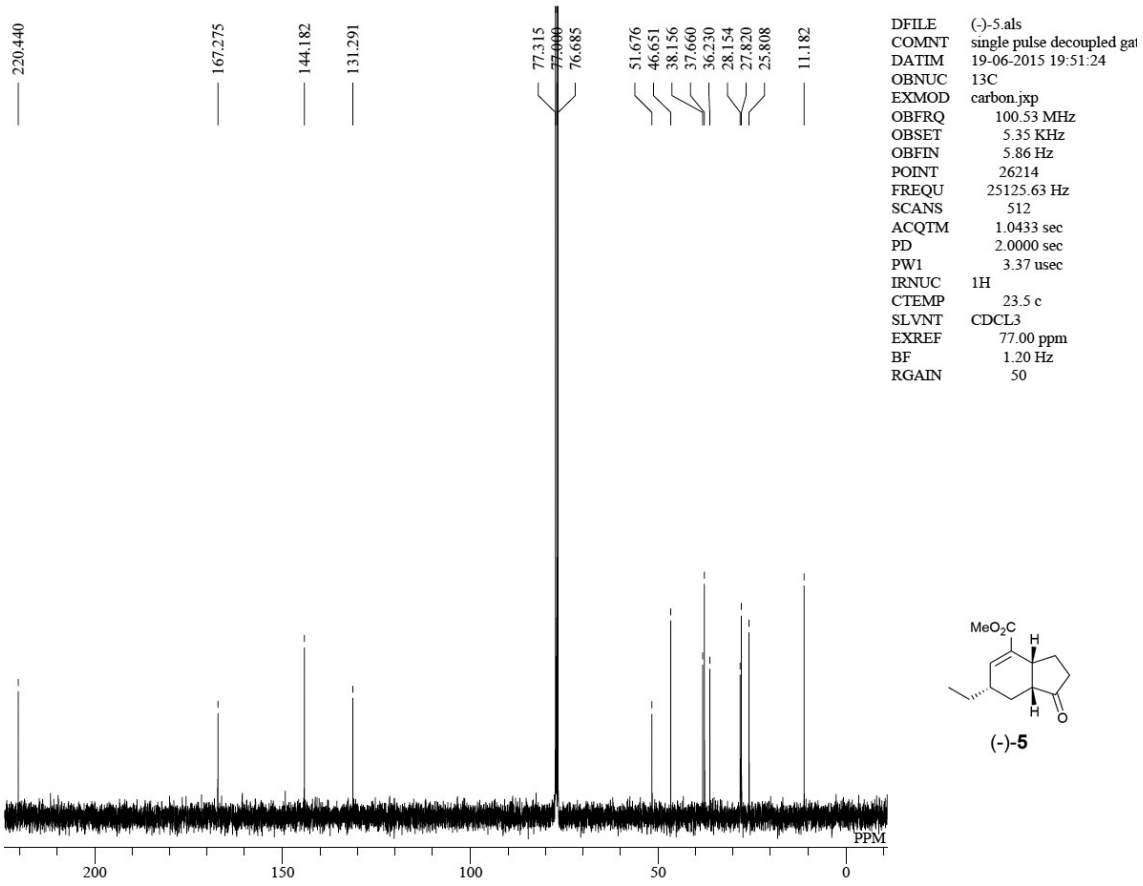
Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.



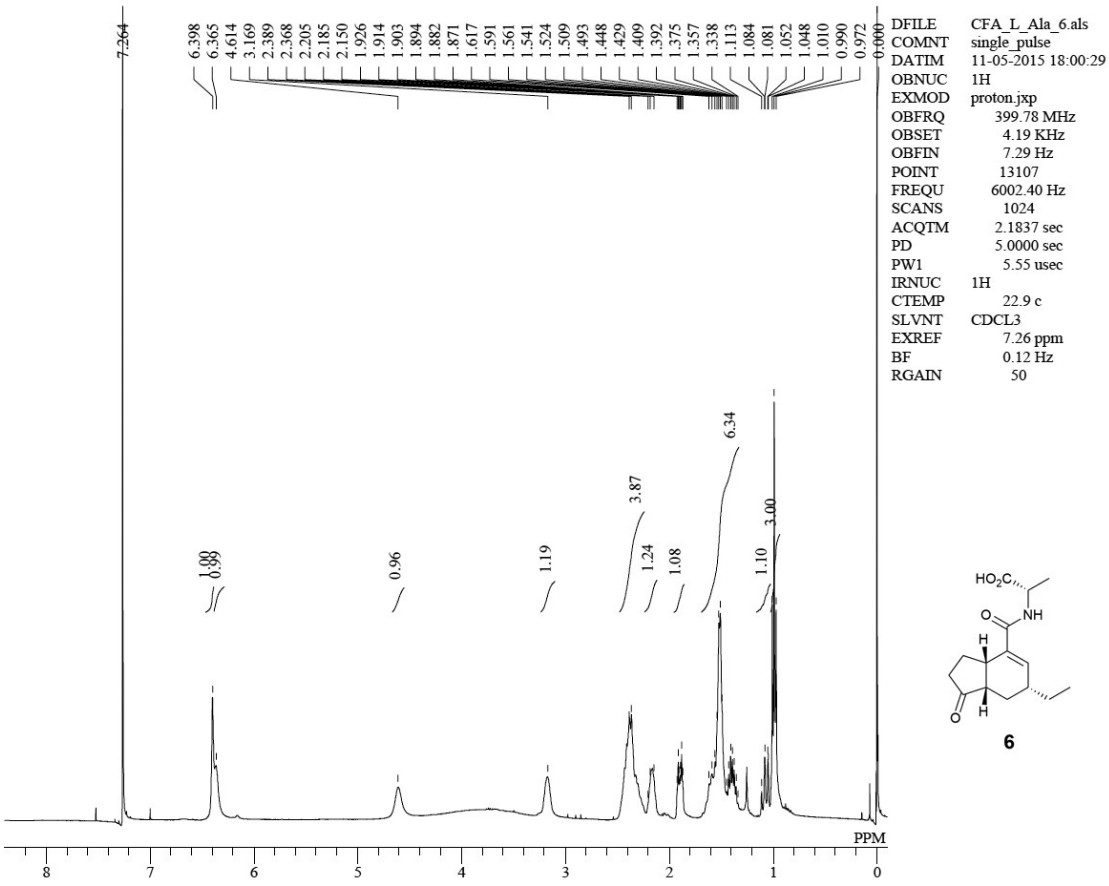
Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.



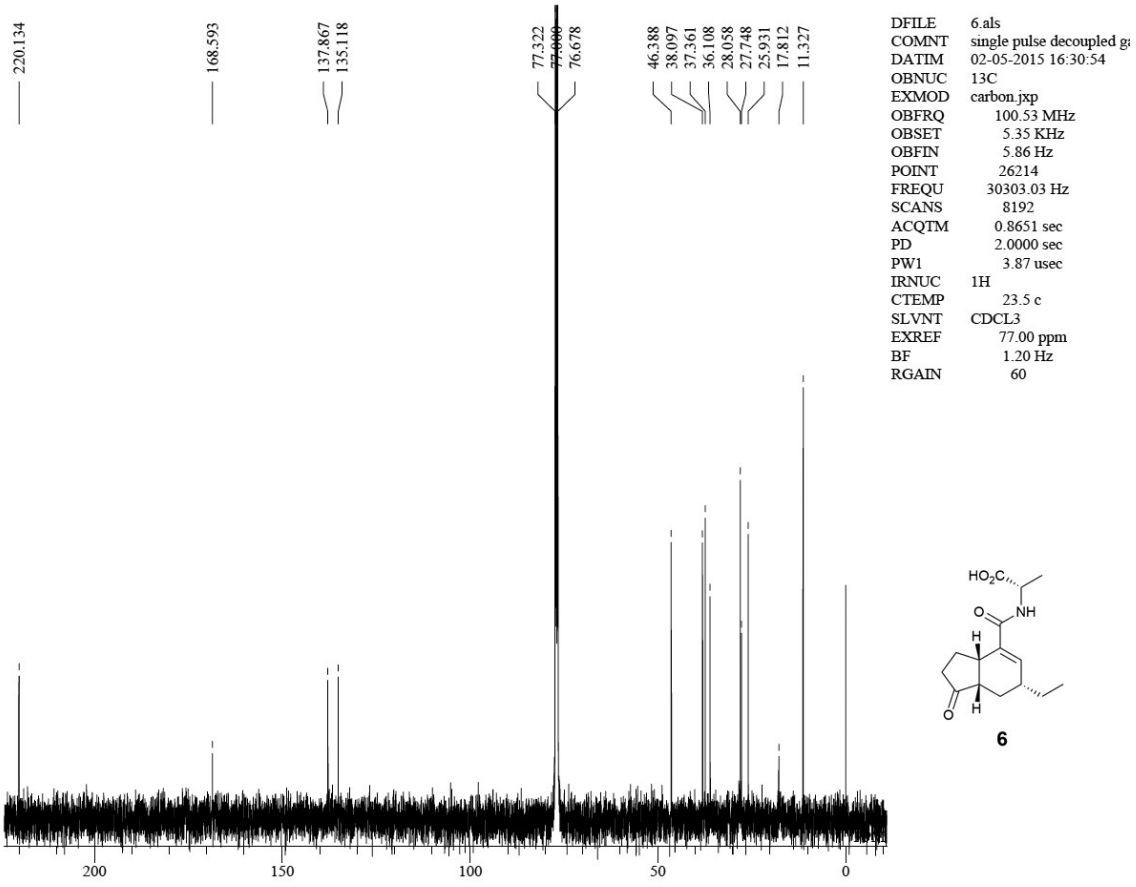
Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.



Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

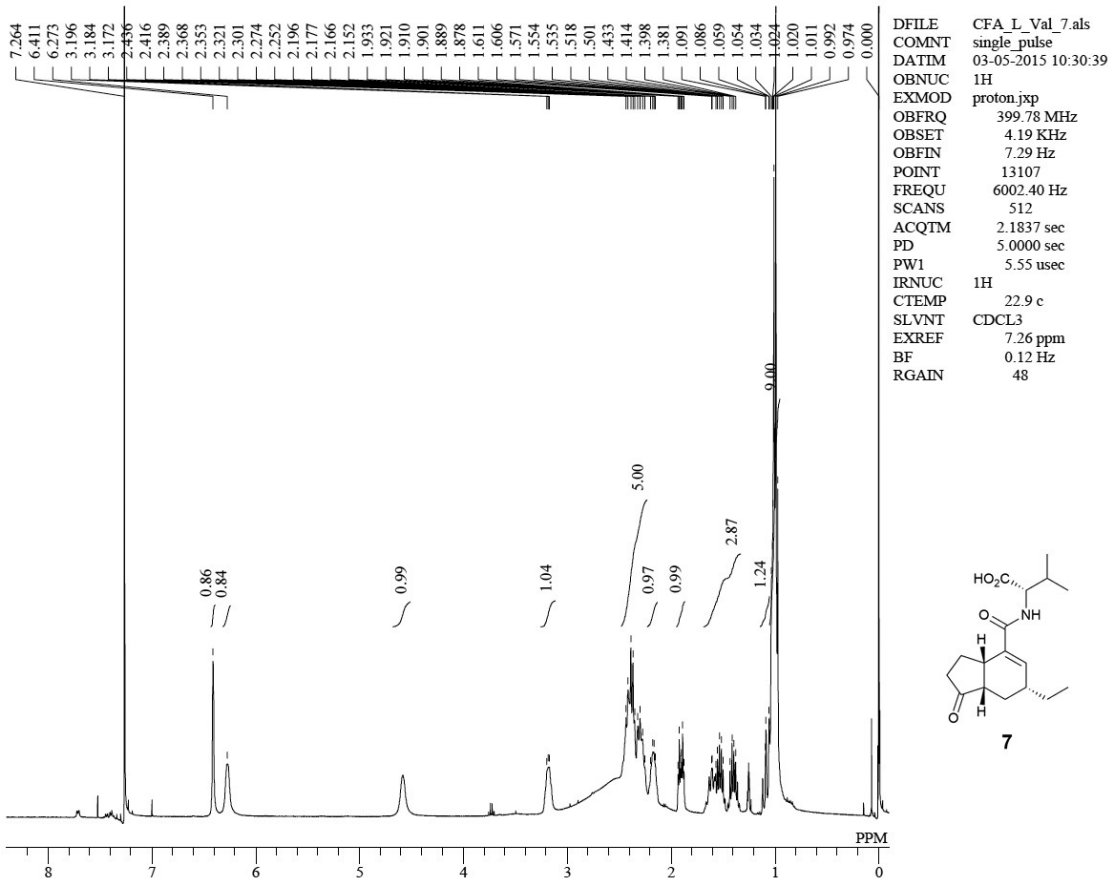


Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.



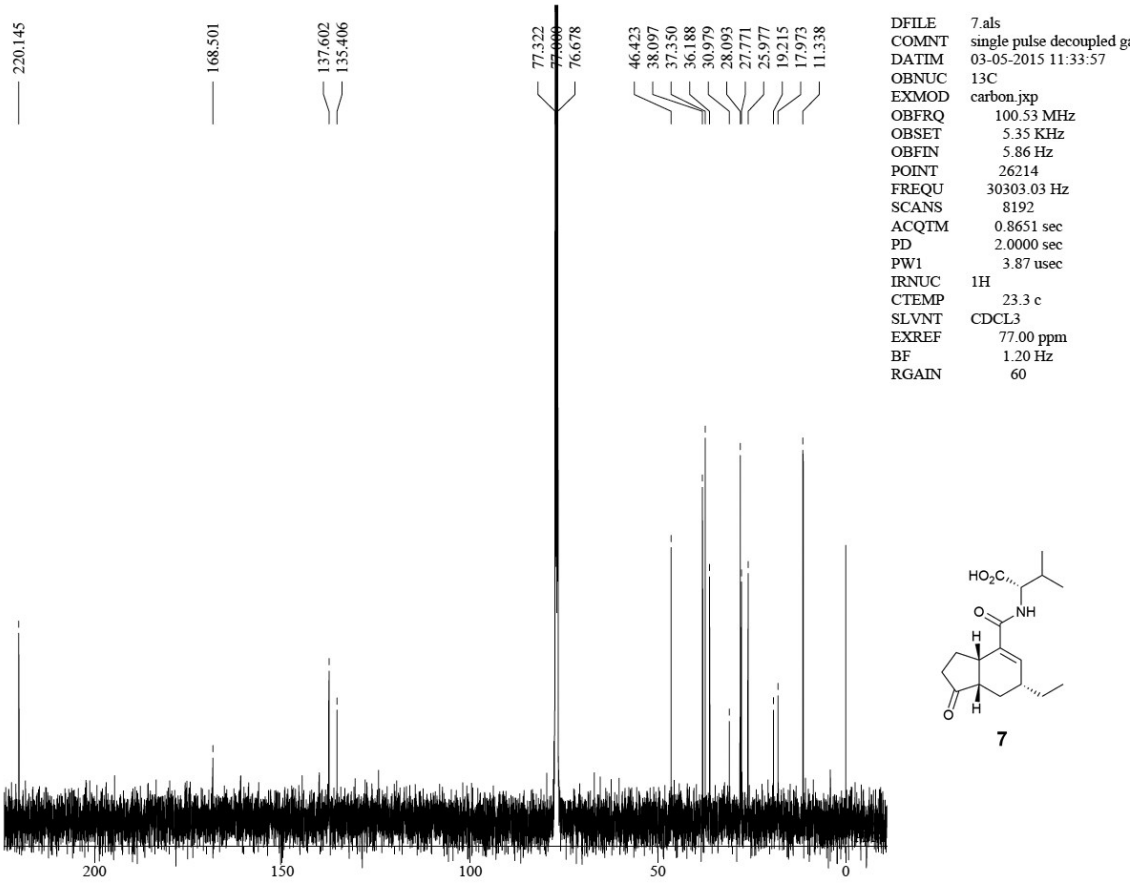
6

Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

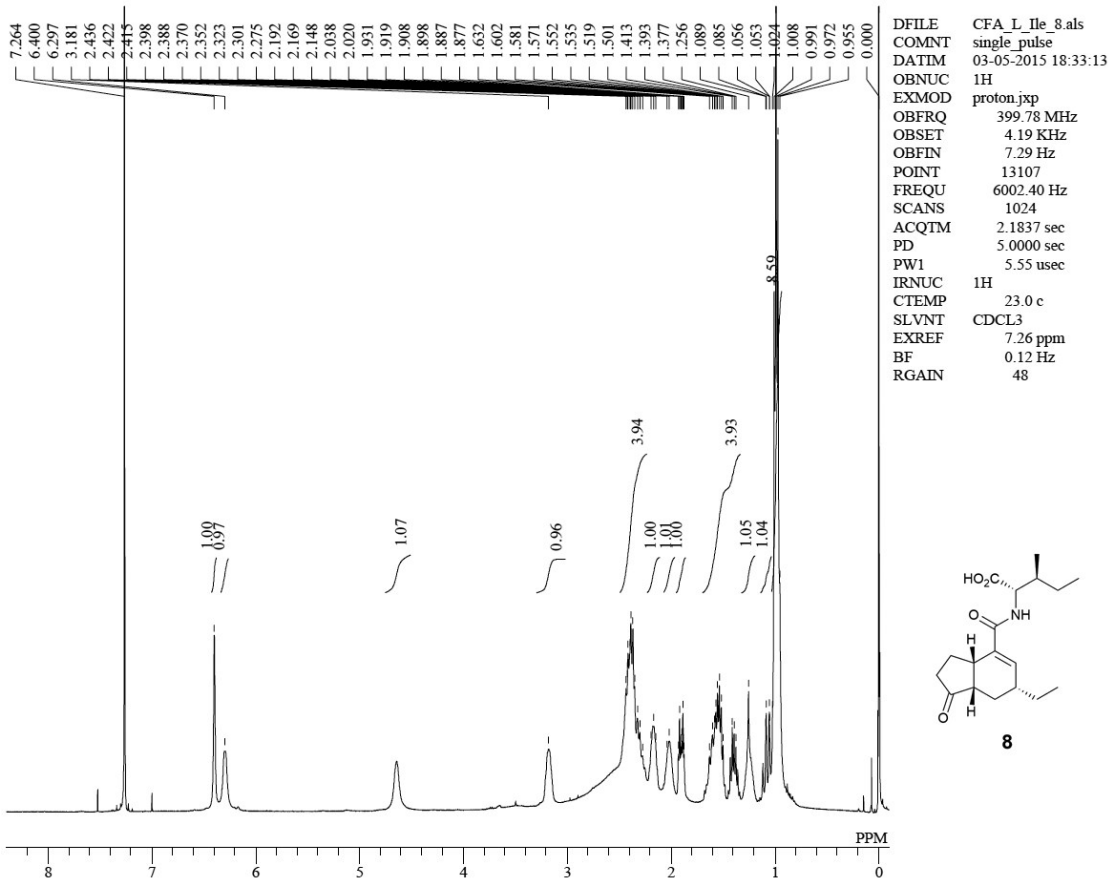


7

Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

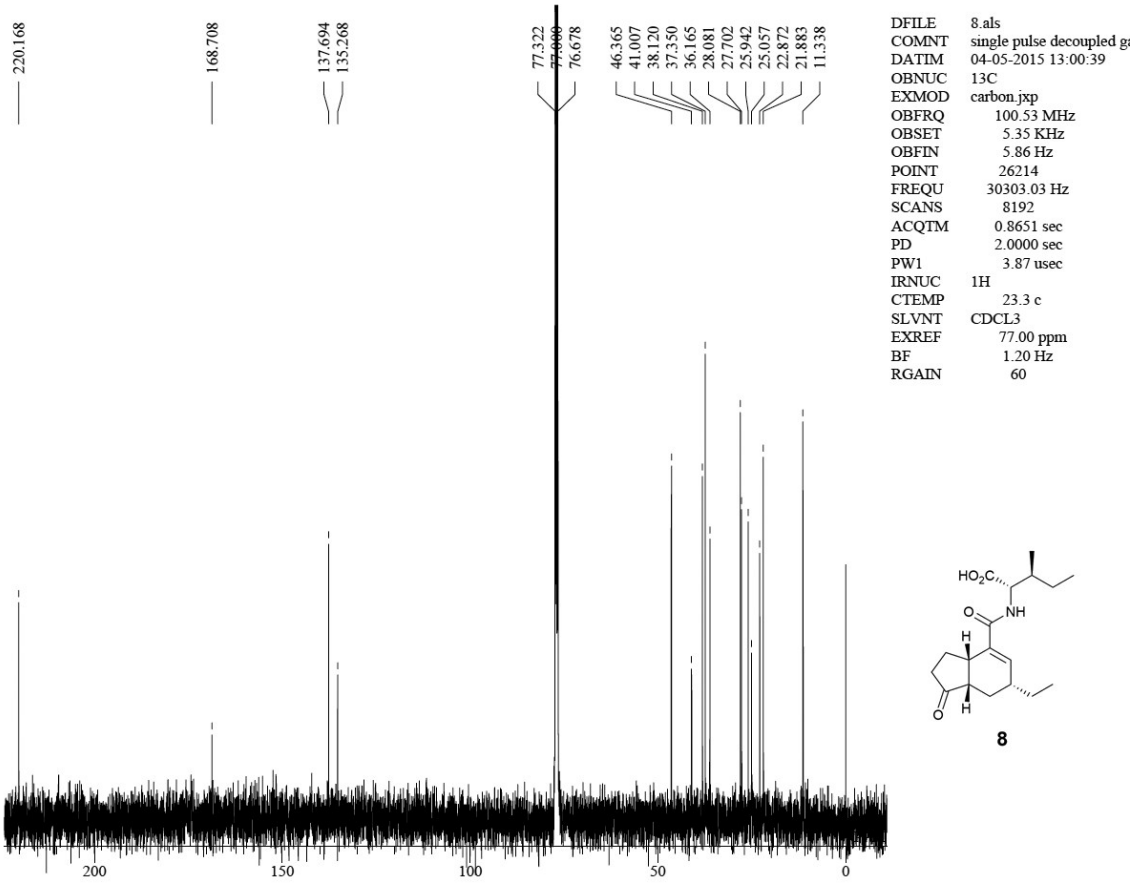


Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.



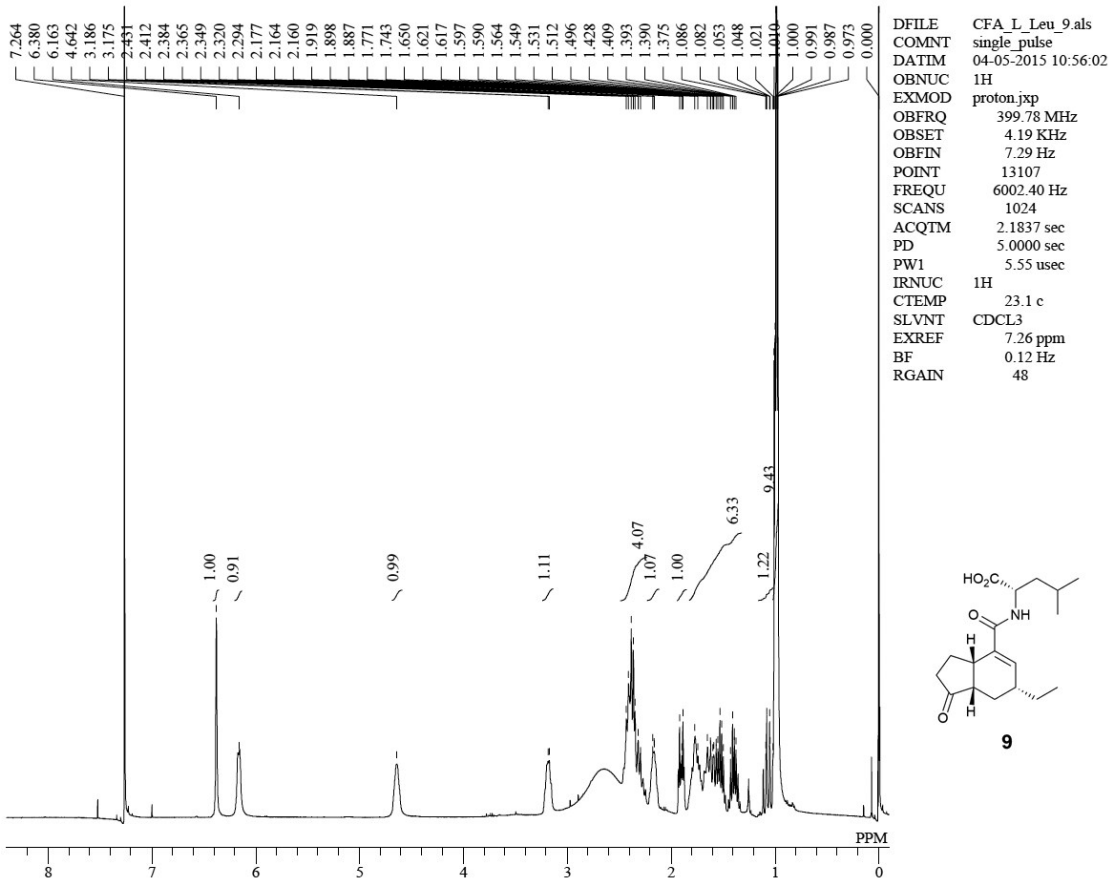
8

Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.



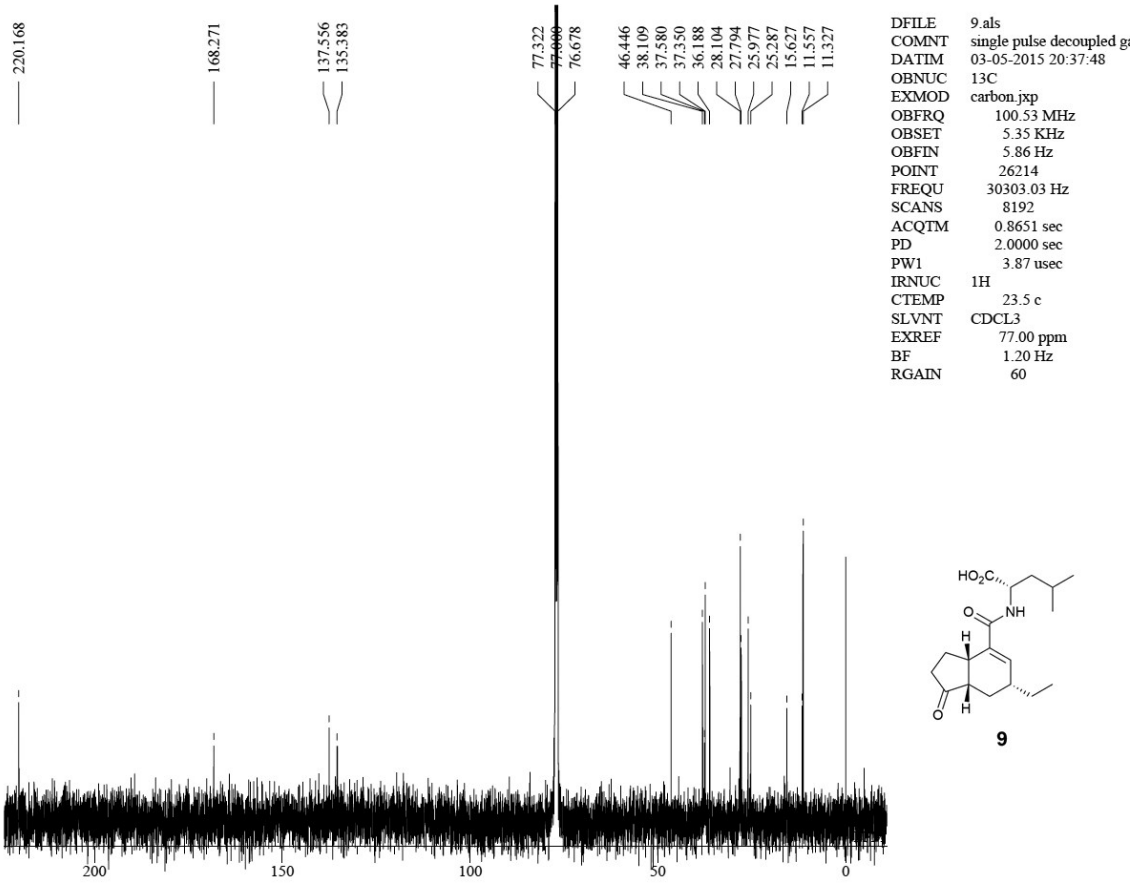
8

Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

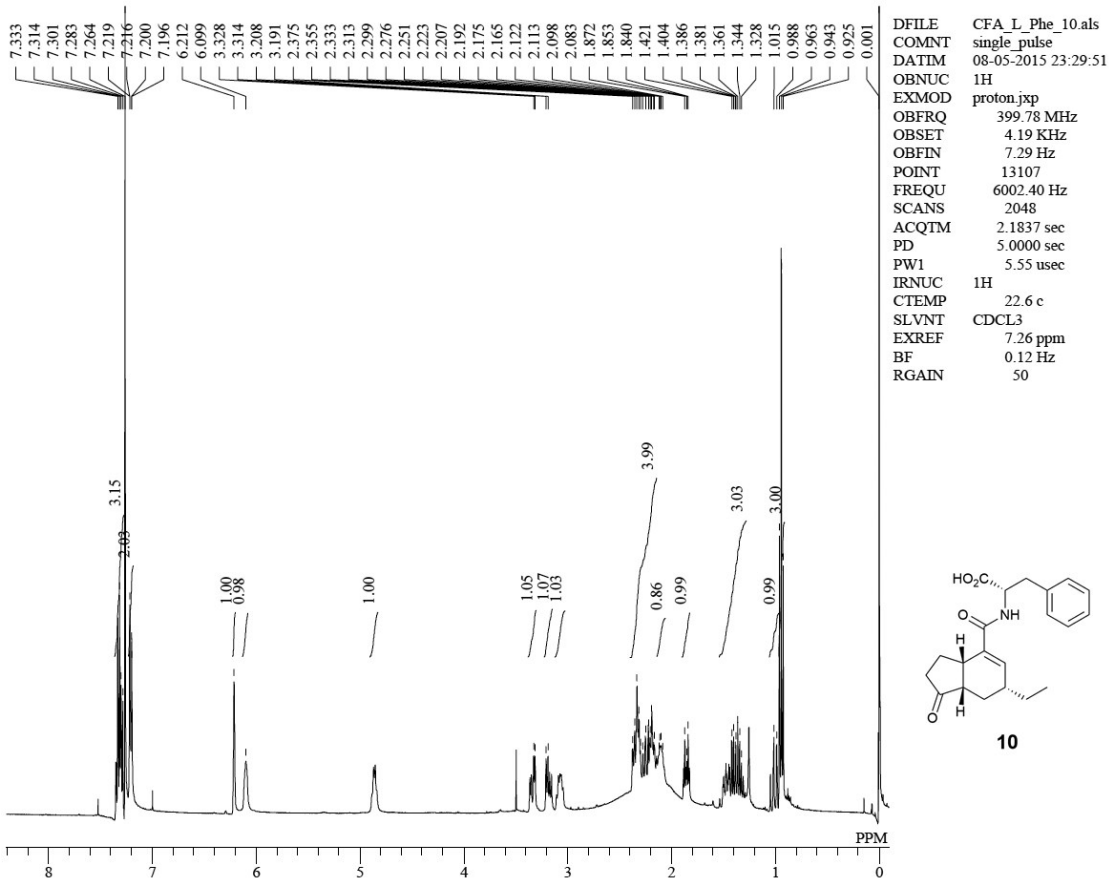


9

Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

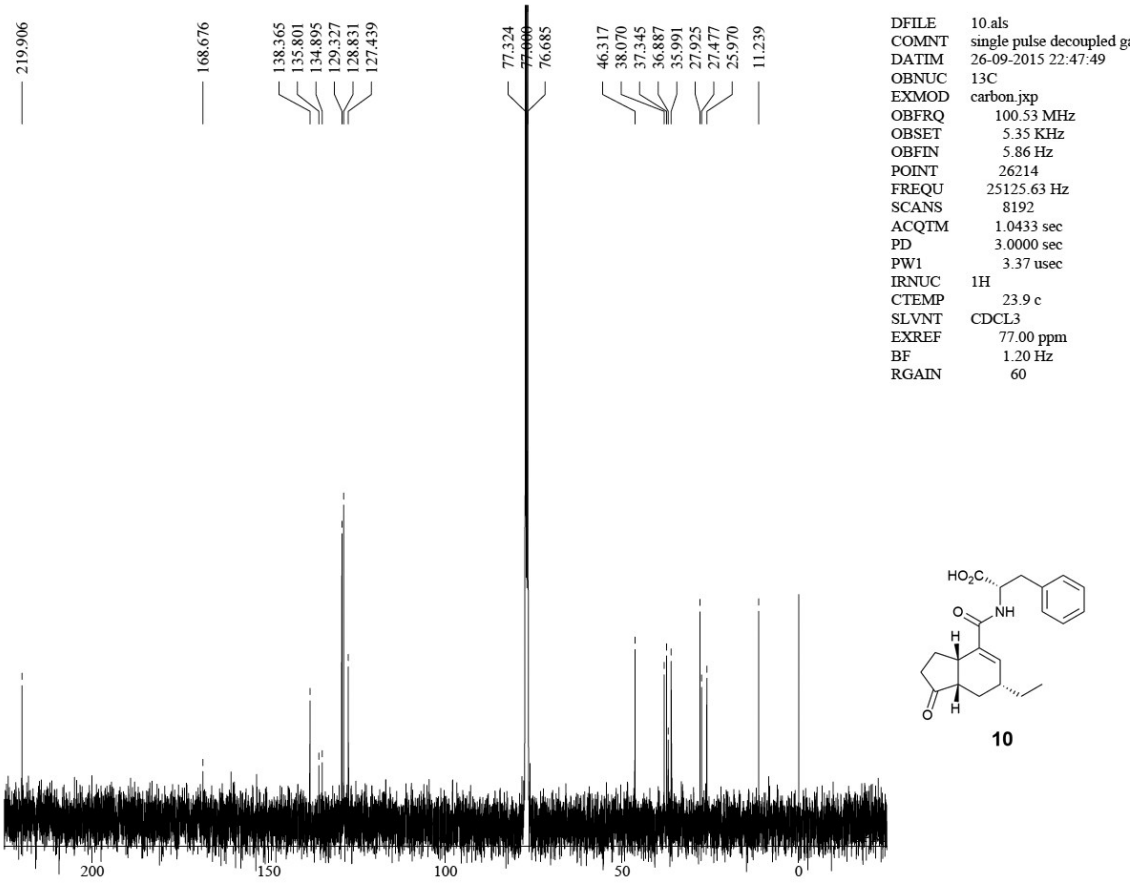


Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

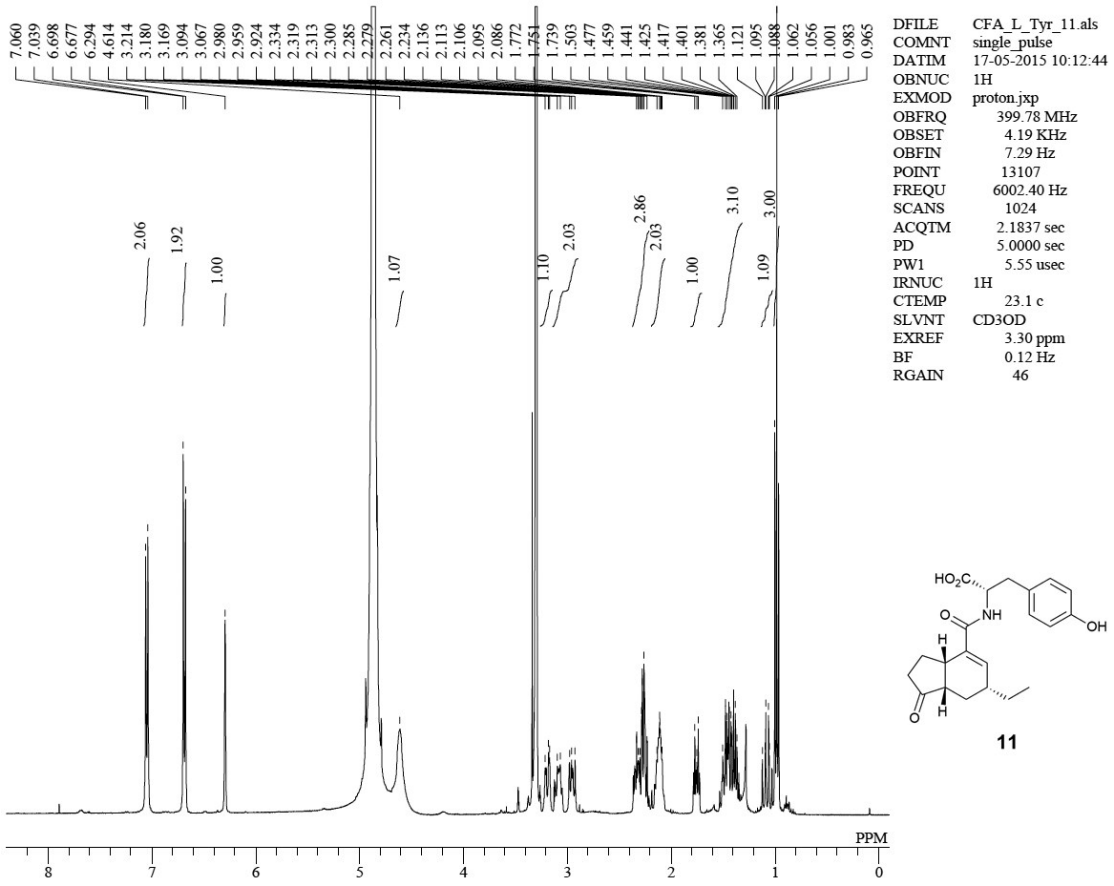


10

Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

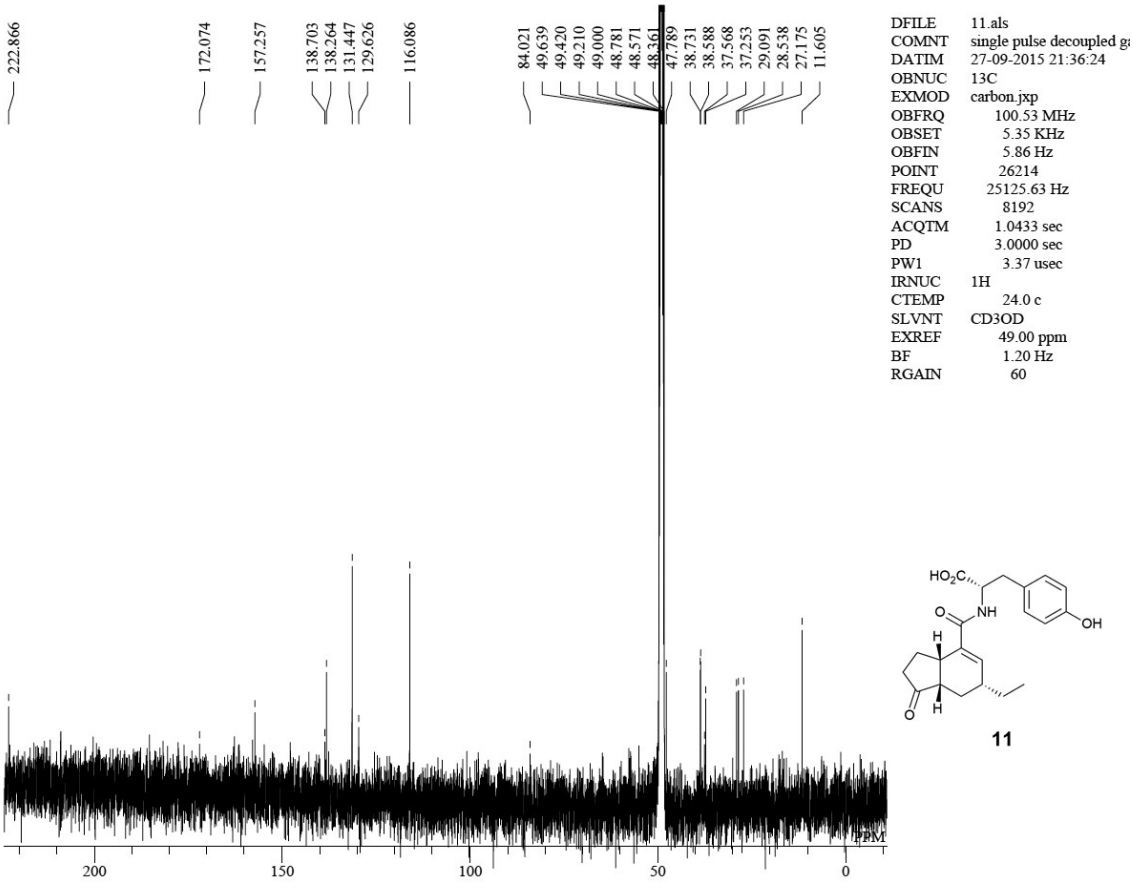


Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

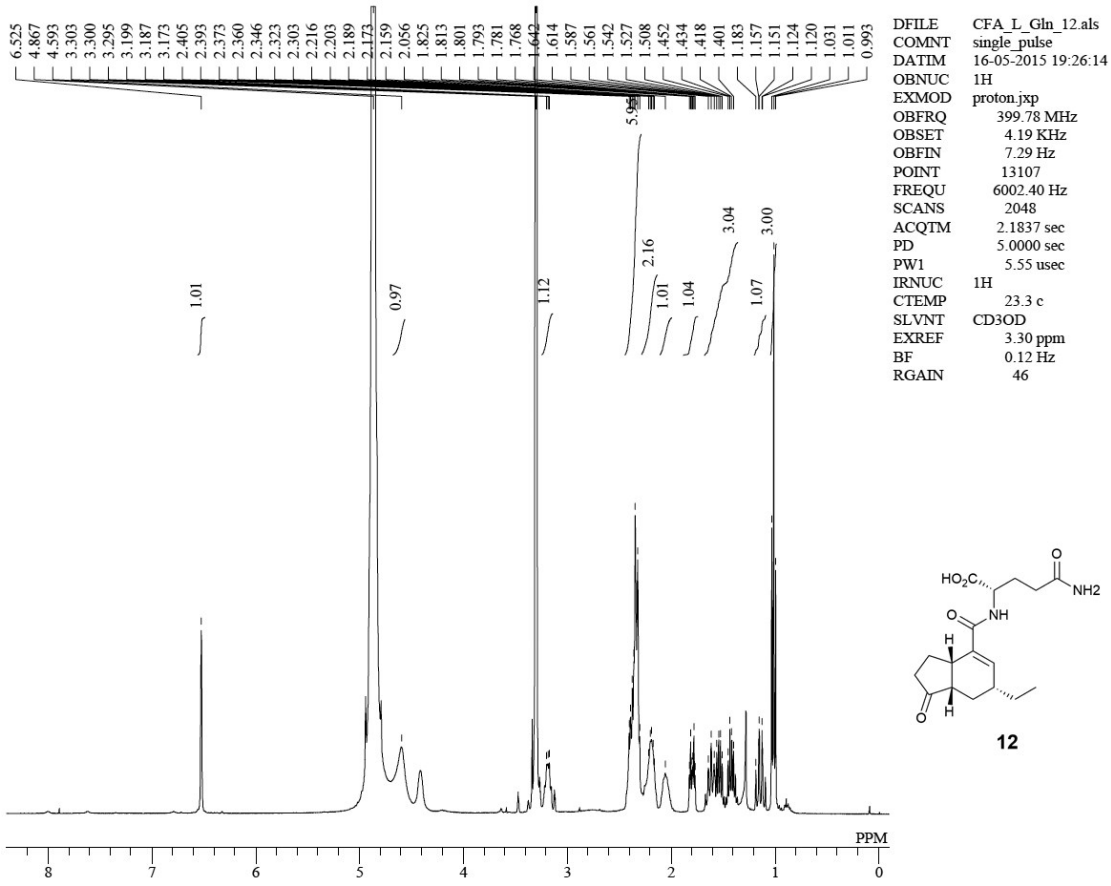


11

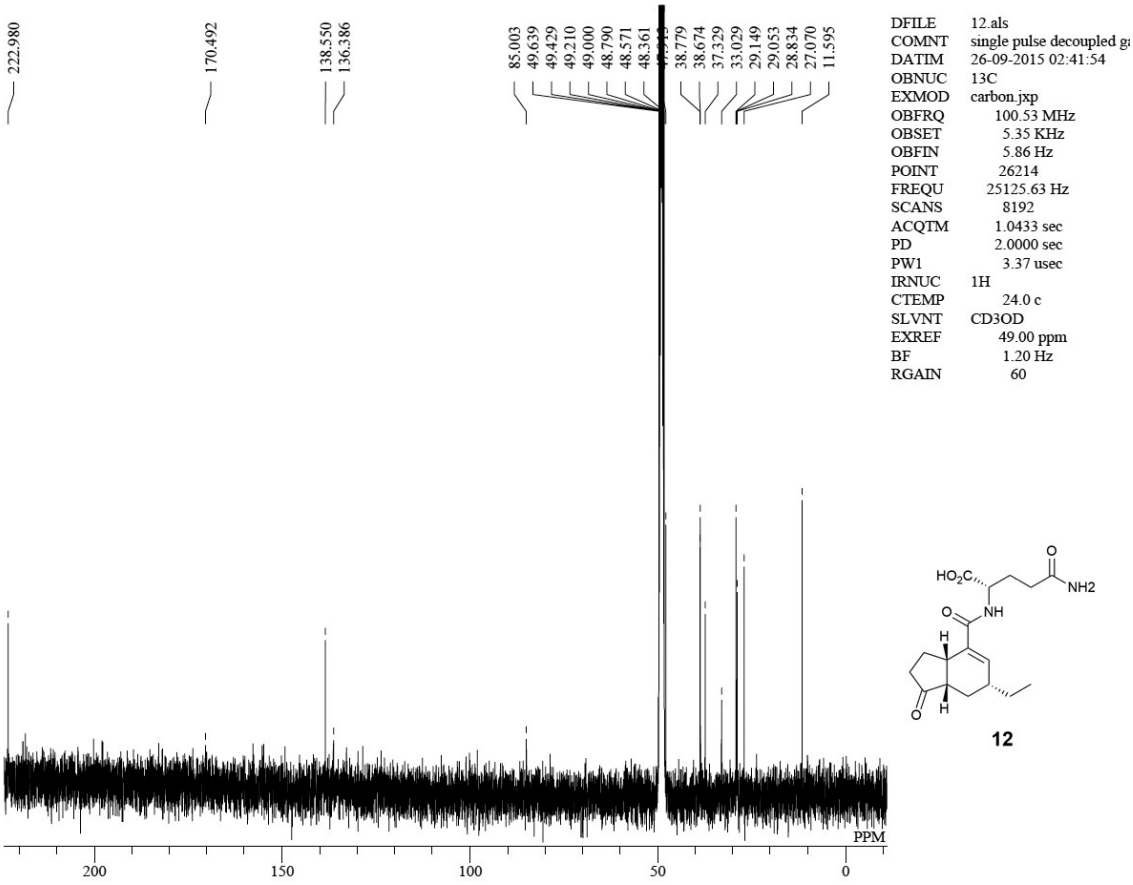
Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.

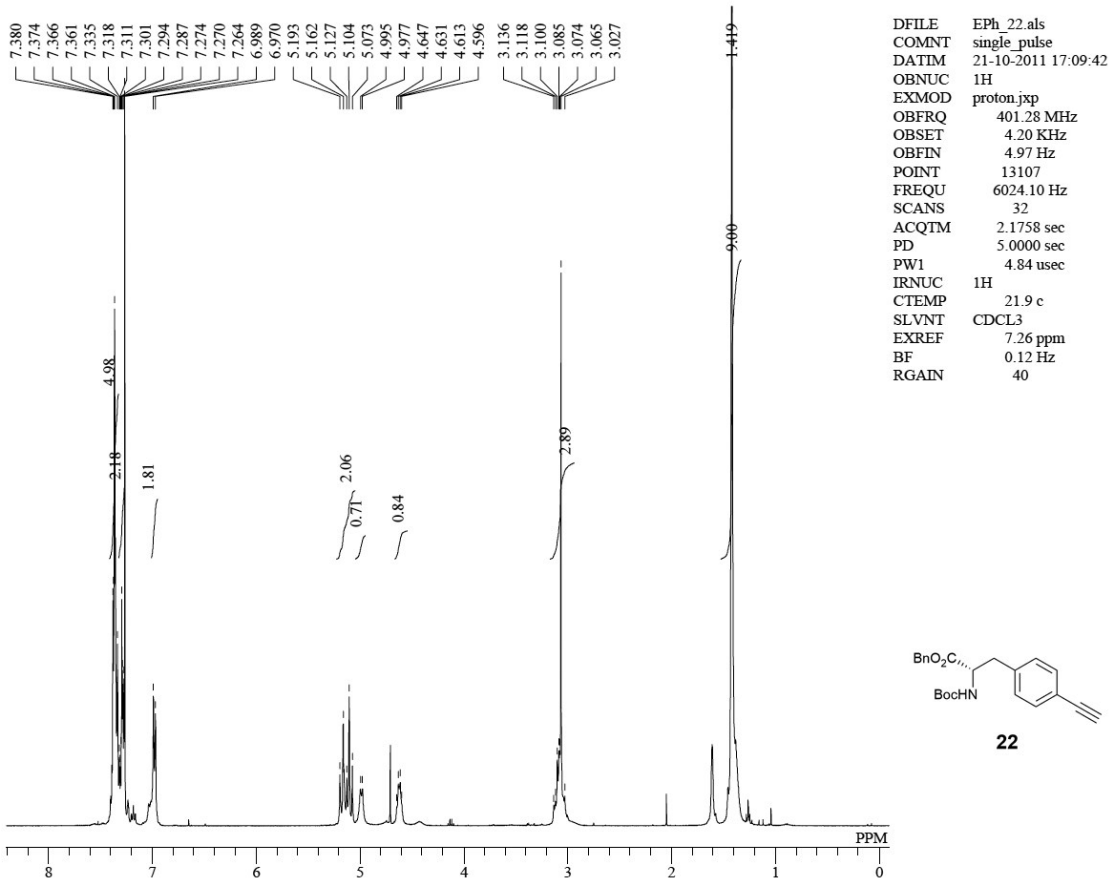


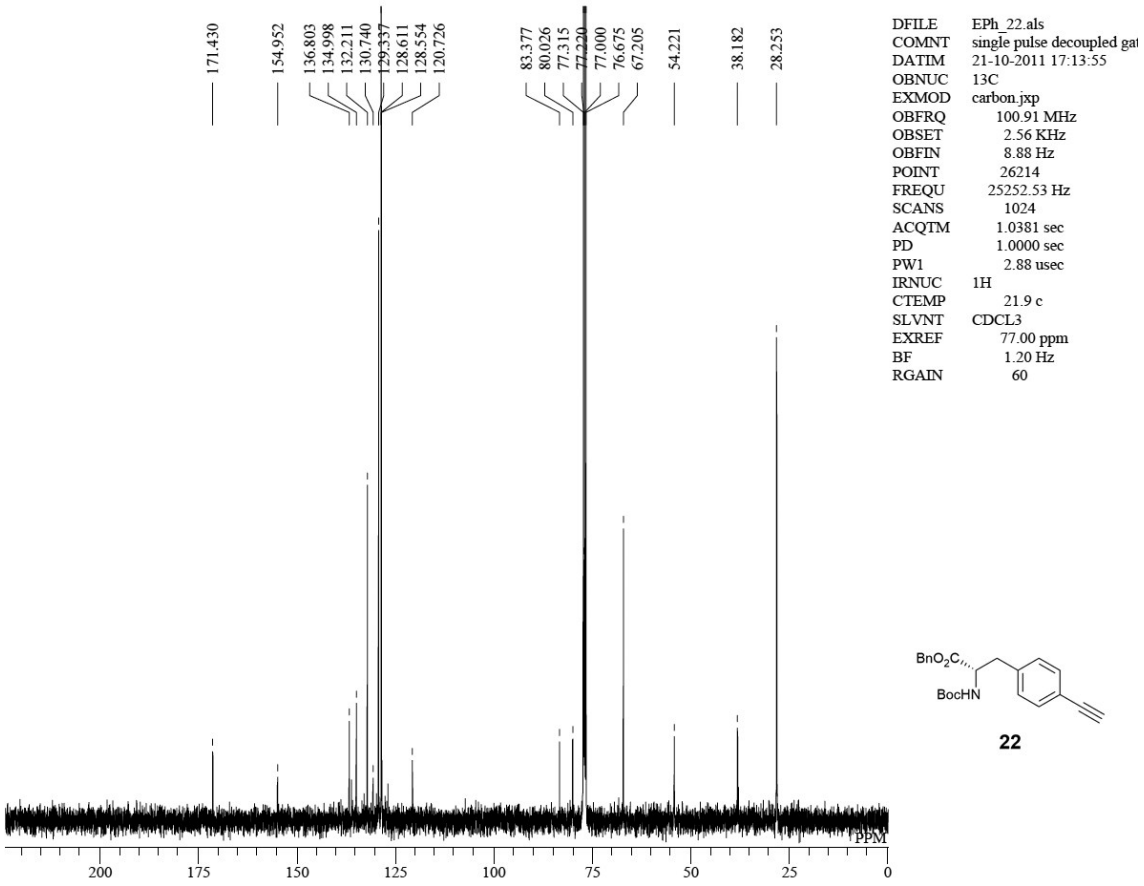
Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.



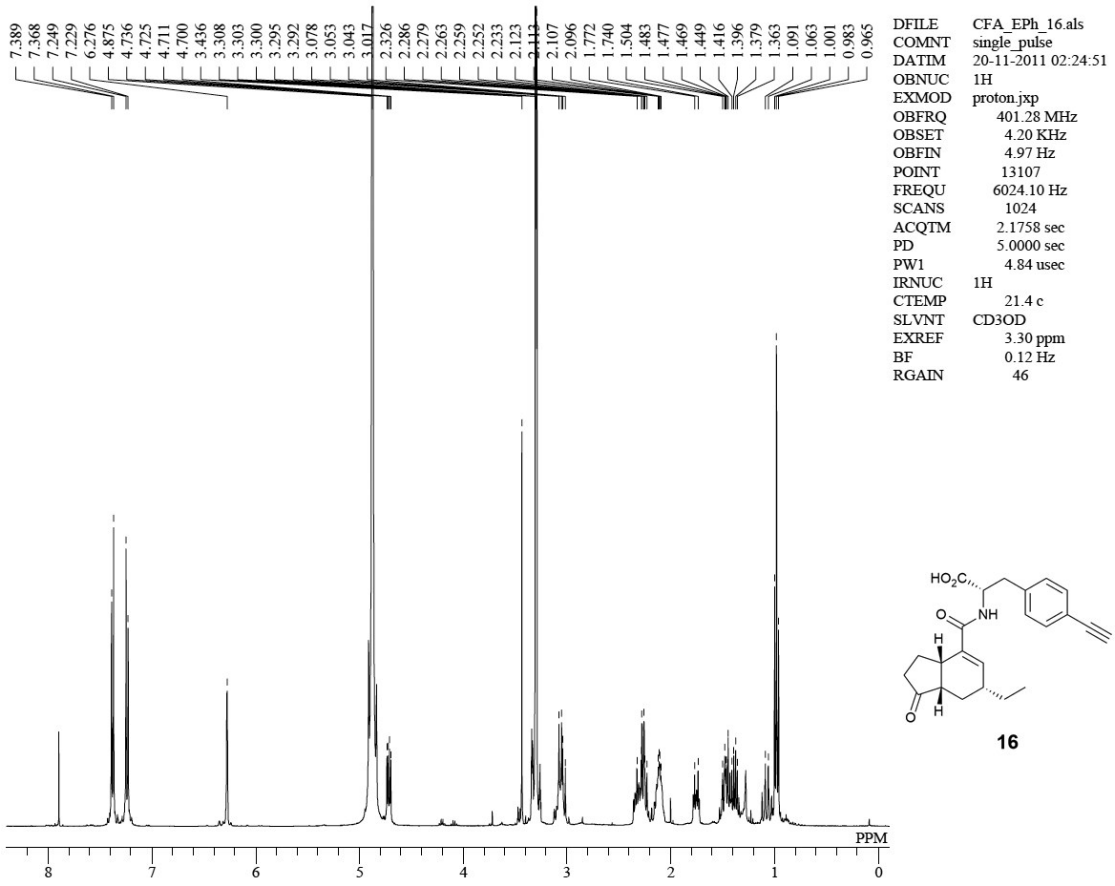
Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.




7.380
7.374
7.366
7.361
7.335
7.318
7.311
7.301
7.294
7.287
7.274
7.270
7.264
6.989
6.970
5.193
5.162
5.127
5.104
5.073
4.995
4.977
4.647
4.631
4.613
4.596
3.136
3.118
3.100
3.085
3.074
3.065
3.027
1.419
4.98
2.18
1.81
2.06
0.71
0.84
2.89
9.00
PPM
8
7
6
5
4
3
2
1
0
DFILE EPh_22.als
COMNT single_pulse
DATIM 21-10-2011 17:09:42
OBNUC 1H
EXMOD proton.jxp
OBFRQ 401.28 MHz
OBSET 4.20 KHz
OBFIN 4.97 Hz
POINT 13107
FREQU 6024.10 Hz
SCANS 32
ACQTM 2.1758 sec
PD 5.0000 sec
PW1 4.84 usec
IRNUC 1H
CTEMP 21.9 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.12 Hz
RGAIN 40
BnO2C
BocHN
22

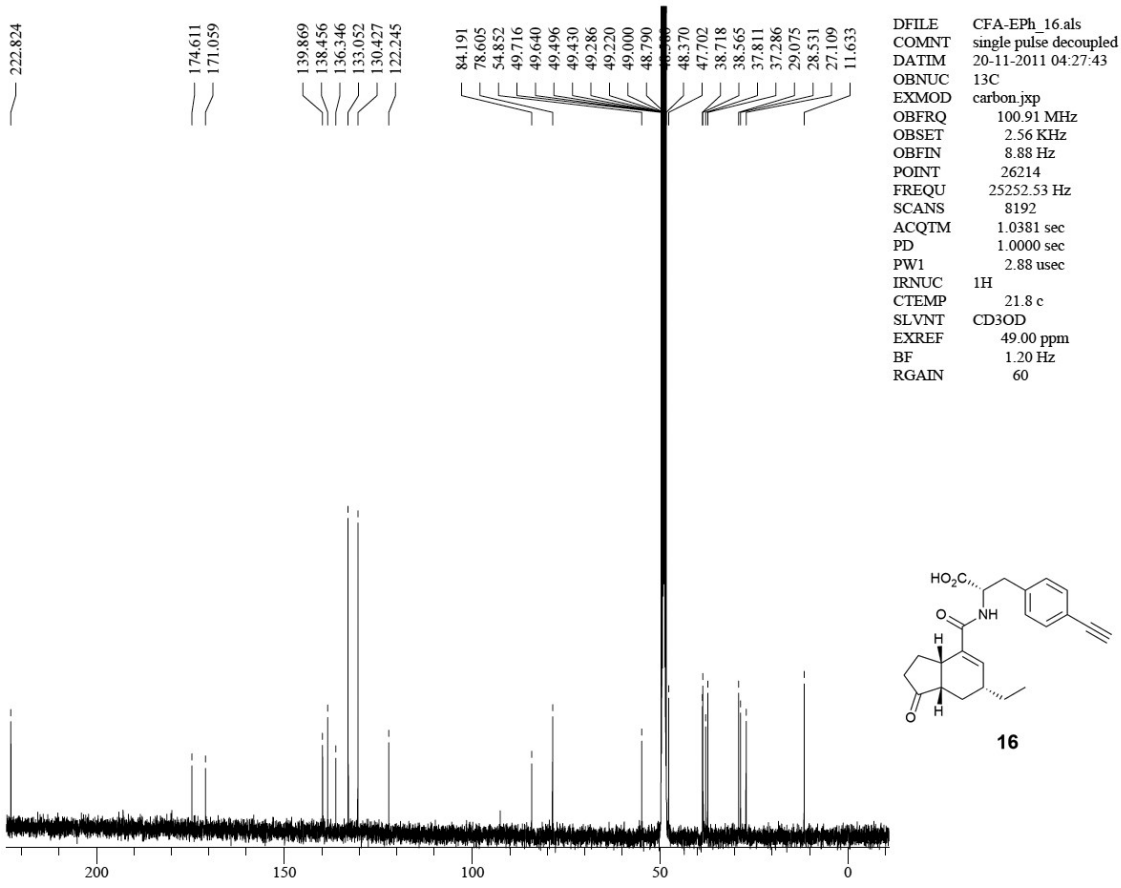

171.430
154.952
136.803
134.998
132.211
130.740
129.337
128.611
128.554
120.726
83.377
80.026
77.315
77.220
77.000
76.675
67.205
54.221
38.182
28.253
DFILE EPh_22.als
COMNT single pulse decoupled gat
DATIM 21-10-2011 17:13:55
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.91 MHz
OBSET 2.56 KHz
OBFIN 8.88 Hz
POINT 26214
FREQU 25252.53 Hz
SCANS 1024
ACQTM 1.0381 sec
PD 1.0000 sec
PW1 2.88 usec
IRNUC 1H
CTEMP 21.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 60
BnO2C
BocHN
22
PPM
200
175
150
125
100
75
50
25
0

Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.



16

Supporting Information for Egoshi, Takaoka, Saito, Nukadzuka, Hayashi, Ishimaru, Yamakoshi, Dodo, Sodeoka and Ueda; Dual function of coronatine as a bacterial virulence factor against plants: possible COI1-JAZ-independent role.



16