Supporting Information for

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Aggregation-induced emission enhancement in halochalcones

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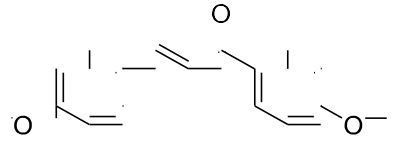
Synthesis

General

Melting points were determined on a BUCHI Melting point apparatus and are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded on Bruker 300 or 500 [300.13 MHz (^{1}H), 75.47 MHz (^{13}C) or 500.13 MHz (^{1}H), 125.77 MHz (^{13}C)] spectrometers with TMS as internal reference. Data for ^{1}H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity [s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet)], coupling constant (*J*, Hz) and integration. Data for ^{13}C NMR are reported in terms of chemical shift (*δ*, ppm). Unequivocal ^{1}H assignments were made with aid of 2D COSY ($^{1}H/^{1}H$), while ^{13}C assignments were made on the basis of 2D HSQC ($^{1}H/^{13}C$) and HMBC experiments. Elemental analyses were obtained with a Carlo Erba 1108 CHNS analyser. High resolution mass spectra analysis (HRMS-ESI) were performed on a microTOF (focus) mass spectrometer (Bruker Daltonics, Bremen, Germany). Ions were generated using an Apollo II (ESI) source. Ionization was achieved by electrospray, using a voltage of 4500 V applied to the needle, and a counter voltage between 100 and 150 V applied to the capillary. Silica gel 60 F254 (Merck) was used for TLC, and the spots were detected with UV light (254 nm). Flash column chromatography was carried out on silica gel 60 (Merck).

(E)-1,3-bis(4-methoxyphenyl)prop-2-en-1-one ***1a***

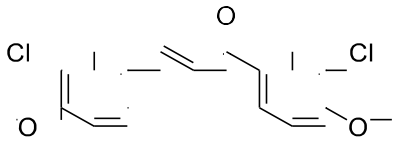


4'-methoxyacetophenone (450 mg, 3 mmol, 1 equiv) and 4-methoxybenzaldehyde (408 mg, 3 mmol, 1 equiv.) were dissolved in MeOH (40 mL). NaOH (240 mg, 6 mmol, 2 equiv) was added slowly. The reaction mixture was stirred at RT during 12 h, then water (10 mL) was added. The solid was collected by filtration, washed with water and methanol, and dried in air. The product was obtained without further purification as a pale yellow solid (437mg, 54%).

Reference for this compound: J. Zheng, D. Zhang, P. Sheng, H. Wang, X. Yao, *Yingyong Huaxue(Chin.) Chin. J. Appl. Chem.* **1992**, *9*, 66-3

^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.04 (d, $^{3}J_{H\text{-}H}$ 8.9 Hz, 2H, Harom), 7.78 (d, $^{3}J_{H\text{-}H}$ 15.6 Hz, 1H, CH=CH), 7.60 (d, $^{3}J_{H\text{-}H}$ 8.8 Hz, 2H, Harom), 7.43 (d, $^{3}J_{H\text{-}H}$ 15.6 Hz, 1H, CH=CH), 6.98 (d, $^{3}J_{H\text{-}H}$ 8.9 Hz, 2H, Harom), 6.94 (d, $^{3}J_{H\text{-}H}$ 8.8 Hz, 2H, Harom), 3.89 (s, 3H, OCH_3), 3.86 (s, 3H, OCH_3).

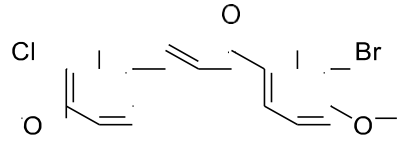
(E)-1,3-Bis(3-chloro-4-methoxyphenyl)prop-2-en-1-one ***1b***



3'-Chloro-4'-methoxyacetophenone (50 mg, 0.27 mmol, 1 equiv) and 3-chloro-4-methoxybenzaldehyde (70 mg, 0.41 mmol, 1.5 equiv.) were dissolved in MeOH (10 mL). NaOH (43 mg, 1.08 mmol, 4 equiv) was added slowly. The reaction mixture was stirred under reflux during 4 h, cooled to room temperature, poured into ice and acidified with dilute HCl. The mixture was extracted with dichloromethane, washed with water, dried over sodium sulfate, and evaporated. The residue was purified by chromatography (dichloromethane/hexane: 2/1) by TLC to give the product as a yellow solid (76mg, 85%).

m.p.: 164-165°C. ESI^+-MS: m/z: 337 $[M+H]^+$ (^{35}Cl, 100%), 339 $[M+H]^+$ ($^{35}Cl^{37}Cl$, 60%), 341 $[M+H]^+$ (^{37}Cl, 10%). Anal Calcd (%) for $C_{17}H_{14}Cl_2O_3.H_2O$ (355.21): C 57.48, H 4.54; found C 57.41, H 4.23. ^1H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.09 (d, $^4J_{H-H}$ 2.1 Hz, 1H, Harom), 7.97 (dd, $^4J_{H-H}$ 2.1, $^3J_{H-H}$ 8.6 Hz, 1H, Harom), 7.72 (d, $^3J_{H-H}$ 15.5 Hz, 1H, CH=CH), 7.71 (d, $^4J_{H-H}$ 2.1 Hz, 1H, Harom), 7.50 (dd, $^4J_{H-H}$ 2.1, $^3J_{H-H}$ 8.5 Hz, 1H, Harom), 7.38 (d, $^3J_{H-H}$ 15.5 Hz, 1H, CH=CH), 7.01 (d, $^3J_{H-H}$ 8.6 Hz, 1H, Harom), 6.96 (d,$^3J_{H-H}$ 8.5 Hz, 1H, H arom), 3.99 (s, 3H, OCH_3), 3.96 (s, 3H, OCH_3). ^{13}C NMR (75 MHz, $CDCl_3$, 25ºC): δ = 56.3 (O**C**H_3), 56.4 (O**C**H_3), 111.4 (**C**Harom), 112.0 (**C**Harom), 120.0 (CH=**C**H), 123.0 (**C**arom), 123.3 (**C**arom), 128.4 (**C**arom), 128.9 (**C**Harom), 129.2 (**C**Harom), 129.5 (**C**Harom), 130.8 (**C**Harom), 131.6 (**C**arom), 143.1 (**C**H=CH), 156.8 (**C**OMe), 158.7 (**C**OMe), 187.4 (**C**=O).

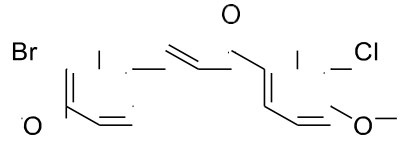
(E)-1-(3-Bromo-4-methoxyphenyl)-3-(3-chloro-4-methoxyphenyl)prop-2-en-1-one ***1c***



3'-Bromo-4'-methoxyacetophenone (50 mg, 0.22 mmol, 1 equiv) and 3-chloro-4-methoxybenzaldehyde (84 mg, 0.33 mmol, 1.5 equiv) were dissolved in MeOH (5 mL). NaOH (34 mg, 0.87 mmol, 4 equiv) was added slowly. The reaction mixture was stirred under reflux during 4 h, cooled to room temperature, poured into ice and acidified with dilute HCl. The mixture was extracted with dichloromethane, washed with water, dried over sodium sulfate, and evaporated. The residue was purified by chromatography (dichloromethane/hexane: 1/1) by TLC to give the product as yellow solid (74 mg, 92 %).

m.p.: 166-168°C. ESI^+-MS: m/z: 381 $[M+H]^+$ ($^{79}Br^{35}Cl$, 100%), 383 $[M+H]^+$ ($^{79}Br,^{37}Cl$ or $^{81}Br^{35}Cl$, 70%), 385 $[M+H]^+$ ($^{81}Br^{37}Cl$, 15%). Anal Calcd (%) for $C_{17}H_{14}BrClO_3.CH_3OH$ (413.69): C 52.26, H 4.39; found C 52.20, H 4.06. ^1H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.26 (d, $^4J_{H-H}$ 1.9 Hz, 1H, Harom), 8.02 (dd, $^4J_{H-H}$ 1.9, $^3J_{H-H}$ 7.4 Hz, 1H, Harom), 7.73 (d, $^4J_{H-H}$ 2.1 Hz, 1H, Harom), 7.73 (d, $^3J_{H-H}$ 15.6 Hz, 1H, CH=CH), 7.50 (dd, $^4J_{H-H}$ 2.1, $^3J_{H-H}$ 7.2 Hz, 1H, Harom), 7.38 (d, $^3J_{H-H}$ 15.6 Hz, 1H, CH=CH), 6.99 (d, $^3J_{H-H}$ 7.4 Hz, 1H, Harom), 6.96 (d,$^3J_{H-H}$ 7.2 Hz, 1H, Harom), 3.99 (s, 3H, OCH_3), 3.96 (s, 3H, OCH_3). ^{13}C NMR (75 MHz, $CDCl_3$, 25ºC): δ = 56.3 (O**C**H_3), 56.5 (O**C**H_3), 111.2 (**C**Harom), 112.0 (**C**Harom), 112.0 (**C**arom), 120.0 (CH=**C**H), 123.3 (**C**arom), 128.4 (**C**arom), 129.2 (**C**Harom), 129.5 (**C**Harom), 129.7 (**C**Harom), 132.1 (**C**arom), 134.0 (**C**Harom), 143.1 (**C**H=CH), 156.8 (**C**OMe), 159.5 (**C**OMe), 187.2 (**C**=O).

(E)-3-(3-Bromo-4-methoxyphenyl)-1-(3-chloro-4-methoxyphenyl)prop-2-en-1-one ***1d***

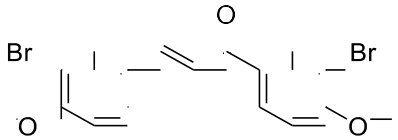


3'-Chloro-4'-methoxyacetophenone (50 mg, 0.27 mmol, 1 equiv) and 3-bromo-4-methoxybenzaldehyde *(*123 mg, 0.54 mmol, 2 equiv) were dissolved in MeOH (10 mL). NaOH (43 mg, 1.08 mmol, 4 equiv) was added slowly. The reaction mixture was stirred under reflux during 4 h, cooled to room temperature, poured into ice and acidified with dilute HCl. The mixture was extracted with dichloromethane, washed with water, dried over sodium sulfate, and evaporated. The residue was purified by chromatography (dichloromethane/hexane: 2/1) by TLC to give the product as a yellow solid (71mg, 71%).

m.p.: 148-150°C. ESI^+-MS: m/z: 381 $[M+H]^+$ ($^{79}Br^{35}Cl$, 100%), 383 $[M+H]^+$ ($^{79}Br^{37}Cl$ or $^{81}Br^{35}Cl$, 70%), 385 $[M+H]^+$ ($^{81}Br^{37}Cl$, 15%). HRMS (ESI^+-MS): calcd. for $C_{17}H_{14}BrClO_3$ $[M+H]^+$ 380.9893;

found 380.9894. ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.09 (d, $^{4}J_{H\text{-}H}$ 2.1Hz, 1H, Harom), 7.97 (dd, $^{4}J_{H\text{-}H}$ 2.1, $^{3}J_{H\text{-}H}$ 8.6 Hz, 1H, Harom), 7.90 (d, $^{4}J_{H\text{-}H}$ 2.1 Hz, 1H, Harom), 7.72 (d, $^{3}J_{H\text{-}H}$ 15.6 Hz, 1H, CH=CH), 7.55 (dd, $^{4}J_{H\text{-}H}$ 2.1, $^{3}J_{H\text{-}H}$ 8.5 Hz, 1H, Harom), 7.38 (d, $^{3}J_{H\text{-}H}$ 15.6 Hz, 1H, CH=CH), 7.02 (d, $^{3}J_{H\text{-}H}$ 8.6 Hz, 1H, Harom), 6.94 (d,$^{3}J_{H\text{-}H}$ 8.5 Hz, 1H, Harom), 4.00 (s, 3H, OCH_3), 3.96 (s, 3H, OCH_3). ^{13}C NMR (75 MHz, $CDCl_3$, 25ºC): δ = 56.4 (O**C**H_3), 56.4 (O**C**H_3), 111.4 (**C**Harom), 111.9 (**C**Harom), 112.4 (**C**arom), 120.0 (CH=**C**H), 123.0 (**C**arom), 128.9 (**C**Harom), 128.9 (**C**arom), 129.9 (**C**Harom), 130.8 (**C**Harom), 131.6 (**C**arom), 132.6 (**C**Harom), 143.0 (**C**H=CH), 157.7 (**C**OMe), 158.7 (**C**OMe), 187.3 (**C**=O).

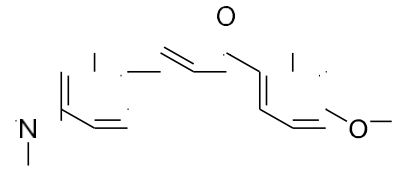
*(E)-1,3-Bis(3-bromo-4-methoxyphenyl)prop-2-en-1-one **1e***



3'-Bromo-4'-methoxyacetophenone (50 mg, 0.22 mmol, 1 equiv) and 3-bromo-4-methoxybenzaldehyde (70 mg, 0.33 mmol, 1.5 equiv) were dissolved in MeOH (10 mL). NaOH (35 mg, 0.87 mmol, 4 equiv) was added slowly. The reaction mixture was stirred under reflux during 4 h, cooled to room temperature, poured into ice and acidified with dilute HCl. The mixture was extracted with dichloromethane, washed with water, dried over sodium sulfate, and evaporated. The residue was purified by chromatography (dichloromethane/hexane: 2/1) by TLC to give the product as a yellow solid (68 mg, 73%).

m.p.: 152-153°C. ESI^{+}-MS: m/z: 427.0 $[M+H]^{+}$ (^{79}Br, 100%), 424.9 $[M+H]^{+}$ (^{79}Br^{81}Br, 50%), 428.0 $[M+H]^{+}$ (^{81}Br, 40%). Anal Calcd (%) for $C_{17}H_{14}Br_2O_3.CH_3OH$ (458.14): C 47.19, H 3.96; found C 47.15, H 3.57. ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.25 (d, $^{4}J_{H\text{-}H}$ 2.1 Hz, 1H, Harom), 8.00 (dd, $^{4}J_{H\text{-}H}$ 2.1, $^{3}J_{H\text{-}H}$ 8.6 Hz, 1H, Harom), 7.89 (d, $^{4}J_{H\text{-}H}$ 2.1 Hz, 1H, Harom), 7.71 (d, $^{3}J_{H\text{-}H}$ 15.5 Hz, 1H, CH=CH), 7.54 (dd, $^{4}J_{H\text{-}H}$ 2.1, $^{3}J_{H\text{-}H}$ 8.5 Hz, 1H, Harom), 7.36 (d, $^{3}J_{H\text{-}H}$ 15.5 Hz, 1H, CH=CH), 6.97 (d, $^{3}J_{H\text{-}H}$ 8.6 Hz, 1H, Harom), 6.92 (d,$^{3}J_{H\text{-}H}$ 8.4 Hz, 1H, Harom), 3.98 (s, 3H, OCH_3), 3.95 (s, 3H, OCH_3). ^{13}C NMR (75 MHz, $CDCl_3$, 25ºC): δ = 56.4 (O**C**H_3), 56.5 (O**C**H_3), 111.2 (**C**Harom), 111.7 (**C**Harom), 112.0 (**C**arom), 112.4 (**C**arom), 120.0 (CH=**C**H), 128.9 (**C**arom), 129.7 (**C**Harom), 129.9 (**C**Harom), 132.1 (**C**arom), 132.7 (**C**Harom), 134.0 (**C**Harom), 143.0 (**C**H=CH), 157.7 (**C**OMe), 159.5 (**C**OMe), 187.2 (**C**=O).

*(E)-3-(4-(dimethylamino)phenyl)-1-(4-methoxyphenyl)prop-2-en-1-one **2a***

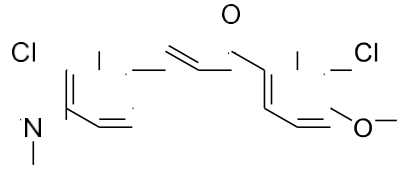


4'-methoxyacetophenone (300 mg, 2 mmol, 1 equiv) and 4-dimethylaminobenzaldehyde (300 mg, 2 mmol, 1 equiv.) were dissolved in MeOH (20 mL). NaOH (160 mg, 4 mmol, 2 equiv) was added slowly. The reaction mixture was stirred at RT during 12 h, then water (10 mL) was added. The solid was collected by filtration, washed with water and methanol. Recrystallization from ethanol gave the pure product as a yellow solid (353mg, 63%).

Reference for this compound: K. Rurack, M. L. Dekhtyar, J. L. Bricks, U. Resch-Genger, W. Rettig, *J. Phys. Chem. A* **1999**, *103*, 9626-9635.
A. C. Grosscurt, R. Van Hes, K. Wellinga, *J. Agric. Food Chem.* **1979**, *27*, 406-409.
J. Wu, J. Li, Y. Cai, Y. Pan, F. Ye, Y. Zhang, Y. Zhao, S. Yang, X. Li, G. Liang, *J. Med. Chem.* **2011**, *54*, 8110-8123.

^{1}H NMR (300 MHz, Acetone-d_6, 25 ºC): δ = 8.12 (d, $^3J_{H\text{-}H}$ 9.0 Hz, 2H, Harom), 7.72 (d, $^3J_{H\text{-}H}$ 15.4 Hz, 1H, CH=CH), 7.66 (d, $^3J_{H\text{-}H}$ 8.9 Hz, 2H, Harom), 7.60 (d, $^3J_{H\text{-}H}$ 15.4 Hz, 1H, CH=CH), 7.05 (d, $^3J_{H\text{-}H}$ 9.0 Hz, 2H, Harom), 6.77 (d, $^3J_{H\text{-}H}$ 8.9 Hz, 2H, Harom), 3.89 (s, 3H, OCH_3), 3.04 (s, 6H, $N(CH_3)_2$).

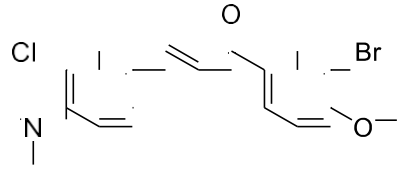
*(E)-3-(3-Chloro-4-(dimethylamino)phenyl)-1-(3-chloro-4-methoxyphenyl)prop-2-en-1-one **2b***



3'-Chloro-4'-methoxyacetophenone (50 mg, 0.27 mmol, 1 equiv) and 3-chloro-4-(dimethylamino)benzaldehyde (74 mg, 0.41 mmol, 1.5 equiv) were dissolved in MeOH (10 mL). NaOH (43 mg, 1.08 mmol, 4 equiv) was added slowly. The reaction mixture was stirred under reflux during 4 h, cooled to room temperature, poured into ice and acidified with dilute HCl. The mixture was extracted with dichloromethane, washed with water, dried over sodium sulfate, and evaporated. The residue was purified by chromatography (dichloromethane/hexane: 2/1) by TLC to give the product as a yellow solid (62 mg, 66%).

m.p.: 111-113°C. ESI$^+$-MS: m/z: 350 $[M+H]^+$ (^{35}Cl, 100%), 352 $[M+H]^+$ ($^{35}Cl^{37}$Cl, 60%), 354 $[M+H]^+$ (^{37}Cl, 10%). Anal Calcd (%) for $C_{18}H_{17}Cl_2NO_2$ (350.24): C 61.73, H 4.89, N 4.00; found C 61.86, H 4.90, N 3.93. ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.09 (d, $^4J_{H\text{-}H}$ 2.1 Hz, 1H, Harom), 7.97 (dd, $^4J_{H\text{-}H}$ 2.1, $^3J_{H\text{-}H}$ 8.6 Hz, 1H, Harom), 7.72 (d, $^3J_{H\text{-}H}$ 15.5 Hz, 1H, CH=CH), 7.67 (d, $^4J_{H\text{-}H}$ 2.0 Hz, 1H, Harom), 7.46 (dd, $^4J_{H\text{-}H}$ 2.0, $^3J_{H\text{-}H}$ 8.4 Hz, 1H, Harom), 7.37 (d, $^3J_{H\text{-}H}$ 15.5 Hz, 1H, CH=CH), 7.04 (d, $^3J_{H\text{-}H}$ 8.4 Hz, 1H, Harom), 7.02 (d,$^3J_{H\text{-}H}$ 8.6 Hz, 1H, Harom), 4.00 (s, 3H, OCH_3), 2.90 (s, 6H, NCH_3). ^{13}C NMR (75 MHz, $CDCl_3$, 25ºC): δ = 44.9 (2 x N**C**H_3), 56.5 (O**C**H_3), 111.4 (**C**Harom), 123.1 (CH=**C**H), 125.9 (**C**arom), 127.6 (**C**Harom), 128.3 (**C**Harom), 128.9 (**C**arom), 129.0 (**C**Harom), 130.9 (**C**Harom), 131.2 (**C**arom), 131.3 (**C**arom), 131.9 (**C**Harom), 141.9 (**C**H=CH), 151.1 (**C**NCH_3), 158.9 (**C**OCH_3), 187.0 (**C**=O).

*(E)-1-(3-Bromo-4-methoxyphenyl)-3-(3-chloro-4-(dimethylamino)phenyl)prop-2-en-1-one **2c***

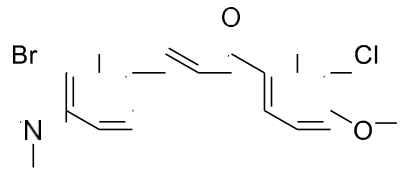


3'-Bromo-4'-methoxyacetophenone (50 mg, 0.22 mmol, 1 equiv) and 3-chloro-4-(dimethylamino)benzaldehyde (60 mg, 0.33 mmol, 1.5 equiv) were dissolved in MeOH (10 mL). NaOH (35 mg, 0.87 mmol, 4 equiv) was added slowly. The reaction mixture was stirred under reflux during 4 h, cooled to room temperature, poured into ice and acidified with dilute HCl. The mixture was extracted with dichloromethane, washed with water, dried over sodium sulfate, and evaporated. The residue was purified by chromatography (dichloromethane/hexane: 2/1) by TLC to give the product as a yellow solid (62 mg, 72%).

m.p.: 108-110°C. ESI$^+$-MS: m/z: 394 $[M+H]^+$ ($^{79}Br^{35}$Cl, 100%), 396 $[M+H]^+$ ($^{79}Br^{37}$Cl or $^{81}Br^{35}$Cl, 70%), 398 $[M+H]^+$ ($^{81}Br^{37}$Cl, 15%). HRMS (ESI$^+$-MS): calcd. for $C_{18}H_{18}BrClNO_2$ $[M+H]^+$

394.0209; found 394.0215. ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.25 (d, $^{4}J_{H-H}$ 2.1 Hz, 1H, Harom), 8.00 (dd, $^{4}J_{H-H}$ 2.1, $^{3}J_{H-H}$ 8.6Hz, 1H, Harom), 7.71 (d, $^{3}J_{H-H}$ 15.5 Hz, 1H, CH=CH), 7.66 (d, $^{4}J_{H-H}$ 2.0 Hz, 1H, Harom), 7.46 (dd, $^{4}J_{H-H}$ 2.0, $^{3}J_{H-H}$ 8.4 Hz, 1H, Harom), 7.37 (d, $^{3}J_{H-H}$ 15.5 Hz, 1H, CH=CH), 7.03 (d, $^{3}J_{H-H}$ 8.4 Hz, 1H, Harom), 6.97 (d,$^{3}J_{H-H}$ 8.6 Hz, 1H, Harom), 3.98 (s, 3H, OCH_3), 2.90 (s, 6H, NCH_3). ^{13}C NMR (75 MHz, $CDCl_3$, 25ºC): δ = 44.0 (N**C**H_3), 44.1 (N**C**H_3), 56.6 (O**C**H_3), 111.3 (**C**Harom), 112.1 (**C**arom), 112.1 (**C**arom), 117.4 (**C**arom), 121.3 (CH=**C**H), 128.9 (**C**Harom), 128.9(**C**Harom), 129.7(**C**Harom), 131.9 (**C**Harom), ,132.0 (**C**arom), 134.0 (**C**Harom), 142.3 (**C**H=CH), 150.5 (**C**NCH_3), 159.6 (**C**OCH_3), 187.0 (**C**=O).

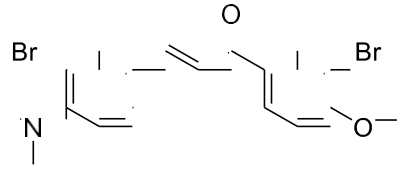
*(E)-3-(3-Bromo-4-(dimethylamino)phenyl)-1-(3-chloro-4-methoxyphenyl)prop-2-en-1-one **2d***



3'-Chloro-4'-methoxyacetophenone (50 mg, 0.27 mmol, 1 equiv) and 3-bromo-4-(dimethylamino)benzaldehyde (123 mg, 0.54 mmol, 2 equiv) were dissolved in MeOH (10 mL). NaOH (43 mg, 1.08 mmol, 4 equiv) was added slowly. The reaction mixture was stirred under reflux during 4 h, cooled to room temperature, poured into ice and acidified with dilute HCl. The mixture was extracted with dichloromethane, washed with water, dried over sodium sulfate, and evaporated. The residue was purified by chromatography (dichloromethane/hexane: 2/1) on TLC to give the product as a yellow solid (63 mg, 63%).

m.p.: 125-127°C. ESI^{+}-MS: m/z: 394 $[M+H]^{+}$ ($^{79}Br^{35}Cl$, 100%), 396 $[M+H]^{+}$ ($^{79}Br^{37}Cl$ or $^{81}Br^{35}Cl$, 70%), 398 $[M+H]^{+}$ ($^{81}Br^{37}Cl$, 15%). Anal Calcd (%) for $C_{18}H_{17}BrClNO_2$ (394.69): C 54.78, H 4.34, N 3.55; found C 54.58, H 4.48, N 3.52. ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.09 (d, $^{4}J_{H-H}$ 2.3 Hz, 1H, Harom), 7.97 (dd, $^{4}J_{H-H}$ 2.3, $^{3}J_{H-H}$ 8.6 Hz, 1H, Harom), 7.88 (d, $^{4}J_{H-H}$ 2.1 Hz, 1H, Harom), 7.72 (d, $^{3}J_{H-H}$ 15.5 Hz, 1H, CH=CH), 7.51 (dd, $^{4}J_{H-H}$ 2.1, $^{3}J_{H-H}$ 8.2 Hz, 1H, Harom), 7.38 (d, $^{3}J_{H-H}$ 15.5 Hz, 1H, CH=CH), 7.06 (d, $^{3}J_{H-H}$ 8.2 Hz, 1H, Harom), 7.02 (d,$^{3}J_{H-H}$ 8.6 Hz, 1H, Harom), 4.00 (s, 3H, OCH_3), 2.89 (s, 6H, NCH_3). ^{13}C NMR (75 MHz, $CDCl_3$, 25ºC): δ = 44.1 (N**C**H_3), 56.4 (O**C**H_3), 111.4 (**C**Harom), 120.0 (CH=**C**H), 123.1 (**C**arom), 128.8 (**C**Harom), 128.8 (**C**arom), 129.0 (**C**Harom), 130.8(**C**Harom), 130.8 (**C**Harom), 131.3 (**C**arom), 131.4 (**C**Harom), 134.4 (**C**arom), 142.0 (**C**H=CH), 152.8 (**C**NCH_3), 158.8 (**C**OCH_3), 187.1 (**C**=O).

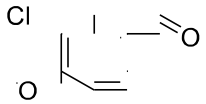
*(E)-3-(3-Bromo-4-(dimethylamino)phenyl)-1-(3-bromo-4-methoxyphenyl)prop-2-en-1-one **2e***



3'-Bromo-4'-methoxyacetophenone (50 mg, 0.22 mmol, 1 equiv) and 3-bromo-4-(dimethylamino)benzaldehyde (75 mg, 0.33 mmol, 1.5 equiv) were dissolved in MeOH (10 mL). NaOH (35 mg, 0.87 mmol, 4 equiv) was added slowly. The reaction mixture was stirred under reflux during 4 h, cooled to room temperature, poured into ice and acidified with dilute HCl. The mixture was extracted with dichloromethane, washed with water, dried over sodium sulfate, and evaporated. The residue was purified by chromatography (dichloromethane/hexane: 2/1) by TLC to give the product as a yellow solid (67 mg, 70%).

m.p.: 124-125°C. ESI$^+$-MS: m/z: 438 $[M+H]^+$ (^{79}Br, 100%), 440 $[M+H]^+$ (^{79}Br^{81}Br, 45%), 442 $[M+H]^+$ (^{81}Br, 40%). Anal Calcd (%) for $C_{18}H_{17}Br_2NO_2.CH_3OH$ (471.18): C 48.43, H 4.49, N 2.97; found C 48.31, H 4.06, N 3.11. ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.26 (d, $^4J_{H\text{-}H}$ 2.1 Hz, 1H, Harom), 8.01 (dd, $^4J_{H\text{-}H}$ 2.1, $^3J_{H\text{-}H}$ 8.6 Hz, 1H, Harom), 7.87 (d, $^4J_{H\text{-}H}$ 2.0 Hz, 1H, Harom), 7.71 (d, $^3J_{H\text{-}H}$ 15.5 Hz, 1H, CH=CH), 7.51 (dd, $^4J_{H\text{-}H}$ 2.0, $^3J_{H\text{-}H}$ 8.4 Hz, 1H, Harom), 7.37 (d, $^3J_{H\text{-}H}$ 15.5 Hz, 1H, CH=CH), 7.05 (d, $^3J_{H\text{-}H}$ 8.4 Hz, 1H, Harom), 6.98 (d,$^3J_{H\text{-}H}$ 8.6 Hz, 1H, Harom), 3.99 (s, 3H, OCH_3), 2.89 (s, 6H, NCH_3). ^{13}C NMR (75 MHz, $CDCl_3$, 25ºC): δ = 44.0 (N**C**H_3), 44.1 (N**C**H_3), 56.6 (O**C**H_3), 111.3 (**C**Harom), 112.0 (**C**arom), 112.1 (**C**arom), 117.4 (**C**arom), 121.3 (CH=**C**H), 128.9 (**C**Harom), 128.9(**C**Harom), 129.7(**C**Harom), 131.9 (**C**Harom), 134.0 (**C**arom), 134.2 (**C**Harom), 142.3 (**C**H=CH), 146.4 (**C**NCH_3), 159.6 (**C**OCH_3), 187.0 (**C**=O).

3-Chloro-4-methoxybenzaldehyde ***4a***

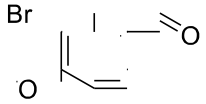


Reference for this compound: Commercial by Aldrich

A mixture of *p*-methoxybenzaldehyde (1.00 mL, 8.2 mmol, 1 equiv) and ammonium nitrate (0.13 g, 1.6 mmol, 0.2 equiv) in acetonitrile (10 mL) was stirred at room temperature. *N*-Chlorosuccinimide (4.36 g, 33 mmol, 4 equiv) was added slowly over 3 days. The solid obtained was filtered and the mixture was extracted with dichloromethane, washed with water and dried over Na_2SO_4. The solvent was then evaporated under reduced pressure, and silica gel flash column chromatography (eluent: dichloromethane/ Hexane: 1/1) of the residue gave the product as a white solid (0.62g, 45%).

^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 9.84 (s, C*H*O) 7.84 (d, $^4J_{H\text{-}H}$ 2.0 Hz, 1H, Harom), 7.77 (dd, $^4J_{H\text{-}H}$ 2.0, $^3J_{H\text{-}H}$ 8.5 Hz, 1H, Harom), 7.04 (d, $^3J_{H\text{-}H}$ 8.5 Hz, 1H, Harom), 3.99 (s, 3H, OCH_3).

3-Bromo-4-methoxybenzaldehyde ***4b***

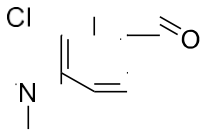


Reference for this compound: Commercial by Aldrich

A mixture of *p*-methoxybenzaldehyde (1.25 mL, 10 mmol, 1 equiv) and ammonium nitrate (0.16 g, 2 mmol, 0.2 equiv) in acetonitrile (10 mL) was stirred at room temperature. *N*-Bromosuccinimide (3.56 g, 20 mmol, 2 equiv) was added slowly over 3 days. The solid obtained was filtered and the mixture was extracted with dichloromethane, washed with water, dried, and evaporated. The residue was purified by chromatography (eluent: dichloromethane) on TLC to give the product as orange solid (0.92 g, 43%).

^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 9.85 (s, 1H, C*H*O), 8.09 (d, $^4J_{H\text{-}H}$ 1.9 Hz, 1 H, Harom), 7.83 (dd, $^4J_{H\text{-}H}$ 1.9, $^3J_{H\text{-}H}$ 8.7 Hz, 1H, Harom), 7.02 (d, $^3J_{H\text{-}H}$ 8.7 Hz, 1H, Harom), 4.00 (s, 3 H, OC*H*$_3$).

3-Chloro-4-(dimethylamino)benzaldehyde ***4c***

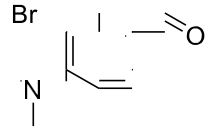


Reference for this compound: D. Ginsburg, *J. Am. Chem. Soc.*, **1951**, *73*, 702-704. S. Guieu, J. Rocha, A. M. S. Silva, *J. Mol. Struct.*, **2013**, 1035, 1-5.

N-Chlorosuccinimide (2.67 g, 20 mmol, 2 equiv) was added to a solution of 4-(dimethylamino)benzaldehyde (1.49 g, 10 mmol, 1 equiv) in dichloromethane (50 mL), and the reaction mixture was stirred at room temperature for 72 h. The solvent was then evaporated under reduced pressure, and silica gel flash column chromatography (eluent: dichloromethane/petroleum ether: 1/1) of the residue gave the product as a colorless liquid (0.98 g, 54%).

^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 9.81 (s, 1H, C*H*O), 7.83 (d, $^4J_{H\text{-}H}$ 2.1 Hz, 1 H, Harom), 7.68 (dd, $^4J_{H\text{-}H}$ 2.1, $^3J_{H\text{-}H}$ 8.4 Hz, 1H, Harom), 7.05 (d, $^3J_{H\text{-}H}$ 8.4 Hz, 1H, Harom), 2.96 (s, 6 H, CH_3).

3-Bromo-4-(dimethylamino)benzaldehyde ***4d***

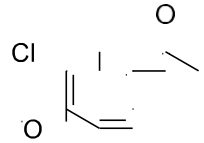


Reference for this compound: B. Das, K. Venkateswarlu, A. Majhi, V. Siddaiah, K.R. Reddy, *J. Mol. Catal. A: Chem.*, **2007**, *267*, 30-33. S. Guieu, J. Rocha, A. M. S. Silva, *J. Mol. Struct.*, **2013**, *1035*, 1-5.

N-Bromosuccinimide (1.78 g, 10 mmol, 1 equiv) was added to a solution of 4-(dimethylamino)benzaldehyde (1.49 g, 10 mmol, 1 equiv) in dichloromethane (50 mL), and the reaction mixture was stirred at room temperature for 72 h. The solvent was then evaporated under reduced pressure, and silica gel flash column chromatography (eluent: dichloromethane/petroleum ether: 1/1) of the residue gave the product as a colorless liquid (1.62 g, 71%).

^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 9.80 (s, 1H, C*H*O), 8.03 (d, $^4J_{H\text{-}H}$ 1.8 Hz, 1 H, Harom), 7.73 (dd, $^4J_{H\text{-}H}$ 1.8, $^3J_{H\text{-}H}$ 8.4 Hz, 1 H, Harom), 7.06 (d, $^3J_{H\text{-}H}$ 8.4 Hz, 1H, Harom), 2.94 (s, 6 H, CH_3).

1-(3-Chloro-4-methoxyphenyl)ethan-1-one ***6a***

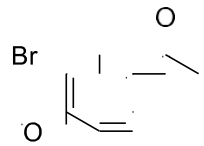


Reference for this compound: Commercial by Aldrich

To a solution of 4'-methoxyacetophenone (1.0 g, 6.66 mmol) in glacial acetic acid (8 mL) was added 5% NaOCl in water (30 mL) dropwise. The mixture was stirred for 30 minutes. A solid was obtained, which was separated by filtration and purified over silica gel flash column chromatography (dichloromethane / petroleum ether 3/1). The solvent was completely evaporated, yielding 3'-chloro-4'-methoxyacetophenone (0.568 g, 3.08 mmol, 46%) as white crystals.

^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.00 (d, $^4J_{H\text{-}H}$ 2.2 Hz, 1H, Harom), 7.87 (dd, $^4J_{H\text{-}H}$ 2.2, $^3J_{H\text{-}H}$ 8.4 Hz, 1H, Harom), 6.97 (d, $^3J_{H\text{-}H}$ 8.4 Hz, 1H, Harom), 3.97 (s, 3H, OCH_3), 2.56 (s, 3H, CCH_3).

1-(3-Bromo-4-methoxyphenyl)ethan-1-one ***6b***



Reference for this compound: Commercial by Aldrich. K. Tanemura, T. Suzuki, Y. Nishida, K. Satsumabayashi, T. Horaguchi, *Chem. Lett.*, **2003**, *32*, 932-933.

A mixture of 4'methoxyacetophenone (1.00 g, 6.6 mmol, 1 equiv) and ammonium nitrate (0.10 g, 1.3 mmol, 0.2 equiv) in acetonitrile (10 mL) was stirred at room temperature. *N*-Bromosuccinimide (3.56 g, 20 mmol, 2 equiv) was added slowly over 3 days. The solid obtained was filtered and the mixture was extracted with dichloromethane, washed with water and dried over Na_2SO_4. The solvent was then evaporated under reduced pressure, and silica gel flash column chromatography (eluent: dichloromethane/ Hexane: 1/1) of the residue gave the product as a white solid (1.07 g, 71%).

^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.17 (d, $^4J_{H-H}$ 2.1 Hz, 1H, Harom), 7.93 (dd, $^4J_{H-H}$ 2.1, $^3J_{H-H}$ 8.6 Hz, 1H, Harom), 6.95 (d, $^3J_{H-H}$ 8.6 Hz, 1H, Harom), 3.98 (s, 3H, OCH_3), 2.57 (s, 3H, CH_3).

NMR spectra

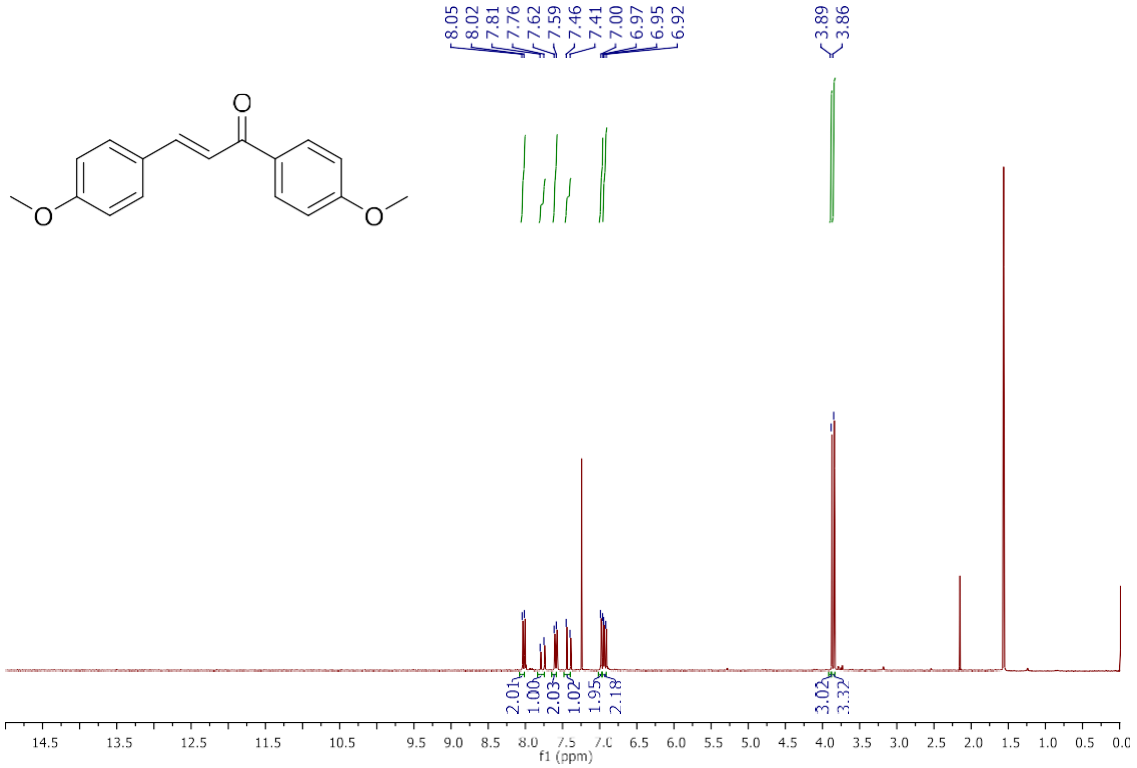


Figure S1. ^{1}H NMR spectrum of (*E*)-1,3-bis(4-methoxyphenyl)prop-2-en-1-one **1a** in $CDCl_3$

Figure S2. ^{1}H NMR spectrum of (*E*)-1,3-bis(3-chloro-4-methoxyphenyl)prop-2-en-1-one **1b** in $CDCl_3$

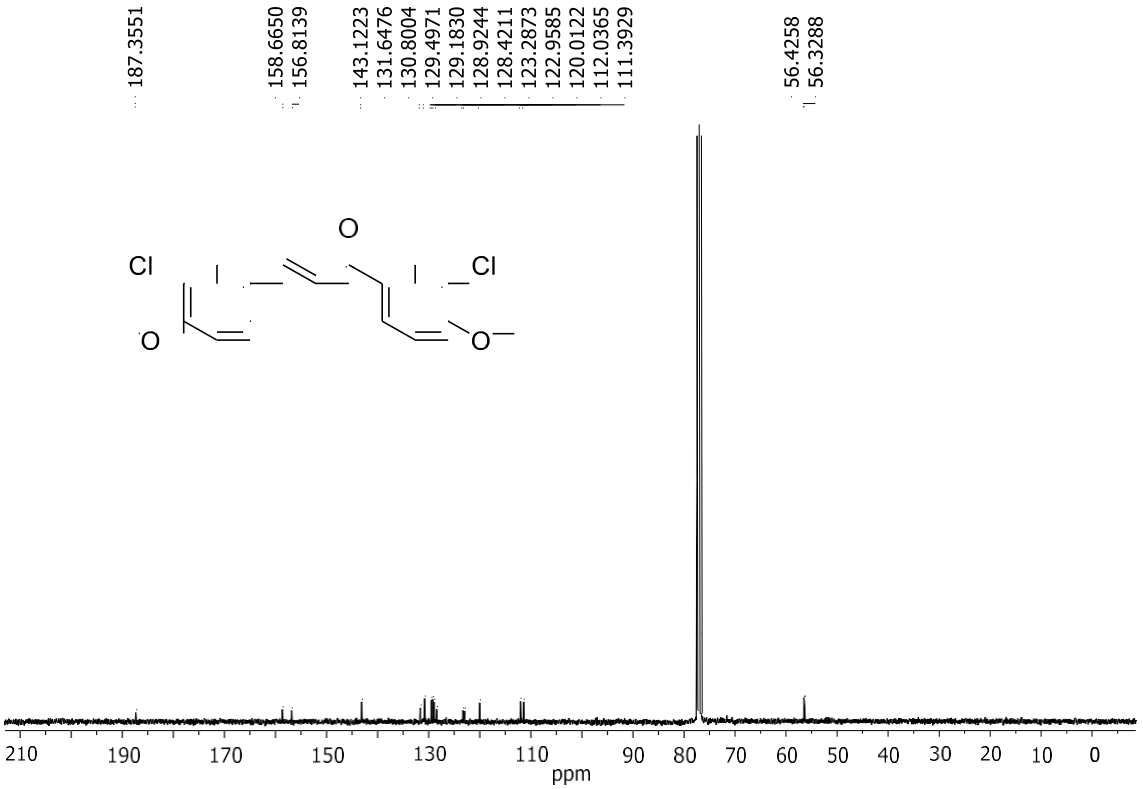


Figure S3. ^{13}C NMR spectrum of (*E*)-1,3-bis(3-chloro-4-methoxyphenyl)prop-2-en-1-one **1b** in $CDCl_3$

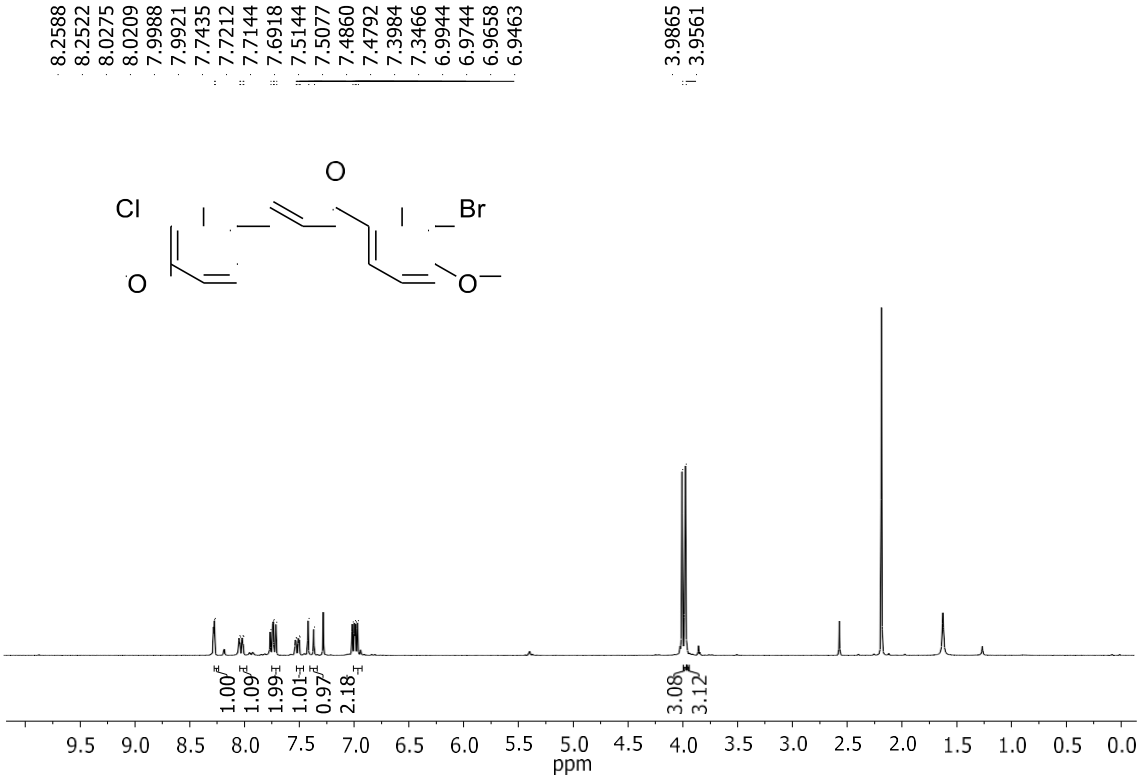


Figure S4. ^{1}H NMR spectrum of (*E*)-1-(3-bromo-4-methoxyphenyl)-3-(3-chloro-4-methoxyphenyl)prop-2-en-1-one **1c** in $CDCl_3$

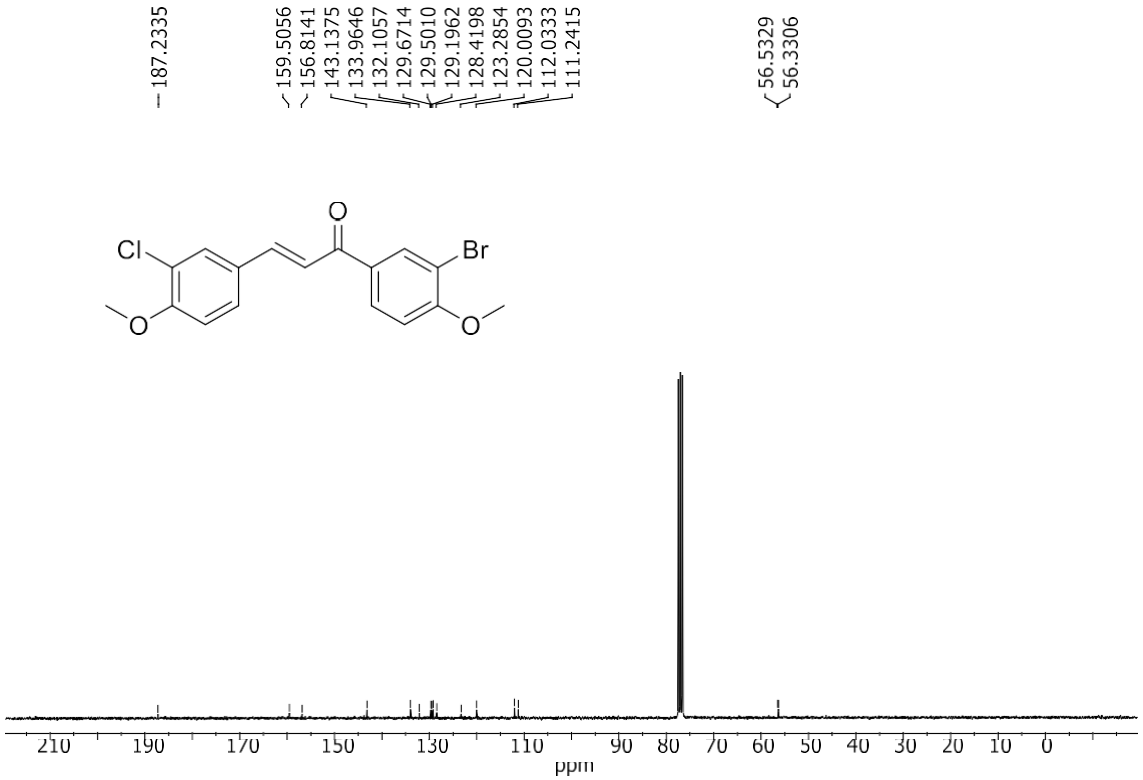


Figure S5. ^{13}C NMR spectrum of (*E*)-1-(3-bromo-4-methoxyphenyl)-3-(3-chloro-4-methoxyphenyl)prop-2-en-1-one **1c** in $CDCl_3$

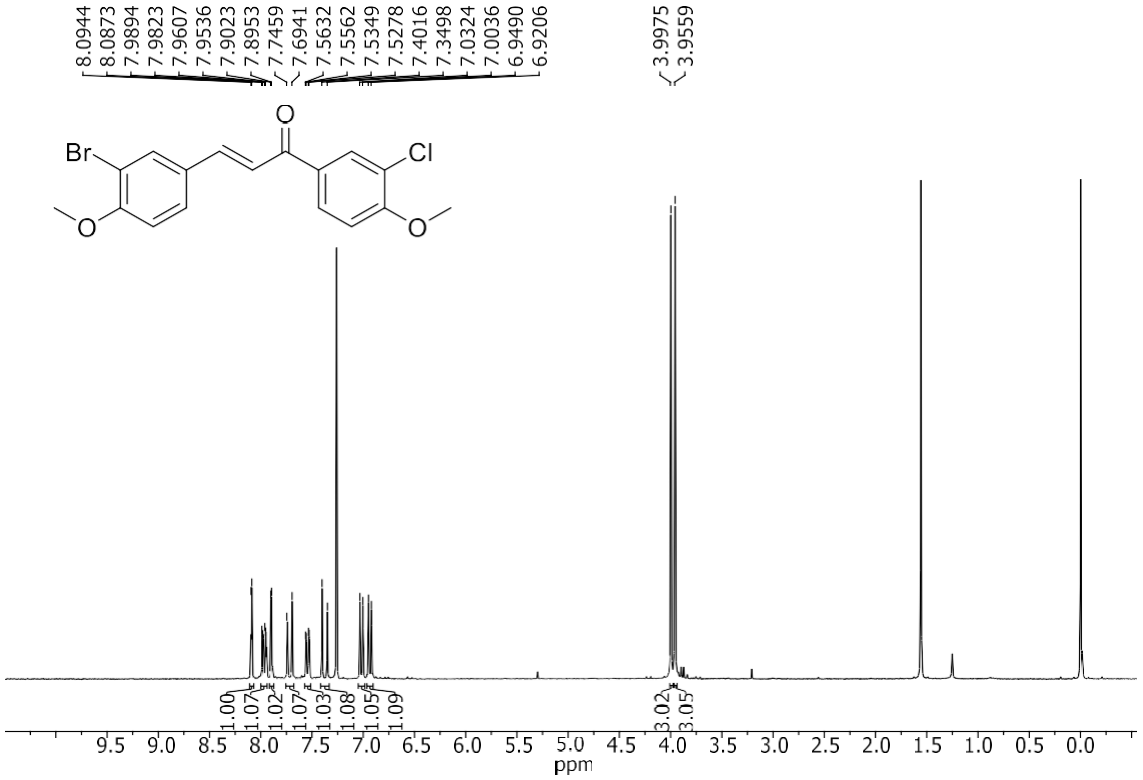


Figure S6. ^{1}H NMR spectrum of (*E*)-3-(3-bromo-4-methoxyphenyl)-1-(3-chloro-4-methoxyphenyl)prop-2-en-1-one **1d** in $CDCl_3$

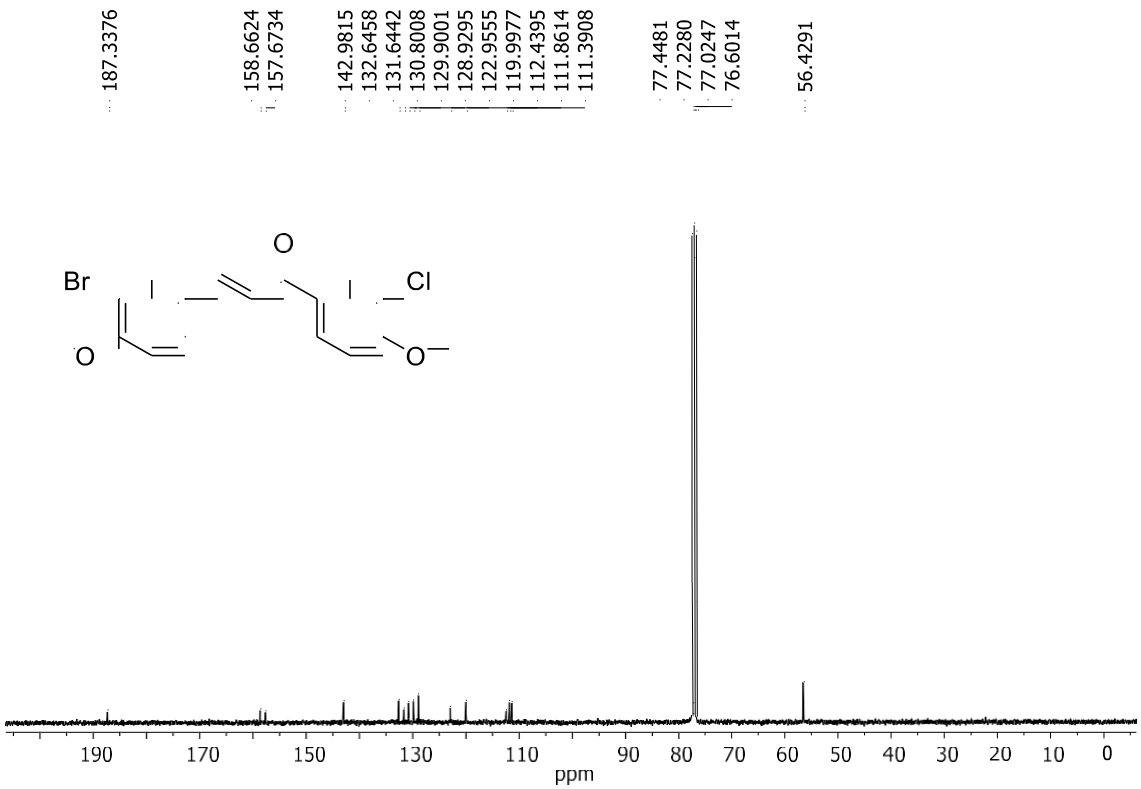


Figure S7. ^{13}C NMR spectrum of (*E*)-3-(3-bromo-4-methoxyphenyl)-1-(3-chloro-4-methoxyphenyl)prop-2-en-1-one **1d** in $CDCl_3$

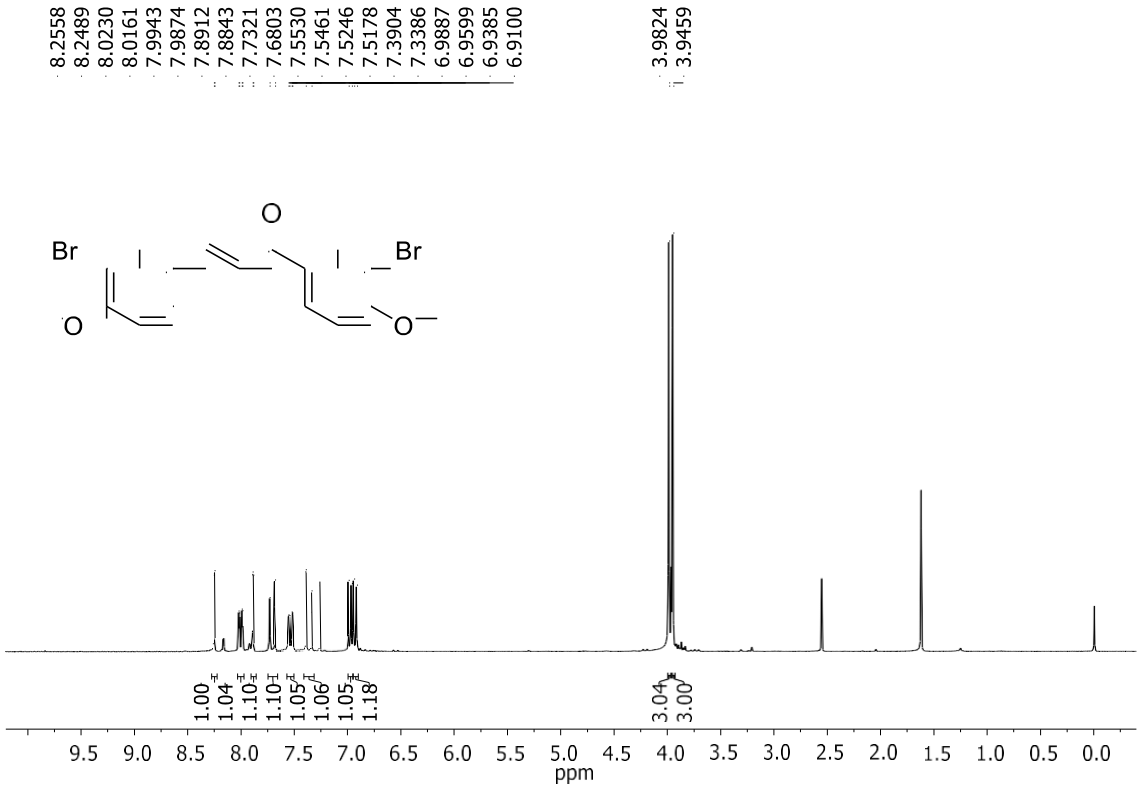


Figure S8. ^{1}H NMR spectrum of (*E*)-1,3-bis(3-bromo-4-methoxyphenyl)prop-2-en-1-one **1e** in $CDCl_3$

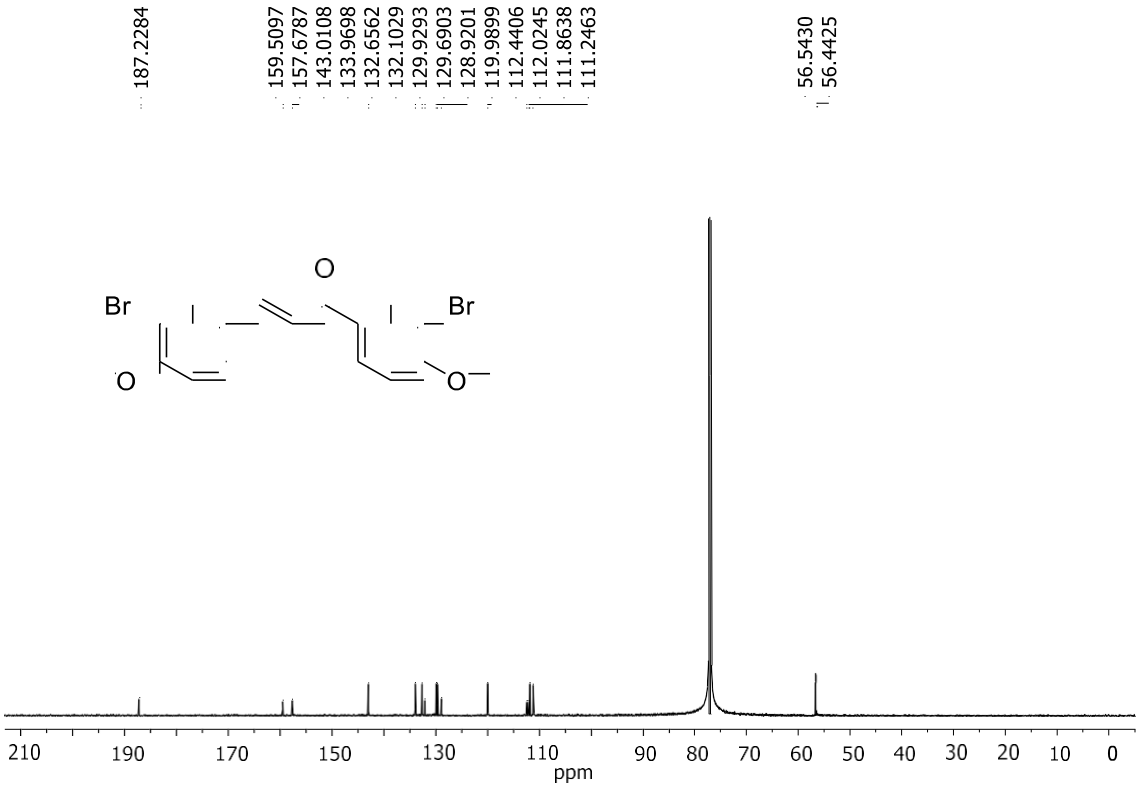


Figure S9. ^{13}C NMR spectrum of (*E*)-1,3-bis(3-bromo-4-methoxyphenyl)prop-2-en-1-one **1e** in $CDCl_3$

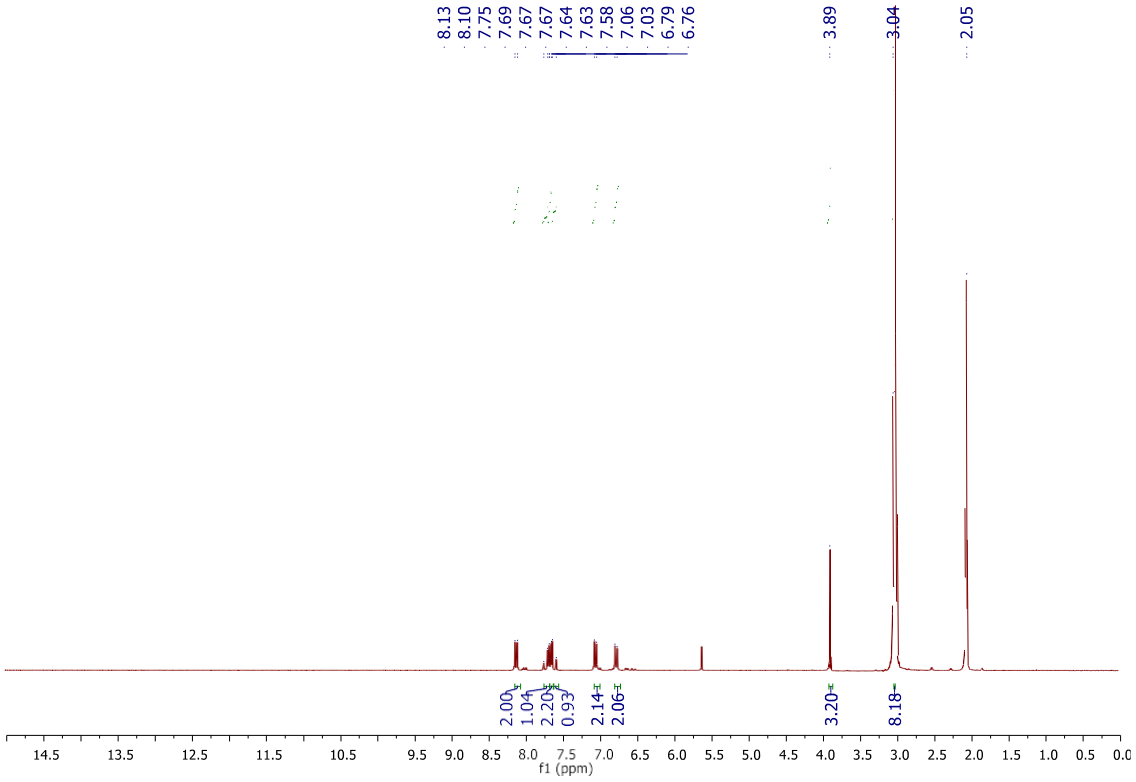


Figure S10. ^{1}H NMR spectrum of (*E*)-3-[4-(dimethylamino)phenyl]-1-(3-chloro-4-methoxyphenyl)prop-2-en-1-one **2a** in Acetone-d_6

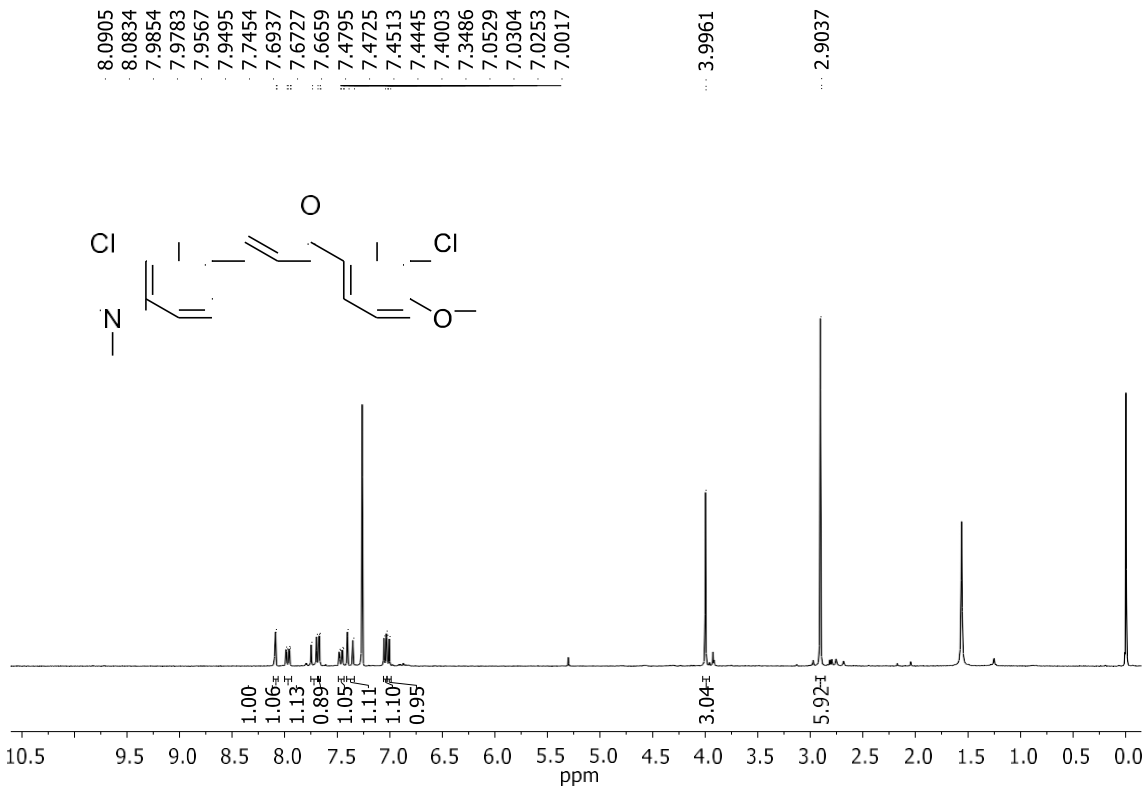


Figure S11. ^{1}H NMR spectrum of (*E*)-3-[3-chloro-4-(dimethylamino)phenyl]-1-(3-chloro-4-methoxyphenyl)prop-2-en-1-one **2b** in $CDCl_3$

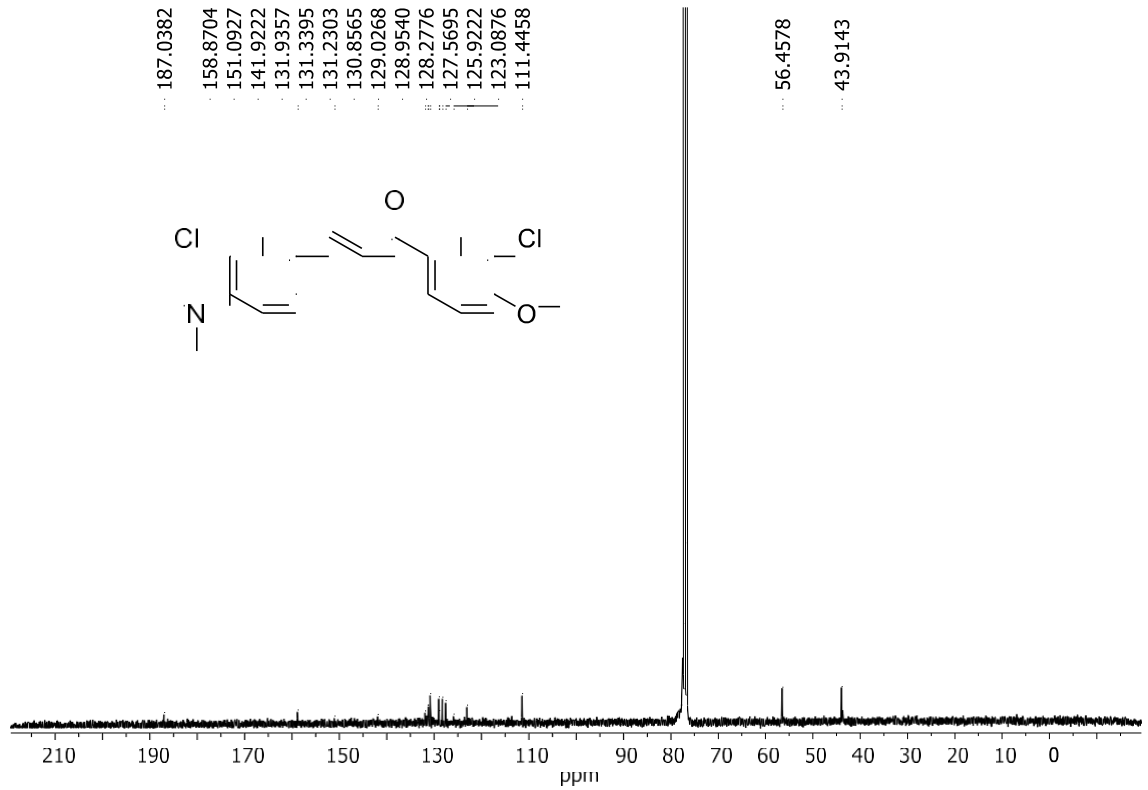


Figure S12. ^{13}C NMR spectrum of (*E*)-3-[3-chloro-4-(dimethylamino)phenyl]-1-(3-chloro-4-methoxyphenyl)prop-2-en-1-one **2b** in $CDCl_3$

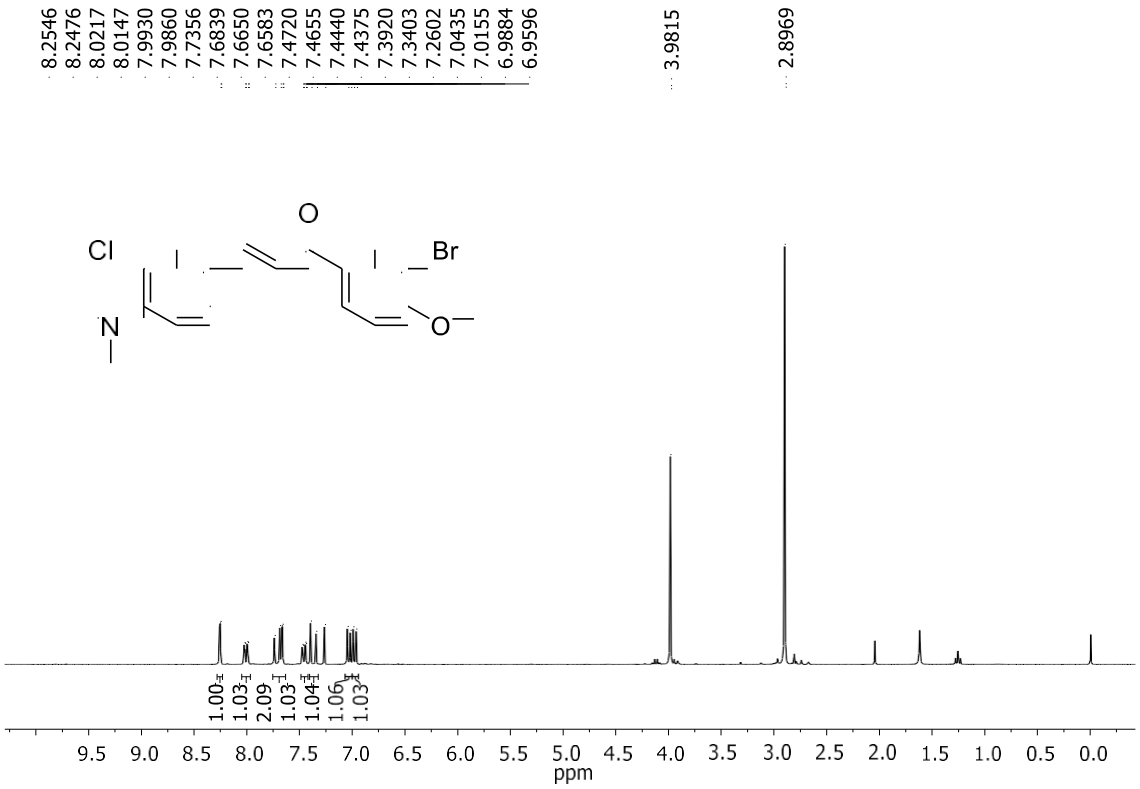


Figure S13. ^{1}H NMR spectrum of (*E*)-1-(3-bromo-4-methoxyphenyl)-3-[3-chloro-4-(dimethylamino)phenyl]prop-2-en-1-one **2c** in $CDCl_3$

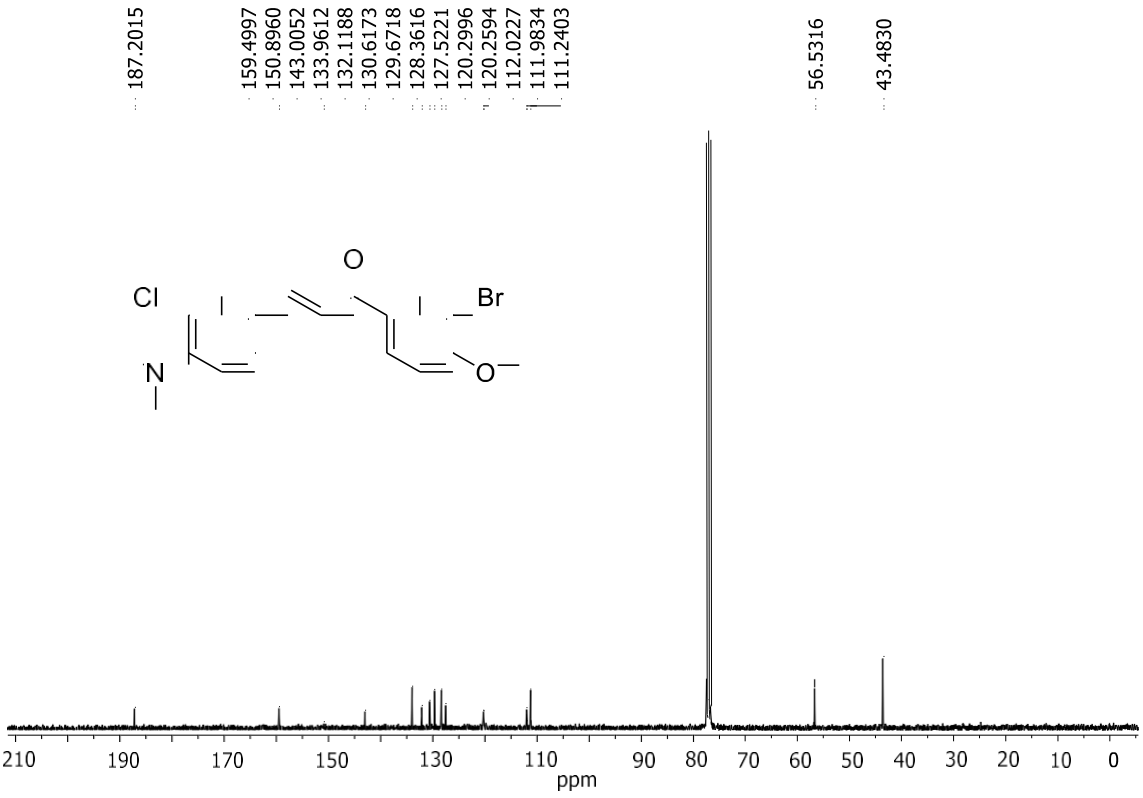


Figure S14. ^{13}C NMR spectrum of (*E*)-1-(3-bromo-4-methoxyphenyl)-3-[3-chloro-4-(dimethylamino)phenyl]prop-2-en-1-one **2c** in $CDCl_3$

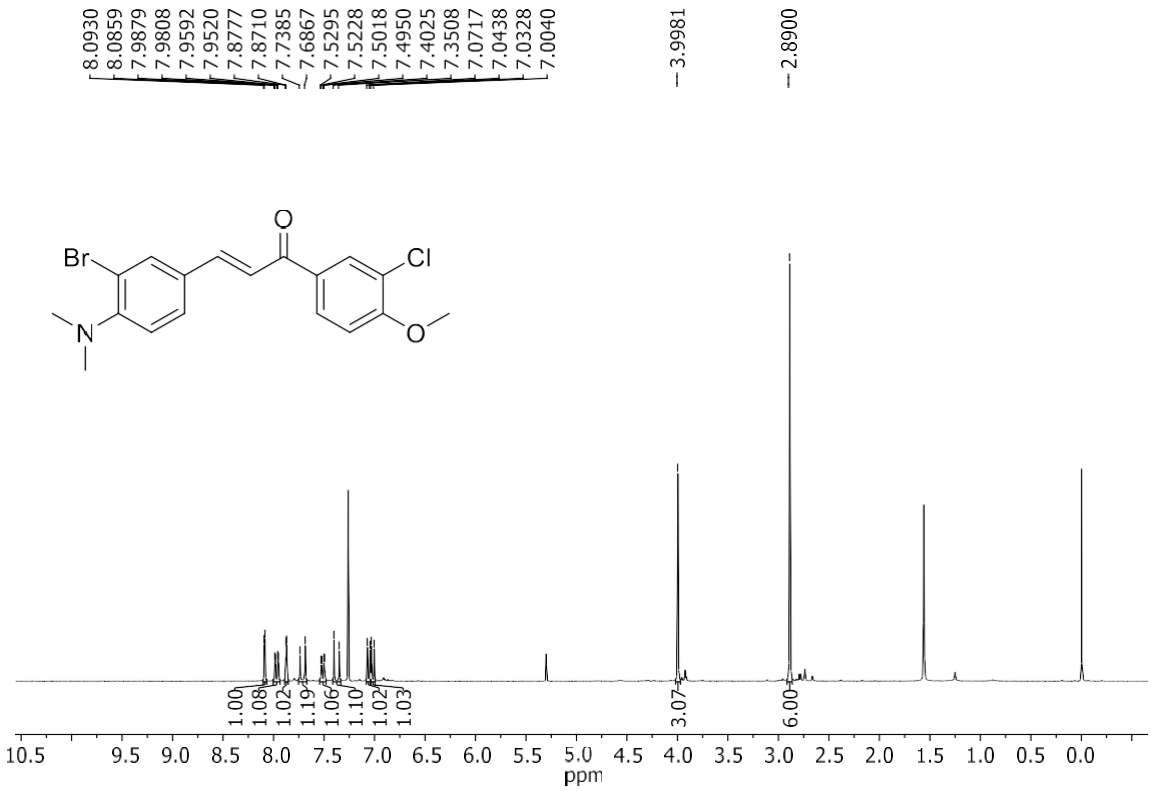


Figure S15. ^{1}H NMR spectrum of (*E*)-3-[3-bromo-4-(dimethylamino)phenyl]-1-(3-chloro-4-methoxyphenyl)prop-2-en-1-one **2d** in $CDCl_3$

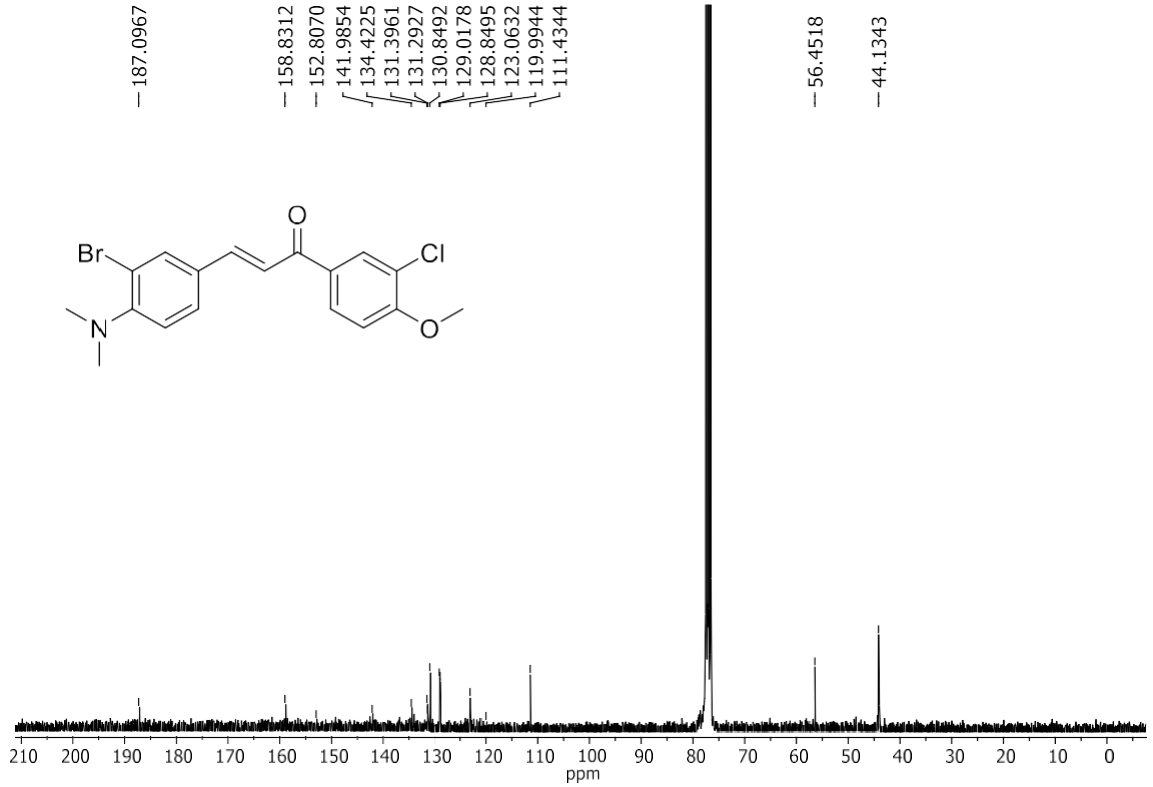


Figure S16. ^{13}C NMR spectrum of (*E*)-3-[3-bromo-4-(dimethylamino)phenyl]-1-(3-chloro-4-methoxyphenyl)prop-2-en-1-one **2d** in $CDCl_3$

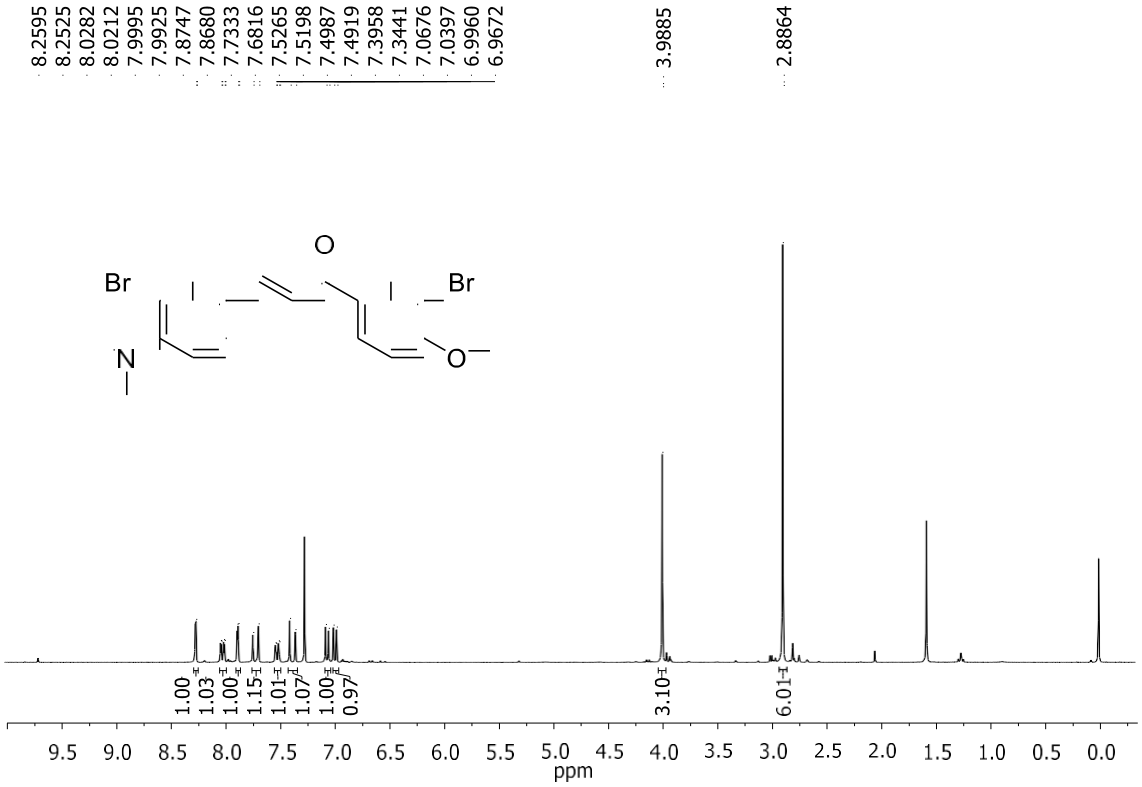


Figure S17. ^{1}H NMR spectrum of (*E*)-3-[3-bromo-4-(dimethylamino)phenyl]-1-(3-bromo-4-methoxyphenyl)prop-2-en-1-one **2e** in $CDCl_3$

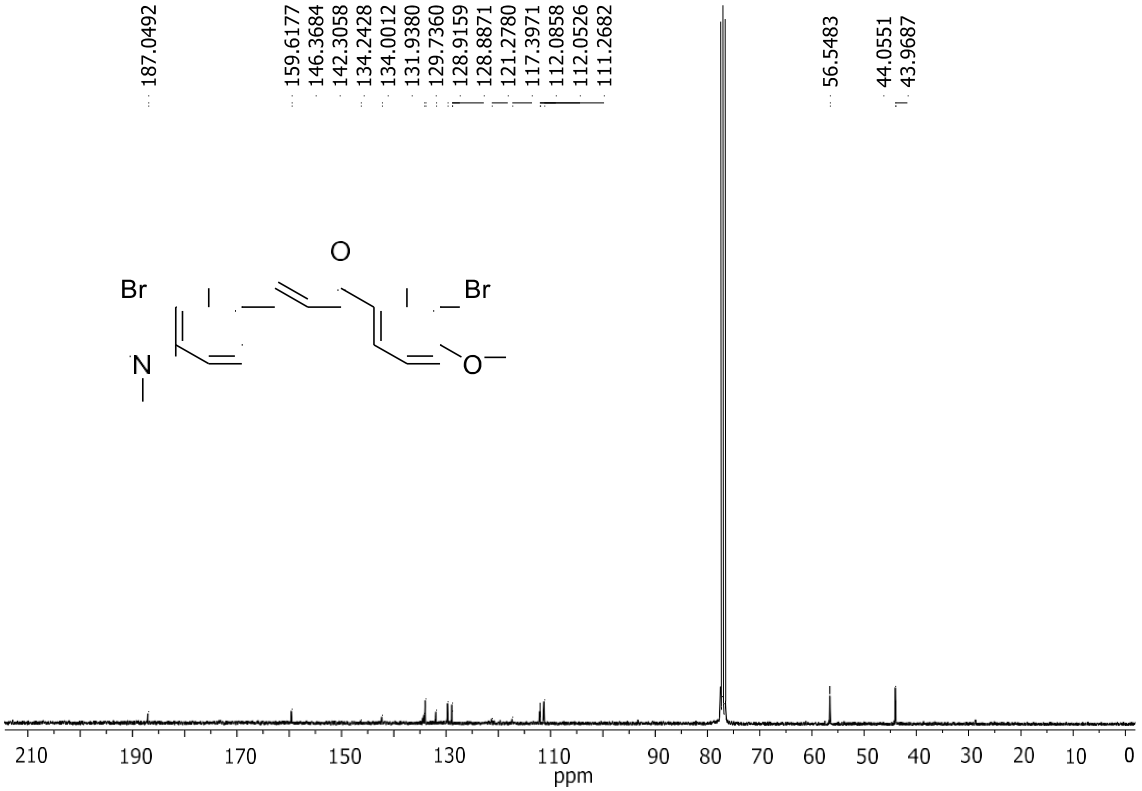


Figure S18. ^{13}C NMR spectrum of (*E*)-3-[3-bromo-4-(dimethylamino)phenyl]-1-(3-bromo-4-methoxyphenyl)prop-2-en-1-one **2e** in $CDCl_3$

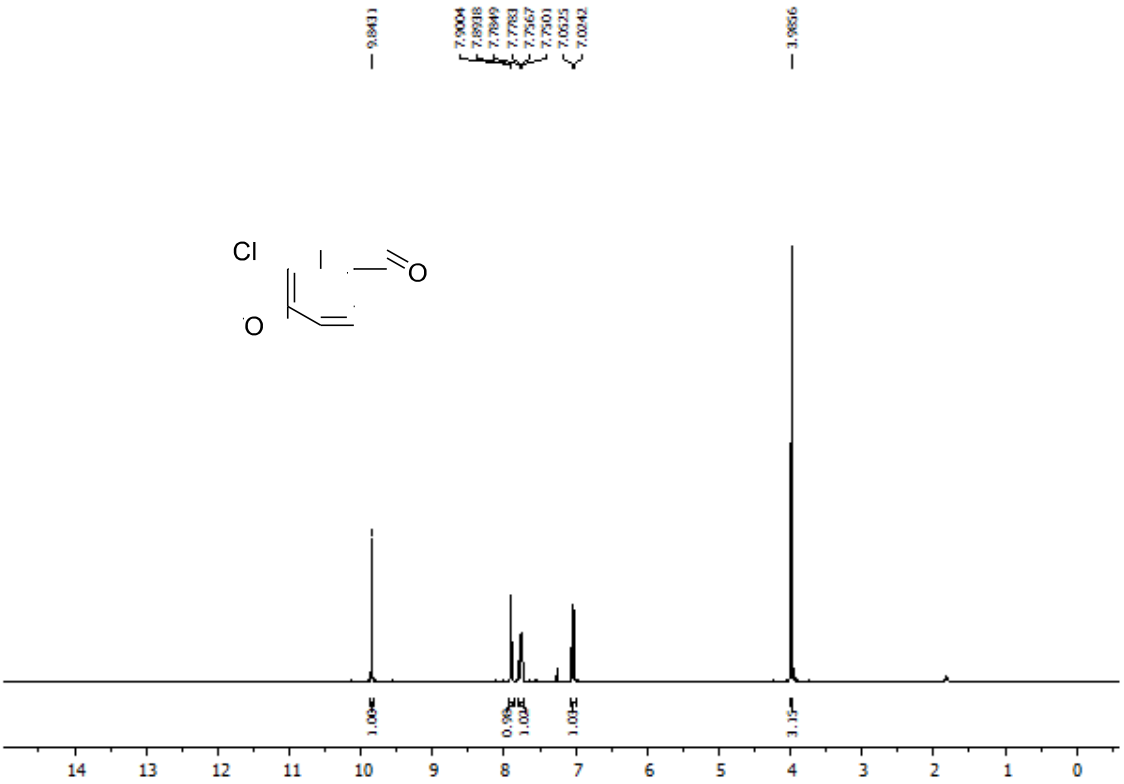


Figure S19. ^{1}H NMR spectrum of 3-chloro-4-methoxybenzaldehyde **4a** in $CDCl_3$

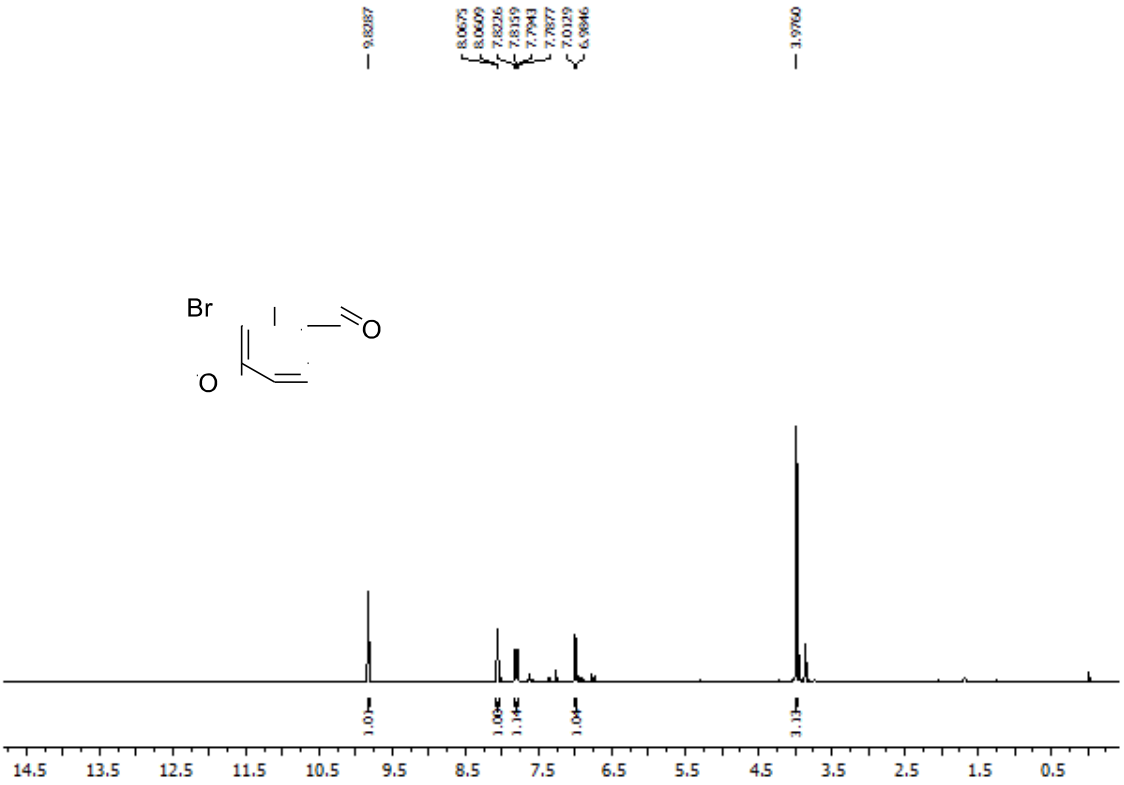


Figure S20. ^{1}H NMR spectrum of 3-bromo-4-methoxybenzaldehyde **4b** in $CDCl_3$

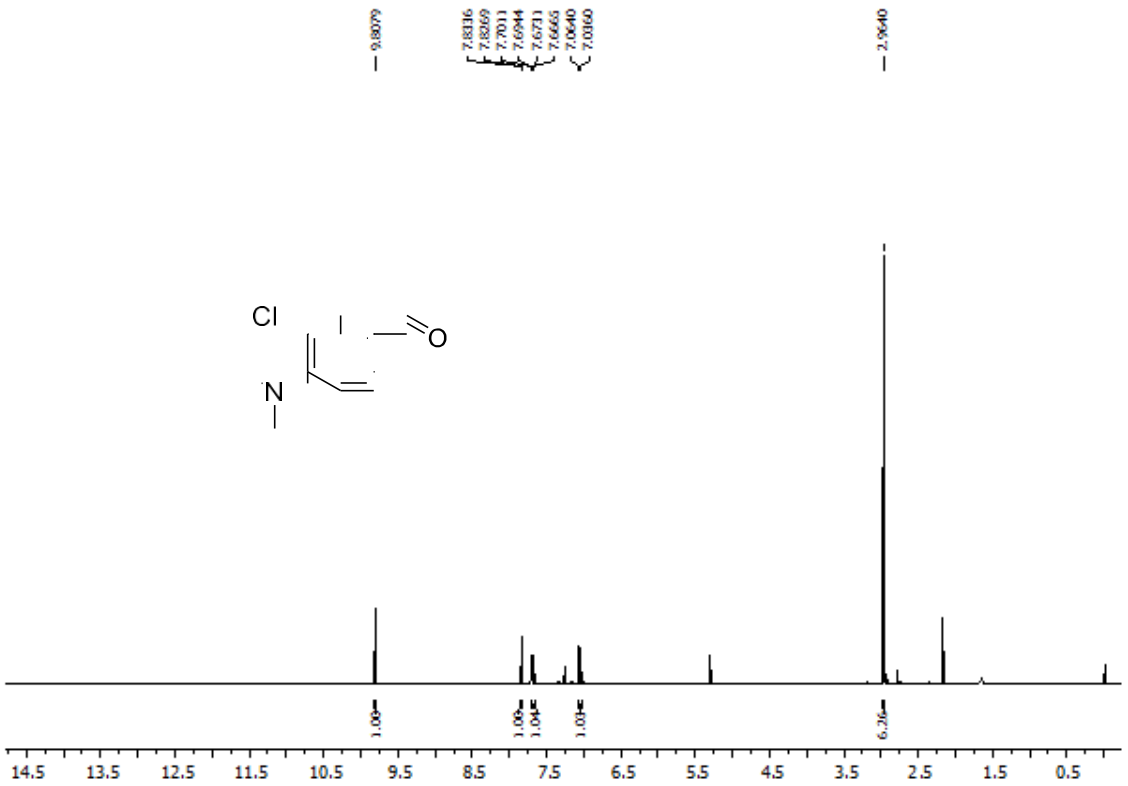


Figure S21. ^{1}H NMR spectrum of 3-chloro-4-(dimethylamino)benzaldehyde **4c** in $CDCl_3$

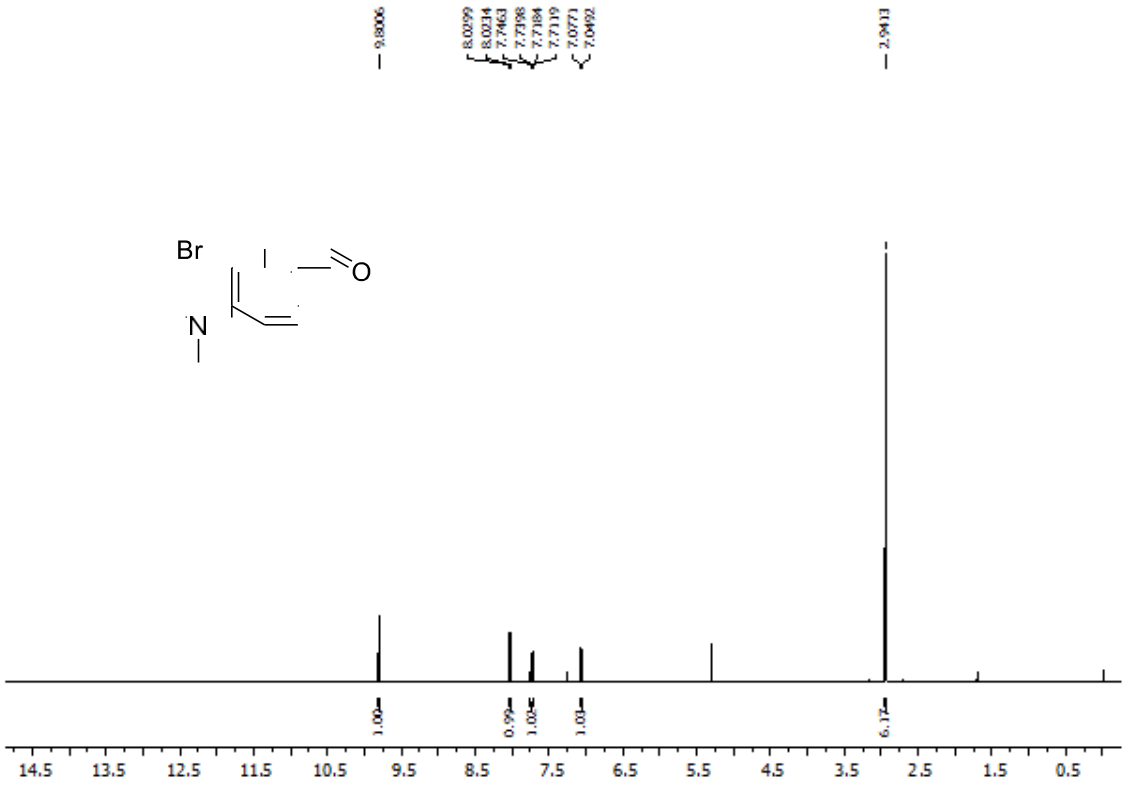


Figure S22. ^{1}H NMR spectrum of 3-bromo-4-(dimethylamino)benzaldehyde **4d** in $CDCl_3$

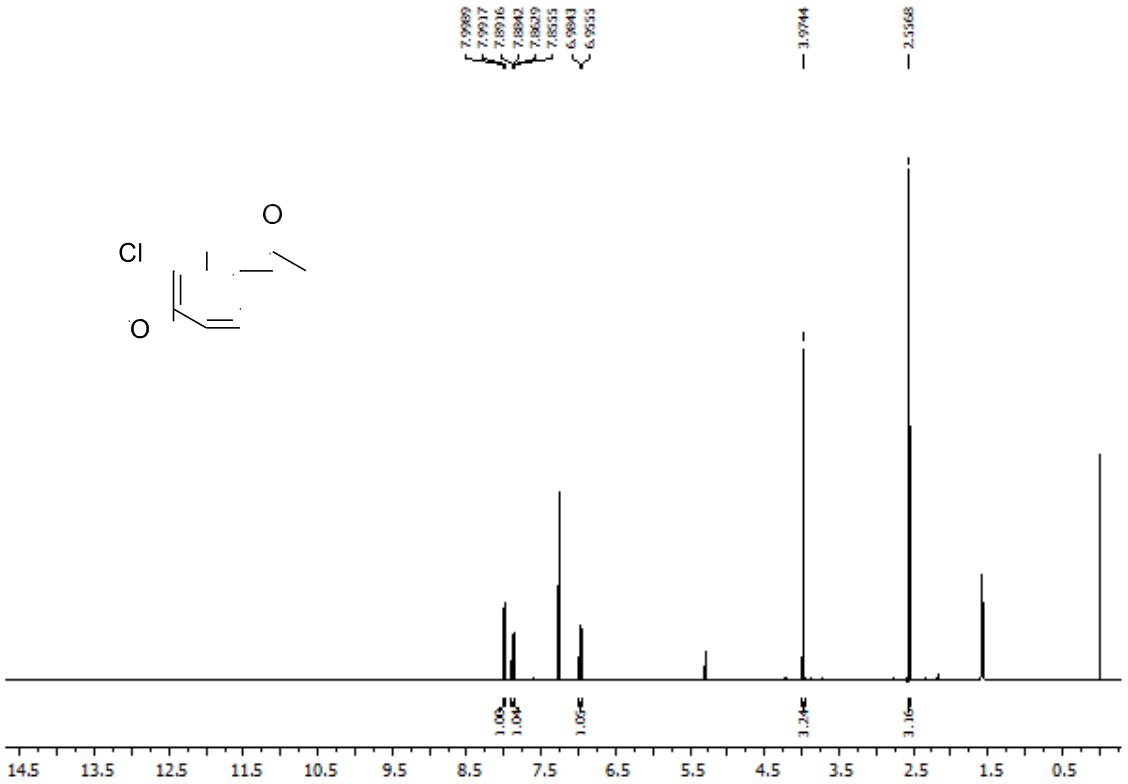


Figure S23. ^{1}H NMR spectrum of 1-(3-chloro-4-methoxyphenyl)ethan-1-one **6a** in $CDCl_3$

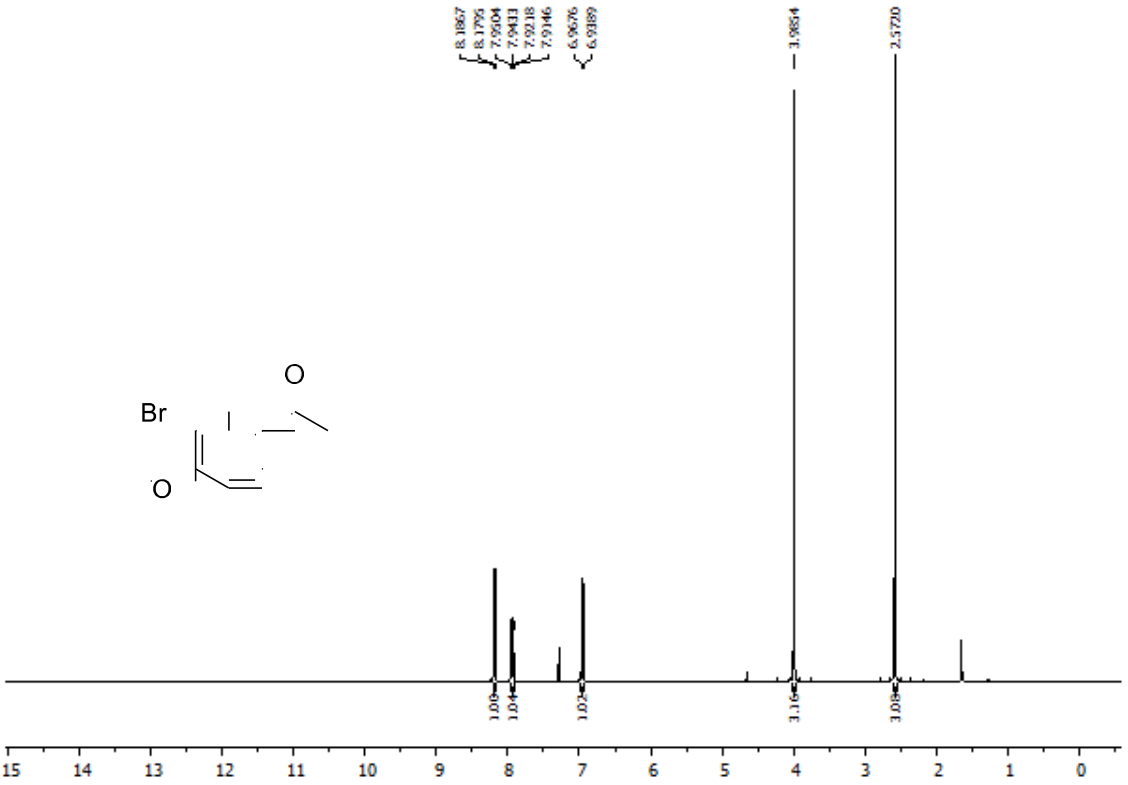


Figure S24. ^{1}H NMR spectrum of 1-(3-bromo-4-methoxyphenyl)ethan-1-one **6b** in $CDCl_3$

Absorption and emission properties

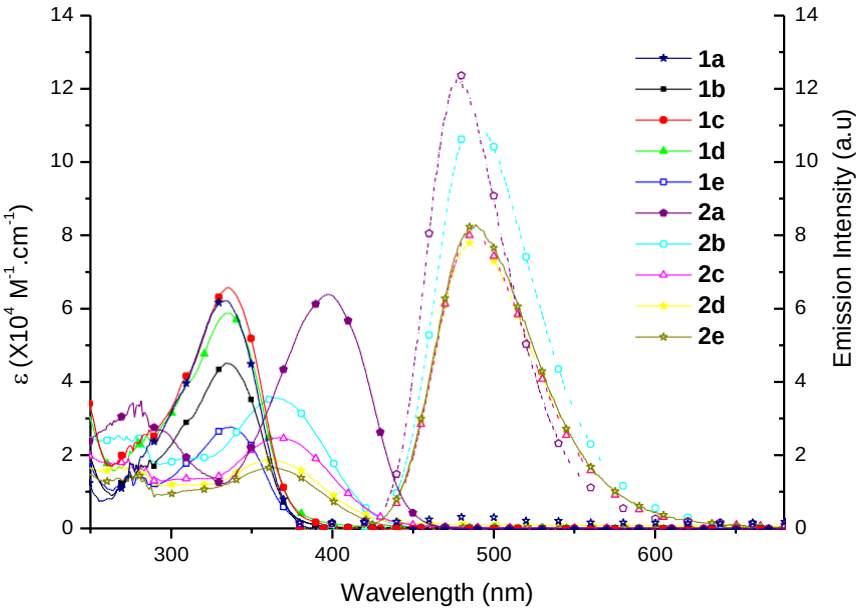


Figure S25. Absorption and emission spectra of chalcones **1a-e,2a-e** in THF solution (at *ca.* 1.10^{-5} mol.L^{-1}). Excitation at 370 nm.

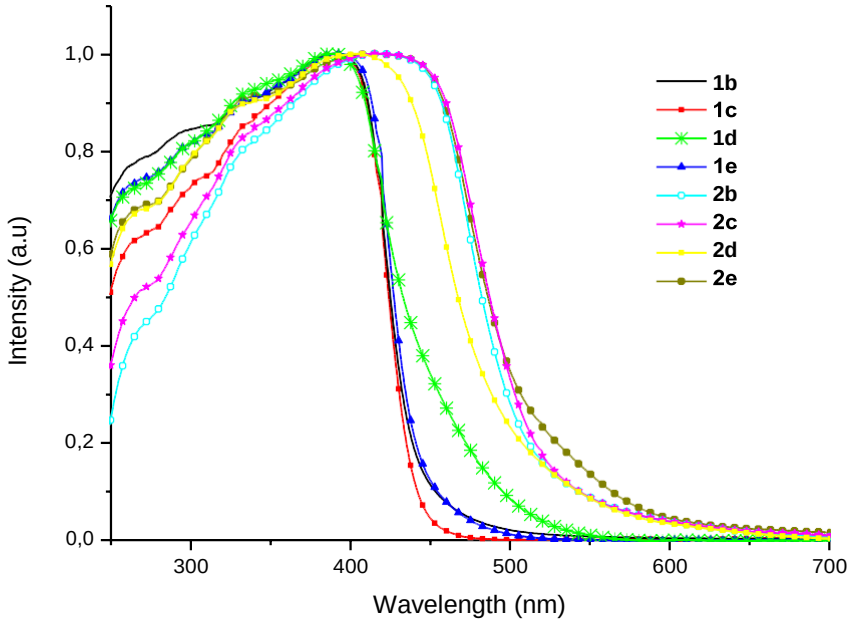


Figure S26. Absorption spectra of chalcones **1b-e,2b-e** in solid state.

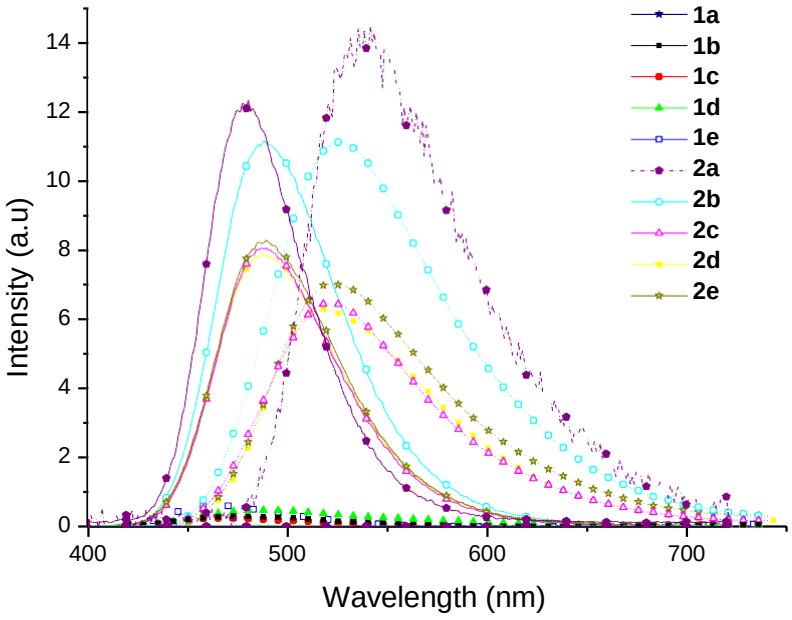


Figure S27. Photoluminescence spectra in solution (*ca.* 10^{-5} mol.L^{-1} in THF, solid lines) and solid state (dotted lines). The excitation wavelength was 365 nm.

Aggregation-Induced Emission Enhancement

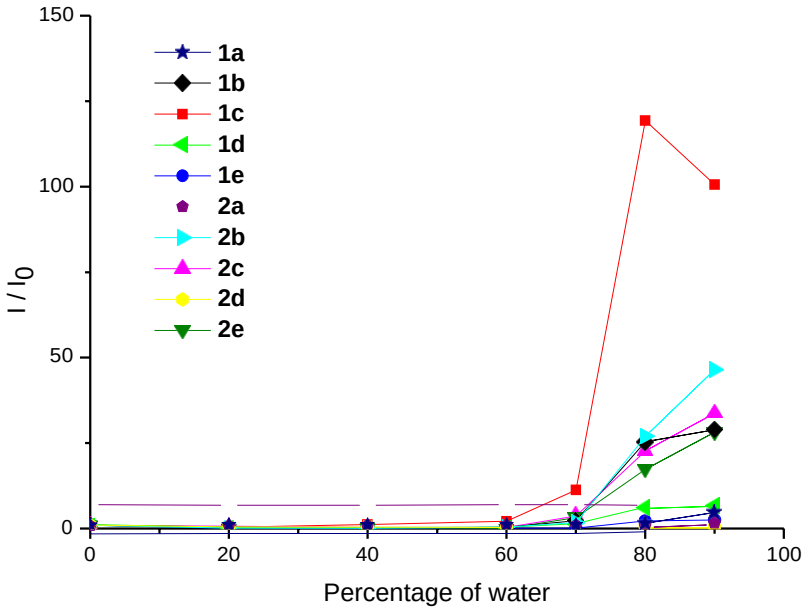


Figure S28. Aggregation-induced emission enhancement of chalcones **1b-e,2b-e** in THF-water.

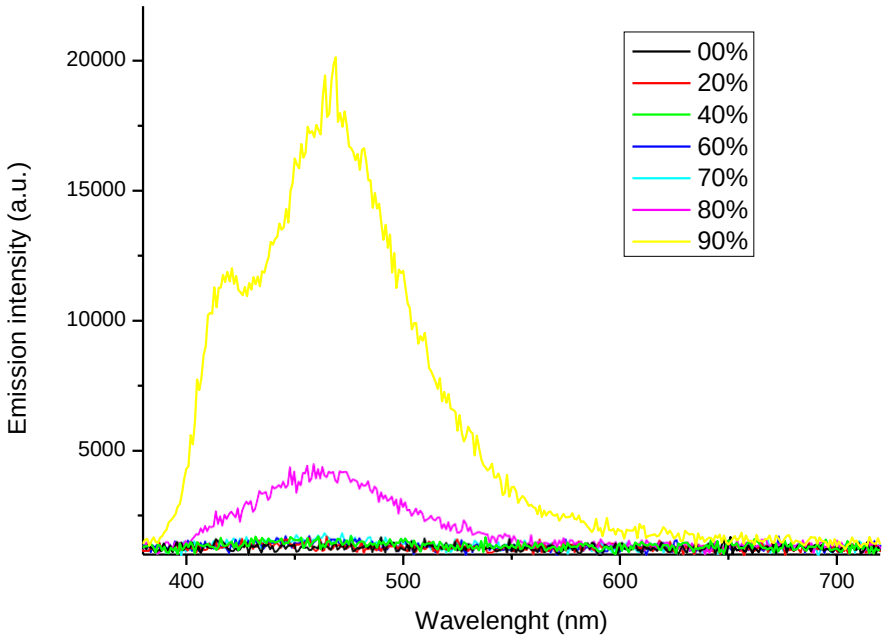


Figure S29. Aggregation-induced emission enhancement of chalcone **1a** in THF-water.

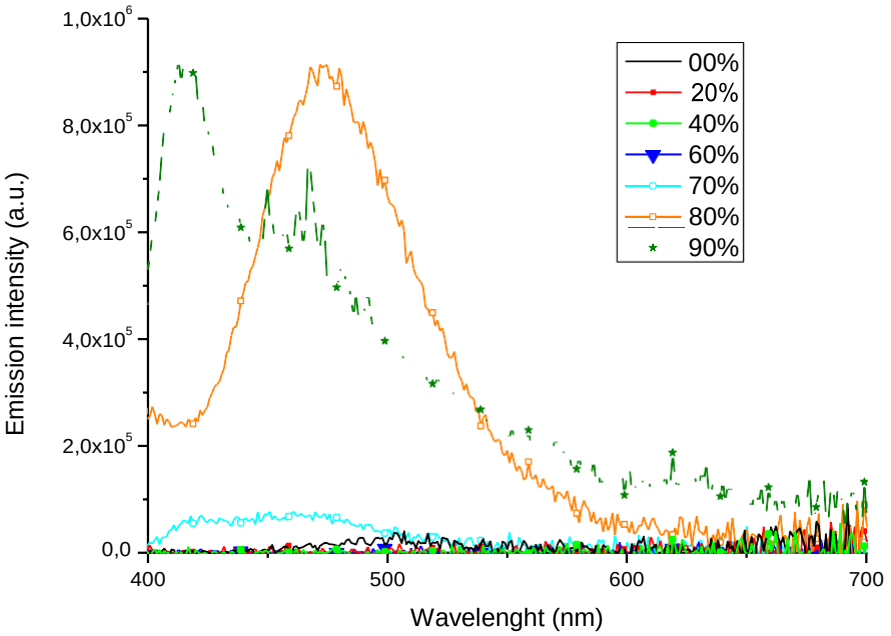


Figure S30. Aggregation-induced emission enhancement of chalcone **1b** in THF-water.

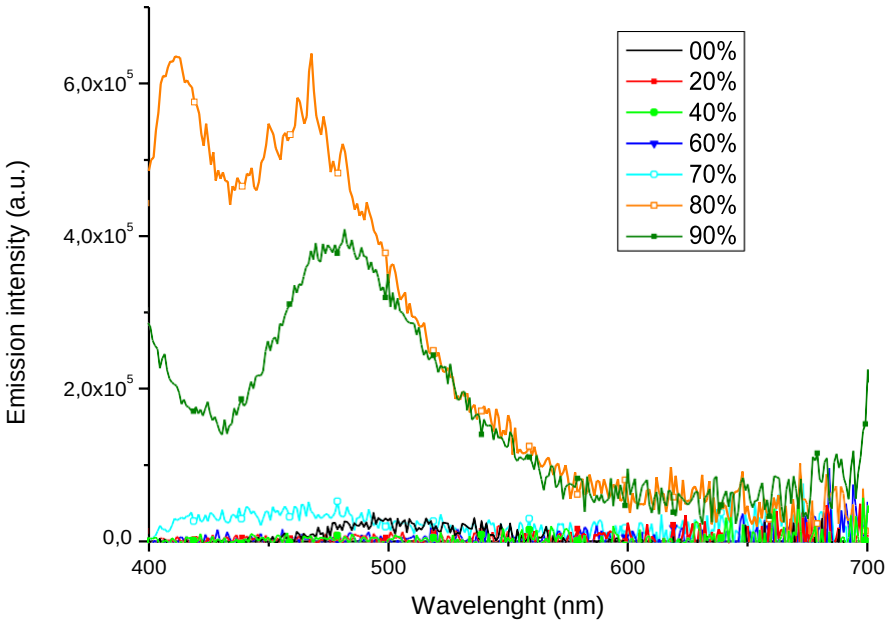


Figure S31. Aggregation-induced emission enhancement of chalcone **1c** in THF-water.

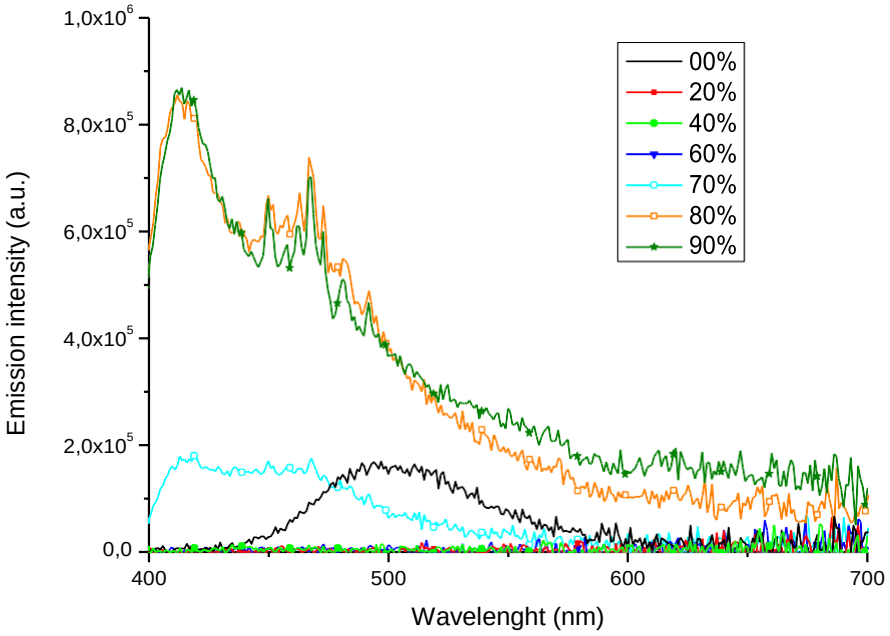


Figure S32. Aggregation-induced emission enhancement of chalcone **1d** in THF-water.

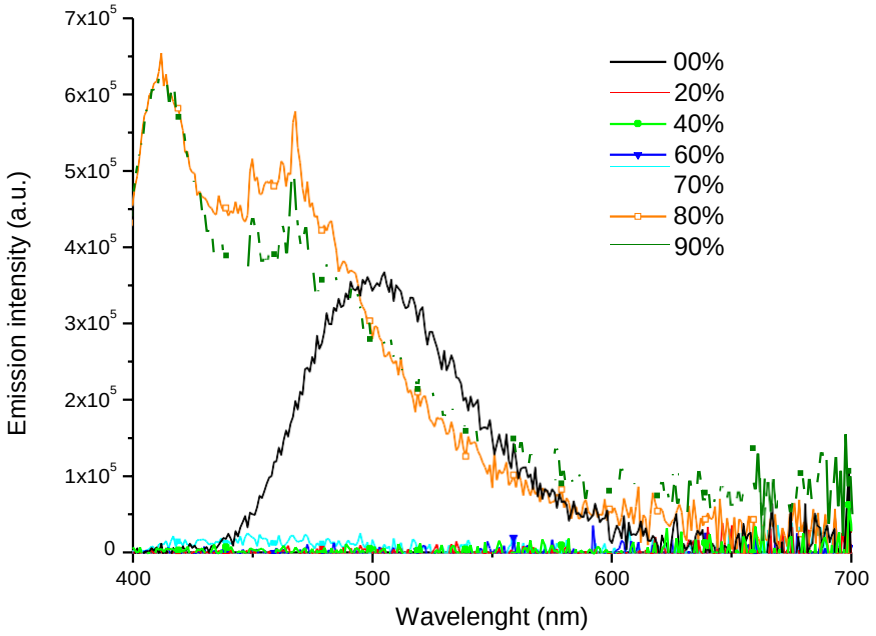


Figure S33. Aggregation-induced emission enhancement of chalcone **1e** in THF-water.

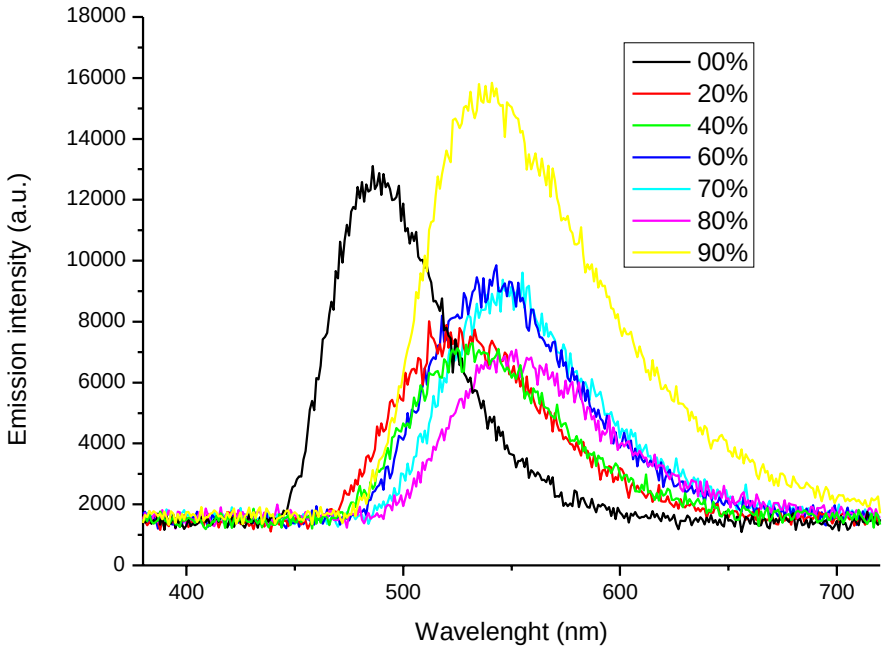


Figure S34. Aggregation-induced emission enhancement of chalcone **2a** in THF-water.

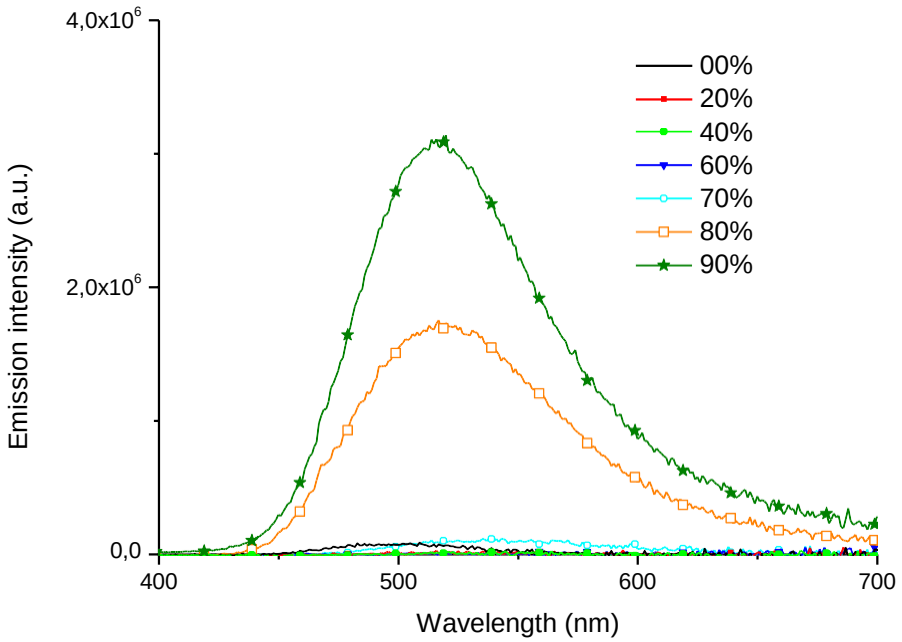


Figure S35. Aggregation-induced emission enhancement of chalcone **2b** in THF-water.

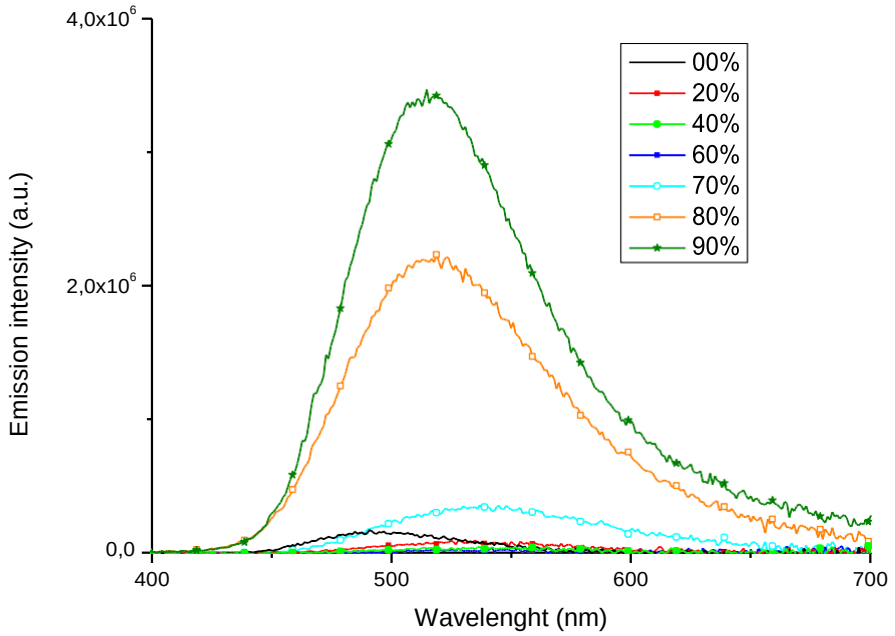


Figure S36. Aggregation-induced emission enhancement of chalcone **2c** in THF-water.

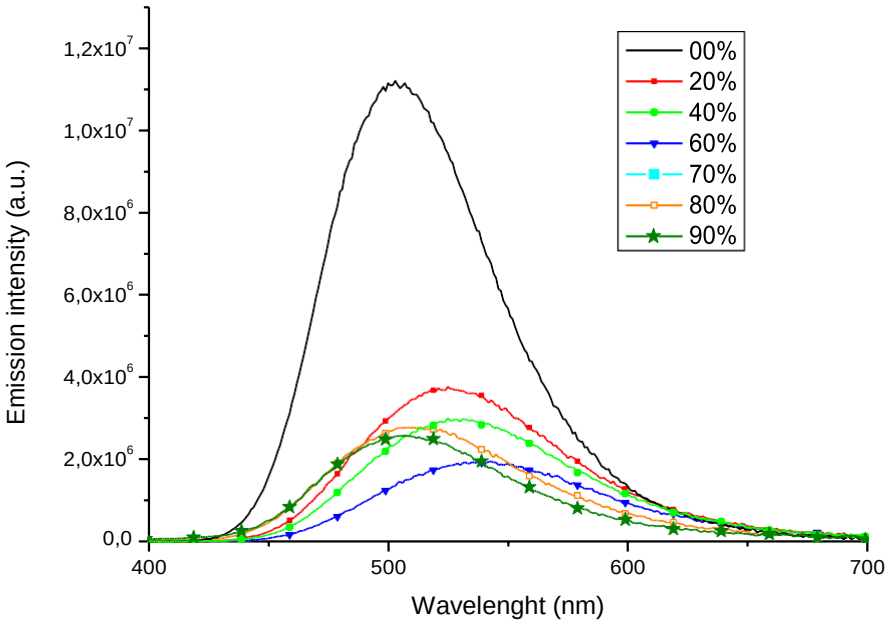


Figure S37. Aggregation-induced emission enhancement of chalcone **2d** in THF-water.

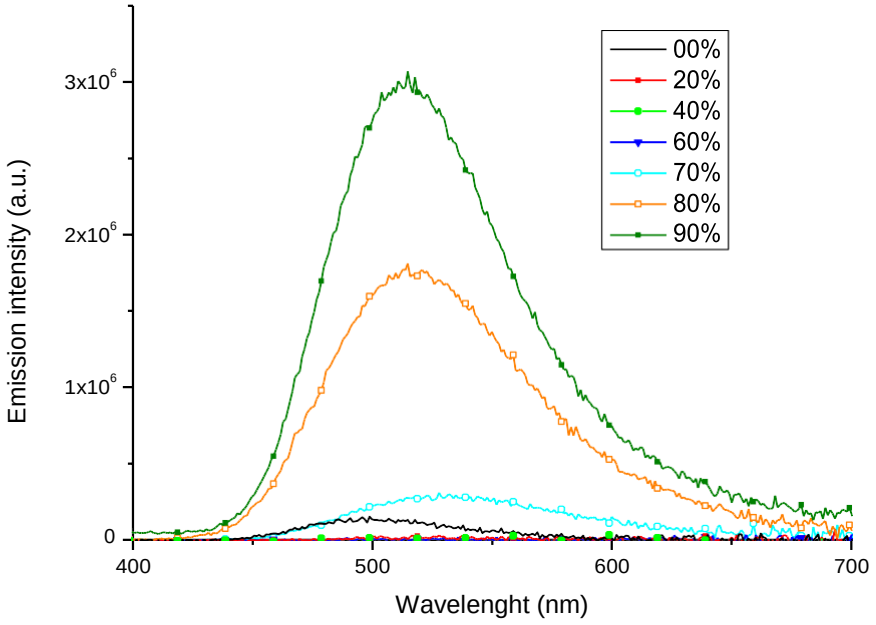


Figure S38. Aggregation-induced emission enhancement of chalcone **2e** in THF-water.

Crystal structures

Single-crystals with block shape of compound **2b** and with needle shape of compound **2d** were manually selected from the crystallization vial. A suitable single-crystal was mounted on a glass fiber with the help of silicon grease. Data were collected at 180(2) K on a Bruker X8 Kappa APEX II charge-coupled device (CCD) area-detector diffractometer (Mo K_a graphite-monochromated radiation, λ = 0.71073 Å) controlled by the APEX2 software package,[1] and equipped with an Oxford Cryosystems Series 700 cryostream monitored remotely using the software interface Cryopad.[2] Images were processed using the software package SAINT+,[3] and data were corrected for absorption by the multi-scan semi-empirical method implemented in SADABS.[4] The structure was solved using the direct methods algorithm implemented in SHELXS-97,[5,6] which allowed the immediate location of the majority of the atoms. All remaining non-hydrogen atoms were located from difference Fourier maps calculated from successive full-matrix least squares refinement cycles on F^2 using SHELXL-97.[5,7] All non-hydrogen atoms were successfully refined using anisotropic displacement parameters.

Hydrogen atoms bound to carbon were located at their idealized positions using appropriate *HFIX* instructions in SHELXL (*43* for the aromatic and vinylic, *23* for the $–CH_2–$ moieties and *13* for the chiral tertiary carbon atoms) and included in subsequent refinement cycles in riding-motion approximation with isotropic thermal displacements parameters (U_{iso}) fixed at 1.2 times U_{eq} of the atom to which they are attached.

Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication No. CCDC 1057223-1057224. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 2EZ, U.K. Fax: (+44) 1223 336033. E-mail: deposit@ccdc.cam.ac.uk.

(1) APEX2, *Data Collection Software Version 2.1-RC13, Bruker AXS, Delft, The Netherlands* **2006**.

(2) Cryopad, *Remote monitoring and control, Version 1.451, Oxford Cryosystems, Oxford, United Kingdom* **2006**.

(3) SAINT$^+$, *Data Integration Engine v. 7.23a* © 1997-2005, *Bruker AXS, Madison, Wisconsin, USA.*

(4) G. M. Sheldrick, *SADABS v.2.01, Bruker/Siemens Area Detector Absorption Correction Program* **1998**, *Bruker AXS, Madison, Wisconsin, USA.*

(5) G. M. Sheldrick, *Acta Cryst. A*, **2008**, *64*, 112-122.

(6) G. M. Sheldrick, *SHELXS-97, Program for Crystal Structure Solution, University of Göttingen* **1997**.

(7) G. M. Sheldrick, *SHELXL-97, Program for Crystal Structure Refinement, University of Göttingen* **1997**.