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## **Graphical Abstract**



# The Influence of the Push-Pull Effect and a π-Conjugated System in Conversion Efficiency of Bis-chalcone Compounds in a Dye Sensitized Solar Cell

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#### 16 Abstract

Chalcone and its related compounds are known to be  $\pi$ -conjugated compounds, which can be 17 potentially used in different electronic areas include dye sensitized solar cell (DSSC). A total of 18 six bis-chalcone compounds (1-6) have been synthesized using a Claisen-Schmidt condensation 19 method under basic conditions. The compounds were used as the dye in DSSC to test their solar 20 conversion efficiency. In the process of solar cell fabrication, titanium(II) oxide (TiO<sub>2</sub>) coated 21 glass was used as the working electrode, whereas the mixture of iodine (I<sub>2</sub>), lithium iodide (LiI), 22 4-tertbutylpyridine 1,2-dimethyl-3-propylimidazolium 23 (4-**TBP**) and (DMPII) in 3-

24	methoxypropionitrile were used as the electrolyte. The DSSC was fabricated by immersing the
25	$TiO_2$ glass into the respective bis-chalcone compound solution and dried into the oven at 45 $^\circ C$
26	for 120 minutes. Lastly, the working electrode and counter electrode were sealed using surlyn of
27	$60 \ \mu m$ thickness. The efficiency test was conducted under AM 1.5G illumination with the
28	incident light intensity of 100 mW/cm <sup>2</sup> . Among the six bis-chalcone derivatives, compound 2,
29	namely 1,4-bis-2-hydroxychalcone, was recorded with the highest efficiency (0.054%) compared
30	to the others (0.022-0.035%). The presence of a $\pi$ -conjugated system and the push-pull effect in
31	the molecule were found to enhance the conversion efficiency of DSSC. Details of the results are
32	discussed in the present paper.
33	
34	Keyword: Bis-chalcone, dye sensitized solar cell (DSSC), $\pi$ -conjugation system, push-pull effect
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37	1. Introduction
38	
39	Solar energy has great potential to be used as a renewable energy source in the future. However,
40	in the current market, over 90% solar cells are made of silicon, which, despite giving high
41	conversion efficiency are expensive [1]. As a result, the organic type dye sensitized solar cell
42	(DSSC) was developed, which offers low cost [2], however, the conversion efficiency is still far
43	lower than the silicon type solar cell [3]. Despite DSSC giving low conversion efficiency, this
44	type of solar cell still attracts attention from different fields of researchers due to several
45	advantages [4]. In addition to the low cost, the organic dye can be coated onto the plastic type

46 substrates which can increase the flexibility of the cell [2]. Moreover, by understanding the

47 structure-property relationship, chemists can structurally design the dyes in order to enhance the48 sun light absorption properties [4].

49 Chalcone is a natural compound found in apple seeds [5]. The structure of chalcone consists of 50 two aromatic rings that linked by  $\alpha,\beta$ -conjugated keto-enol group (**Fig. 1**).



#### 51

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Fig. 1. Structure of chalcone

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Chalcone and its derivatives are widely used in non-linear optics (NLO), optical computing, 54 optical communication, optical limiting, photoinitiated polymerization, electrochemical sensing 55 and Langmuir films [6-8]. According to Kamath and co-workers, chalcones are used as NLO due 56 to their good optical power limiting properties and third-order nonlinearity. In general, chalcones 57 offer large nonlinear coefficients due to the fact that they consist of a conjugated double bond in 58 between two planar benzene rings [9]. The delocalization of  $\pi$ -electrons within these double 59 bond and benzene rings are the one that responsible for the third order nonlinear optical 60 responses. Furthermore, the effect can also be increased by enhancing the ability of electron 61 62 donating groups [10].

In fact, some researchers found that small molecules containing donor (D)-acceptor (A) groups connected by  $\pi$ -conjugated system can pose high solar conversion efficiency [11-14]. For this reason, Chambon and co-workers have synthesized a series of 2'-hydroxychalcones coordinated to borondifluoride, a strong  $\pi$ -acceptor, in order to enhance the push-pull character by having donor-acceptor (D-A) groups in the molecule. The group was able to achieve an efficiency conversion of 1.13% when the boron-chalcones complexes were used as donor materials while

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69 [6,6]phenyl-C61-butyric acid methyl ester ( $PC_{61}BM$ ) as the electron accepting material in the 70 solar cells [15]. In addition, flavonoid, which is a natural pigment from the same family with 71 chalcone, and its' application in DSSC has been reported [16].

Herein, we report the solar conversion efficiency of six bis-chalcone compounds (**Fig.2**). The synthesis, photophysical properties [8], and the biological activities [17-21] of compounds **1-4** have already been reported, whereas compounds **5-6** are novel compounds. To our knowledge, none of these compounds have been reported concerning their solar conversion efficiency in DSSC.



77

Fig. 2. Bis-chalcone compounds 1-6 that have been tested for conversion efficiency in DSSC

The influence of the push-pull effect in conversion efficiency can be observed by comparing compounds **3** and **4** to compounds **1** and **2**. There are two methoxy groups present at the 2 and 5 positions at the central phenyl ring, which act as electron donor in compounds **3** and **4**. Meanwhile, the bis-chalcone analogues in compounds **5** and **6** are located at the *meta*-position in order to reduce  $\pi$ -conjugated effect along the molecule.

85

#### 86 2. Experimental

All chemicals used for the synthesis of compounds 1-6 were purchased from Fluka, Aldrich and
Acros-organic. Unless otherwise stated, the chemicals and solvents were used without further
purification.

Ethanol (1.00 L) was purified by mixing with 1.5 g of iodine and 3.5 g of magnesium turning in
a round bottom flask. The mixture was refluxed until its colour changed from dark brown to
colourless and then collected *via* distillation to obtain dry ethanol.

93

#### 94 2.1 Characterization

The IR spectra of bis-chalcone compounds were recorded using a Thermo Scientific Fourier 95 transform infrared spectrometer (FTIR) model - NICOLET iS10 in KBr dish in the range of 96 4000-400 cm<sup>-1</sup>. The resolution used for obtaining the IR spectra was 4.000 with the scan's 97 number of 36 in a deuterated triglycine sulphate (DTGS) KBr detector. The <sup>1</sup>H NMR spectra 98 99 were recorded by using JEOL, 500 MHz FT-NMR spectrometer, and the chemical shifts were reported relative to TMS internal standard and referenced via residual proton NMR resonances 100 of the deuterated solvent (CDCl<sub>3</sub>:  $\delta_H$  7.26;  $\delta_C$  77.7 ppm). The absorption spectra were recorded 101 102 with JASCO V-630 spectrophotometer. The elemental analysis of carbon, hydrogen, and nitrogen were carried out by using CHN analyzer Thermo-flash EA 1112 Series. Melting points 103 were determined using open capillary in Stuart MP3 melting point apparatus. 104

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#### 106 2.2 General procedures for the preparation of bischalcone

107 The procedures of preparing bis-chalcone compounds are similar to those reported in the 108 literature [8]. Compounds 1-4 have been reported in literature [8, 17-23], while compounds 5 and 109 6 were newly synthesized. The general procedures of bis-chalcone compounds 1-4 preparation are described as below, whereas the spectroscopic data of compounds 1-4 can be found in S.I orour earlier publication [8].

Two equivalent molar amount of R-acetophenone [where R=H (1 & 3) and ortho-OH (2 & 4)] 112 was added into 100 mL beaker and was dissolved in 20 mL of ethanol. 10 mL of 10 % aqueous 113 KOH was poured gently into the beaker containing R-acetophenone and the mixture was stirred 114 for about 10 minutes. 1,4-terephthaldehyde (0.67 g, 0.0050 mol) and 2,5-dimethoxy-1,4-115 terephthaldehyde (0.20 g, 0.0010 mol) were added into beaker (1 & 3) and (2 & 4), respectively. 116 The mixture was stirred vigorously under room temperature for 4 hours. After that, 3M HCl was 117 added until the solution was neutralized. The obtained precipitate was filtered, rinsed with 118 119 distilled water and ethanol. The washed precipitate was allowed to air dried. Finally, the precipitate was purified *via* slow evaporation by using THF. 120

For compounds **5** and **6**, precaution steps were taken as the precipitate easily agglomerate during the neutralization process. Therefore, the neutralization process was carried out under cold condition. The preparation procedures and spectroscopic data of compounds **5** and **6** are as described below:

Acetophenone (0.360 g, 3.0 mmole for compound 5) and 2-hydroxyacetophenone (0.408 g, 3.0 125 mmole for compound 6) was dissolved in 20 mL of ethanol, respectively. 10 mL of 10% aqueous 126 KOH was added gently into the solution and the mixture was stirred for about 10 minutes. Iso-127 terephthaldehyde (0.200 g, 1.5 mmol) was added into the mixture and stirred vigorously at room 128 temperature for 4 hours. After that, the reaction flask was immersed into ice bath and 3M HCl 129 was added until the solution was neutralized. The obtained precipitate was filtered, rinsed with 130 distilled water and ethanol. The washed precipitate was allowed to air dried. The precipitate was 131 purified using recrystallization via slow evaporation in tetrahydrofuran (THF). 132

- 134 2.2.1 (2E,2'E)-3,3'-(1,3-phenylene)bis(1-phenylprop-2-en-1-one), 5
- 135 White solid. Yield: 0.530 g, 95%. M.P.: 136.4-137.3 °C. IR (KBr, cm<sup>-1</sup>): 1660 ( $\nu$ C=O), 1607 136 ( $\nu$ C=C), 1442 and 1420 ( $\nu$ C=C, aromatic ring). <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$ : 8.05 (d, 4H, J = 8
- 137 Hz, Ar-H), 7.89 (d, 2H, J = 16 Hz, CH=CH<sub> $\beta$ </sub>), 7.82 (s, 1H, Ar-H), 7.69 (d, 2H, J = 8 Hz, Ar-H), 138 7.60 (d, 2H, J = 16 Hz, CH<sub> $\alpha$ </sub>=CH), 7.62 (t, 2H, 8Hz, Ar-H), 7.53 (m, 5H, Ar-H). <sup>13</sup>C-NMR (125
- 139 MHz, CDCl<sub>3</sub>) δ: 190.5, 143.9, 138.1, 135.8, 133.1, 130.3, 129.7, 128.8, 128.7, 128.4 and 123.1.
- 140 UV-Vis (DCM) ( $\lambda_{max}$ /nm): 261 and 307. Anal. Cal. for C<sub>24</sub>H<sub>18</sub>O<sub>2</sub>: C, 85.18; H, 5.36; Found: C,
- 141 85.62; H, 5.43.
- 142
- 143 2.2.2 (2E,2'E)-3,3'-(1,3-phenylene)bis[1-(2-hydroxyphenyl)prop-2-en-1-one), 6

Yellow solid. Yield: 0.161 g, 27%. M.P.: 178-180 °C. IR (KBr, cm<sup>-1</sup>): 3455 (vOH), 1639 144 (vC=O), 1575 (vC=C), 1487 and 1441 (vC=C, aromatic ring). <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) δ: 145 12.74 (s, 2H, OH), 7.96 (d, 2H, J = 6 Hz, Ar-H), 7.95 (d, 2H, J = 15 Hz, CH<sub>a</sub>=CH), 7.91 (s, 1H, 146 Ar-H), 7.74 (d, 2H, J = 5 Hz, Ar-H), 7.72 (d, 2H, J = 15 Hz, CH=CH<sub>B</sub>), 7.53 (t, 3H, J = 8Hz, Ar-147 H), 7.05 (d, 2H, J = 8 Hz, Ar-H), 6.98 (t, 2H, J = 7 Hz, Ar-H). <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$ : 148 193.59, 163.74, 144.39, 136.75, 135.61, 130.56, 129.79, 128.91, 121.37, 120.01, 119.08 149 and118.82. UV-Vis (DCM) (\lambda\_max/nm): 260, 315 and 351. Anal. Cal. for C<sub>24</sub>H<sub>18</sub>O<sub>4</sub>: C, 77.82; H, 150 4.90; Found: C, 77.84; H, 4.95. 151

- 152
- 153 2.3 Dye sensitized solar cell (DSSC) fabrication

154 The fabrication method of DSSC followed that reported in the literature [24] with slight 155 modification. **Fig. 3** shows a schematic assembly of DSSC, whereas the completed DSSC is shown in Fig.4. The preparation procedures of each individual component as described in thefollowing sub-sections 2.3.1-2.38.



170 completion, it was treated under UV light for 30 minutes. The treated FTO glass was directly 171 used for the TiO<sub>2</sub> coating by using the doctor blade technique. The TiO<sub>2</sub> coating was started from 172 the thickness of 5  $\mu$ m, followed by 10, 15, 20, 35, 40, 45 and lastly 50  $\mu$ m. Each coat was kept 173 for 60 minutes interval gap. The excess TiO<sub>2</sub> was scraped out using microscopic slide to create a 174 dimension of 0.5 cm×0.5 cm as a working electrode. The film was treated to 150 °C for 90 175 minutes and annealed to 450 °C for 30 minutes.

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177 2.3.3 Preparation of standard dye cis-[bis(isothiocyanato)bis(2,2'-pyridinyl-4,4'-dicarboxylic
178 acid)ruthenium(II)](N3) solution

The standard dye namely N3 (0.0223 g, 0.03 mmol) was dissolved into a mixture of 50 mL acetonitrile and 50 mL *tert*-butylalcohol in a beaker. Lights were turned off during the preparation due to light sensitive nature of N3. The mixture was capped and sonicated for about 30 minutes. The beaker was covered with aluminium foil to avoid direct contact with light.

183

184 2.3.4 Preparation of bis-chalcone compounds as organic dye

185 Respective bis-chalcone compound (0.03 mmol) was dissolved into 20 mL of acetonitrile and 20
186 mL of tertbutylalcohol in a beaker. The mixture was capped and sonicated for 30 minutes.

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188 2.3.5 Preparation of Pt counter electrode

The electron beams evaporation technique (**Fig. 5**) was used to coat the Pt counter electrode. This technique involves the use of electricity to generate an electron beam in a high pressure vacuum chamber of about  $7.5 \times 10^{-5}$  Torr ( $10^{-2}$  Pa) and control of magnetic field to deflect the beams by 180° or 270° onto the evaporation material. The kinetic energy produced from the

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electricity drives the generated electron beams and upon contact with the evaporation material, it is converted into thermal energy producing heat to melt or sublimate it. Once sufficient heat and pressure were reached, the vapour evaporated upwards and formed a thin layer film on the substrate that is attached onto the substrate dome.

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Fig. 5. Electron beams evaporation technique

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200 2.3.6 Preparation of Electrolyte

The electrolyte consists of 0.05 mol iodine ( $I_2$ ), 0.5 mol lithium iodide (LiI), 0.5 mol 4tertbutylpyridine (4-TBP) and 1 mol 1,2-dimethyl-3-propylimidazolium (DMPII) in 15 mL 3methoxypropionitrile (MPN).

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207 2.3.7 Preparation of dye-sensitized working electrode

The  $TiO_2$  working electrode was immersed into the  $N_3$  dye in a dark room and put into the oven at 45 °C for 120 minutes. Upon completion, the film was taken out and dipped into the acetonitrile solution three times. It was allowed to air dried.

211 For the bis-chalcone organic dye, the prepared  $TiO_2$  working electrode was immersed into the

respective bis-chalcone compound and put into the oven at 45 °C overnight. Upon completion,

the film was take out and was allowed to dry in air.

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215 2.3.8 Sealing of Dye-sensitized solar cell

The working electrode and counter electrode were sealed using the surlyn of 60  $\mu$ m thickness (surlyn 60  $\mu$ m). Electrolyte was injected into the small drilled hole. The hole was sealed with another piece of small glass using the surlyn 60  $\mu$ m. Silver paste was applied on both of the conductive sides.

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221 2.4 Conversion efficiency measurement

The incident photon to current efficiency (IPCE) was measured under light illumination of air mass 1.5 global (AM 1.5G) with the incident light intensity of 100 mW/cm<sup>2</sup>. The IPCE data were recorded using Keithley 2400 source meter with illuminating monochromatic light on the solar cells. The working dimension for the solar cell was set at 0.25 cm<sup>2</sup>. The *J/V* measurement graph of solar circuit current density (*Jsc*, mA/cm<sup>2</sup>) against voltage (V) was plotted using the Origin8 Pro SR4 software. The power conversion efficiency of the solar cell can be calculated using the equation as shown in Eq. 1 below:

$$\eta = \frac{J_{sc} \ x \ V_{oc} \ x \ FF}{P_{in}} \quad ---- \quad \text{Eq. 1}$$

where

 $J_{sc}$  = short circuit current (mA/cm<sup>2</sup>)  $V_{oc}$  = open circuit photovoltage (V) FF = fill factor (%)  $P_{in}$  = incident light intensity (100 mW/cm<sup>2</sup>)  $\eta$  = power conversion efficiency (%)

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231 2.5 Electrochemical setup

The electrochemical experiments were carried out via electron impedance spectroscopy (EIS) 232 which comprises three-electrode system; glassy carbon electrode (GCE) as working electrode, 233 platinum wire as counter electrode and Ag/AgCl as reference electrode. The system was 234 connected to AUTOLAB PGSTAT302 model potentiostat driven by General Purpose 235 236 Electrochemical System (GPES) software. These experiments were carried out in dichloromethane solution containing 0.1 M tetrabutylammonium hexafluorophosphate 237 [NBu<sub>4</sub>]PF<sub>6</sub> as supporting electrolyte and sample concentration of  $1 \times 10^{-3}$  M. All measurements 238 239 were performed at room temperature.

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241

242 3. Results and discussion

243 3.1 Synthesis and spectroscopic characterization

The bis-chalcone compounds **1-6** were synthesized through Claisen-Schmidt condensation. The reactions were carried out under basic conditions for 6-12 hours and neutralized using 3M HCl upon the completion of the reaction. For compounds **5** and **6**, precautionary steps were taken as the precipitate easily agglomerate during the neutralization process. Therefore, neutralization process was carried out under cold condition in order to avoid the agglomeration problem.

The formation of bis-chalcone compounds can be confirmed from the presence of C=C-C=O conjugation stretching band at 1600-1700 cm<sup>-1</sup> in the IR spectra (See SI under **Fig. S1-S6**) [8]. Meanwhile, another strong stretching band appears at 1570 - 1600 cm<sup>-1</sup> is attributed to the aliphatic C=C bond in the structure. For bis-chalcone compounds **2**, **4** and **6**, a broad signal presents at the region of 3300 - 3400 due to the presence of OH group at the *ortho* position of wing phenyl rings.

Furthermore, in the <sup>1</sup>H NMR spectra (see SI under **Fig. S7-S12**), a pair of doublets can be observed at 8.05-7.80 ppm and 7.71-7.51 ppm with the coupling constant, *J*, values of 16 Hz. The pair of doublets are attributed to the  $\alpha$ - and  $\beta$ -protons located in the C $_{\beta}$ =C $_{\alpha}$ -C=O moiety, confirming the *trans* conformation of the bis-chalcone compounds were obtained.

For the UV-Vis spectra (SI under **Fig. S19-S24**), all the bis-chalcone compounds show two absorption bands namely 268–278 nm for the  $\pi \rightarrow \pi^*$  transition in the phenyl ring and 333-383 nm for the  $n \rightarrow \pi^*$  in the C=O moiety (**Fig. 6**). As well as these two absorption bands, compounds **3-4** also have another additional absorption band at 421 nm attributed to intra-molecule charge transfer (ICT) due to the electron transfer from ethylenic  $\pi$ -orbitals to the carbonyl  $\pi$ -orbital [8].



#### Fig. 6 UV-Vis spectrum of compound 2

266 *3.2 Application of bis-chalcone in solar cell efficiency* 

The standard dye, *cis*-[bis(isothiocyanato)bis(2,2'-pyridinyl-4,4'-dicarboxylicacid)ruthenium(II)] complex (N3), was used in order to ensure the consistency of our solar cell fabrication as well as the measurement. The test was conducted in triplicates and a power conversion efficiency of 4.57, 4.52 and 4.59% was recorded for trials 1, 2 and 3, respectively. The small standard deviation (±0.04) indicating the fabrication technique and measurements were consistent.

Fig. 7 shows the J/V measurement of the bis-chalcone series which was divided into two 272 categories, with and without -OH substituted compounds. From the results obtained (Table 1), 273 274 compound 2 showed the best solar conversion efficiency of 0.054%, which is due to the good absorption of the compound 2 dye in the  $TiO_2$  layer, where a yellow color can be clearly seen on 275 the surface. The result is also supported by the fill factor (FF) value which measured up to 276 277 51.604%. Fill factor is generally defined as the ideal of the device system work. Several factors that can affect the FF value include the thickness of TiO<sub>2</sub>, the electrolyte, the resistance of the 278 cell and also the conversion of photocurrent absorbed by the dye [25]. Thus, the better absorption 279 of the dye sensitizer allows for more photons are being absorbed, which results in a greater 280 photocurrent that could be transported to the nanocrystalline TiO<sub>2</sub> layer and therefore increase 281 the overall performance. 282

On the other hand, the effect of a substituent can be clearly observed. The structure of compound with an -OH substituent on both ends of the molecule promotes the charge transfer within the molecule and delivers the electron towards the TiO<sub>2</sub> semiconductor layer leading to a solar conversion efficiency of 0.054%. In comparison with compound **1**, which does not contain -OH 287 groups in the molecule, a much lower solar conversion efficiency with only 0.030% was288 recorded.

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Fig. 7 J/V measurement of bis-chalcone compounds (without –OH substituent, compounds 1, 3 and 5, left); (with –OH substituent, compounds 2, 4 and 6, right)

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Table 1: Summary of power conversion efficiency of bis-chalcone compounds

Compound	$V_{oc}(\mathbf{V})$	$J_{sc}$ (mA/cm <sup>2</sup> )	Fill factor (%)	Efficiency (%)
1	0.410	0.144	50.649	0.030
2	0.460	0.225	51.604	0.054
3	0.440	0.150	48.570	0.032
4	0.370	0.193	43.970	0.032
5	0.361	0.144	41.620	0.022
6	0.390	0.182	49.423	0.035

297

Furthermore, the presence of  $\pi$ -conjugation in the structure also plays a vital role in solar conversion efficiency. This effect was observed when we changed the substitution position on the central phenyl ring from *para* (compound **2**) to *meta*-position (compound **6**). Compound **6** showed 20% lower solar conversion efficiency (0.035%) compared to compound **2** (0.054%), despite also having the –OH substituted functional group. According to He and coworkers, the  $\pi$ -

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303 conjugation effect in the molecule bonded by a phenyl *meta*-branching point is destroyed, 304 causing the localization of the electron-hole pair and electronic decoupling [26]. Hence, this 305 affects the overall performance of the dye-sensitizer to facilitate the transfer of the electron to the 306 semiconductor layer. Due to this reason, the conversion efficiency for compound **5** is the lowest 307 with a solar efficiency of only 0.022%.

Compounds 3 and 4 were synthesized with two methoxy groups attached at 2 and 5 positions of 308 309 the central phenyl ring at the *para*-branching point. The initial aim of introducing methoxy groups to the central phenyl ring of compounds 3 and 4 was to induce push-pull effect along the 310 molecule. Interestingly, compound **3** is highly luminescent with the  $\lambda$  emission centered at 505 311 312 nm and the  $\Phi$  of 0.57 in DCM solution [8]. Indeed, compound 3 showed slightly higher conversion efficiency compared with compounds 1 and 5, and a higher  $V_{oc}$  and  $J_{sc}$  value were 313 recorded. However, compound 4, which has both methoxy and hydroxyl substituent groups, 314 315 showed the least efficiency in comparison with compounds 2 and 6. This may due to the poor solubility of compound 4 in the solvent system, where the crystal of compound 4 was found to 316 reform on top of the TiO<sub>2</sub> surface. This caused an increase in the thickness of the dye sensitizer 317 layer and the direct contact with the counter electrode would results in an increase in cell 318 resistance and impacting the  $V_{oc}$  and  $J_{sc}$  values. 319

320

321 *3.5 Electrochemistry* 

The electrochemical behaviours of bis-chalcone compounds **2**, **4** and **5** were investigated further by using cyclic voltammetry analysis in order to determine the redox reaction and potential range of different electrochemical processes. Cyclic voltammograms of **2**, **4** and **5** at glassy carbon electrode were recorded in dichloromethane solution using 0.1 M  $[NBu_4]PF_6$  as supporting electrolyte in the potential range -3.0 V to 3.0 V as depicted in **Fig. 8**.

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Fig. 8 Cyclic Voltamograms of bis-chalcone 2, 4 and 5 in DCM/0.1M [NBu<sub>4</sub>]PF<sub>6</sub> at 0.05 V s<sup>-1</sup> scan rate.

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332 Fig. 8 shows the redox potential behaviour with the presence of oxidation and reduction peaks for all three compounds. The anodic peak which corresponded to bis-chalcone oxidation 333 appeared at around 1.74 V to 2.05 V due to the consumption of adsorbed chalcone and/or its 334 oxidative product occurs on the electrode surface [27, 28]. For electrochemical reduction, cyclic 335 voltammogram of 2 reveals well defined quasi-reversible reduction in the range -0.5 V to -2.3 V. 336 The quasi-reversibility of the reduction process is confirmed with the corresponding peak 337 separation value [29] between the catholic peak potential ( $E_{pc}$ = -1.58 V) and the two anodic peak 338 potential ( $E_{pa}$ = -1.79 V) and ( $E_{pa}$ = -1.23 V). The existence of this cyclic voltammetry (CV) wave 339

may be ascribed to the reduction of C=O group [27,30] and showed a mixed adsorptive and diffusive response for the system [31]. These findings were supported by previous literatures describing on similar type of molecular frameworks where they focused on proton coupled electron transfers leading to the reduction of the carbonyl bond to form the hydroxyl and hydrogenation of the vinylic bond [27, 31]. In conclusion, the behaviour of compounds **2**, **4** and **5**, and the existence of redox potential subsequently gave ideal characteristics for potential of the fabrication of DSSC.

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#### 349 **4.** Conclusion

Six bis-chalcone compounds were synthesized and their solar conversion efficiencies in DSSC were measured. Compound 2 gave the highest conversion efficiency (0.054%) compared to the others (0.022-0.035%). The higher efficiency of compounds 1 and 2 compared to compounds 5 and 6, respectively, indicates the importance of  $\pi$ -conjugation system in conversion efficiency. In addition, the presence of push-pull effect in compound 3 also resulted a higher conversion efficiency compared to compounds 1 and 5.

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### Highlights

- The influence of  $\pi$ -conjugated system and push-pull effect to DSSC' efficiency
- The synthesis and characterization of bis-chalcone compounds
- Fabrication of DSSC and the conversion efficiency measurement