#### ORIGINAL PAPER

## A one-pot multicomponent reaction for synthesis of 1-amidoalkyl-2-naphthols catalyzed by PEG-based dicationic acidic ionic liquids under solvent-free conditions

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**Abstract** A mild and efficient method was developed for preparation of amidoalkyl naphthols via one-pot threecomponent condensation of aldehydes with amides and 2-naphthol in the presence of polyethylene glycol (PEG)based dicationic acidic ionic liquid as a powerful catalyst under solvent-free conditions. Excellent yields, short reaction time, simple work-up, and reusable catalyst are advantages of this procedure.

**Keywords** Amidoalkyl naphthols · PEG-based acidic ionic liquid · Solvent-free · One-pot · Multicomponent reaction

#### Introduction

Multicomponent reactions (MCRs) are very elegant and efficient methods to access complex structures in a single synthetic operation from three or more reactants. High atom economy, great synthetic efficiency, and procedural convenience in the construction of multiple new bonds in a one-pot procedure are the advantages of MCRs [1–4]. Thus, the discovery of novel MCRs and development of known MCRs are popular areas of research in current organic chemistry.

Compounds containing a 1,3-arrangement of amino and oxygenated functional groups are commonly found in various biologically important natural products and potent drugs [5–7]. It is noteworthy that 1-amidoalkyl-2-naphthol derivatives can be converted to useful synthetic building

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blocks and important bioactive 1-aminomethyl-2-naphthols by an amide hydrolysis reaction. Their hypotensive and bradycardiac effects in humans have been evaluated [8]. Preparation of 1-amidoalkyl-2-naphthols can be carried out by three-component condensation of aldehydes, 2-naphthols, and amides in the presence of Lewis or Brønsted acidic catalysts such as montmorillonite K10 [9], p-TSA [10], iodine [11],  $Fe(HSO_4)_3$  [12],  $K_5CoW_{12}O_{40}\cdot 3H_2O_{40}\cdot 3H_2O_$ [13], HClO<sub>4</sub>–SiO<sub>2</sub> [14], cation-exchange resins [15], silica sulfuric acid [16], 2,4,6-trichloro-1,3,5-triazine (TCT) [17], thiamine hydrochloride [18], [TEBSA][HSO<sub>4</sub>] [19], zwitterionic salt [20], and [FemSILP]-L-prolinate [21]. However, many of the reported methods suffer from limitations such as high reaction temperature, prolonged reaction time, use of toxic solvent, and additional microwave or ultrasonic irradiation. Moreover, most of them are limited to only aromatic aldehydes, and the reactions with aliphatic aldehydes were reported to suffer from low yields and harsh reaction conditions. Therefore, identification of a green and ecofriendly protocol that uses a highly efficient and reusable catalyst for preparation of amidoalkyl naphthols is still desirable.

Ionic liquids (ILs), as ecofriendly reaction media or catalysts, have attracted increasing attention due to their particular properties such as undetectable vapor pressure, high thermal stability, excellent solubility, and ease of recovery and reuse [22–25]. Among them, Brønsted acidic ILs used in some acid-catalyzed processes have aroused considerable interest because they combine the advantages of solid acids and mineral acids [26–28]. Recently, we synthesized a new class of Brønsted acidic ILs, PEG-based dicationic acidic ionic liquids (PEG-DAILs), which were found to be very effective for synthesis of benzopyrans [29] and esters [30]. As part of our ongoing work on development of efficient and environmental benign

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Scheme 1





procedures using acidic ILs, we report herein a simple and efficient procedure for one-pot three-component synthesis of amidoalkyl naphthols using PEG-DAIL as an effective and reusable catalyst under solvent-free conditions (Scheme 1).

#### **Results and discussion**

To find the optimum conditions, a model reaction of 3-nitrobenzaldehyde (1 mmol), 2-naphthol (1 mmol), and acetamide (1.2 mmol) in the presence of PEG-DAIL was performed under solvent-free conditions at 80 °C (Table 1). In the absence of any catalyst, no desirable product could be detected (entry 1), whereas good results were obtained in the presence of PEG-DAIL (entries 2–8). All kinds of PEG-DAILs proved to be very active (entries 4, 6–8), and the optimum amount of PEG<sub>1,000</sub>-DAIL was 3 mol% (entry 4). No visible improvement in the reaction results was observed by increasing the amount of PEG<sub>1,000</sub>-DAIL to 5 mol% (entry 5).

The recyclability of the  $PEG_{1,000}$ -DAIL was also investigated using the above model reaction. After completion of the reaction, the mixture was poured into water

 
 Table 1
 Effect of PEG-DAILs on the model reaction of 3-nitrobenzaldehyde, 2-naphthol, and acetamide

Entry	Catalyst (mol%)	Time (min)	Yield (%) <sup>a</sup>
1	_	30	0
2	PEG <sub>1,000</sub> -DAIL (1)	10	69
3	PEG <sub>1,000</sub> -DAIL (2)	8	85
4	PEG <sub>1,000</sub> -DAIL (3)	5	95
5	PEG <sub>1,000</sub> -DAIL (5)	5	94
6	PEG <sub>800</sub> -DAIL (3)	5	94
7	PEG <sub>400</sub> -DAIL (3)	5	93
8	PEG <sub>200</sub> -DAIL (3)	5	94

<sup>a</sup> Isolated yield



Fig. 1 Recycling experiment of the PEG<sub>1,000</sub>-DAIL

and stirred thoroughly. The solid product was isolated by filtration, and the filtrate containing ionic liquid was extracted with ethyl acetate  $(3 \times 5 \text{ cm}^3)$  to remove nonionic organic impurities. Then the water was evaporated under reduced pressure and the recovered catalyst was dried at 70 °C under vacuum for 2 h and reused in the next reaction. The procedure was repeated, and the results indicated that the PEG<sub>1,000</sub>-DAIL could be recycled with slight loss of catalytic activity for eight times (Fig. 1). Only 6.4% weight loss was observed after eight times recycling.

This three-component condensation of various aldehydes and amides with 2-naphthol catalyzed by  $PEG_{1,000}$ -DAIL was then explored under the optimized reaction conditions described above. The results are summarized in Table 2.

As can be seen from Table 2, the reactions were carried out efficiently and the desired products were obtained in good to excellent yield (80-98%) and very short reaction time (3-15 min). Particularly, this procedure was uniformly effective for both aliphatic and aromatic aldehydes. The aliphatic aldehydes such as *n*-butyraldehyde, valeraldehyde, and isovaleraldehyde were all converted to the

A	one-pot	multicomponent	reaction
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 $\label{eq:Table 2} \textbf{Table 2} \ \textbf{One-pot preparation of 1-amidoalkyl-2-naphthols with different aldehydes and amides catalyzed by PEG_{1,000}-DAIL$ 

Comp.	Aldehyde R <sup>1</sup>	Amide R <sup>2</sup>	Time (min)	Product	Yield (%) <sup>a</sup>	M.p. (°C)
1	n-C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	5	NHCOCH <sub>3</sub> OH	85	221–222 222–223 [34]
2	<i>n</i> -C <sub>3</sub> H <sub>7</sub>	Ph	5	NHCOPh OH	83	218–220 220–222 [34]
3	<i>n</i> -C <sub>3</sub> H <sub>7</sub>	CH2=CH	3	NHCOCH=CH <sub>2</sub>	81	190–191
4	n-C <sub>4</sub> H <sub>9</sub>	CH <sub>3</sub>	6	NHCOCH <sub>3</sub> OH	84	188–190
5	i-C <sub>4</sub> H <sub>9</sub>	CH <sub>3</sub>	6	NHCOCH <sub>3</sub> OH	86	195–197
6	Ph	CH <sub>3</sub>	5		91	242–244 245–246 [14]
7	4-Me-C <sub>6</sub> H <sub>4</sub>	CH <sub>3</sub>	10	NHCOCH <sub>3</sub> OH	86	221–223 222–223 [14]
8	4-MeO–C <sub>6</sub> H <sub>4</sub>	CH3	15	MeO NHCOCH <sub>3</sub> OH	82	181–183 183–185 [12]

Table 2 continued

Comp.	Aldehyde R <sup>1</sup>	Amide R <sup>2</sup>	Time (min)	Product	Yield (%) <sup>a</sup>	M.p. (°C)
9	3-MeO–C <sub>6</sub> H <sub>4</sub>	CH <sub>3</sub>	10	MeO NHCOCH <sub>3</sub>	86	203–205 201–204 [12]
10	4-Br–C <sub>6</sub> H <sub>4</sub>	CH3	10	Br NHCOCH <sub>3</sub> OH	89	228–230 228–230 [17]
11	4-Cl-C <sub>6</sub> H <sub>4</sub>	CH3	10		90	226–228 228–229 [17]
12	3-Cl-C <sub>6</sub> H <sub>4</sub>	CH3	15	CI NHCOCH <sub>3</sub> OH	87	237–238
13	3-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>	CH <sub>3</sub>	5	O <sub>2</sub> N NHCOCH <sub>3</sub> OH	95	241–242 241–242 [12]
14	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>	CH3	5	O <sub>2</sub> N NHCOCH <sub>3</sub> OH	97	243–245 248–250 [12]
15	4-Me–C <sub>6</sub> H <sub>4</sub>	Ph	10	NHCOPh OH	87	213–215 215–216 [17]

Comp.	Aldehyde R <sup>1</sup>	Amide R <sup>2</sup>	Time (min)	Product	Yield (%) <sup>a</sup>	M.p. (°C)
16	4-Br–C <sub>6</sub> H <sub>4</sub>	Ph	10	Br NHCOPh OH	89	181–183 182–184 [19]
17	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>	Ph	5	O <sub>2</sub> N NHCOPh OH	96	231–232 228–229 [35]
18	3-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>	Ph	5	O <sub>2</sub> N NHCOPh OH	94	240–242 242–243 [35]
19	4-Me-C <sub>6</sub> H <sub>4</sub>	CH <sub>2</sub> =CH	8	NHCOCH=CH <sub>2</sub> OH	89	214–216
20	4-BrC <sub>6</sub> H <sub>4</sub>	CH <sub>2</sub> =CH	5	Br NHCOCH=CH OH	93	220–222
21	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>	CH <sub>2</sub> =CH	5	O <sub>2</sub> N NHCOCH=CH OH	98	223–225
22	Ph	NH <sub>2</sub>	10		81	175–177 176–178 [19]
23	4-Cl-C <sub>6</sub> H <sub>4</sub>	NH <sub>2</sub>	10	CI NHCONH <sub>2</sub> OH	80	170–171 169–170 [17]

Table 2 continued

Table 2 continued							
Comp.	Aldehyde R <sup>1</sup>	Amide R <sup>2</sup>	Time (min)	Product	Yield (%) <sup>a</sup>	M.p. (°C)	
24	3-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>	NH <sub>2</sub>	6	O <sub>2</sub> N NHCONH <sub>2</sub> OH	84	191–193 184–186 [15]	

<sup>a</sup> Isolated yield

corresponding products 1–5 in good yields. Although some papers have described three-component synthesis of amidoalkyl naphthols using aliphatic aldehydes [10, 16, 20, 31-33], actually only few methods were effective for aliphatic aldehydes [16, 20, 32]. However, those methods were not good enough due to long reaction time and relatively large amount of catalyst.

Furthermore, aromatic aldehydes with electron-donating or electron-withdrawing groups underwent smooth transformation under the reaction conditions (compounds **6–24**). It was shown that aromatic aldehydes with electron-withdrawing groups reacted faster than aromatic aldehydes with electron-donating groups, as would be expected [12]. In all cases, 1-amidoalkyl-2-naphthols were the sole products and no by-product was observed. Thus, PEG<sub>1,000</sub>-DAIL was a highly efficient, general, and green catalyst for preparation of 1-amidoalkyl-2-naphthols.

As shown in Scheme 2, we suppose that the reaction proceeds via *ortho*-quinone methides (*o*-QMs) [10], which form by nucleophilic addition of 2-naphthol to the aldehyde, assisted by PEG-DAIL. The *o*-QMs then react with amides via Michael addition to afford the expected products. The PEG-DAIL could provide multi-acidic sites for activating aldehydes efficiently, thus facilitating the reaction.

To show the merit of  $PEG_{1,000}$ -DAIL in comparison with other reported catalysts, we summarize several results for the preparation of N-[(3-nitrophenyl)(2-hydroxynaphthalen-1-yl)methyl]acetamide from 3-nitrobenzaldehyde, 2-naphthol, and acetamide in Table 3. It is very obvious that

 $PEG_{1,000}$ -DAIL showed much higher catalytic activity in terms of much shorter reaction time and milder conditions than other catalysts used in references.

In conclusion, we have demonstrated that PEG-based dicationic acidic ionic liquids (PEG-DAILs) are a novel class of Brønsted acid catalysts for synthesis of 1-amid-oalkyl-2-naphthols through one-pot three-component reaction under solvent-free conditions. The procedure is equally effective for aliphatic and aryl aldehydes. The notable advantages of this method are high catalytic activity, short reaction time, excellent yields, simple work-up, reusable catalyst, mild reaction conditions, and environmental benignancy. Therefore, this procedure will be a better and more practical alternative to the existing methods.

#### Experimental

Melting points were determined on a PerkinElmer differential scanning calorimeter. <sup>1</sup>H and <sup>13</sup>C nuclear magnetic resonance (NMR) spectra were recorded on a Bruker DRX500 (500 and 125 MHz, respectively). Mass spectra were obtained with an automated FINNIGAN TSQ Advantage mass spectrometer. PEG-DAIL was synthesized according to our previous method [29]. All other chemicals (AR grade) were commercially available and used without further purification.

Scheme 2



Table 3	Comparison of	different catalysts for	one-pot three-compone	nt reaction of 3-nitrobenzaldehyde,	2-naphthol, and acetamide
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Entry	Catalyst (mol%)	Temp. (°C)	Time (min)	Yield (%)	References
1	TCT (5)	100	40	95	[17]
2	$Fe(HSO_4)_3$ (5)	85	25	97	[12]
3	<i>p</i> -TSA (10)	125	240	90	[10]
4	Iodine (5)	125	300	81	[11]
5	$K_5CoW_{12}O_{40}\cdot 3H_2O(1)$	125	180	78	[13]
6	Montmorillonite K10 (0.1 g)	125	30	96	[ <mark>9</mark> ]
7	[FemSILP]-L-prolinate (0.05 g)	100	300	87	[21]
8	Zwitterionic salt (10)	80	90	88	[20]
9	$[TEBSA][HSO_4]$ (5)	120	10	89	[19]
10	PEG <sub>1,000</sub> -DAIL (3)	80	5	95	This work

#### General procedure for synthesis of 1-amidoalkyl-2-naphthols

A mixture of aldehyde (1 mmol), 2-naphthol (1 mmol), amide (1.2 mmol), and PEG<sub>1,000</sub>-DAIL (0.03 mmol) was stirred at 80 °C in an oil bath for 5–20 min as indicated by thin-layer chromatography (TLC) for a complete reaction. The reaction mixture was poured into ice-cold water and stirred thoroughly for 10 min. The solid product was isolated by filtration and then recrystallized from ethanol. The products were characterized by spectral data and comparison of their physical data with literature data.

# *N-[1-(2-Hydroxynaphthalen-1-yl)butyl]propenamide* (**3**, C<sub>17</sub>H<sub>19</sub>NO<sub>2</sub>)

<sup>1</sup>H NMR (500 MHz, DMSO- $d_6$ ):  $\delta = 9.88$  (s, 1H), 8.30 (s, 1H), 8.15 (d, J = 8.6 Hz, 1H), 7.77 (d, J = 7.8 Hz, 1H), 7.68 (d, J = 8.8 Hz, 1H), 7.45 (t, J = 7.4 Hz, 1H), 7.27 (t, J = 7.4 Hz, 1H), 7.17 (d, J = 8.8 Hz, 1H), 6.43–6.38 (m, 1H), 6.02 (dd,  $J_1 = 17.0$  Hz,  $J_2 = 2.1$  Hz, 1H), 5.87 (q, J = 7.6 Hz, 1H), 5.52 (dd,  $J_1 = 10.2$  Hz,  $J_2 = 2.1$  Hz, 1H), 2.07–2.04 (m, 1H), 1.89–1.84 (m, 1H), 1.38–1.36 (m, 1H), 1.21–1.18 (m, 1H), 0.87 (t, J = 7.4 Hz, 3H) ppm; <sup>13</sup>C NMR (125 MHz, DMSO- $d_6$ ):  $\delta = 164.3$ , 153.5, 132.8, 132.6, 129.0, 128.9, 128.7, 126.6, 125.3, 123.0, 122.7, 120.1, 119.0, 46.2, 36.1, 20.0, 14.3 ppm; ESI–MS: m/z = 270.1 ([M + H]<sup>+</sup>).

#### *N-[1-(2-Hydroxynaphthalen-1-yl)pentyl]acetamide* (**4**, C<sub>17</sub>H<sub>21</sub>NO<sub>2</sub>)

<sup>1</sup>H NMR (500 MHz, DMSO- $d_6$ ):  $\delta = 9.87$  (s, 1H), 8.11 (d, J = 8.6 Hz, 1H), 8.03 (s,1H), 7.77 (d, J = 7.9 Hz, 1H), 7.67 (d, J = 8.8 Hz, 1H), 7.45 (t, J = 7.4 Hz, 1H), 7.26 (t, J = 7.4 Hz, 1H), 7.16 (d, J = 8.8 Hz, 1H), 5.77 (q, J = 7.9 Hz, 1H), 2.02–1.98 (m, 1H), 1.89–1.84 (m, 4H), 1.34–1.24 (m, 3H), 1.15–1.10 (m, 1H), 0.81 (t, J = 7.2 Hz, 3H) ppm; <sup>13</sup>C NMR (125 MHz, DMSO- $d_6$ ):  $\delta = 168.9$ , 153.5, 132.8, 129.0, 128.8, 128.7, 126.6, 123.0, 122.7, 120.3, 119.1, 46.3, 33.9, 29.1, 23.2, 22.5, 14.4 ppm; ESI–MS:  $m/z = 272.2 ([M + H]^+).$ 

### N-[1-(2-Hydroxynaphthalen-1-yl)-3-methylbutyl]-

acetamide (5, C<sub>17</sub>H<sub>21</sub>NO<sub>2</sub>)

<sup>1</sup>H NMR (500 MHz, DMSO- $d_6$ ):  $\delta = 9.86$  (s, 1H), 8.11 (d, J = 8.5 Hz, 1H), 8.01 (s, 1H), 7.77 (d, J = 8.1 Hz, 1H), 7.67 (d, J = 8.8 Hz, 1H), 7.46 (t, J = 7.5 Hz, 1H), 7.27 (t, J = 7.4 Hz, 1H), 7.15 (d, J = 8.8 Hz, 1H) 5.89–5.85 (m, 1H), 2.04–1.98 (m, 1H), 1.87 (s, 3H), 1.62–1.52 (m, 2H), 0.89 (d, J = 6.3 Hz, 6H) ppm; <sup>13</sup>C NMR (125 MHz, DMSO- $d_6$ ):  $\delta = 168.9$ , 153.5, 132.6, 129.0, 128.8, 128.7, 126.6, 122.9, 122.7, 120.6, 119.1, 44.5, 43.4, 25.4, 23.5, 23.2, 22.6 ppm; ESI–MS: m/z = 272.2 ([M + H]<sup>+</sup>).

#### N-[(3-Chlorophenyl)(2-hydroxynaphthalen-1-

*yl*)*methyl*]*acetamide* (**12**, C<sub>19</sub>H<sub>16</sub>ClNO<sub>2</sub>)

<sup>1</sup>H NMR (500 MHz, DMSO- $d_6$ ):  $\delta = 10.08$  (s, 1H), 8.51 (d, J = 8.1 Hz, 1H), 7.83–7.78 (m, 3H), 7.40 (t, J = 7.2 Hz, 1H), 7.30–7.21 (m, 5H), 7.13–7.07 (m, 2H), 2.00 (s, 3H) ppm; <sup>13</sup>C NMR (125 MHz, DMSO- $d_6$ ):  $\delta = 169.9$ , 153.7, 145.9, 133.3, 132.7, 130.4, 130.0, 129.0, 128.9, 127.0, 126.5, 126.2, 125.3, 123.4, 123.0, 118.9, 118.7, 48.0, 23.1 ppm; ESI–MS: m/z = 326.1 ([M + H]<sup>+</sup>).

#### N-[(2-Hydroxynaphthalen-1-yl)(4-methyl-

phenyl)methyl]propenamide (19, C<sub>21</sub>H<sub>19</sub>NO<sub>2</sub>)

<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  = 9.99 (s, 1H), 8.68 (d, *J* = 8.0 Hz, 1H), 7.86–7.76 (m, 3H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.28–7.17 (m, 3H), 7.08–7.04 (m, 4H), 6.62–6.57 (m, 1H), 6.13 (dd, *J*<sub>1</sub> = 17.0 Hz, *J*<sub>2</sub> = 2.0 Hz, 1H), 5.61 (dd, *J*<sub>1</sub> = 10.0 Hz, *J*<sub>2</sub> = 2.0 Hz, 1H), 2.24 (s, 3H) ppm; <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  = 164.9, 153.6, 139.6, 135.6, 132.8, 132.3, 129.7, 129.1, 129.0, 126.7, 126.5, 126.0, 123.8, 122.8, 119.1, 118.9, 48.3, 21.0 ppm; ESI–MS: *m/z* = 318.1 ([M + H]<sup>+</sup>). N-[(4-Bromophenyl)(2-hydroxynaphthalen-1-

yl)methyl]propenamide (20, C<sub>20</sub>H<sub>16</sub>BrNO<sub>2</sub>)

<sup>1</sup>H NMR (500 MHz, DMSO- $d_6$ ):  $\delta = 10.07$  (s, 1H), 8.74 (d, J = 8.1 Hz, 1H), 7.83–7.78 (m, 3H), 7.46 (d, J = 8.0 Hz, 2H), 7.40 (t, J = 7.2 Hz, 1H), 7.28 (t, J = 7.4 Hz, 1H), 7.23 (d, J = 8.8 Hz, 2H), 7.16 (d, J = 8.1 Hz, 1H), 7.09 (d, J = 8.3 Hz, 1H), 6.63–6.58 (m, 1H), 6.15 (dd,  $J_1 = 17.0$  Hz,  $J_2 = 2.0$  Hz, 1H), 5.63 (dd,  $J_1 = 10.2$  Hz,  $J_2 = 2.0$  Hz, 1H) ppm; <sup>13</sup>C NMR (125 MHz, DMSO- $d_6$ ):  $\delta = 165.1$ , 153.8, 142.3, 132.7, 132.1, 131.4, 130.1, 129.1, 128.9, 128.8, 127.0, 126.3, 123.5, 123.0, 119.4, 118.9, 118.5, 48.1 ppm; ESI–MS: m/z = 382.0, 384.0 ([M + H]<sup>+</sup>).

#### N-[(2-Hydroxynaphthalen-1-yl)(4-nitrophenyl)methyl]propenamide (**21**, C<sub>20</sub>H<sub>16</sub>N<sub>2</sub>O<sub>4</sub>)

<sup>1</sup>H NMR (500 MHz, DMSO- $d_6$ ):  $\delta = 10.16$  (s, 1H), 8.85 (d, J = 7.8 Hz, 1H), 8.16 (d, J = 8.7 Hz, 2H), 7.85–7.82 (m, 3H), 7.43–7.39 (m, 3H), 7.31–7.22 (m, 3H), 6.66–6.61 (m, 1H), 6.18 (dd,  $J_1 = 17.0$  Hz,  $J_2 = 1.8$  Hz, 1H), 5.66 (dd,  $J_1 = 10.2$  Hz,  $J_2 = 1.8$  Hz, 1H) ppm; <sup>13</sup>C NMR (125 MHz, DMSO- $d_6$ ):  $\delta = 165.3$ , 153.9, 151.2, 146.4, 132.7, 131.8, 130.5, 129.2, 128.9, 127.6, 127.3, 126.6, 123.8, 123.3, 123.1, 118.9, 118.0, 48.5 ppm; ESI–MS: m/z = 349.1 ([M + H]<sup>+</sup>).

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