Supporting Informations

Visible-light-mediated synthesis of β -keto sulfones using g-C₃N₄ as recyclable photocatalyst under sustainable conditions

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General information:

All the reagents were commercially available (Sigma-Aldrich, Alfa-Aesar, Fisher Scientific or TCI chemicals) and used without further purification. Reactions were monitored by thin-layer chromatography (TLC) on 0.25 mm silica gel plates (60 F₂₅₄) and visualized under UV illumination at 254 nm. Organic extracts were dried over anhydrous sodium sulfate (Na₂SO₄). Column chromatography was performed to purify the crude product on silica gel 60–120 mesh using a mixture of hexane and ethyl acetate as eluent. Isolated compounds were characterized by spectroscopic [¹H, ¹³C{1H}, ¹⁹F NMR, IR] techniques and HRMS analysis. NMR spectra were recorded in deuterochloroform (CDCl₃) or deuterated dimethyl sulfoxide (DMSO-d₆). ¹H, ¹³C{¹H} were recorded in 500 (125) or 400 (100) MHz spectrometer and calibrated using tetramethylsilane or residual undeuterated solvent for ¹H NMR, deuterochloroform for ¹³C NMR as an internal reference {Si(CH₃)₄: 0.00 ppm or CHCl₃: 7.260 ppm for ¹H NMR, 77.230 ppm for ¹³C NMR or (CH₃)₂SO: 2.50 ppm for ¹H NMR, 39.50 ppm for ¹³C{1H}NMR. ¹⁹F NMR was calibrated without any internal standard in CDCl₃ in 500 MHz spectrometers. The chemical shifts are quoted in δ units, parts per million (ppm). ¹H NMR data is represented as follows: Chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), integration and coupling constant(s) J in hertz (Hz).

High-resolution mass spectra (HRMS) were recorded on a mass spectrometer using electrospray ionization-time of flight (ESI-TOF) reflection experiments. FT-IR spectra were recorded in KBr or neat and reported in the frequency of absorption (cm^{-1}). Further, Energy Dispersive X-ray (EDX), Transmission Electron Microscope (TEM), Field Emission Scanning Electron Microscope (FE-SEM) and Thermo Gravimetric analysis (TGA) were also recorded for the characterization of g-C₃N₄.

General procedure for the synthesis of graphitic carbon nitride (g-C₃N₄):

Graphitic carbon nitride was synthesized by thermal treatment of Urea crystal (10 g) in a crucible with cover. At first, urea was dried under an oven at 80 °C and then put in a muffle furnace [MAC JGJ-22 (SB)]. This was then heated to 550 °C for 3 h to complete the reaction. The yellow-colored product was then washed with HNO₃ (0.1 mol L⁻¹) and distilled water to remove residual alkaline species like ammonia adsorbed on the surface of the sample. This was then dried at 80 °C for 24 h and finally, 0.4 g of yellow-colored g-C₃N₄ was collected.^{1,2}

References:

X. Chen, S. Lu, Y. Zheng, J. Wang, L. Yang and P. Sun, *Adv. Synth. Catal.*, 2022, 364, 1757.
J. Liu, T. Zhang, Z. Wang, G. Dawson and W. Chen, *J. Mater. Chem.*, 2011, 21, 14398.
General procedure for the Synthesis of β-keto sulfone (1a) from phenylacetylenes (1):



Scheme S1 General procedure for the Synthesis of β -keto sulfone (1a).

To an oven-dried 10 mL borosilicate vial, phenyl acetylene (1) (0.5 mmol, 51 mg), sodium sulfinate salts (a) (0.5 mmol, 89 mg), potassium iodide (0.5 mmol, 83 mg) and g-C₃N₄ (6 mg) were taken. After that 2 mL EtOH was added and the reaction mixture was stirred at room temperature for 3 h, tentatively at a distance of ~6–8 cm from two 10W blue LED bulbs. After completion of the reaction (monitored by TLC analysis), catalyst g-C₃N₄ was separated from the reaction mixture by centrifugation. After centrifugation, we were left with the residue containing g-C₃N₄ and the organic layer containing the desired product. The solvent (EtOH) was then evaporated from the organic layer and to it 25 mL of ethyl acetate was added followed by washing with a 5% solution of aqueous Na₂S₂O₃ (1 x 5 mL). The ethyl acetate layer was dried over anhydrous Na₂SO₄, and the solvent was evaporated under reduced pressure. The crude residue thus obtained was purified by column chromatography over silica gel (60-120 mesh) using hexane and ethyl acetate (17:3) as eluent to afford the desired β -keto sulfones (1a) in 78% (107 mg) yield. The identity and purity of the product was confirmed by spectroscopic analysis.

General procedure for the synthesis of β -keto sulfone (1a) from acetophenone (1'):



Scheme S2 General procedure for the synthesis of β -keto sulfone (1a) from acetophenone (1').

To an oven-dried 10 mL borosilicate vial, acetophenone (1') (0.5 mmol, 60 mg), sodium sulfinate salts (a) (0.5 mmol, 89 mg), potassium iodide (0.5 mmol, 83 mg) and g-C₃N₄ (6 mg) were taken. After that 2 mL EtOH was added and the reaction mixture was stirred at room temperature for 3 h, tentatively at a distance of ~6–8 cm from two 10W blue LED bulbs. After completion of the reaction (monitored by TLC analysis), catalyst g-C₃N₄ was separated from the reaction mixture by centrifugation. After centrifugation, we were left with the residue containing g-C₃N₄ and the organic layer containing the desired product. The solvent (EtOH) was then evaporated from the organic layer and to it 25 mL of ethyl acetate was added followed by washing with a 5% solution of aqueous Na₂S₂O₃ (1 x 5 mL). The ethyl acetate layer was dried over anhydrous Na₂SO₄, and the solvent was evaporated under reduced pressure. The crude residue thus obtained was purified by column chromatography over silica gel (60-120 mesh) using hexane and ethyl acetate (17:3) as eluent to afford the desired *β*-keto sulfones (**1a**) in 80% (110 mg) yield. The identity and purity of the product was confirmed by spectroscopic analysis.



Fig. S1. Photochemical reaction Set-up (a) front view. (b) top view.

Light Information:

Two 10W blue LEDs (Philips) were used as a light source for this light-promoted reaction. We have not used any filters. Range of wavelength 450–495 nm, borosilicate glass was used as a reaction vessel. Distance from the light source to the irradiation vessel \sim 6–8 cm.

Regular fan was used for proper aeration in order to maintain the temperature 28–30 °C (Fig. S1).

General procedure for 3 mmol scale reaction for synthesizing 9a from 9:

To an oven-dried 50 mL borosilicate round bottom flask, 1-bromo-4-ethynylbenzene (**9**) (3 mmol, 0.543 g), sodium *p*-tolylsulfinate (**a**) (3 mmol, 0.534 g), KI (0.498 g) and g-C₃N₄ (36 mg) were taken. After that 12 mL, EtOH was added and the reaction mixture was stirred at room temperature for 24 h, tentatively at a distance of ~6–8 cm from two 10W blue LED bulbs. After completion of the reaction (monitored by TLC analysis), the catalyst was separated from the reaction mixture by centrifugation, then EtOH was evaporated and to the reaction mixture, 30 mL of ethyl acetate was added followed by washing with a 5% solution of aqueous Na₂S₂O₃ (1 x 5 mL). The organic layer was dried over anhydrous Na₂SO₄, and the solvent was evaporated under reduced pressure. The crude residue thus obtained was purified by column chromatography over silica gel (60-120 mesh) using hexane and ethyl acetate as eluent to afford *1-(4-bromophenyl)-2-tosylethan-1-one* (**9a**). The identity and purity of the product was confirmed by spectroscopic analysis.

General procedure for 3 mmol scale reaction for synthesizing 9a from 9':

To an oven-dried 50 mL borosilicate round bottom flask, 4-bromoacetophenone (**9'**) (3 mmol, 0.597 g), sodium *p*-tolylsulfinate (**a**) (3 mmol, 0.534 g), KI (0.498 g) and g-C₃N₄ (36 mg) were taken. After that, 12 mL EtOH was added and the reaction mixture was stirred at room temperature for 20 h, tentatively at a distance of ~6–8 cm from two 10W blue LED bulbs. After completion of the reaction (monitored by TLC analysis), the catalyst was separated from the reaction mixture by centrifugation, then EtOH was evaporated from the reaction mixture and to it, 30 mL of ethyl acetate was added followed by washing with a 5% solution of aqueous Na₂S₂O₃ (1 x 5 mL). The organic layer was dried over anhydrous Na₂SO₄, and the solvent was evaporated under reduced pressure. The crude residue thus obtained was purified by column chromatography over silica gel (60-120 mesh) using hexane and ethyl acetate as eluent to afford *1-(4-bromophenyl)-2-tosylethan-1-one* (**9a**). The identity and purity of the product was confirmed by spectroscopic analysis.

General procedure for catalyst recyclability:

After completion of the reaction, the catalyst was separated from the reaction mixture by simple centrifugation. After centrifugation, we were left with the residue containing $g-C_3N_4$ and

the organic layer containing desired product. The residue containing $g-C_3N_4$ was then carefully washed with distilled water (3 x 1 mL), and EtOH (3 x 1 mL) and dried at 80 °C for 12 h. For performing the reusability test of the photocatalyst, it was recovered from the large scale reactions, and then reused for further runs or for further analyses.

Crystallographic description:

Sample preparation: Compounds (**5a**, 25 mg) and (**2b**, 30 mg) were dissolved separately in 1 mL of DCM and 0.5 mL of MeOH in two separate glass vials (5 mL) and kept at room temperature for slow evaporation. The vial was covered with a cap having a small hole in it for the slow evaporation. It was observed that after 24 h needle-shaped crystals appeared.

For **5a** diffraction data were collected at 293 K with MoK α radiation ($\lambda = 0.71073$ Å) using a BRUKER D8 QUEST diffractometer. The APEX software was used for data collection and for indexing the reflections and determining the unit cell parameters. Data reduction and cell refinement were performed using SHELXL-2019/1.¹ The structures were solved by direct methods and refined by full-matrix least-squares calculations using SHELXL-2019/1 software.

For **2b** diffraction data were collected at 293 K using BRUKER D8 VENTURE SC-XRD system, equipped dual X-ray sources (Mo and Cu), Photon II detector. APEX3 software was used for data collections and refinement was done by using SHELXL-2019/1.¹ The structures were solved by direct methods and refined by full-matrix least-squares calculations using SHELXL-2019/1 software.

Crystallographic description of 1-(4-fluorophenyl)-2-tosylethan-1-one (5a):

M.F. = C₁₅H₁₃FO₃S, crystal dimensions 0.25 x 0.11 x 0.18 mm, $M_r = 292.31$, triclinic space, group P -1, a = 5.6822 (4), b = 9.1526 (6), c = 14.0751 (10) Å, $\alpha = 108.654^{\circ}$ (2), $\beta = 100.575^{\circ}$ (2) , $\gamma = 91.470^{\circ}$ (2), V = 678.97(8) Å³, Z = 2, $\rho_{calcd} = 1.430$ g/cm³, $\mu = 0.254$ mm⁻¹, F(000) = 304.0, final *R* indices [$I > 2\sigma$ (I)]: R_1 0.1031(1821), $wR_2 = 0.2627$ (2323), goodness of fit = 1.224. **CCDC** No = 2177792 for I-(4-fluorophenyl)-2-tosylethan-1-one (5a) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.



Fig. S2. ORTEP diagram of (5a) (CCDC 2177792).

Crystallographic description of 2-(phenylsulfonyl)-1-(p-tolyl)ethan-1-one (2b):

M.F. = C₁₅H₁₄O₃S, crystal dimensions 0.20 x 0.16 x 0.17 mm, $M_r = 274.32$, orthorhombic, space group - P, a = 11.5468 (16), b = 10.2038 (11), c = 22.824 (3) Å, $\alpha = 90^{\circ}$, $\beta = 90^{\circ}$, $\gamma = 90^{\circ}$, V = 2689.2(6) Å³, Z = 8, $\rho_{calcd} = 1.355$ g/cm³, $\mu = 0.241$ mm⁻¹, F(000) = 1152.0, final *R* indices [*I* > 2 σ (*I*)]: $R_1 = 0.0621(1600)$, $wR_2 = 0.2039$ (3152), goodness of fit = 1.060. CCDC No = **2177795** for 2-(*phenylsulfonyl*)-1-(*p*-tolyl)*ethan*-1-one (**2b**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via <u>www.ccdc.cam.ac.uk/data_request/cif</u>.



Fig. S3. ORTEP diagram of (2b) (CCDC 2177795).

Reference:

- 1. G. M. Sheldrick, Acta Crystallogr., 2008, A64, 112–122.
- **1. Radical-trapping experiments:**



Scheme S3. Radical-trapping experiments.

(i) To prove the photocatalytic radical pathway, a radical trapping experiment was conducted between (1 or 1'), and (a), in the presence of BHT (2 equiv) under the standard reaction condition. It was observed that, tosyl radical was trapped and adduct (**M**) was obtained in 61% yield (with 1) and 75% yield (with 1') thereby confirming the radical nature of the present protocols.

The adduct (**M**) was purified by column chromatography over silica gel (60-120 mesh) using hexane and ethyl acetate (9:1) as eluent to afford the 2,6-di-*tert*-Butyl-4-(tosylmethyl)phenol (**M**) in 61% yield (with **1**) and 75% yield (with **1'**). The identity and purity of the product was confirmed by spectroscopic (¹H, ¹³C{1H}, & HRMS) analyses.



Fig. S4 HRMS spectra of intermediate M.



Fig. S5 1 H spectra of intermediate M.



Fig. S6 ${}^{13}C{}^{1}H$ spectra of intermediate M.





Fig. S7 HRMS spectra of intermediate B.



Fig. S8 ¹H spectra of intermediate B.



Fig. S9 ${}^{13}C{}^{1}H$ spectra of intermediate **B**.

Post-synthetic applications:

(a) Synthesis of Quinoline-(P) from $1a^1$



Scheme S4. Synthesis of Quinoline-(P) from 1a.

To an oven-dried 5 mL round bottom flask, *1-phenyl-2-tosylethanone* (**1a**) (44 mg, 0.16 mmol), 2-amino-5-chlorobenzophenone (37 mg, 0.16 mmol), *p*-TsOH. H₂O (0.025 mmol) and 2 mL of toluene were taken. The flask was fitted with a condenser and the reaction mixture was stirred in a preheated oil bath at 120 °C for 4 h. Next, the reaction mixture was cooled to room temperature and admixed with ethyl acetate (10 mL). The organic layer was washed with

saturated sodium bicarbonate solution (2 x 5 mL) and dried over Na₂SO₄ and the solvent was removed under reduced pressure. The crude product so obtained was purified over a column of silica gel (hexane: ethyl acetate, 9.4:0.6) to afford the *6-chloro-2,4-diphenyl-3-tosylquinoline* (**P**) (51 mg, yield 73%). The identity and purity of the product were confirmed by spectroscopic analysis.

(**b**) Synthesis of Oxime (**Q**) from **1a**.²



Scheme S5. Synthesis of Oxime (Q) from 1a.

To an oven-dried 10 mL round bottom flask, *1-phenyl-2-tosylethanone* (**1a**) (274 mg, 1 mmol), NH₂OH. HCl (105 mg, 1.5 mmol), anhydrous NaOAc (123 mg, 1.5 mmol) and 5 mL of EtOH were taken. The flask was fitted with a condenser and the reaction mixture was stirred in a preheated oil bath at 80 °C for 1 h. Next, the reaction mixture was cooled to room temperature. Following that, it was poured into cold water and the solid product was filtered off and washed with water to afford (*E*)-1-phenyl-2-tosylethanone oxime (**Q**) (200 mg, yield 69.20%) (**Q**). Identity and purity of the product were confirmed by spectroscopic analysis.

Reaction in presence of Et₃N instead of KI

To support the mechanistic path, the standard reaction was carried out using triethyl amine as the sacrificial reducing agent, instead of KI. The desired β -keto sulfone (**1a**) was obtained in 42% yield after 3 h. No substantial improvement in the product was observed after carrying out the reaction till 6 h. However, in this case, the reaction proceeds *via* the following mechanism. Initially, in the presence of blue LEDs, the graphitic carbon nitride (g-C₃N₄) gets photo-excited and generates a hole and electron pair. Then, triethyl amine gets converted to its radical cation to neutralize the hole of the g-C₃N₄. Then the sulfonyl anion obtained from the sodium sufinate is oxidized by the radical cation of triethyl amine to generate sulfonyl radical thereby regenerating the triethyl amine. This sulfonyl radical adds to the terminal alkyne to generate a vinyl sulfonyl radical intermediate (**A**) which is trapped by the O₂ to generate intermediate (**X**). This is then reduced by the electron pair of the g-C₃N₄ to an anionic intermediate (**C**), which undergoes tautomerization giving the desired product **1a**. Similar reductive cleavage of peroxide using benezene sulfinic acid is reported by Lei *et al.* (J. Am. Chem. Soc., 2013, 135, 11481-11484).



Proposed mechanism in the presence of sacrificial reducing agent Et₃N



Scheme S6. Synthesis of 1a by Et₃N in presence of g-C₃N₄

Calculation of Green Chemistry Metrics.

Table S1 Evaluation of green chemistry metrics for the synthesis of 9a from 1-bromo-4-ethynylbenzene (9)

E-factor (Enviromental factor)	$= \frac{\text{Mass of waste}}{\text{Mass of product}} \text{Atom economy (\%)} =$	$(AE) = \frac{Molec}{Mol}$) = <u>Molecular mass of desired product</u> x 100 Molecular mass of all reactants			
tom efficiency (%)=	Yield of the product (%) Atom economy (%)	iency (%) =	Total no. of C in reactants Total no. of C in products x 100			
React	ionmass economy (%) = (RME) = $\frac{Mass}{Mass}$	of desired product s of all reactants	— x 100			
Reactant 1	1-bromo-4-ethynylbenzene	0.543g	3 mmol	FW 181.03		
Reactant 2	Sodium 4-methylbenzene Sulfinate	0.534g	3 mmol	FW 178.18		
Solvent	Ethanol	9.468g				
Additive (KI)	Potassium Iodide	0.498g	3 mmol	FW 166.00		
Product	1-(4-bromophenyl)-2-tosylethanone	0.686g	1.9 mmol	FW 352.98		
<pre>'roduct yield = 65% E-factor = (0.543+ 0.5 Atom economy = (352 Atom efficiency = 65% Carbon efficiency = 1;</pre>	34+0.498+9.468 - 0.686)/0.686 = 15.09 Kg .98/359.21) x100 = 98.26% 5 x 98.26% /100 = 63.70% 5/15 x100= 100%	waste/1Kg produ	ict.	·		

E-factor (Enviromental factor)	$= \frac{\text{Mass of waste}}{\text{Mass of product}} \text{Atom economy (\%)} = (A)$) = Molecular mass of desired product Molecular mass of all reactants			
Atom efficiency $(\%) = \frac{1}{2}$	Atom economy (%) x 100 Carbon e	- x 100 Carbon efficiency (%) = -		Total no. of C in reactants Total no. of C in products x 100		
Reacti	onmass economy $(\%) = (\mathbf{RME}) = \frac{1}{M}$	lass of all reac	tants	x 100		
Reactant 1	4-Bromoacetophenone	0.	597g	3 mmol	FW 199.04	
Reactant 2	Sodium 4-methylbenzene	0.	534g	3 mmol	FW 178.18	
	Sulfinate					
Solvent	Ethanol	9.	468g			
		(12	2 mL)			
Additive (KI)	Potassium Iodide	0.	498g	3 mmol	FW 166.00	
Product	Product 1-(4-bromophenyl)-2-tosylethanone			2.08 mmol	FW 352.98	
Product yield = 69%	L					
E-factor= (0.597+ 0.534	+0.498+9.468 - 0.733)/0.733 = 14.15 K	g waste/1Kg	product.			
Atom economy = (352.9)	98/377.22) x100 = 93.57%					
Atom efficiency = 69%	x 93.57% /100 = 64.56%					
Carbon efficiency = 15/	15 x100= 100%					
Reaction mass efficienc	$v = 0.733/(0.597 + 0.534)g \times 100 = 64.80$)%				

Table S2 Evaluation of green chemistry metrics for the synthesis of 9a from 4-Bromoacetophenone (9')

E-factor	Mass of waste	A tom according $(9/) = (AE)$	Molec	Molecular mass of desired product			
(Enviromental factor)	$= \frac{1}{\text{Mass of product}} \text{Atom economy}(\%) = (AE) = 1$) = Mol	Molecular mass of all reactants			
Atom efficiency (%)=	Yield of the product (% Atom economy (%	6) x 100 Carbon efficiency	v (%) =	Total no. of C in react	tants ducts x 100		
Reactionmass economy (%) = (RME) = $\frac{\text{Mass of desired product}}{\text{Mass of all reactants}} \times 100$							
Reactant 1	1-bromo-4	-ethynylbenzene	0.831g	3 mmol	FW 277.00		
Reactant 2	Sodium 4	-methylbenzene	0.534g	3 mmol	FW 178.18		
Solvent		DMF	11.33g				

FW 352.98

Table S3 Evaluation of green chemistry metrics for the synthesis of 9a by known procedure³

		(12 mL)						
Product	1-(4-bromophenyl)-2-tosylethanone	0.705g	2 mmol					
Product yield = 67%								
E-factor= (0.831+ 0.534+11.33- 0.705)/0.705 = 17 Kg waste/1Kg product.								
Atom economy = (352.98/455.18) x100 = 77.54%								
$A = -\frac{1}{2} \frac{1}{2} \frac{1}{2}$								

Atom efficiency = 67% x 77.54% /100 = 51.95%

Carbon efficiency = 15/15 x100= 100%

Reaction mass efficiency = 0.705/(0.831+0.534)g x 100 = 51.64%

	Parameters									
Method	E-factor		Atom economy (%)		Atom efficiency (%)		Carbon efficiency(%)		RME (%)	
	With 1-bromo-4- ethynylbenz ene	4- Bromo- acetophe none	1- bromo- 4- ethynylb enzene	4- Bromo- acetophe none	1- bromo- 4- ethynyl benzen e	4- Bromo - acetop henon e	1- bromo- 4- ethynyl benzen e	4- Brom o- acetop henon e	1- bromo- 4- ethynyl benzen e	4- Brom o- acetop henon e
Photoch emical	15. 09 Kg waste/ 1Kg product	14.15Kg waste/ 1Kg product	98.26	93.57	63.70	64.56	100	100	63.69	64.80
Thermal	17 Kg waste/ 1Kg product		77.	.54	51.	95	10	0	51.	64

Table S4 Comparison of photochemical and thermal method green chemistry metrics

Reference:

1. C-K. Chan, C-Y. Lai, W-C. Lo, Y-T. Cheng, M-Y. Chang and C-C. Wang, Org. Biomol. Chem., 2020, 18, 305.

2. H. A. A. Aziz, K. A. A. Rashood, K. H. El-Tahir and G. M. Suddek, *Eur. J. Med. Chem.*, 2014, **80**, 416.

3. J. Xiang, M. Ipek, V. Suri, M. Tam, Y. Xing, N. Huang, Y. Zhang, J. Tobin, T. S. Mansoura and J. McKew, *Bioorg. Med. Chem.*, 2007, **15**, 4396.

Table S5. Eco-scale calculation for reaction with 1-ethynyl-4-bromo benzene (9) for synthesis of9a:

Ecoscale = 100 – Sum of individu	al penalties
Score on EcoScale: > 75, Excellent; >50, Acce	ptable; <50, Inadequate
A) Calculation of penalty points:	
Parameters	Penalty points
1. Yield (100-65)/2 =	17.5
2. Price of reaction components	
(To obtain 10 mmol of end product)	
a. 1-ethynyl-4-bromo benzene=2.85 g= \$111.41	
b. Sodium 4-methylbenzene Sulfinate=2.81g = \$2.02	
c. $KI = 2.619g = $ \$1.09	
f. $EtOH = 60mL = $ \$0.78	
Total price (USD) = \$115.30	
Thus, expensive (>\$50)	5
3. Safety	
Reagent:	
<u>1-bromo-4-ethynylbenzene</u>	
N (dangerous for environment)	5
Ethanol	
Highly Flammable	5
4. Technical Setup	
Unconventional activation technique	2
(Photochemical activation)	
5. Temperature and time	
Room temperature and <24h	1
6. Workup and purification	
Removal of solvent with bp <150°C	0
Classical Chromatography	10
Total penalty points:	45.5

Eco-scale value for synthesis of 9a by present photochemical procedure = (100-45.5)= 54.5 (Since > 50, so **acceptable** synthesis)

Table S6. Eco-scale calculation with 4-bromoacetophenone (9') for synthesis of 9a:

A) Calculation of penalty points:	
Parameters	Penalty points
1. Yield (100-69)/2 =	15.5
2. Price of reaction components	
(To obtain 10 mmol of end product)	
a. 4-bromoacetophenone=2.869 g= \$1.96	
b. Sodium 4-methylbenzene Sulfinate=2.56g = \$1.84	
c. $KI = 2.38g = $ \$1.00	
f. $EtOH = 60mL = $ \$0.78	
Total price $(USD) = 5.58	
Thus, inexpensive (<\$10)	3
3.Safety	
Reagent:	
<u>Ethanol</u>	
Highly Flammable	5
4. Technical Setup	
Unconventional activation technique	
(Photochemical activation)	2
5. Temperature and time	
Room temperature and <24h	1
6. Workup and purification	
Removal of solvent with bp <150°C	0
Classical Chromatography	10
Total penalty points:	36.5

Eco-scale value for synthesis of 9a by present photochemical procedure = (100-36.5) = 63.5 (Since >50, so **acceptable** synthesis)

Spectral Data

1-Phenyl-2-tosylethanone (1a):



Yield: 78% (107 mg) as white solid; mp 123–125 °C; ¹H NMR (CDCl₃, 400 MHz) δ 7.94 (dd, 2H J_1 = 8.4, J_2 = 1.2 Hz), 7.76 (d, 2H, J = 8.4 Hz), 7.63–7.59 (m, 1H), 7.48 (t, 2H, J = 8.0 Hz), 7.33 (d, 2H, J = 8.0 Hz), 4.72 (s, 2H), 2.44 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 100 MHz) δ 188.3, 145.6, 136.0, 135.9, 134.5, 130.0, 129.5, 129.0, 128.8, 63.8, 21.9; IR (KBr, cm⁻¹): 3368, 2925, 2852, 1672, 1595, 1450, 1151, 1025; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₅O₃S, [M + H]⁺: 275.0736, found 275.0701.

1-(p-Tolyl)-2-tosylethan-1-one (2a):



Yield: 80% (115 mg) as a white solid; mp 121–123 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.84 (d, 2H, *J* = 8.0 Hz), 7.75 (d, 2H, *J* = 8.0 Hz), 7.33 (d, 2H, *J* = 8.0 Hz), 7.27 (t, 2H, *J* = 8.0Hz), 4.68 (s, 2H), 2.44 (s, 3H), 2.42 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 187.9, 145.8, 145.5, 136.1, 133.7, 130.0, 129.8, 129.7, 128.8, 63.9, 22.0, 21. 9; IR (KBr, cm⁻¹): 3042, 2932, 1660, 1511, 1449, 1149, 1054; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₆H₁₇O₃S, [M + H]⁺: 289.0893, found 289.0867.

1-(4-(tert-Butyl)phenyl)-2-tosylethan-1-one (3a):



Yield: 74% (122 mg) as brown gummy; mp 100-102 °C; ¹H NMR (CDCl₃, 500 MHz): δ 7.88 (d, 2H, J = 8.5 Hz), 7.76 (d, 2H, J = 8.5 Hz), 7.48 (d, 2H, J = 8.5 Hz), 7.33 (d, 2H, J = 8.0 Hz), 4.69 (s, 2H), 2.44 (s, 3H), 1.34 (s, 9H); ¹³C{¹H} NMR (125 MHz, CDCl₃) δ 187.8, 158.6, 145.5, 136.0, 133.5, 130.0, 129.6, 128.8, 126.0, 63.8, 35.5, 31.2, 21.9; IR (KBr, cm⁻¹): 3052, 2960, 2930, 1676, 1152, 1085; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₉H₂₃O₃S, [M + H]⁺: 331.1362, found 331.1338.



Yield: 82% (124 mg) as white solid; mp 125–127 °C; ¹H NMR (CDCl₃, 400 MHz) δ 7.88 (d, 2H, *J* = 9.2 Hz), 7.70 (d, 2H, *J* = 8.0 Hz), 7.29 (d, 2H, *J* = 8.0 Hz), 6.90 (d, 2H, *J* = 8.8 Hz), 4.63 (s, 2H), 3.84 (s, 3H), 2.16 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 100 MHz) δ 186.4, 164.6, 145.4, 135.9, 132.0, 129.9, 129.0, 128.6, 114.2, 63.6, 55.7, 21.8; IR (KBr, cm⁻¹): 3011, 2925, 1745, 1591, 1443, 1152, 1027; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₆H₂₀NO₄S, [M + NH₄]⁺: 305.0842, found 305.0834.

1-(4-Fluorophenyl)-2-tosylethan-1-one (5a):



Yield: 79% (115 mg) as white solid; mp 140–142 °C; ¹H NMR (CDCl₃, 500 MHz) δ 8.01 – 7.98 (m, 2H), 7.75 (d, 2H, *J* = 8.5 Hz), 7.34 (d, 2H, *J* = 8.0 Hz), 7.16 (t, 2H, *J* = 8.5 Hz), 4.68 (s, 2H), 2.45 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 186.8, 166.7 (d, *J* = 258.4 Hz), 145.7, 135.9, 132.5, 132.4, 130.1, 128.8, 116.3 (d, *J* = 22.1 Hz), 64.0, 21.9; ¹⁹F (CDCl₃, 471 MHz) δ –102.5; IR (KBr, cm⁻¹): 3076, 2949, 2922, 1676, 1593, 1460, 1413, 1148, 1084; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₄FO₃S, [M + H]⁺: 293.0642, found 293.0640.

1-(3-Fluorophenyl)-2-tosylethan-1-one (6a):



Yield: 76% (110 mg) as white solid; mp 135–137 °C; ¹H NMR (CDCl₃, 400 MHz) δ 7.76 (d, 3H, J = 8.5 Hz), 7.63 – 7.59 (m, 1H), 7.51-7.45 (m, 1H), 7.36 – 7.32 (m, 3H), 4.69 (s, 2H), 2.45 (s, 3H).; ¹³C{¹H} NMR (CDCl₃, 100 MHz) δ 187.3, 164.2, 161.8, 145.8, 135.7, 130.8 (d, J = 7.7 Hz), 130.1, 128.2, 125.6 (d, J = 22.9 Hz), 121.7 (d, J = 21.4 Hz), 116.1 (d, J = 22.9 Hz), 64.0, 21.9.; ¹⁹F (CDCl₃, 376 MHz) δ –111.0; IR (KBr, cm⁻¹): 3078, 2944, 2912, 1672, 1498, 1153, 1062; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₄FO₃S, [M + H]⁺: 293.0642, found 293.0653.



Yield: 80% (123 mg) as white solid; mp 136–138 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.90 (d, 2H, *J* = 9.0 Hz), 7.74 (d, 2H, *J* = 8.0 Hz), 7.46 (d, 2H, *J* = 8.5 Hz), 7.34 (d, 2H, *J* = 8.0 Hz), 4.67 (s, 2H), 2.45 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 187.2, 145.8, 141.3, 135.8, 134.3, 131.0, 130.1, 129.4, 128.8, 64.0, 21.9; IR (KBr, cm⁻¹): 3065, 2927, 1676, 1439, 1147, 1025; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₄ClO₃S, [M + H]⁺: 309.0347, found 309.0356.

1-(3-Chlorophenyl)-2-tosylethan-1-one (8a):



Yield: 71% (109 mg) as light yellow solid; mp 127–129 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.85 (d, 2H, *J* = 8.5 Hz), 7.75 (d, 2H, *J* = 8.0 Hz), 7.58 (d, 1H, *J* = 7.0 Hz), 7.44 (t, 1H, *J* = 8.0 Hz), 7.35 (d, 2H, *J* = 8.0 Hz), 4.68 (s, 2H), 2.45 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 187.2, 145.8, 137.5, 135.7, 135.5, 134.4, 130.4, 130.1, 129.4, 128.8, 127.8, 64.0, 21.9; IR (KBr, cm⁻¹): 3000, 2912, 1680, 1421, 1150, 1110, 1012; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₄ClO₃S, [M + H]⁺: 309.0347, found 309.0355.

1-(4-Bromophenyl)-2-tosylethan-1-one (9a):



Yield: 78% (138 mg) as white solid; mp 144–146 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.82 (d, 2H, J = 8.5 Hz), 7.74 (d, 2H, J = 8.0 Hz), 7.63 (d, 2H, J = 9.0 Hz), 7.34 (d, 2H, J = 8.0 Hz), 4.67 (s, 2H), 2.45 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz): δ 187.5, 155.2, 134.8, 134.7, 132.5, 131.0, 130.1, 130.03, 128.8, 64.0, 21.9; IR (KBr, cm⁻¹): 3005, 2918, 1677, 1417, 1178, 1098; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₄BrO₃S, [M + H]⁺: 352.9842, found 352.9858.

1-(4-Nitrophenyl)-2-tosylethan-1-one (10a):



Yield: 64% (102 mg) as white solid; mp 145–147 °C; ¹H NMR (CDCl₃, 500 MHz) δ 8.34 (d, 2H, *J* = 9.0 Hz), 8.15 (d, 2H, *J* = 8.5 Hz), 7.74 (d, 2H, *J* = 8.0 Hz), 7.37 (d, 2H, *J* = 8.0 Hz), 4.74 (s, 2H), 2.47 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 187.3, 151.1, 146.4, 140.2, 135.6, 130.7, 130.3, 128.7, 124.2, 64.4, 22.0; IR (KBr, cm⁻¹): 3061, 2922, 1688, 1328, 1161, 1078; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₃NO₅SNa [M + Na]⁺: 342.0407, found 342.0370.

1-(2-Nitrophenyl)-2-tosylethan-1-one (11a):



Yield: 58% (93 mg) as light yellowish solid; mp 138–140 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.15 (d, 1H, *J* = 9.0 Hz), 7.80 (dd, 3H, *J*₁ = 13.5 Hz, *J*₂ = 7.5 Hz), 7.69-7.63 (m, 2H), 7.38 (d, 2H, *J* = 8.0 Hz), 4.59 (s, 2H), 2.47 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz): δ 190.1, 145.9, 145.5, 136.6, 136.1, 135, 131.7, 130.2, 129.3, 128.6, 124.4, 67.1, 21.9; IR (KBr, cm⁻¹): 3063, 2926, 2855, 1708, 1597, 1265, 1002; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₃ NO₅SNa [M + Na]⁺: 342.0407, found 342.0381.

1-(Thiophen-2-yl)-2-tosylethanone (12a):



Yield: 69% (97 mg) as dark brown solid; mp 124-126 °C; ¹H NMR (CDCl₃, 500 MHz): δ 7.81 (d, 1H, *J* = 4.0 Hz), 7.75 (t, 3H, *J* = 8.5 Hz), 7.34 (d, 2H, *J* = 8.0 Hz), 7.16 (t, 1H, *J* = 4.5 Hz), 4.60 (s, 2H), 2.44 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz): δ 180.5, 145.7, 143.4, 136.5, 135.8, 135.4, 130.1, 129.0, 128.8, 65.0, 21.9; IR (KBr, cm⁻¹): 3096, 2954, 2919, 1410, 1139, 1081; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₃H₁₃O₃S₂, [M + H]⁺: 281.0301, found 281.0306.

1-phenyl-2-tosylpropan-1-one (13"a):



Yield: 66% (95 mg) as brown gummy; mp 123–125 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.89 (d, 2H, *J* = 8.0 Hz), 7.58 (d, 2H, *J* = 8.0 Hz), 7.53 (t, 1H, *J* = 7.0 Hz), 7.40 (t, 2H, *J* = 7.7 Hz), 7.22 (d, 2H, *J* = 8.0 Hz), 5.09-5.06 (q, *J* = 6.8 Hz, 1H), 2.34 (s, 3H), 1.48 (d, 3H, *J* = 7.0 Hz); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 191.6, 144.3, IR (KBr, cm⁻¹): 3028, 2925, 1671, 1590, 1453, 1150, 1025; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₆H₁₆O₃S, [M + H]⁺: 289.0898, found 289.0911.

1-Phenyl-2-(phenylsulfonyl)ethanone (1b):



Yield: 73% (95 mg) as white solid; mp 117-119 °C; ¹H NMR (CDCl₃, 500 MHz,) δ 7.94 (d, 2H, *J* = 8.0 Hz), 7.90 (d, 2H, *J* = 8.0 Hz), 7.67 -7.60 (m, 2H), 7.55 (t, 2H, *J* = 8.0 Hz), 7.48 (t, 2H, *J* = 7.5 Hz), 4.73 (s, 2H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 188.2, 139.0, 136.0, 134.6, 134.4, 129.5, 129.4, 129.1, 128.8, 63.7; IR (KBr, cm⁻¹): 3022, 2939, 1665, 1455, 1153, 1021; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₄H₁₆NO₃S, [M + NH₄]⁺: 261.0580, found 261.0586.

2-((4-Chlorophenyl)sulfonyl)-1-phenylethanone (1c):



Yield: 69% (102 mg) as white solid; mp 132–134 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.94 (d, 2H, *J* = 7.5 Hz), 7.83 (d, 2H, *J* = 8.5 Hz), 7.64 (t, 1H, *J* = 7.5 Hz), 7.51 (dd, 4H, *J*₁ = 16.0, *J*₂ = 8.5 Hz), 4.73 (s, 2H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 188.1, 141.4, 137.4, 135.9, 134.8, 130.4, 129.8, 129.5, 129.2, 63.6; IR (KBr, cm⁻¹): 3028, 2918, 2859, 1676, 1447, 1089; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₄H₁₂ClO₃S, [M + H]⁺: 295.019, found 295.011.

2-(4-Bromophenylsulfonyl)-1-phenylethanone (1d):



Yield: 64% (108 mg) as white solid; mp 130–132 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.93 (d, 2H, *J* = 7.5 Hz), 7.76 (d, 2H, *J* = 9.0 Hz), 7.69 (d, 2H, *J* = 8.5 Hz), 7.64 (t, 1H, *J* = 7.5 Hz), 7.49 (t, 2H, *J* = 8.0 Hz), 4.73 (s, 2H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 188.1, 137.9, 135.8, 134.7, 132.7, 130.4, 130.0, 129.5, 129.1, 63.6; IR (KBr, cm⁻¹): 3361, 2908, 1687, 1567, 1461, 1395, 1309, 1199, 1137, 1059, 1009, 821, 768, 689; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₄H₁₂BrO₃S, [M + H]⁺: 338.9685, found 338.9671.

2-(Methylsulfonyl)-1-phenylethanone (1e):



Yield: 53% (52 mg) as brown solid; mp 115–117 °C; ¹H NMR (CDCl₃, 400 MHz,) δ 8.01 (d, 2H, *J* = 7.2 Hz), 7.67 (t, 1H, *J* = 8.0 Hz), 7.53 (t, 2H, *J* = 8.0 Hz), 4.60 (s, 2H), 3.16 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 100 MHz) δ 189.4, 135.8, 135.0, 129.5, 129.3, 61.5, 42.0; IR (KBr, cm⁻¹): 3028, 2927, 1675, 1452, 1149, 987; HRMS (ESI/Q-TOF) (m/z): calcd for C₉H₁₀O₃SNa, [M + Na]⁺: 221.0243, found 221.0205.

2-(Phenylsulfonyl)-1-(p-tolyl)ethan-1-one (2b):



Yield: 72% (99 mg) as white solid; mp 119–121 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.89 (t, 2H, *J* = 7.0 Hz), 7.84 (d, 2H, *J* = 8.0 Hz), 7.66 (t, 1H, *J* = 7.5 Hz), 7.54 (t, 2H, *J* = 7.5 Hz), 7.27 (t, 2H, *J* = 8.0Hz), 4.70 (s, 2H), 2.42 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 187.7, 145.8, 139.1, 134.4, 133.6, 129.8, 129.7, 129.4, 128.8, 63.7, 22.0; IR (KBr, cm⁻¹): 3012, 2929, 1678, 1596, 1451, 1317, 1143, 1071, 1013, 767; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₅O₃S, [M + H]⁺: 275.0736, found 275.0742.

2-((4-Chlorophenyl)sulfonyl)-1-(4-methoxyphenyl)ethan-1-one (4c):



Yield: 71% (115 mg) as white solid; mp 168-170 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.92 (d, 2H, J = 8.5 Hz), 7.81 (d, 2H, J = 8.5 Hz), 7.51 (d, 2H, J = 8.5 Hz), 6.95 (d, 2H, J = 8.9 Hz), 4.68 (s, 2H), 3.89 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 186.3,

165.0, 141.2, 137.4, 132.1, 130.4, 129.7, 128.9, 114.4, 63.6, 55.9; IR (KBr, cm⁻¹): 3053, 2953, 2910, 1672, 1470, 1391, 1307, 1169, 1022; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₄ClO₄S, [M + H]⁺: 325.0296, found 325.0264.

1-(4-Fluorophenyl)-2-(phenylsulfonyl)ethanone (5b):



Yield: 68% (94 mg) as white solid; mp 119–121 °C; ¹H NMR (CDCl₃, 500 MHz) δ 8.00 (dd, 2H, $J_1 = 8.5$ Hz, $J_2 = 5.5$ Hz), 7.88 (d, 2H J = 7.5 Hz), 7.68 (t, 1H, J = 7.4 Hz), 7.56 (t, 2H, J = 7.5 Hz), 7.16 (t, 2H, J = 8.5 Hz), 4.70 (s, 2H).; ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 186.6, 167.8, 165.7, 138.9, 134.6, 132.4 (d, J = 9.7 Hz), 129.5, 128.8, 116.3 (d, J = 22.0Hz), 64.0; ¹⁹F (CDCl₃, 471 MHz) δ –102.3; IR (KBr, cm⁻¹): 3005, 2920, 1676, 999; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₄H₁₁O₃SFNa, [M + Na]⁺: 301.0305, found 301.0307.

2-(4-Bromophenylsulfonyl)-1-(thiophen-2-yl)ethanone (12d):



Yield: 63% (109 mg) as white solid; mp 116– 118 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.81 (d, 1H, J = 3.9 Hz), 7.78 – 7.74 (m, 3H), 7.70 (d, 2H, J = 8.5 Hz), 7.19 (t, 1H, J = 4.5 Hz), 4.63 (s, 2H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 180.02, 143.0, 137.3, 136.7, 135.2, 132.6, 130.2, 129.9, 128.8, 64.4; IR (KBr, cm⁻¹): 3088, 2954, 2919, 1655, 1409, 1148, 1062; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₂H₉BrO₃S₂Na, [M + Na]⁺: 366.9069, found 366.9058.

With acetophenones:

1-Phenyl-2-tosylethanone (1a):



Yield: 80% (110 mg) as white solid, mp 123–125 °C; ¹H NMR (CDCl₃, 400 MHz) δ 7.95 (dd, 2H, $J_1 = 8.0$, $J_2 = 0.8$ Hz), 7.76 (d, 2H, J = 8.4 Hz), 7.62 (t, 1H, J = 7.6 Hz), 7.48 (t, 2H, J = 8.0 Hz), 7.34 (d, 2H, J = 8.0 Hz), 4.72 (s, 2H), 2.44 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 100 MHz) δ 188.4, 145.6, 136.0, 135.9, 134.5, 130.1, 129.5, 129.1, 128.8, 63.8, 21.9; IR (KBr, cm⁻¹): 3353, 2925, 1670, 1610, 1511, 1451, 1309, 1268, 1157, 1022, 665; HRMS (ESI/Q-TOF) (m/z): calcd for $C_{15}H_{15}O_3S$, $[M + H]^+$: 275.0736, found 275.0749.

1-(p-Tolyl)-2-tosylethan-1-one (2a):



Yield: 80% (115 mg) as white solid; mp 121–123 °C; ¹H NMR (CDCl₃, 400 MHz) δ 7.85 (d, 2H, *J* = 8.0 Hz), 7.76 (d, 2H, *J* = 8.4 Hz), 7.34 (d, 2H, *J* = 8.0 Hz), 7.28 (d, 2H, *J* = 8.0 Hz), 4.68 (s, 2H), 2.44 (s, 3H), 2.42 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 100 MHz) δ 187.6, 145.5, 145.3, 135.7, 133.3, 129.8, 129.57, 129.53, 128.6, 63.6, 21.8, 21.7; IR (KBr, cm⁻¹): 3029, 2948, 1668, 1591, 1448, 1151, 1013; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₆H₁₇O₃S, [M + H]⁺: 289.0893, found 289.0881.

1-(4-Methoxyphenyl)-2-tosylethan-1-one (4a):



Yield: 82% (125 mg) as white solid; mp 125–127 °C; ¹H NMR (CDCl₃, 400 MHz) δ 7.88 (d, 2H, *J* = 9.0 Hz), 7.70 (d, 2H, *J* = 8.3 Hz), 7.29 (d, 2H, *J* = 8.0 Hz), 6.90 (d, 2H, *J* = 9.0 Hz), 4.63 (s, 2H), 3.84 (s, 3H), 2.40 (s, 3H).; ¹³C{¹H} NMR (CDCl₃ + DMSOd₆, 100 MHz) δ 186.4, 164.6, 145.4, 135.9, 132.0, 129.9, 129.0, 128.6, 114.2, 63.6, 55.7, 21.8; IR (KBr, cm⁻¹): 3006, 2925, 1665, 1433, 1010; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₆H₂₀NO₄S, [M + NH₄]⁺: 305.0842, found 305.0861.

1-(4-Fluorophenyl)-2-tosylethanone (5a):



Yield: 79% (115 mg) as white solid; m.p 142-144; ¹H NMR (CDCl₃, 500 MHz) δ 8.01 – 7.98 (m, 2H), 7.75 (d, 2H, *J* = 8.0 Hz), 7.34 (d, 2H, *J* = 8.0 Hz,), 7.16 (t, 2H, *J* = 8.5 Hz), 4.68 (s, 2H), 2.45 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 186.8, 167.7 (d, *J* = 256.1 Hz), 145.7, 135.8, 132.8, 132.5 (d, *J* = 9.3 Hz), 130.1, 128.8, 116.3 (d, *J* = 22.0 Hz), 64.0, 21.9; ¹⁹F NMR (CDCl₃, 471

MHz) δ –102.4; IR (KBr, cm⁻¹): 3063, 2950, 2919, 1677, 1413, 1153, 1089; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₄FO₃S, [M + H]⁺: 293.0642, found 293.0648.

1-(3-Chlorophenyl)-2-tosylethan-1-one (7a):



Yield: 78% (120 mg) as yellow solid; m.p 125-127 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.85 (d, 2H, *J* = 8.0 Hz), 7.75 (d, 2H, *J* = 8.2 Hz), 7.58 (d, 1H, *J* = 8.1 Hz), 7.44 (t, 1H, *J* = 7.8 Hz), 7.34 (d, 2H, *J* = 8.0 Hz), 4.68 (s, 2H), 2.45 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 187.0, 145.6, 137.2, 135.6, 135.3, 134.2, 130.1, 129.9, 129.1, 128.6, 127.5, 63.7, 21.7; IR (KBr, cm⁻¹): 3003, 2920, 1685, 1421, 1165, 1089; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₄O₃SCl, [M + H]⁺: 309.0347, found 309.0359.

1-(4-Bromophenyl)-2-tosylethanone (9a):



Yield: 80% (141 mg) as white solid; mp145–147 °C; ¹H NMR (CDCl₃, 400 MHz) δ 7.82 (d, 2H, *J* = 8.4 Hz), 7.74 (d, 2H, *J* = 8.4 Hz), 7.63 (d, 2H, *J* = 8.8 Hz), 7.34 (d, 2H, *J* = 8.0 Hz), 4.67 (s, 2H), 2.45 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 100 MHz) δ 187.5, 145.8, 135.7, 134.7, 132.4, 131.0, 130.2, 130.1, 128.7, 63.9, 21.9; IR (KBr, cm⁻¹): 3009, 2916, 1678, 1403, 1399, 1301, 1095; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₇BrNO₃S, [M + NH₄]⁺: 352.9842, found 352.9820.

1-(4-Nitrophenyl)-2-tosylethanone (10a):



Yield: 75% (120 mg) as white solid; mp 145–147 °C; ¹H NMR (CDCl₃, 500 MHz) δ 8.34 (d, 2H, *J* = 9.0 Hz), 8.15 (d, 2H, *J* = 8.5 Hz), 7.74 (d, 2H, *J* = 8.0 Hz), 7.37 (d, 2H, *J* = 8.0 Hz), 4.74 (s, 2H), 2.47 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 187.2, 151.1, 146.1, 140.2, 135.6, 130.7, 130.3, 128.7, 124.2, 64.4, 22.0; IR (KBr, cm⁻¹): 3063, 2943, 1690, 1155, 1079; HRMS (ESI/Q-

TOF) (m/z): calcd for $C_{15}H_{13}$ NO₅SNa [M + Na]⁺: 342.0407, found 342.0389.

1-(2-Nitrophenyl)-2-tosylethanone (11a):



Yield: 73% (117 mg) as white solid; mp 139–141 °C; ¹H NMR (CDCl₃, 500 MHz) δ 8.15 (d, 1H, *J* = 8.5 Hz), 7.81 – 7.77 (m, 3H), 7.69 – 7.63 (m, 2H), 7.38 (d, 2H, *J* = 8.0 Hz), 4.59 (s, 2H), 2.47 (s, 3H).; ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 190.1, 145.9, 145.5, 136.6, 136.1, 135.1, 131.7, 130.2, 129.3, 128.6, 124.4, 67.1, 21.9; IR (KBr, cm⁻¹): 3063, 2926, 2855, 1708, 1345, 1152, 1002; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₃ NO₅SNa [M + Na]⁺: 342.0407, found 342.0417.

1-(Thiophen-2-yl)-2-tosylethanone (12a):



Yield: 74% (104 mg) as dark brown solid; mp 123–125 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.81 (d, 1H, *J* = 4.0 Hz,), 7.75 (t, 3H, *J* = 8.0 Hz), 7.34 (d, 2H, *J* = 8.0 Hz), 7.17 (t, 1H, *J* = 4.5 Hz), 4.60 (s, 2H), 2.44 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 180.5, 145.7, 143.4, 136.6, 135.7, 135.4, 130.0, 128.9, 128.8, 65.0, 21.9; IR (KBr, cm⁻¹): 3093, 2955, 2919, 1655, 1410, 1357, 1139, 1080; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₃H₁₃O₃S₂, [M + H]⁺: 281.0301, found 281.0314.

1-(Furan-2-yl)-2-tosylethanone (13a):



Yield: 72% (95 mg) as white solid, mp 116–118 °C; ¹H NMR (CDCl₃, 400 MHz,) δ 7.76 (d, 2H, J = 8.4 Hz), 7.61 (dd, 1H, $J_1 = 1.6$ Hz, $J_2 = 0.8$ Hz), 7.34 – 7.32 (m, 3H), 6.58 (dd, 1H, $J_1 = 3.6$ Hz, $J_2 = 2.0$ Hz), 4.56 (s, 2H), 2.44 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 100 MHz) δ 176.1, 152.1, 148.3, 145.6, 135.9, 130.0, 128.78, 120.6, 113.4, 63.8, 21.9; IR (KBr, cm⁻¹): 3015, 2985, 2930, 1644,

1462, 1310, 1149, 1083, 1012; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₃H₁₃O₄S [M + H]⁺: 265.0529, found 265.0479.

1-(2-Hydroxy-5-methoxyphenyl)-2-tosylethan-1-one (14a):



Yield: 64% (103 mg) as brown solid; mp 108–110 °C; ¹H NMR (CDCl₃, 400 MHz) δ 12.28 (s, 1H), 7.35 (d, 2H, *J* = 8.0 Hz), 7.17 (dd, 2H, *J*₁ = 6.8 Hz, *J*₂ = 3.2 Hz), 6.93 (d, 1H, *J* = 9.6), 4.69 (s, 2H), 3.81 (s, 3H), 2.46 (s, 3H).; ¹³C{¹H} NMR (CDCl₃, 100 MHz) δ 193.0, 158.2, 152.2, 145.9, 135.6, 130.2, 128.8, 126.9, 119.8, 113.3, 64.4, 56.2, 21.9; IR (KBr, cm⁻¹): 3341, 2957, 1638, 1461, 1084; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₆H₁₇O₅S, [M + H]⁺: 321.0791 found 321.0747.

1-(Naphthalen-2-yl)-2-tosylethanone (15a):



Yield: 71% (116 mg) as white solid; mp 150–152 °C; ¹H NMR (CDCl₃, 400 MHz) δ 8.45 (s, 1H), 9.97 (d, 1H, J = 1.6Hz), 7.95 (d, 1H, J = 1.6 Hz), 7.88 (d, 2H, J₁ = 8.8 Hz, J₂ = 4.0 Hz), 7.77 (d, 2H, J = 8.4 Hz), 7.66-7.62 (m, 1H), 7.60-7.56 (m, 1H), 7.31 (d, 2H, J = 8.0 Hz), 4.84 (s, 2H), 2.41 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 100 MHz) δ 188.2, 145.6, 136.2, 135.9, 133.3, 132.5, 132.4, 130.1, 130.0, 129.6, 129.0, 128.8, 128.0, 127.3, 124.1, 64.0, 21.9; IR (KBr, cm⁻¹): 3027, 2931, 1674, 1627, 1448, 1150, 1089, 1012; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₉H₁₇O₃S, [M + H]⁺: 325.0893, found 325.0870.

1-(Benzo[d][1,3]dioxol-5-yl)-2-tosylethanone (16a):



Yield: 70% (111 mg) as white solid; mp 156-158 °C; ¹H NMR (CDCl₃, 400 MHz) δ 7.75 (d, 2H, J = 8.4 Hz) 7.58 (dd, 1H, $J_1 = 8.2$, Hz, $J_2 = 1.8$ Hz), 7.39 (d, 1H, J = 1.8 Hz), 7.34 (d, 2H, J = 8.0 Hz), 6.87 (d, 1H, J = 8.2 Hz), 6.07 (s, 2H), 4.63 (s, 2H), 2.44 (s, 3H);

¹³C{¹H} NMR (CDCl₃, 100 MHz) δ 186.1, 153.2, 148.7, 145.5, 135.9, 130.9, 130.0, 128.8, 127.0, 108.7, 108.3, 102.4, 63.8, 21.9; IR (KBr, cm⁻¹): 3068, 3008, 2954, 1656, 1446, 1146, 1082; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₆H₁₅O₅S, [M + H]⁺: 319.0635, found 319.0605.

(S)-2-Tosyl-3,4-dihydronaphthalen-1(2H)-one (17a):



Yield: 60% (90 mg) as brown solid; mp 120-122 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.98 (d, 1H, J = 8.0 Hz), 7.79 (d, 2H, J = 8.5 Hz,), 7.53-7.49 (m, 1H), 7.36 (d, 2H, J = 8.0 Hz), 7.31 (t, 1H, J = 7.5 Hz), 7.27 (s, 1H), 4.08 (t, 1H, J = 5.5 Hz), 3.55 – 3.49 (m, 1H), 3.01 – 2.95 (m, 1H), 2.89-2.83 (m, 1H), 2.68-2.61 (m, 1H), 2.46 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 189.0, 145.3, 143.8, 136.2, 134.7, 132.0, 129.9, 129.3, 129.1, 128.2, 127.2, 69.9, 26.8, 23.9, 21.9; IR (KBr, cm⁻¹): 2957, 2921, 1675, 1434, 1167, 1080; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₇H₁₇OS, [M + H]⁺: 301.0893, found 301.0872.

2-Tosylcyclohexan-1-one (18a):



Yield: 54% (68 mg) as gummy; mp 92-94 °C; ¹H NMR (CDCl₃, 400 MHz) δ 7.58 (d, 2H, *J* = 8.0 Hz), 7.31 (d, 2H, *J* = 8.0 Hz,), 4.11-4.05 (m, 1H), 2.41 (s, 3H), 1.26-1.23 (m, 8H); ¹³C{¹H} NMR (CDCl₃, 100 MHz) δ 204.9, 142.8, 142.1, 129.8, 125.4, 60.9, 29.86, 21.6, 15.7, 14.9, 14.2.; IR (KBr, cm⁻¹): 2987, 2931, 1715, 1424, 1157, 1074; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₃H₁₆O₃S, [M + H]⁺: 253.0893, found 253.0872.

1-Phenyl-2-(phenylsulfonyl)ethanone (1b):



Yield: 71% (92 mg) as white solid, mp 117-119 °C; ¹H NMR (CDCl₃, 500 MHz,) δ 7.94 (d, 2H, J = 8.0 Hz), 7.90 (d, 2H, J = 7.5 Hz), 7.68 -7.60 (m, 2H), 7.56 (t, 2H, J = 7.5 Hz), 7.49 (t, 2H, J = 7.5 Hz), 4.73 (s, 2H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 187.9,

138.8, 135.7, 134.3, 134.2, 129.3, 129.2, 128.8, 128.6, 63.5; IR (KBr, cm⁻¹): 3031, 2942, 1668, 1451, 1151, 1020; HRMS (ESI/Q-TOF) (m/z): calcd for $C_{14}H_{16}NO_3S$, $[M + NH_4]^+$: 261.0580, found 261.0597.

2-((4-Chlorophenyl)sulfonyl)-1-phenylethanone (1c):



Yield: 72% (106 mg) as white solid; mp 134–136 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.94 (d, 2H, *J* = 7.5 Hz), 7.84 (d, 2H, *J* = 8.5 Hz), 7.65 (t, 1H, *J* = 7.5 Hz), 7.53-7.48 (m, 4H), 4.73 (s, 2H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 188.0, 141.1, 137.1, 135.6, 134.5, 130.2, 129.5, 129.2, 129.0, 63.4; IR (KBr, cm⁻¹): 3045, 2930, 2861, 1689, 1448, 1089; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₄H₁₂ClO₃S, [M + H]⁺: 295.019, found 295.023.

2-(4-Bromophenylsulfonyl)-1-phenylethanone (1d):

Yield: 68% (115 mg) as white solid; mp 128–130 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.93 (d, 2H, *J* = 8.0 Hz), 7.76 (d, 2H, *J* = 8.5 Hz), 7.69 (d, 2H, *J* = 8.5 Hz), 7.65 (t, 1H, *J* = 7.5 Hz), 7.51 (t, 2H, *J* = 7.7 Hz), 4.73 (s, 2H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 187.8, 137.7, 135.6, 134.5, 132.5, 130.2, 129.7, 129.2, 129.0, 63.3; IR (KBr, cm⁻¹): 3354, 2901, 1673, 1565, 1461, 1399, 1308, 1200, 1135, 1055, 1001, 820, 770, 691; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₄H₁₂BrO₃S, [M + H]⁺: 338.9685, found 338.9664.

2-(Methylsulfonyl)-1-phenylethanone (1e):

Yield: 59% (58 mg) as brown solid; mp 116–118 °C; ¹H NMR (CDCl₃, 500 MHz,) δ 8.01 (d, 2H, *J* = 8.0 Hz), 7.67 (t, 1H, *J* = 7.2 Hz), 7.54 (t, 2H, *J* = 7.5 Hz), 4.60 (s, 2H), 3.16 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 189.1, 135.7, 135.0, 129.2, 129.0, 61.3, 42.0; IR (KBr, cm⁻¹): 3027, 2920, 1673, 1450, 1149, 981; HRMS (ESI/Q-TOF) (m/z): calcd for C₉H₁₀O₃SNa, [M + Na]⁺: 221.0243, found 221.0209.

Yield: 73% (100 mg) as white solid; mp 120-122; ¹H NMR (CDCl₃, 500 MHz) δ 7.89 (d, 2H, *J* = 7.3 Hz), 7.84 (d, 2H, *J* = 8.1 Hz), 7.66 (t, 1H, *J* = 8.0 Hz), 7.55 (t, 2H, *J* = 7.8 Hz,), 7.27 (t, 2H, *J* = 8.5 Hz), 4.71 (s, 2H), 2.42 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 126 MHz) δ 187.7, 145.8, 139.0, 134.4, 133.6, 129.8, 129.7, 129.4, 128.8, 63.7, 22.0; IR (KBr, cm⁻¹): 3014, 2927, 1675, 1451, 1109, 1078; calcd for C₁₅H₁₅O₃S, [M + H]⁺: 275.0736, found 275.0743.

1-(4-bromophenyl)-2-(thiophen-2-ylsulfonyl)ethan-1-one (9f):

Yield: 64% (111 mg) as white solid; mp 115–117 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.82 (d, 2H, 8.5 Hz), 7.76 (d, 1H, *J* = 5 Hz), 7.68 (d, 1H, 3.5 Hz), 7.64 (d, 2H, *J* = 8.5 Hz), 7.15 (t, 1H, *J* = 4.25 Hz), 4.78 (s, 2H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 187.0, 139.2, 135.5, 135.1, 134.4, 132.3, 130.7, 130.1, 128.0, 64.5; IR (KBr, cm⁻¹): 3082, 2945, 2929, 1657, 1400, 1143, 1047; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₂H₉BrO₃S₂Na, [M + Na]⁺: 366.9069, found 366.9081.

2-(4-Bromophenylsulfonyl)-1-(thiophen-2-yl)ethanone (12d):

Yield: 66% (114 mg) as white solid; mp 118–120 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.81 (d, 1H, *J* = 3.5 Hz), 7.78 – 7.74 (m, 3H), 7.70 (d, 2H, *J* = 8.0 Hz), 7.19 (t, 1H, *J* = 3.75 Hz), 4.63 (s, 2H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 180.0, 143.0, 137.4, 136.7, 135.2, 132.5, 130.2, 129.9, 128.8, 64.4; IR (KBr, cm⁻¹): 3088, 2952, 2920, 1653, 1408, 1150, 1060; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₂H₉BrO₃S₂Na, [M + Na]⁺: 366.9069, found 366.9055.

1-(p-Tolyl)-2-tosylethan-1-one (16b):

Yield: 65% (99 mg) as brown gummy; mp 134-136 °C; ¹H NMR (CDCl₃, 400 MHz) δ 7.89 (d, 1H, J = 7.2 Hz), 7.69 – 7.64 (m, 1H), 7.57 (dd, 3H, J_1 = 8.2 Hz, J_2 = 1.6 Hz), 7.39 (d, 1H, J = 2.0 Hz), 6.87 (d, 1H, J = 8.4 Hz), 6.07 (s, 2H), 5.30 (s, 1H), 4.65 (s, 2H);

¹³C{¹H} NMR (CDCl₃, 100 MHz) δ 186.0, 153.3, 148.7, 138.9, 134.4, 130.9, 129.4, 128.8, 127.0, 108.7, 108.3, 102.4, 63.7; IR (KBr, cm⁻¹): 3332, 3003, 2917, 1667, 1442, 1149, 1033; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₂O₅SNa, [M + Na]⁺: 327.0298, found 327.0307.

(S)-2-(Phenylsulfonyl)-3,4-dihydronaphthalen-1(2H)-one (17b):

Yield: 58% (83 mg) as a reddish gummy; mp 99-101 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.99 (d, 1H, *J* = 8.0 Hz), 7.93 (d, 2H, *J* = 7.0 Hz), 7.69 (t, 1H, *J* = 7.5 Hz), 7.59 (t, 3H, *J* = 8.0 Hz), 7.53-7.50 (m, 1H),7.33 (t, 1H, *J* = 7.5 Hz), 4.12 (t, 1H, *J* = 6.0 Hz), 3.54-3.48 (m, 1H), 3.02-2.97 (m, 1H), 2.90-2.84 (m, 1H), 2.70-2.63 (m, 1H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 188.8, 143.8, 139.2, 134.7, 134.2, 132.0, 129.3, 129.2, 129.16, 128.2, 127.3, 69.9, 26.8, 23.8; IR (KBr, cm⁻¹): 3064, 2924, 1680, 1448, 1237, 1142, 1083; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₆H₁₅O₃S, [M + H]⁺: 287.0736, found 287.0730.

((2-Iodo-2-phenylvinyl)sulfonyl)-4-methylbenzene (B):

Obtained as brown solid; mp 78–80 °C; ¹H NMR (CDCl₃, 500 MHz): δ , 7.39 (d, 2H, J = 8.0 Hz), 7.28 (s, 1H), 7.23 (dd, 3H, $J_1 = 10.0$ Hz, $J_2 = 8.0$ Hz), 7.16 (d, 2H, J = 7.0 Hz), 7.11 (d, 2H, J = 7.5 Hz), 2.31 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 144.8, 141.5, 139.9, 137.5, 129.9, 129.86, 128.1, 128.07, 127.9, 114.3, 21.82.; IR (KBr, cm⁻¹): 3038, 2923, 2847, 1585, 1443, 1149, 1084; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₃IO₂S, [M + H]⁺: 384.9754, found 384.9750.

2,6-Di-tert-butyl-4-(tosylmethyl)phenol (M):

Yield: 61%, (115 mg, with phenylacetylene), 75% (141 mg, with acetophenone) as white solid, mp 101–103 °C; ¹H NMR (CDCl₃, 500 MHz) δ 7.44 (d, 2H, *J* = 8.5 Hz), 7.21 (d, 2H, *J* = 8.0 Hz), 6.73
(s, 2H), 5.23 (s, 1H), 4.19 (s, 2H), 2.40 (s, 3H), 1.32 (s, 18H).; $^{13}C\{^{1}H\}$ NMR (CDCl₃, 125 MHz) δ 154.4, 144.5, 136.2, 135.2, 129.5, 129.1, 127.9, 119.2, 63.5, 34.2, 30.2, 21.7.; IR (KBr, cm⁻¹): 3629, 3583, 2950, 1598, 1441, 1311, 1295, 1148, 1082; HRMS (ESI/Q-TOF) (m/z): calcd for C₂₂H₃₀O₃S, [M + Na]⁺: 397.1808, found 397.1787.

6-Chloro-2,4-diphenyl-3-tosylquinoline (P):



Yield: 73% (51 mg) as light greenish yellow solid; mp 288-290 °C; ¹H NMR (CDCl₃, 500 MHz) δ 8.11 (d, 1H, *J* = 9.0 Hz), 7.74 (dd, 1H, *J*₁ = 9.0 Hz, *J*₂ = 2.5 Hz), 7.55 (d, 2H, *J* = 6.5 Hz), 7.49 (t, 1H, *J* = 7.5 Hz), 7.43 – 7.39 (m, 4H), 7.39 – 7.35 (m, 2H), 7.25 (t, 2H, *J* = 7.0 Hz), 6.94 (d, 2H, *J* = 8.0 Hz), 6.87 (d, 2H, *J* = 8.0 Hz), 2.30 (s, 3H).; ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 158.3, 150.6, 146.2, 143.3, 140.9, 139.0, 134.5, 134.49, 133.9, 133.1, 131.3, 130.3, 129.6, 129.1, 129.06, 128.9, 128.2, 128.0, 127.6, 127.4, 126.2, 21.7; IR (KBr, cm⁻¹): 3037, 2952, 2922, 2853, 1538, 1467, 1153, 1078; HRMS (ESI/Q-TOF) (m/z): calcd for C₂₈H₂₁ClNO₂S, [M + H]⁺: 470.0976, found 470.0998.

(E)-1-phenyl-2-tosylethanone oxime (Q):



Yield: 69% (200 mg) as white solid; mp ¹H NMR (DMSO-d₆, 500 MHz) δ 11.73 (s, 1H), 7.64 (q, 4H, $J_1 = 10.0$ Hz, $J_2 = 6.4$ Hz), 7.35 (t, 5H, J = 5.5 Hz), 4.92 (s, 2H), 2.37 (s, 3H).; ¹³C{¹H} NMR (DMSO-d₆, 125 MHz) δ 145.7, 144.4, 136.9, 134.6, 129.5, 129.0, 128.2, 127.9, 126.4, 51.5, 21.12; IR (KBr, cm⁻¹): 3275, 3184, 3054, 1635, 1464, 1380, 1147, 1054; HRMS (ESI/Q-TOF) (m/z): calcd for C₁₅H₁₆NO₃S, [M + H]⁺: 290.0845, found 290.081



1-Phenyl-2-tosylethanone (1a): ¹H NMR (CDCl₃, 400 MHz)

1-Phenyl-2-tosylethanone (1a): ¹³C{¹H} NMR (CDCl₃, 100 MHz)



1-(p-Tolyl)-2-tosylethan-1-one (2a):¹H NMR (CDCl₃, 500 MHz)







1-(p-Tolyl)-2-tosylethan-1-one (2a):¹³C¹_{¹H} NMR (CDCl₃, 125 MHz)

1-(4-(tert-Butyl)phenyl)-2-tosylethan-1-one (3a): ¹H NMR (CDCl₃, 500 MHz)











S43



1-(4-Methoxyphenyl)-2-tosylethan-1-one (4a): ¹H NMR (CDCl₃, 400 MHz)



1-(4-Methoxyphenyl)-2-tosylethan-1-one (4a): ¹³C{¹H} NMR (CDCl₃, 100 MHz)



1-(4-Fluorophenyl)-2-tosylethan-1-one (5a): ¹H NMR (CDCl₃, 500 MHz)



1-(4-Fluorophenyl)-2-tosylethan-1-one (5a): ¹³C{¹H} NMR (CDCl₃, 125 MHz)



1-(4-Fluorophenyl)-2-tosylethan-1-one (5a): ¹⁹F NMR (CDCl₃, 471 MHz)











1-(3-Fluorophenyl)-2-tosylethan-1-one (6a): ¹³C{¹H} NMR (CDCl₃, 100 MHz)





20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -11 f1 (ppm)	10 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22















7,859 7,741 7,741 7,593 7,593 7,593 7,593 7,454 7,428 7,428 7,428 7,428 7,428 7,428 7,428 7,428 7,428





____2.453





1-(4-Bromophenyl)-2-(methylsulfonyl)ethan-1-one (9a): ¹H NMR (CDCl₃, 500 MHz)





-4.665





1-(4-Nitrophenyl)-2-tosylethan-1-one (10a): ¹H NMR (CDCl₃, 500 MHz)

-2.466 -2.466 -2.466























-2.440















210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 f1 (ppm)



1-Phenyl-2-(phenylsulfonyl)ethanone (1b): ¹H NMR (CDCl₃, 500 MHz)





2-(4-Chlorophenyl)sulfonyl)-1-phenylethanone (1c):¹H NMR (CDCl₃, 500 MHz)







2-(4-Bromophenylsulfonyl)-1-phenylethanone (1d): ¹H NMR (CDCl₃, 500 MHz)







2-(4-Bromophenylsulfonyl)-1-phenylethanone (1d): ¹³C{¹H} NMR (CDCl₃, 125 MHz)

-188.094

916 7532 7532 7532 753 753 753 753 7753 775	84 76 71
37.5 332.1 29.52	6.97 3.5





.016

586 567







-3.161


2-(Methylsulfonyl)-1-phenylethanone (1e):¹³C¹_lH} NMR (CDCl₃, 100 MHz)







2-(Phenylsulfonyl)-1-(p-tolyl)ethan-1-one (2b): ¹³C{¹H} NMR (CDCl₃, 125 MHz)

2-((4-Chlorophenyl)sulfonyl)-1-(4-methoxyphenyl)ethan-1-one (4c): ¹H NMR (CDCl₃, 500 MHz)





2-((4-Chlorophenyl)sulfonyl)-1-(4-methoxyphenyl)ethan-1-one (4c): ¹³C{¹H} NMR (CDCl₃, 125 MHz)

1-(4-Fluorophenyl)-2-(phenylsulfonyl)ethanone (5b):¹H NMR (CDCl₃, 500 MHz)





1-(4-Fluorophenyl)-2-(phenylsulfonyl)ethanone (5b):¹³C{¹H} NMR (CDCl₃, 125 MHz)





-5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 fl (ppm)







2-(4-Bromophenylsulfonyl)-1-(thiophen-2-yl)ethanone (12d): ¹³C{¹H} NMR (CDCl₃, 125 MHz)

With Acetophenone:

1-Phenyl-2-tosylethanone (1a): ¹H NMR (CDCl₃, 400 MHz)





1-Phenyl-2-tosylethanone (1a): ¹³C{¹H} NMR (CDCl₃, 100 MHz)



1-(p-Tolyl)-2-tosylethan-1-one (2a): ¹H NMR (CDCl₃, 400 MHz)

Z 7.389 Z 7.839 Z 7.839 Z 7.344 Z 7.344 Z 7.324 Z 7.324 Z 7.324 Z 7.324





<2.444 <2.426



1-(p-Tolyl)-2-tosylethan-1-one (2a): ¹³C{¹H} NMR (CDCl₃, 100 MHz)



1-(4-Methoxyphenyl)-2-tosylethan-1-one (4a): ¹H NMR (CDCl₃, 400 MHz)



1-(4-Methoxyphenyl)-2-tosylethan-1-one (4a):¹³C{¹H} NMR (CDCl₃, 100 MHz)





-2.451







1-(4-Fluorophenyl)-2-tosylethanone (5a): ¹³C{¹H} NMR (CDCl₃, 125 MHz)















1-(3-Chlorophenyl)-2-tosylethan-1-one (6a): ¹³C¹_lH} NMR (CDCl₃, 125 MHz)

1-(4-Bromophenyl)-2-tosylethanone (9a): ¹H NMR (CDCl₃, 400 MHz)







-2.448





1-(4-Nitrophenyl)-2-tosylethanone (10a): ¹H NMR (CDCl₃, 500 MHz)







-2.466







1-(2-Nitrophenyl)-2-tosylethanone (11a):¹H NMR (CDCl₃, 500 MHz)

1-(2-Nitrophenyl)-2-tosylethanone (11a):¹³C{¹H} NMR (CDCl₃, 125 MHz)





















1-(Furan-2-yl)-2-tosylethanone (13a): ¹³C{¹H} NMR (CDCl₃, 100 MHz)

1-(2-Hydroxy-5-methoxyphenyl)-2-tosylethan-1-one (14a): ¹H NMR (CDCl₃, 400 MHz)





1-(2-Hydroxy-5-methoxyphenyl)-2-tosylethan-1-one (14a): ¹³C{¹H} NMR (CDCl₃, 100 MHz)

1-(Naphthalen-2-yl)-2-tosylethanone (15a): ¹H NMR (CDCl₃, 400 MHz)





1-(Naphthalen-2-yl)-2-tosylethanone (15a): ¹³C{¹H} NMR (CDCl₃, 100 MHz)






1-(Benzo[d][1,3]dioxol-5-yl)-2-tosylethanone (16a):¹³C{¹H} NMR (CDCl₃, 100 MHz)

(S)-2-Tosyl-3,4-dihydronaphthalen-1(2H)-one (17a):¹³C{¹H} NMR (CDCl₃, 500 MHz)











2-Tosylcyclohexan-1-one (18a): ¹H NMR (CDCl₃, 400 MHz)



2-Tosylcyclohexan-1-one (18a): ¹³C{¹H} NMR (CDCl₃, 100 MHz)



1-Phenyl-2-(phenylsulfonyl)ethanone (1b): ¹H NMR (CDCl₃, 500 MHz)





1-Phenyl-2-(phenylsulfonyl)ethanone (1b): ¹³C{¹H} NMR (CDCl₃, 125 MHz)



2-(4-Chlorophenyl)sulfonyl)-1-phenylethanone (1c):¹H NMR (CDCl₃, 500 MHz)









2-(4-Chlorophenyl)sulfonyl)-1-phenylethanone (1c):¹³C{¹H} NMR (CDCl₃, 125 MHz)

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)

2-(4-Bromophenylsulfonyl)-1-phenylethanone (1d): ¹H NMR (CDCl₃, 500 MHz)







2-(4-Bromophenylsulfonyl)-1-phenylethanone (1d): ¹³C{¹H} NMR (CDCl₃, 125 MHz)







2-(Methylsulfonyl)-1-phenylethanone (1e):¹³C¹_lH} NMR (CDCl₃, 125 MHz)



5.0 4.5 f1 (ppm)

4.0

3.5

3.0

1-(p-Tolyl)-2-tosylethan-1-one (2b):¹H NMR (CDCl₃, 500 MHz)

10.0

9.5

9.0

8.5

8.0

7.5

7.0

6.5

6.0

5.5

2.5

2.0

1.5

1.0

0.5

0.0





1-(4-bromophenyl)-2-(thiophen-2-ylsulfonyl)ethan-1-one (9f): ¹H NMR (CDCl₃, 500 MHz)

7,829 7,739 7,631 7,636 7,636 7,145 7,145 7,145





1-(4-bromophenyl)-2-(thiophen-2-ylsulfonyl)ethan-1-one (9f): ¹³ C {¹/₄H} NMR (CDCl₃, 125 MHz)

135,518 135,518 135,518 135,518 135,518 135,130 136,130 130,136





2-(4-Bromophenylsulfonyl)-1-(thiophen-2-yl)ethanone) (12d):¹H NMR (CDCl₃, 500 MHz)







1-(Benzo[d][1,3]dioxol-5-yl)-2-(phenylsulfonyl)ethan-1-one (16b):¹H NMR (CDCl₃, 400 MHz)





1-(Benzo[d][1,3]dioxol-5-yl)-2-(phenylsulfonyl)ethan-1-one (16b): ¹³C{¹H} NMR (CDCl₃, 100 MHz)

(R)-2-(Phenylsulfonyl)-3,4-dihydronaphthalen-1(2H)-one (17b): ¹H NMR (CDCl₃, 500 MHz)







2-Iodo-2-phenylvinyl)sulfonyl)-4-methylbenzene (B):¹H NMR (CDCl₃, 400 MHz)







2-Iodo-2-phenylvinyl)sulfonyl)-4-methylbenzene (B): ¹³C¹_lH} NMR (CDCl₃, 125 MHz)





2,6-Di-tert-Butyl-4-(tosylmethyl)phenol (M):¹H NMR (CDCl₃, 500 MHz)

2,6-Di-tert-Butyl-4-(tosylmethyl)phenol (M):¹³C{¹H} NMR (CDCl₃, 125 MHz)

























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