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Supporting Information

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1. Experimental procedure

General methods

All reactions were carried out under nitrogen atmosphere, with dry, freshly distilled solvents. All chemicals (2-hydroxy-1,4-naphthoquinone, 5-hydroxy-1,4-naphthoquinone, alkynes, sulfonyl chlorides, metal salts and NH₄Y) were used as commercially available without further purification unless otherwise noted. NMR spectra were registered on Bruker DRX spectrometer operating at 300 & 400 MHz for ¹H and 75 &100 MHz for ¹³C. All ¹H NMR and ¹³C NMR spectra were measured in CDCl₃ with TMS as the internal standard. High resolution mass spectra were obtained by Orbitrap Elite. Purifications by column chromatography were performed on 60-120 mesh silica gel. The XRD pattern of the catalyst samples was measured with a PW3050/60 (XPERT-PRO Diffractometer system) instrument using a Cu K α radiation at room temperature. Sulfonyl azides ¹ were prepared according to the published methods.

Preparation of Cu^I-Y zeolite

Cu^I -Y zeolite was prepared according to the reported procedure by Li et al.² A mixture of CuCl and HY (obtained from deammonification of NH₄Y at 450°C for 6h) was ground by pestle and mortar, it was heated in flowing nitrogen atmosphere at a heating rate of 10°C/min. The ion-exchange of Cu(I) in solid CuCl with H⁺ in HY zeolite occurred at over 300°C and the maximum ion-exchange rate was reached at 340°C with the consequent release of HCl gas. Cu^I -Y was prepared at two different temperatures *via* heating the mixture of CuCl/HY at 350°C for 15 h and 450°C for 6 h under nitrogen atmosphere. After the preparation was over, the Cu^I -Y was kept under high vacuum. The prepared Cu^I -Y zeolite was characterized by powder XRD, and EDX which was found to be in good agreement with the literature.³ The total copper content in the samples was determined by EDX analysis and it was found to be 13.09 wt% (Fig S2).



Figure S1. Powder XRD pattern of Cu^I Y zeolite



Element	AN	Series	[wt.%]	[norm. wt.%]	[norm. at.%]	Error in wt.% (1 Sigma)
Oxygen	8	K- Series	54.47932	51.35877	65.27364	7.017194
Silicon	14	K- Series	23.17572	21.84822	15.81834	1.066766
Carbon	12	K- Series	4.961082	4.676914	7.917848	1.456259
Aluminium	13	K- Series	9.572342	9.024042	6.800821	0.5178
Copper	29	K- Series	13.88753	13.09205	4.189349	0.387437
		Sum:	106.076	100.00	100.00	

Figure S2. EDX spectrum of Cu^I Y zeolite



Figure S3. Ultra Violet- Diffuse Reflectance spectrum of Cu^IY zeolite

General procedure for the synthesis of naphtho[2,1-*b*]furan-2,5-diones

A solution of alkyne (1.0 mmol) was added slowly to a mixture of Cu^IY- zeolite (10 mol%), sulfonyl azide (1.0 mmol), 2-hydroxy-1,4-naphthoquinone (1.0 mmol), triethylamine (2.0 mmol) and 4Å molecule sieves (100 mg) taken in 3 mL of 1,4-dioxane under nitrogen atmosphere at room temperature for the 30 minutes, after the completion of reaction the 1,4-dioxane was evaporated under reduced pressure then reaction mixture was diluted with ethyl acetate (5 mL). The catalyst was separated by filtration, followed by solvent evaporation under reduced pressure, the resulting crude product was finally purified by column chromatography by using silica gel (60-120 mesh), ethyl acetate and petroleum ether mixture (5%). The recovered catalyst was thoroughly washed with ethyl acetate and used it for next run.

The crystal structures of compound **4a** has been deposited at the Cambridge Crystallographic Data Centre and allocated the deposition number **CCDC 1465059**.



General procedure for the synthesis of benzo[de]chromene-2,6-diones

A solution of alkyne (1.0 mmol) was added slowly to a mixture of Cu^{I} Yzeolite (10 mol %), sulfonyl azide (1.0 mmol), 5-hydroxy-1,4-naphthoquinone (1.0 mmol), triethylamine (2.0 mmol) and 4Å molecule sieves (100 mg) taken in 3 mL of 1,4-dioxane under nitrogen atmosphere at room temperature for the 1 h, after the completion of reaction the 1,4-dioxane was evaporated under reduced pressure then reaction mixture was diluted with ethyl acetate (5 mL). The catalyst was separated by filtration, followed by solvent evaporation under reduced pressure, the resulting crude product was finally purified by column chromatography by using silica gel (60-120 mesh), ethyl acetate and petroleum ether mixture (5%).

The crystal structures of compound **7d** has been deposited at the Cambridge Crystallographic Data Centre and allocated the deposition number **CCDC 1456377**.



Table 1. Optimization in sulfonyl azides. ^a

$1 + $ 2 3 $Conditions$ $Conditions$ $4a$ SO_2NH_2 $Conditions$ 5					
Entry	R		Yield(%) ^b		
1	$4-CH_3-C_6H_{4-}$	2a	63		
2	C ₆ H ₅ -	2b	56		
3	$4-NO_2-C_6H_4-$	2c	36		
4	2,4,5-Cl ₃ -C ₆ H ₂ -	2e	52		
5	$4-Br-C_6H_4-$	2d	48		
6	2-Naphthyl-	2f	31		
^a Reaction conditions: Sulfonyl azide (1.0 mmol), phenylacetylene					
(1.0 mmol), 2-hydroxy-1,4-naphthoquinone $(1.0 mmol)$, Et ₃ N (2.0					
mmol), Cu ¹ Y (10 mol%), molecular sieves (100mg), 1,4-dioxane (3.0					
mL), rt, N ₂ , 30 minutes. ^b Isolated yield.					

Table 2. Reusability of Cu^{I} Y zeolite in the cascade synthesis of naphtho[2,1-*b*]furan-2,5-dione.^a

Reuse	1st	2nd	3rd	4th			
Yield ^b	63	61	58	53			
^a Reaction conditions: Phenylacetylene (5.0 mmol, 0.6g), p-Toluenesulfonyl azide (5.0 mmol, 1.0 g), 2-							
hydroxy-1,4-naphthoquinone (5.0 mmol, 0.89 g), TEA (10 mmol, 1.35 mL), catalyst (10 mol %), 4Å							
molecular sieves (500 mg) solvent (10 ml), rt, 30 minutes. ^b Isolated yield.							

Table 3. Absorbance and florescence values of naphtho[2,1-*b*]furan-2,5-dione and benzo[de]chromene-2,6-dione derivatives

S. No	Compound	Absorbance maximum (nm)	Excitation (nm)	Emission Maximum (nm) (λ emission)
1.	4a	372	380	454,558
2.	4b	380	390	453,585
3.	4c	388	400	507,590
4.	4d	390	400	455,611
5.	4e	438	450	578
6.	4f	440	450	487,527,565
7.	4g	420	430	528,564,607
8.	4h	548	560	-
9.	4i	372	380	453,539
10.	7a	387	400	546
11.	7b	389	400	543
12.	7c	410	420	543
13.	7d	390	400	544
14.	7e	385	400	543
15.	7f	383	390	545

MTT assay studies

Liver cancer cell line Hep3B and breast cancer cell line MB231 were maintained in MEM and DMEM-Higlucose media respectively along with 10 % fetal bovine serum and other supplements (Himedia). MTT assay was performed as described earlier (Denizot and Lang, 1986).⁴ About 8000 cells were seeded per well in 96 well cell culture dishes. After 24hrs of incubation, cells were treated with seven different concentrations of drugs with DMSO as a vehicle control and further incubated for 36 hrs. Subsequently, MTT (3-(4,5-Dimethylthiazol-2-yl)-2,5-Diphenyltetrazolium Bromide) (Himedia, India) was added to the cells and incubated for 4hrs. The formed formazon was dissolved in DMSO and readings were taken calorimetrically at 570nm and 630nm. Optical density values were calculated as percentage of cell viability in comparison to the control cells.







B-231- Breast Cell line



AGS-Gastric Cell line







Hep3B Cell line

town sown town 200m 200m

120

Control

NFD-3

they tony John

MB231 Cell Line



н₃со́



Hep3B Cell line















Table 4. Cell viability results

Compound	Hep3B	MB 231	AGS
code	at	at	at
	10 µM	10 µM	10 µM
	Cell Vial	bility (%)	
4 a	94	104	88
4f	41	85	
4 i	66	89	
7a	59	94	84
7c	52	68	
7e	26	70	

Characterization Data













¹H and ¹³ C-NMR spectra and Mass analysis





























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