

Figure S1. The wild type CHO cells do not adhere to collagen I, and neither do CHO- $\alpha 2$ or CHO-wt cells adhere to plastic.

1 Materials and Methods

2 Molecular modeling

All molecules during the development process were sketched by using Sybyl 7 (Tripos Inc., St. Louis, MO, USA), and energy minimized using the Merck molecular force field (MMFF94)¹ and conjugate gradient method until the energy gradient was less than 0.05 kcal/mol. Energy minimized molecules were docked to the closed conformation of α 21 domain with Gold3.1.1.² using search area of a 15 Å radius sphere centered at the Mg²⁺ ion. Gold was selected for this study, because the scoring function has been developed by using the small molecule crystal structure data, and the metal coordination geometries are properly described. Protein structures were acquired from the PDB ³. Hydrogen atoms were added to the protein structure with Sybyl. Protonation of histidines was selected on the basis of hydrogen bonding with nearby atoms. All docking results were visually inspected by using Bodil Modeling Environment⁴.

11 Structural characterization

NMR measurements were done with Bruker Avance DRX 500 (¹H-NMR 500 MHz and ¹³C-NMR 126 MHz) using dimethylsulfoxide-d6 (DMSO-d₆) as the solvent. The mass spectrometry was done with Micromass ESI TOF spectrometer using methanol as solvent. Melting points were measured using Stuart Scientific melting point apparatus and are uncorrected. All compounds have purities >95% determined by elemental analyses (using Bruker Quantax400 EDS).

16 Cell adhesion assay

17 CHO (Chinese hamster ovarian cells), were obtained from the American type Culture Collection (ATCC). CHO cells were 18 transfected to express either wild-type (wt) human α^2 or α^1 integrin⁵⁶. Shortly, integrin α^2 cDNA was linked to pAWneo2 19 expression vector (Ohashi et al, 1985) Integrin al cDNA was linked to pcDNA3.1. Cells chosen to adhesion tests are controlled 20 to have similar integrin overexpression. In adhesion assays CHO- $\alpha 2$ or - $\alpha 1$ cells (150 000/well) were allowed to attach on rat tail 21 collagen I or on collagen IV (respectively, Becton Dickinson Labware) for 2 h at 37°C. Number of adherent cells was measured 22 with WST-1 (Roche Applied Science) according to the manufacturer's protocol. WST-1 measures the amount of live cells. The 23 stable tetrazolium salt WST-1 is cleaved to a soluble formazan that occurs primarily at the cell surface. This is dependent on the 24 production of NAD(P)H in viable cells. Therefore, the amount of formazan dye formed directly correlates to the number of 25 metabolically active cells in the culture. The EC₅₀ (concentration required for half maximal effect) and I_{max} (maximal inhibitory 26 effect) values were determined using Graph Pad Prism (Graph Pad Software Inc). Based on our previous study, sulfonamides do 27 not inhibit CHO wild type adhesion to collagen 1^7 . In addition, CHO wt cells do not adhere to collagen I, and neither do CHO- $\alpha 2$ 28 or CHO-wt cells adhere to plastic (supplementary Fig. S2). The $\alpha 2$ vs $\alpha 1$ selectivity was determined by comparing EC₅₀ values 29 of CHO- α 2 and - α 1 adhesion assays.

30 Cytotoxicity assay

S1 Cytotoxicity of compounds were measured with CytoTox-ONETM (Promega, Madison, WI, USA) by following the manufacturer's protocol. The protocol is based on determining the release of lactate dehydrogenase from cells with a damaged membrane. An enzymatic assay that converts resazurin into a fluorescent resorufin is measured after 10 minutes. The amount of fluorescent resorufin is proportional to the number of dead cells. As mentioned in Table 1, **5-20** were not toxic at $\leq 200\mu$ M, **4** was not toxic at $\leq 200\mu$ M, and **21** was not toxic at $\leq 100\mu$ M.

36 Figures

Figs. 2A, 3, and 4 were prepared by using $Bodil^4$, $Molscript v2.1.2^8$ and $Raster3D^9$.

38 Synthesis.

General procedures. Sulfonamides were synthesized with one step synthesis from commercially available starting materials. General procedure a (compounds 4-7 and 12-20; Scheme S1:a): Corresponding amine (2 mmol) and sulfonyl chloride (2.2 mmol.) were dissolved in 30 mL of acetone with 1 mL of pyridine and stirred at room temperature for 10-16 hours. 10 mL of 2 M HCl was added to the reaction mixture to precipitate crude product. Recrystallization was done from ethanol/water mixture using following procedure: Crude product was dissolved to hot 2:1 Ethanol/water mixture. Water was added to the hot mixture until short precipitation happened. The reaction mixture was cooled slowly to 4-6 °C, precipitated product was filtered of and washed

45 several time with water to give the pure product.

Methylation of sulfonamides was done using following process (general procedure **b**; compounds **8-10**; Scheme S1: b) 1 eqv. of corresponding sulphonamide (compounds **4-6**), 2 eqv of iodomethane and 3 eqv of potassium carbonate in dimethylformamide (10 mL) were stirred under nitrogen atmosphere for 72 hours. The mixture was diluted in dichloromethane and hydrolized with 10% hydrochloric acid. Water phase was extracted with dichloromethane, organic layers were combined, dried over magnesium sulfate and solvent was evaporated. Recrystallization was done from ethanol/water mixture as described above.

Preparation of sulfonates (general procedure c; compounds 11 and 21; Scheme S1:c): Corresponding phenol (2 mmol) and trethylamine (3 mmol) in 30mL of acetone. Corresponding sulfonylchloride (2 mmol) in 10mL of acetone was added drop wise to the reaction mixture. The reaction mixture was stirred with a magnetic stir bar under nitrogen gas for 5 hours. Recrystallization was done from ethanol/water mixture as described above.



Scheme 1. a) pyridine, acetone, RT 12-16h b) K2CO3, DMF, RT 70h c) triethylamine, acetone, RT 12-14h

LogP Screening

The LogP value (octanol/water partition coefficient) of a drug compound reflects the lipophilicity of the compound.

RP-LC technique (Reverse-Phase Liquid Chromatography) was used for the determination. An Agilent 1100-series HPLCsystem (Agilent Technologies, Waldbronn, Germany) with UV- and mass-selective detection was used for the measurement. The used column was a double-encapped C18-column (Zorbax XDB-C18, 3.0 mm x 100 mm, 3.5 μM, Agilent Technologies) and the mobile phase was a mixture of water and acetonitrile.

Compounds with known LogP values were used as the reference compounds. The retention times of the compounds were measured. Capacity factors (k') were calculated to generate the calibration curve (LogP versus logk'). Log P value of the compound JYV-149 was then was then extrapolated from the calibration curve.

- Capacity factor: k' = (tr t0)/t0tr= retention time of the analyte
- $t_0 = retention time of uncetained solvent$

Compound characterization data

4 General procedure a:

N-4-benzoylphenyl-2,4-dichlorobenzenesulfonamide 4: Yield 54 %; mp: 123-125 °C; ¹H NMR (500MHz, DMSO- d₆): 11.32(s, 1H), 8.14(d, 1H, J = 8.6 Hz), 7.87(d, 2H, J = 1.9 Hz), 7.67-7.61(m, 6H), 7.52(t, 2H, J = 7.8 Hz), 7.24(d, 2H, J = 8.8

- Hz); ¹³C NMR (126MHz, DMSO- d₆): 194.3, 141.0, 138.9, 137.2, 135.3, 132.9, 132.2, 131.9, 131.8, 131.5, 131.4, 129.3, 128.4,
- 128.1, 117.5; ESI-TOF-MS (m/z): $[M]^-$ calcd. for C₁₉H₁₅Cl₂NO₃S-H, 403.99; found 403.95; elemental analysis (calcd., found for

1 C₁₉H₁₃Cl₂NO₃S: C(56.17, 56.12), H(3.23, 3.26), N (3.45, 3.36).

2 3 N-3-benzoylphenyl-2,4-dichlorobenzenesulfonamide, 5: Yield 48 %; mp: 136-137 °C; ¹H NMR (500MHz, DMSO- d₆): 10.97(s, 1H), 8.00(d, 1H, J = 8.6 Hz), 7.88(d, 1H, J = 1.9 Hz), 7.69(tt, 1H, J = 7.3 Hz), 7.63-7.60(m, 3H), 7.55(t, 2H, J = 7.8 Hz), 7.69(tt, 2H, J 4 5 6 7 Hz), 7.45-7.44(m, 2H), 7.40-7.37(m, 2H); ¹³C NMR (126MHz, DMSO- d₆): 194.9, 138.8, 137.8, 137.0, 136.6, 135.3, 132.7, 131.9, 131.4, 129.6, 129.4, 128.5, 128.0, 125.2, 123.3, 120.1; ESI-TOF-MS (m/z): [M]⁻ calcd. for C₁₉H₁₅Cl₂NO₃S-H, 403.99;

found 403.95; elemental analysis (calcd., found for C₁₉H₁₅Cl₂NO₃S: C(56.17, 56.17), H(3.23, 3.16), N (3.45, 3.46).

N-(9-okso-9H-fluoren-2-yl)-2,4dichlorobenzenesulfonamide, 6: Yield 57 % mp: 186-187 °C; ¹H NMR (500MHz, DMSO- d₆): 8 9 11.05(s, 1H), 8.07(d, 1H, J = 8.6 Hz), 7.87(d, 1H, J = 2.0 Hz), 7.66-7.62(m, 3H), 7.57-7.54(m, 2H), 7.24-7.27(m, 3H); ¹³C NMR (126MHz, DMSO- d₆): 192.3, 143.5, 139.3, 138.9, 137.9, 135.5, 135.2, 134.4, 133.2, 132.8, 131.9, 128.9, 128.0, 124.9, 124.0, 10 122.1, 120.8, 114.6; ESI-TOF-MS (m/z): $[M]^-$ calcd. for $C_{19}H_{11}Cl_2NO_3S$ -H, 401.98; found 401.95; elemental analysis (calcd. ,

11 found for C₁₉H₁₁Cl₂NO₃S: C(56.45, 56.29), H(2.74, 2.78), N (3.46, 3.55). 12

N-(4-acetylphenyl)-2,4-dichlorobenzenesulfonamide, 7: Yield 47 %; mp: 204-206 °C; ¹H NMR (500MHz, DMSO- d₆): 11.27 13 (s, 1H), 8.12 (d, 1H, J = 8.6 Hz), 7.85-7.82 (m, 3H), 7.65 (dd, 1H J = 8.6 Hz, J = 2.1 Hz), 7.18 (d, 2H, J = 8.8 Hz), 2.46 (s, 3H);

14 13C NMR (126MHz, DMSO- d₆): 196.32, 141.19, 138.96, 135.16, 132.98, 132.08, 131.93, 131.47, 129.78 (2C), 128.03, 117.50 15 (2C), 26.30; ESI-TOF-MS (m/z): $[M]^{-}$ calcd. for $C_{14}H_{11}Cl_2NO_3S-H$, 341.99; found 342.10; elemental analysis (calcd., found for

16 $C_{14}H_{11}Cl_2NO_3S \cdot \frac{1}{2}C_3H_6O$: C(49.87, 49.50), H(3.78, 3.27), N (3.75, 3.87).

17 N-(9H-fluoren-2-yl)-2,4-dichlorobenzenesulfonamide, 12 Yield 48 %, mp: 177-178 °C ¹H NMR (500MHz, DMSO- d₆): 10.72 18 (s, 1H), 8.03 (d, 1H, J = 8.6Hz), 7.83 (d, 1H, J = 2.0Hz), 7.76-7.72 (m, 2H), 7.58 (dd, 1H, J = 8.6Hz, J = 2.0Hz), 7.51 (d, 1H, J = 2.0Hz), 7.51 (d, 1H, J = 2.0Hz), 7.51 (d, 2H), 7.51 19 7.4 Hz), 7.34-7.32 (m, 2H), 7.25 (td, 1H, J = 7.5Hz, J = 1.2Hz) 7.12 (dd, 1H, J = 8.5Hz, J = 2.0Hz); ¹³C NMR (126MHz, DMSO-20 d₆): 194.3, 141.0, 138.9, 137.2, 135.3, 132.9, 132.2, 131.9, 131.8, 131.5, 131.4, 129.3, 128.4, 128.1, 117.5; ESI-TOF-MS (m/z): 21 [M]⁻ calcd. for C₁₉H₁₃Cl₂NO₂S-H 388.00; found 387.97; elemental analysis (calcd. , found for C₁₉H₁₃Cl₂NO₂S: C(58.47, 58.54), 22 H(3.36, 3.38), N (3.59, 3.61)

23 N-(3-benzoylphenyl)-benzenesulfonamide 13: Yield 70 %; mp: 101-103 °C; ¹H NMR (500MHz, DMSO- d₆): 10.52(s, 1H), 24 7.76(m, 2H), 7.70-7.62(m, 1H), 7.60-7.54(m, 6H), 7.43-7.41(m, 4H); ¹³C NMR (126MHz, DMSO- d₆): 195.0, 139.2, 137.8, 25 137.7, 136.6, 133.0, 132.7, 129.5, 129.4, 129.3, 128.5, 126.6, 125.2, 124.1, 120.8; ESI-TOF-MS (m/z): [M]⁻ calcd. for 26 C19H15NO3S-H, 336.07; found 336.09; elemental analysis (calcd., found for C19H15NO3S: C(67.64, 67.65), H(4.48, 4.42), N 27 (4.15, 4.04).

28 N-(4-benzoylphenyl)-benzenesulfonamide 14: Yield 35 %; mp: 102-104 °C; ¹H NMR (500MHz, DMSO- d₆): 10.89(s, 1H), 29 7.86(d, 2H, J = 8.9 Hz), 7.66-7.57(m, 8H), 7.52(t, 2H, J = 7.0 Hz), 7.26 (d, 2H, J = 8.6 Hz); ¹³C NMR (126MHz, DMSO-30 d₆):194.3, 142.0, 139.4, 137.2, 133.2, 132.2, 131.6, 131.3, 129.4, 129.2, 128.4, 126.6, 117.9; ESI-TOF-MS (m/z): [M]⁻ calcd. for 31 $C_{19}H_{15}NO_3S-H$, 336.07; found 336.09; elemental analysis (calcd., found for $C_{19}H_{15}NO_3S-\frac{1}{2}C_2H_6O$: C(66.65, 66.54), H(5.03, 10.10) 32 33 4.62), N (3.89, 3.72).

N-(4-benzoylphenyl)-4-methylbenzenesulfonamide 15: Yield 28 %; mp: 180-181 °C; ¹H NMR (500MHz, DMSO- d₆): 10.83(s, 34 1H), 7.74(d, 2H, J = 8.0 Hz), 7.66-7.62(m, 5H), 7.52(t, 2H, J = 7.3Hz), 7.38(d, 2H, J = 8.0 Hz), 7.25 (d, 2H, J = 7.3Hz), 2.34 (s, 35 1H); ¹³C NMR (126MHz, DMSO- d₆): 194.3, 143.6, 137.3, 136.5, 132.2, 131.5, 131.3, 129.8, 129.22, 128.4, 126.6, 117.8, 20.8; 36 ESI-TOF-MS (m/z): $[M]^{-}$ calcd. for C₂₀H₁₇NO₃S-H, 350.09; found 350.11; elemental analysis (calcd., found for C₂₀H₁₇NO₃S: 37 C(68.36, 67.80), H(4.88, 4.68), N (3.99, 3.95)

38 N-(3-benzovlphenyl)-4-methylbenzenesulfonamide 16: Yield 21 %; mp: 118-119 °C; ¹H NMR (500MHz, DMSO- d₆): 10.44(s, 39 1H), 7.68(m, 1H), 7.64(d, 2H, J = 8.5 Hz), 7.62-7.58(m, 2H), 7.56-7.53(m, 2H), 7.43-7.42(m, 2H), 7.40-7.36(m, 4H), 2.35(s, 40 3H); ¹³C NMR (126MHz, DMSO- d₆): 195.0, 143.4, 138.0, 137.7, 136.6, 136.4, 132.7, 129.7, 129.5, 129.4, 128.5, 126.6, 125.0, 41 123.8, 120.6, 20.9; ESI-TOF-MS (m/z): [M]⁻ calcd. for C₂₀H₁₇NO₃S-H, 350.01; found 350.01; elemental analysis (calcd., found 42 for C₂₀H₁₇NO₃S: C(68.36, 68.26), H(4.88, 4.74), N (3.99, 3.86).

43 N-(3-benzoylphenyl)-4-bromobenzenesulfonamide 17: Yield 47 %; mp: 127-130; ¹H NMR (500MHz, DMSO- d₆): 44 10,59(s,1H), 7.80(dt, 2H, J = 8.7 Hz, J = 2.5Hz), 7.68(m, 3H), 7.60(m, 2H), 7.54(m,2H), 7,44(m,4H); ¹³C NMR (126MHz, 126MHz), 7.54(m,2H), 7.54(45 DMSO- d₆): 194.9, 138.4, 137.8, 137.5, 136.6, 132.7, 132.4, 129.7, 129.4, 128.6, 128.5, 126.9, 125.5, 124.4, 121.1; ESI-TOF-MS 46 (m/z): $[M]^{-}$ calcd. for $C_{19}H_{14}BrNO_3S$ -H, 416,29; found 415.94; elemental analysis (calcd. , found for $C_{19}H_{14}BrNO_3S$: C(54.73, 47 54.82), H(3.39, 3.43), N (3.36, 3.25)

48 N-(4-benzoylphenyl)-4-bromobenzenesulfonamide, 18: Yield 39 %; mp: 173-175 °C; ¹H NMR (500MHz, DMSO- d₆): 49 10.96(s, 1H), 7.82-7.76(m, 4H), 7.68-7.64(m, 5H), 7.53(t, 2H, J = 7.8 Hz), 7.26(d, 2H, J = 8.6 Hz); ¹³C NMR (126MHz, 12.60)

50 DMSO- d₆): 194.3, 141.6, 138.6, 137.2, 132.5, 132.2, 131.9, 131.4, 129.2, 128.6, 128.4, 127.1, 118.2; ESI-TOF-MS (m/z): [M]⁻

51 calcd. for $C_{19}H_{14}BrNO_3S$ -H, 415.98; found 416.01; elemental analysis (calcd., found for $C_{19}H_{14}BrNO_3S$: C(54.82, 54.82), 52 H(3.39, 3.27), N (3.36, 3.38)

53 N-(4-benzoylphenyl)-4-iodobenzenesulfonamide, 19: Yield 33.1 %; mp: 167-168 °C; ¹H NMR (500MHz, DMSO- d₆): 54 10.94(s, 1H), 7.98(dt, 2H, J = 8.6 Hz, J = 2.0 Hz), 7.68-7.62(m, 5H), 7.60(dt, 2H, J = 8.6 Hz, J = 2.0 Hz), 7.53(t, 2H, J = 7.6Hz),

55 7.25(d, 2H, *J* = 8.7 Hz); ¹³C NMR (126MHz, DMSO- d₆): 194.3, 141.7, 139.0, 138.3.0, 137.2, 132.2, 131.9, 131.4, 129.2, 128.4,

56 128.2, 118.1; ESI-TOF-MS (m/z): [M]⁻ calcd. for C₁₉H₁₅INO₃S-H, 461.96; found 461.96; elemental analysis (calcd., found for 1 C₁₉H₁₄INO₃S: C(49.26, 49.06), H(3.05, 2.96), N (3.02, 2.91).

2 3 N-(3-benzoylphenyl)-4-iodobenzenesulfonamide 20: Yield 55 %; mp: 134-135 °C; ¹H NMR (500MHz, DMSO- d₆): 10.56(s,

- 1H), 7.97(dt, 2H, 8.6Hz), 7.70-7.66(t, 1H, 7.3Hz), 7.61-7.52(m, 4H) 7.55(dt, 2H, 8.6Hz), 7.48-7.40(m, 4H); ¹³C NMR (126MHz,
- DMSO- d₆): 194.9, 138.8, 138.2, 137.8, 137.5, 136.6, 132.7, 129.6, 129.4, 128.5, 128.2, 125.4, 124.3, 121.0, 101.3; ESI-TOF-MS
- (m/z): [M]⁻ calcd. for C₁₉H₁₄INO₃S-H, 461.97; found 461.96; elemental analysis (calcd., found for C₁₉H₁₄INO₃S: C(49.26,
- 4 5 6 7 49.58), H(3.05, 3.05), N (3.02, 2.91).
- General procedure b:

8 9 N-methyl-N-4-benzoylphenyl-2,4-dichlorobenzenesulfonamide 8: Yield 84 %; mp: 108-109 °C; ¹H NMR (500MHz, DMSOd₆): 7.95(d, 1H, J = 8.6 Hz), 7.92(d, 1H, J = 1.9Hz), 7.72(d, 2H, J = 8.5 Hz), 7.70-7.66 (m, 3H₂), 7.64 (dd, 1H, J = 8.6Hz, J =

- 1.9Hz), 7.56 (t, 2H, 7.8Hz) 7.45 (d 2H, J = 8.5 Hz) 3.39(s, 3H); ¹³C NMR (126MHz, DMSO- d₆): 194.7, 144.1, 139.0, 136.8, 10
- 134.6, 134.2, 133.3, 132.6, 132.3, 131.8, 130.5, 129.4, 128.5, 128.0, 124.5, 37.4; ESI-TOF-MS (m/z): [M]⁺ calcd. for 11
- 12 $C_{20}H_{15}Cl_2NO_3SNa$, 442.00; found 441.93; elemental analysis (calcd., found for $C_{20}H_{15}Cl_2NO_3S : C(57.15, 57.19)$, H(3.60, 3.61),
- 13 N (3.33, 3.25).
- 14 N-methyl-N-3-benzoylphenyl-2,4-dichlorobenzenesulfonamide 9: Yield 73 %; mp: 76-77 °C; ¹H NMR (500MHz, DMSO- d₆): 15 7.91(d, 1H, *J* = 1,9 Hz), 7.86(d, 1H, *J* = 8,6 Hz), 7.69(t, 1H, *J* = 7.8Hz), 7.66-7.64(m, 3H), 7.61(dd, 1H, *J* = 8,6 Hz, *J* = 1,9 Hz),
- 16 7.59-7.53(m 4H), 7.51(s, 1H), 3.35(s, 3H); ¹³C NMR (126MHz, DMSO- d₆): 194.7, 140.4, 138.9, 137.8, 136.4, 134.2, 133.3,
- 17 132.9, 132.3, 131.7, 130.2, 129.6, 129.5, 128.5, 128.2, 128.0, 126.9, 38.3; ESI-TOF-MS (m/z): [M]⁺ calcd. for
- 18 $C_{20}H_{15}Cl_2NO_3SNa, 442,00$; found 441,93; elemental analysis (calcd., found for $C_{20}H_{15}Cl_2NO_3S : C(57.15, 57.07), H(3.60, 3.53)$,
- 19 N (3.33, 3.23).

20 *N*-methyl-*N*-(9-okso-9*H*-fluoren-2-yl)-2,4dichlorobenzenesulfonamide, 10: Yield 74 %; mp: 132-133 °C; ¹H NMR (500MHz, 21 DMSO- d₆): 7.91(d, 1H, J = 1.9 Hz), 7.87(d, 1H, J = 8.6 Hz), 7.78-7.76(m, 2H), 7.63-7.60(m, 3H), 7.47(d, 1H, J = 2.0 Hz), 22 7.45(s, 1H), 7.38(d, 1H J = 7.3 Hz), 3.34(s, 3H); ¹³C NMR (126MHz, DMSO- d₆): 192.1, 143.1, 142.2, 141.4, 138.9, 135.5, 23 134.0, 133.5, 133.3, 132.5, 132.4, 131.8, 129.5, 128.0, 124.0, 121.7, 121.5, 121.4, 38.2; ESI-TOF-MS (m/z): [M]⁺ calcd. for 24 $C_{20}H_{13}Cl_2NO_3SNa, 439,99$; found 440,05; elemental analysis (calcd., found for $C_{20}H_{15}Cl_2NO_3S$: C(57.43, 57.27), H(3.13, 3.13), N (3.35, 3.30).

General procedure c:

25 26 27 4-benzoylphenyl-2,4-dichlorobenzenesulfonate, 11: Yield 86 %; mp: 97-98 °C; ¹H NMR (500MHz, DMSO- d₆): 8.09(d, 1H,

- 28 J = 1.9 Hz), 7.97(d, 1H, J = 8.6 Hz), 7.78(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 8.8 Hz), 7.78(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 7.7 Hz), 7.33(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 8.8 Hz), 7.78(dt, 2H, J = 8.8 Hz), 7.78(dt, 2H, J = 8.8 Hz), 7.77-7.64(m, 4H), 7.54(dt, 2H, J = 8.8 Hz), 7.78(dt, 2H, J = 8.8 Hz), 7.88(dt, 2H, J = 8.8 Hz), 7. 29
- Hz); ¹³C NMR (126MHz, DMSO- d₆): 194.3, 151.3, 140.9, 136.4, 136.2, 133.4, 133.1, 132.8, 132.2, 131.8, 131.1, 129.5, 128.5, 30 128.4, 121.8; ESI-TOF-MS (m/z): [M]⁻ calcd. for C₁₉H₁₂Cl₂O₄SNaCH₃OH, 461,00; found 461.07; elemental analysis (calcd.,
- 31 found for C₁₉H₁₂Cl₂O₄S: C(56.03, 56.10), H(2.97, 2.89), N (0.00, 0.00).

32 4-benzoylphenyl-3,5-dichloro-2-hydroxybenzenesulfonate 21: Yield 17 %; mp: 150 - 151 °C; ¹H NMR (500MHz, DMSO-

33 d₆): 11.86 (br, 1H), 8.03 (d, 1H, J = 2.6 Hz), 7.80 (dt, 2H, J = 9.0 Hz, J = 2.7 Hz, J = 2.0 Hz), 7.73-7.66 (m, 3H), 7.62 (d, 1H, J = 34 2.6 Hz), 7.56(t, 2H, J = 7.6 Hz), 7.34 (dt, 2H, J = 9.0 Hz, J = 2.7 Hz, J = 2.0 Hz); ¹³C NMR (126MHz, DMSO- d₆): 194.4, 151.7,

- 35 136.5, 136.0, 135.9, 132.8, 131.7, 129.5, 128.6, 128.4, 125.3, 124.7, 124.5, 122.9, 121.9; ESI-TOF-MS (m/z): [M]⁻ calcd. for
- 36 $C_{19}H_{12}C_{12}O_5S$, 420,98; found 420.95; elemental analysis (calcd., found for $C_{19}H_{12}C_{12}O_5S$; C (53.91, 54.19), H (2.86, 2.79), N
- 37 (0.00, 0.00).
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