Supporting Information for

Phenylcinnamides as novel antimitotic agents

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**Biological Evaluation**

**Biological Materials.** Purified bovine brain tubulin was a gift of Prof. Tim Mitchison. Before use, polymerization-competent tubulin was repurified following Mitchison’s polymerization/depolymerization cycling protocol and quantitated spectrophotometrically using $\varepsilon_{280\text{ nm}} = 115,000\ \text{M}^{-1}\text{cm}^{-1}$. MTS/PMS CellTiter 96 cell proliferation assay reagent was purchased from Promega (Madison, WI). Fetal bovine serum was purchased from Biomeda (Foster City, CA). FITC-conjugated mouse anti- $\alpha$-tubulin antibody, Sulforhodamine B sodium salt, formaldehyde (37% solution in water), glutaraldehyde (50% aqueous solution, photographic grade) were purchased from Sigma-Aldrich (St. Louis, MO). Goat anti-mouse IgG, Alexa-Fluor 488 conjugate and propidium iodide were from Molecular Probes (Eugene, OR). Goat serum (10% solution) was from Invitrogen (Carlsbad, CA). Vectashield mounting medium was from Vector Laboratories (Burlingame, CA). RPMI-1640 cell culture medium was obtained from the UIUC School of Chemical Sciences Cell Media Facility. Microtiter plates (96-well, tissue culture-treated), microscope slides, No. 1 microscope coverslips, eppendorf tubes, and all other reagents were purchased from Fisher (Chicago, IL).

**Cell Culture.** HeLa and U-937 cell lines were purchased from American Type Culture Collection (Manassas, VA). HL-60 and HL-60/VCR cell lines were a generous gift from Dr. Russell J. Mumper. For all experiments, cell lines were cultured in RPMI-1640 supplemented with 10% FBS and 1% penicillin/streptomycin in tissue-culture treated flasks and Petri dishes and maintained at 37°C in a humidified 5% CO$_2$ incubator.

**Flow Cytometric Analysis.** HeLa cells were synchronized in G1/S following a standard double thymidine-block protocol. Arrested cells were released by washing three times with thymidine-free medium, and immediately harvested by trypsinization, counted using a hemocytometer, and plated (1.5 x 10$^6$ per plate) in 10 cm cell-culture-treated Petri dishes containing 12 mL cell growth medium. 8H (25 µM), colchicine (100 nM), cycloheximide (2.5 µM) or an equal volume of DMSO vehicle as added and cells were incubated for 9 h at 37°C in a humidified 5% CO$_2$ incubator. Cells were rapidly harvested by scraping, washed with PBS pH 7.4,
and fixed for 10 min in 500 µL PBS pH 7.4 containing 3% formaldehyde in sealed 1.7 mL Eppendorf tubes in a 37°C water bath. After fixation, cells were incubated on ice for 1 min, centrifuged 5 min at 200 x g, and PBS was removed via aspiration. Cells were gently resuspended in 300 µL MeOH by dropwise addition of ice-cold 100% MeOH to a gently vortexed tube. Cell suspensions were incubated on ice for 30 min and stored overnight at -20 °C to permeabilize cells. Permeabilized cells were then washed twice with blocking solution (0.5% BSA in PBS pH 7.4) to remove MeOH, and resuspended in 500 µL blocking solution and incubated at 25 °C for 10 min. Blocking solution was removed by aspiration and cells were resuspended in 100 µL blocking solution containing mouse anti-phospho(Ser10) histone H3 antibody (Cell Signaling Technology) at 1:25 dilution and incubated for 30 min at 25 °C. A portion of the 8H-treated cells (0.5 x 10⁶) were separated before treatment and were incubated in blocking solution alone as a control for nonspecific 2° antibody binding. After incubation, cells were washed 3 x 1 mL in blocking solution and were resuspended in 200 µL blocking solution containing goat anti-mouse IgG, Alexa-Fluor 488 conjugate (1:1000) and incubated for 30 min at 25 °C. After washing 3 x 1 mL in blocking solution, cells were resuspended in 200 µL PBS containing 100 µg/mL RNase A and incubated for 30 min at 25 °C, at which point 100 µL propidium iodide (1 mg/mL in PBS) was added and incubated for an additional 30 min. Cells were washed 3 x 1 mL PBS, resuspended in 400 µL PBS and immediately analyzed on a BD Biosciences LSR II flow cytometer using a 488 nm excitation laser, monitoring green and red channels with 530 ± 15 nm and 695 ± 20 nm bandpass filters, respectively.

**Assessment of Cell Viability via Sulforhodamine B Assay.** Cytotoxicity against the HeLa cell line was assessed using the sulforhodamine B (SRB) assay in 96-well plate format using the optimized protocol of Vichai and Kirtikara. Briefly, two µL of a dilution series of each compound dissolved in DMSO were added to 98 µL of appropriate growth medium at five replicates per concentration. Then, cells suspended in 100 µL growth medium at a concentration of 5 x 10⁴ cells/mL were added and the plate was incubated in a 5% CO₂ incubator 72 h at 37 °C. After 72 h, media was removed from the plates and cells were fixed by addition of 100 µL ice-cold 10% (w/v) trichloroacetic acid (TCA) in water and placed in a refrigerator. After overnight incubation, TCA was removed by washing plates four times with distilled water and plates were allowed to dry.
at room temperature overnight. Sulforhodamine B, sodium salt (100 µL of 0.06% w/v solution dissolved in 1% acetic acid) was added to each well and the plates incubated at room temperature for 30 min, after which time unbound sulforhodamine B was removed by washing 4 times with 1% acetic acid. SRB bound to proteins was released by addition of 200 µL 10 mM Tris, pH 10.5, and absorbance of each well was measured at 510 nm on a Molecular Devices SpectraMax 384 plus plate reader after 30 min incubation at room temperature. Each plate contained internal positive (known cytotoxic compound at 100 µM) and negative (DMSO vehicle) controls for calibration of the percentage of cell death observed in each well, which was used to construct a dose-response curve and calculate an LC₅₀.

**Assessment of Cell Viability via MTS Assay.** Cytotoxicity of compounds against the U-937, HL-60, and HL-60/VCR cell lines was assessed using the MTS assay according to the manufacturer’s specifications (Promega). Briefly, two µL of a dilution series of each compound dissolved in DMSO were added to 98 µL of appropriate growth medium at five replicates per concentration. Then, cells suspended in 100 µL growth medium at a concentration of 1 x 10⁵ (U-937 and HL-60) or 1 x 10⁶ (HL-60/VCR) cells/mL were added and the plate was incubated in a 5% CO₂ incubator at 37 °C. After 72 h, plates were removed and processed as per the MTS protocol, wherein a 20 µL solution of MTS ((3-(4,5-dimethylthiazol-2-yl)-5-(3-carboxymethoxyphenyl)-2-(4-sulfophenyl)-2H-tetrazolium, inner salt) and PMS (phenazine methosulfate) in PBS was added to each well, and plates were returned to a 5% CO₂ incubator until signal from vehicle-treated cells reached the upper end of the linear range of the assay (O.D. ~ 1.5, roughly 30 min for U-937 and HL-60 cell lines, up to 2 h for HL-60/VCR cell line). Absorbance of each well was measured at 490 nm on a Molecular Devices SpectraMax 384 plus plate reader. Each plate contained internal positive (known cytotoxic compound at 100 µM) and negative (DMSO vehicle) controls for calibration of the percentage of cell death observed in each well, which was used to construct a dose-response curve and calculate an LC₅₀.

**Tubulin Polymerization Assay.** Polymerization of tubulin was monitored by measuring absorbance at 340 nm in a 384-well plate Molecular Devices Spectramax 384 plus spectrophotometer (Sunnydale, CA) preheated to 37 °C. To a 0.5 mL polypropylene tube on ice was added 40 µL ice-cold 1.25X BRB-80 buffer (100 mM
PIPS/pH 6.8, 1.25 mM MgCl₂, 1.25 mM EGTA, 1.25 µM GTP (added from 100 mM stock immediately before use), 6.25% v/v glycerol). To individual aliquots of buffer was also added DMSO or compound in DMSO (DMSO 0.6 % final in buffer, paclitaxel and nocodazole at 10 µM, 8H at 25 and 100 µM). To this solution was rapidly added 10 µL 15 mg/mL polymerization-competent tubulin in ice-cold 500 mM K-PIPS, pH 6.8, 0.5 mM MgCl₂, buffer, which had been thawed on ice immediately before use. Solutions were mixed rapidly on ice and then immediately transferred to a 384-well plate. Final concentrations of reagents in polymerization reaction were as follows: 80 mM PIPES/pH 6.8, 1.0 mM MgCl₂, 1.0 mM EGTA, 1.0 µM GTP, 5% glycerol, 0.5% DMSO, 3 mg/mL tubulin. Turbidity at 340 nm corresponding to polymerization was assessed every 60 sec. for 60 min.

**Laser Fluorescence Confocal Microscopy.** For laser fluorescence confocal microscopy, HeLa cells were grown on nitric acid-washed No. 1 coverslips overnight in a 5% CO₂ incubator h at 37 °C. Compound in DMSO or DMSO vehicle alone (0.2% DMSO final) was added to the cells at 40 or 70% confluency, and further incubated for 6 h (70% confluent cells) or 16 h (40% confluent cells). Cells were washed briefly with BRB-80 and fixed for 10 min with 0.5% glutaraldehyde in BRB-80, then permeabilized for 15 min in 1% Triton X-100 in PBS. After washing three times in PBS/pH 8.0, unreacted aldehydes were reduced with three seven min incubations of 1 mg/mL NaBH₄ dissolved in PBS/pH 8 immediately before use. Cells were given 3 rinses with a solution of 0.1% Triton X-100 in PBS/pH 8.0 (PBST) and blocked 20 min in 10% goat serum. FITC-conjugated anti-α-tubulin was added at a 1:100 dilution in 10% goat serum and the cells incubated for 1 h, then washed 3 x 10 min in PBST. Goat anti-mouse IgG, Alexa-Fluor 488 conjugate was diluted 1:200 in 10% goat serum and incubated with cells for 1 h, then washed three times with PBST. Cells were incubated in PBS containing 10 µg/mL propidium iodide and 1 µg/mL RNAse A for 15 min, washed twice with PBS, once with dH₂O, and mounted onto microscope slides using 8 µL Vectashield mounting medium and sealed with colorless nail polish. Samples were visualized immediately on a Zeiss LSM 510 laser scanning confocal microscope, 63X oil DIC objective, 1.4 NA. Widefield images were acquired by moving the stage to 10-15 random locations on each slide, thereafter only adjusting the stage in the z-direction to bring a maximal number of cells into focus.
**In silico prediction of biological properties.** SMILES formulae for all new compounds were generated in Chemdraw (Cambridgesoft Corp. Cambridge, MA, USA). SMILES formulae for known antimitotics were downloaded from the PubChem database.\(^4\) Values for calculated partition coefficient octanol/water \((C_{\text{log}P})\) and topological polar surface area \((\text{TPSA})\) were calculated using Daylight software (Daylight Chemical Information Systems, Inc., Aliso Viejo, CA, USA) which contains implementations of \(C_{\text{log}P}\)\(^5\) (BioByte Corp., Claremont, CA, USA) and TPSA\(^6\) algorithms. Predicted \(\log BB\) was calculated using the formula \(\log BB = -0.0148 \text{TPSA} + 0.152 C_{\log P} + 0.139\).\(^5\)

**Chemistry**

**Method A. Two-step synthesis of phenylcinnamides.** All reactions were run on a scale calculated to provide a theoretical yield of roughly 50 mg (~0.1-0.2 mmol) amide product. In an oven-dried microwave tube, a given carboxylic acid was dissolved in 2.0 mL anhydrous \(\text{CH}_2\text{Cl}_2\). To the tube was added oxalyl chloride (2 eq.) and one drop of anhydrous \(N,N\)-dimethylformamide and the tube was stirred lightly capped at room temperature overnight. After acid chloride formation was complete as judged by TLC, all volatiles were evaporated to dryness under a steady stream of dry \(N_2\). The resulting acid chloride was then immediately redissolved in 2.0 mL anhydrous \(\text{MeCN}\). An amine (1.5 eq.) was added, followed by DIPEA (2.0 eq.). The solution was capped and the tube was heated in a CEM discover multimode reaction microwave, holding at 150 °C for 90 minutes. After cooling, the reaction mixture was evaporated to dryness and the crude reaction mixture redissolved in 20 mL EtOAc and extracted 3 x 15 mL 1M HCl, 3 x 15 mL 1 M NaOH, then 1 x 15 mL brine. The organic layer was dried over \(\text{MgSO}_4\), filtered and adsorbed onto silica gel. The silica was then loaded into a purification cartridge and the crude mixture was separated over a 0-100% hexanes-ethyl acetate gradient on an Isco Companion automated chromatography system.

**Method B. One-step synthesis of phenylcinnamides.** All reactions were run on a scale calculated to provide a theoretical yield of roughly 50 mg (~0.1-0.2 mmol) amide product. In an oven-dried microwave tube, a given
carboxylic acid was dissolved in 2.0 mL anhydrous MeCN. An amine (1.5 eq.) was added, followed by HATU (1.5 eq.) and DIPEA (2.0 eq.). The solution was capped and the tube was heated in a CEM discover multimode reaction microwave, holding at 150 °C for 90 minutes. After cooling, the reaction mixture was evaporated to dryness and the crude reaction mixture redissolved in 20 mL EtOAc and extracted 3 x 15 mL 1M HCl, 3 x 15 mL 1 M NaOH, then 1 x 15 mL brine. The organic layer was dried over MgSO₄, filtered and adsorbed onto silica gel. The silica was then loaded into a purification cartridge and the crude mixture was separated over a 0-100% hexanes-ethyl acetate gradient on an Isco Companion automated chromatography system.
Yield and analytical HPLC purity analysis of library compounds

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NA = no melting point (oil).
NMR analysis of library members

Compound 8H

3-(3-Methoxy-phenyl)-N-(3,4,5-trimethoxy-phenyl)-acrylamide

\[
\begin{align*}
\text{NMR }^1\text{H (500 MHz, CDCl}_3\text{)} & \delta \text{ ppm 8.59 (br s, 1H) ppm 7.69 (d, 1H, J=15.5 Hz), 7.20 (t, 1H, J=7.9 Hz), 7.03} \\
& \text{ (s, 1H), 7.00 (d, 1H, J=7.7 Hz), 6.94 (s, 1H), 6.85 (dd, 1H, J=2.2 Hz, J=8.1 Hz), 6.68 (d, 1H, J=15.5 Hz), 3.80} \\
& \text{(s, 3H) ppm 3.729 (s, 3H), 3.725 (s, 6H).}
\end{align*}
\]

**NMR** $^{13}\text{C (125 MHz, CDCl}_3\text{)} \delta \text{ ppm: 164.35, 159.73, 153.12, 141.92, 135.82, 134.67, 134.21, 129.76, 121.26,} \\
\text{120.24, 115.39, 113.19, 97.49, 60.86, 55.77, 55.08.}

$R_f=12\text{mm/53mm (EtOAc/Hexanes=50/50);}$

IR (thin film, cm$^{-1}$): 3313, 2938, 2836, 1663, 1607, 1546, 1507, 1452, 1432, 1411, 1332, 1290, 1234, 1210, 1128, 1044, 980, 913, 837, 776;

**MS** (FAB): 344.22(M+1, 57.77), 222.14(16.66), 195.11(10.18), 184.15(100), 168.13(59.86), 161.12(47.20);

**HRMS** (FAB): found: 344.1500 (M+1); calc. for C$_{19}$H$_{22}$NO$_5$: 344.149798

Compound 6

\[
\begin{align*}
(\text{E})-3-(3\text{-trifluoromethoxyphenyl})-\text{N-(3,4,5-trimethoxyphenyl)}\text{-acrylamide}
\end{align*}
\]
**Compound 1**

(E)-N-(2-methoxyphenyl)-3-(3-(trifluoromethoxy)phenyl)acrylamide

![Structural formula of compound 1](image)

**NMR $^1H$ (500 MHz, CD$_3$OD)** δ ppm: 7.62 (d, 1H, J=15.78Hz), 7.54 (d, 1H, J=7.75Hz), 7.48 (m, 2H), 7.28 (d, 1H, J=8.17Hz), 7.05 (s, 2H), 6.78 (d, 1H, J=15.66Hz), 3.82 (s, 6H), 3.74 (s, 3H).

**NMR $^{13}C$ (500 MHz, CD$_3$OD)** δ ppm: 164.61, 153.34, 149.79, 139.58, 137.42, 135.11, 134.62, 130.54, 126.61, 123.18, 121.93, 119.75, 97.73, 60.04, 55.33.

**Compound 7**

(3E)-N-(2-methoxyphenyl)-3-(3-(trifluoromethoxy)phenyl)acrylamide

![Structural formula of compound 7](image)

**NMR $^1H$ (500 MHz, CD$_3$OD)** δ ppm: 8.12 (dd, 1H, J=9.4 Hz, J=1.4 Hz), 7.63 (d, 1H, J=15.7 Hz), 7.59 (d, 1H, J=7.6 Hz), 7.53 (s, 1H), 7.49 (t, 1H, J=8.0 Hz), 7.29 (d, 1H, J=8.2 Hz), 7.09 (m, 2H), 7.02 (dd, 1H, J=8.2 Hz, J=1.1 Hz), 6.93 (td, 1H, J=7.7 Hz, J=1.1 Hz), 3.90 (s, 3H).

**NMR $^{13}C$ (500 MHz, CD$_3$OD)** δ ppm: 164.90, 150.14, 149.80, 139.59, 137.59, 130.52, 127.14, 126.73, 125.08, 123.42, 121.90, 121.87, 120.32, 119.79, 110.57, 55.07.

**Compound 8**

(E)-3-(3-hydroxyphenyl)-N-(3,4,5-trimethoxyphenyl)acrylamide

![Structural formula of compound 8](image)

**NMR $^1H$ (500 MHz, CD$_3$OD)** δ ppm: 7.57 (d, 1H, J=15.6Hz), 7.21 (t, 1H, J=7.8Hz), 7.06 (s, 2H), 6.82 (d, 1H, J=7.9Hz), 6.69 (d, 1H, J=15.6Hz), 3.82 (s, 6H) 3.74 (s, 3H).
**NMR $^{13}$C (500 MHz, CD$_3$OD)** $\delta$ ppm: 166.07, 158.54, 153.98, 142.45, 136.98, 135.90, 135.16, 130.49, 121.60, 120.03, 117.69, 114.77, 98.42, 60.75, 56.02.

**Compound 9**

$N$-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)cinnamamide

![Diagram of Compound 9]

**NMR $^1$H (500 MHz, CD$_3$OD)** $\delta$ ppm: 7.62 (d, 1H, $J=15.7$ Hz), 7.51 (m, 2H), 7.33 (m, 3H), 7.04 (s, 2H), 6.72 (d, 1H, $J=15.7$ Hz), 3.77 (s, 6H), 3.72 (s, 3H).

**NMR $^{13}$C (500 MHz, CD$_3$OD)** $\delta$ ppm: 165.26, 153.31, 141.56, 135.23, 134.95, 134.47, 129.86, 128.82, 127.81, 121.11, 97.74, 60.11, 55.34.

**Compound 10**

(E)-N,3-bis(3,4,5-trimethoxyphenyl)acrylamide

![Diagram of Compound 10]

**NMR $^1$H (500 MHz, (CD$_3$)$_2$CO)** $\delta$ ppm: 7.61 (d, 1H, $J=15.5$ Hz), 7.21 (s, 2H), 6.94 (s, 2H), 6.78 (d, 1H, $J=15.5$ Hz), 3.89 (s, 6H), 3.82 (s, 6H), 3.77 (s, 3H), 3.71 (s, 3H).

**NMR $^{13}$C (500 MHz, (CD$_3$)$_2$CO)** $\delta$ ppm: 163.69, 153.95, 153.66, 141.02, 140.14, 135.82, 134.73, 130.85, 121.47, 105.48, 97.41, 59.99, 59.96, 55.79, 55.65.

**Compound 11**

(E)$-N$-(3,5-dimethoxyphenyl)-3-(3,4,5-trimethoxyphenyl)acrylamide
NMR $^1$H (500 MHz, CD$_3$OD) δ ppm: 7.57 (d, 1H, J=15.6 Hz), 6.91 (s, 4H), 6.68 (d, 1H, J=15.6 Hz), 6.26 (s, 1H), 3.88 (s, 6H), 3.78 (m, 9H).

NMR $^{13}$C (500 MHz, CD$_3$OD) δ ppm: 165.49, 161.30, 153.63, 141.67, 140.44, 139.75, 130.90, 120.51, 105.19, 98.20, 96.18, 60.00, 55.46, 54.56.

Compound 12

(E)-N-(3-methoxyphenyl)-3-(3,4,5-trimethoxyphenyl)acrylamide

NMR $^1$H (500 MHz, CD$_3$OD) δ ppm: 8.17 (d, 1H, J=7.9 Hz), 7.55 (d, 1H, J=15.6 Hz), 7.10 (m, 1H), 7.02 (m, 1H), 6.94 (m, 4H), 3.90 (s, 3H), 3.87 (s, 6H), 3.79 (s, 3H).

NMR $^{13}$C (500 MHz, CD$_3$OD) δ ppm: 165.54, 153.59, 149.96, 141.55, 139.60, 131.04, 127.32, 124.84, 121.61, 120.80, 120.34, 110.53, 105.20, 60.00, 55.44, 55.09.

Compound 13

(E)-N-(2-methoxyphenyl)-3-(3,4,5-trimethoxyphenyl)acrylamide

NMR $^1$H (500 MHz, CD$_3$OD) δ ppm: 7.57 (d, 1H, J=15.6 Hz), 7.40 (s, 1H), 7.22 (t, 1H, J=8.1 Hz), 7.14 (d, 1H, J=8.1 Hz), 6.90 (s, 1H), 6.68 (d, 1H, J=15.5 Hz), 6.68 (dd, 1H, J=2.4 Hz, J=7.9 Hz), 3.87 (s, 6H), 3.79 (s,

Compound 14

(E)-N-phenyl-3-(3,4,5-trimethoxyphenyl)acrylamide

![Chemical Structure of Compound 14]

NMR $^1$H (500 MHz, CD$_3$OD) δ ppm: 7.65 (d, 2H, J=8.2), 7.57 (d, 1H, J=15.6 Hz), 7.32 (t, 2H, J=8.3 Hz), 7.10 (t, 1H, J=7.4 Hz), 6.89 (s, 2H), 6.71 (d, 1H, J=15.6), 3.86 (s, 6H), 3.79 (s, 3H).

NMR $^{13}$C (500 MHz, CD$_3$OD) δ ppm: 165.20, 156.78, 153.61, 141.14, 139.64, 131.82, 130.98, 121.63, 120.56, 113.83, 105.13, 60.00, 55.45, 54.67.

Compound 15

(E)-N-(4-methoxyphenyl)-3-(3,4,5-trimethoxyphenyl)acrylamide

![Chemical Structure of Compound 15]

NMR $^1$H (500 MHz, CD$_3$OD) δ ppm: 7.54 (m, 3H), 6.88 (m, 4H), 6.67 (d, 1H, J=15.6 Hz), 3.86 (s, 6H), 3.79 (s, 3H), 3.77 (s, 3H).

NMR $^{13}$C (500 MHz, CD$_3$OD) δ ppm: 165.20, 156.78, 153.61, 141.14, 139.64, 131.82, 130.98, 121.63, 120.56, 113.83, 105.13, 60.00, 55.45, 54.67.
Compound 16

\((E)-3\text{-}(2\text{-methoxyphenyl})-N\text{-}(3,4,5\text{-trimethoxyphenyl})\text{acrylamide}\)

\[
\begin{align*}
\text{NMR }^{1}H \text{ (500 MHz, CD}_{2}\text{OD)} \delta \text{ ppm: } 7.95 \text{ (d, 1H, J=15.8 Hz)}, & \quad 7.52 \text{ (d, 1H, J=6.8 Hz)}, \quad 7.33 \text{ (t, 1H, J=7.1 Hz)}, \\
& \quad 7.06 \text{ (s, 2H)}, \quad 7.00 \text{ (d, 1H, J=8.3 Hz)}, \quad 6.94 \text{ (t, 1H, J=7.5 Hz)}, \quad 6.82 \text{ (d, 1H, J=15.8 Hz)}, \quad 3.87 \text{ (s, 3H)}, \quad 3.81 \text{ (s, 6H)}, \\
& \quad 3.73 \text{ (s, 3H)}.
\end{align*}
\]

\[
\begin{align*}
\text{NMR }^{13}C \text{ (500 MHz, CD}_{2}\text{OD)} \delta \text{ ppm: } 166.00, & \quad 158.57, \quad 153.30, \quad 137.03, \quad 135.35, \quad 134.42, \quad 131.24, \quad 128.49, \quad 123.57, \\
& \quad 121.38, \quad 120.60, \quad 111.24, \quad 97.71, \quad 60.05, \quad 55.32, \quad 54.85.
\end{align*}
\]

Compound 17

\((E)-N,3\text{-bis(2-methoxyphenyl)}\text{acrylamide}\)

\[
\begin{align*}
\text{NMR }^{1}H \text{ (500 MHz, CD}_{2}\text{OD)} \delta \text{ ppm: } 8.12 \text{ (d, 1H, J=7.7 Hz)}, & \quad 7.98 \text{ (d, 1H, J=15.8 Hz)} \quad 7.61 \text{ (d, 1H, J=7.5 Hz)}, \\
& \quad 7.35 \text{ (t, 1H, J=7.1Hz)}, \quad 7.10 \text{ (t, 1H, J=7.3 Hz)}, \quad 6.98 \text{ (m, 5H)}, \quad 3.90 \text{ (s, 6H)}.
\end{align*}
\]

\[
\begin{align*}
\text{NMR }^{13}C \text{ (500 MHz, CD}_{2}\text{OD)} \delta \text{ ppm: } 166.16, & \quad 158.51, \quad 150.24, \quad 136.89, \quad 131.20, \quad 128.23, \quad 127.28, \quad 124.92, \quad 123.71, \\
& \quad 122.06, \quad 121.32, \quad 120.59, \quad 120.29, \quad 111.22, \quad 110.57, \quad 55.06, \quad 54.86.
\end{align*}
\]

Compound 18

\((E)-3\text{-}(4\text{-hydroxyphenyl})-N\text{-}(3,4,5\text{-trimethoxyphenyl})\text{acrylamide}\)
NMR $^1$H (500 MHz, DMSO-d6) δ ppm: 9.92 (s br, 1H), 7.42 (m, 3H), 7.07 (s, 2H), 6.81 (d, 2H, J=8.5 Hz), 6.56 (d, 1H, J=15.6 Hz), 3.74 (s, 6H), 3.61 (s, 3H).

NMR $^{13}$C (500 MHz, DMSO-d6) δ ppm: 164.56, 159.88, 153.40, 140.90, 136.30, 134.00, 130.18, 126.36, 119.23, 116.54, 97.52, 60.79, 56.35.

Compound 19

(E)-N-(3,5-dimethoxyphenyl)-3-(4-hydroxyphenyl)acrylamide

NMR $^1$H (500 MHz, CD$_3$OD) δ ppm: 7.57 (d, 1H, J=15.6 Hz), 7.45 (d, 2H, J=8.5 Hz), 6.90 (dd, 1H, J=1.7 Hz, J=5.1 Hz), 6.81 (d, 2H, J=8.5 Hz), 6.57 (d, 1H, J=15.6 Hz), 6.25 (d, 1H, J=1.7 Hz), 5.48 (br s, 1H), 3.77 (s, 6H).

NMR $^{13}$C (500 MHz, CD$_3$OD) δ ppm: 166.15, 161.28, 159.63, 141.90, 140.50, 129.60, 126.44, 117.53, 115.60, 98.20, 96.10, 54.55.

Compound 20

(E)-3-(3-(prop-2-ynyloxy)phenyl)-N-(3,4,5-trimethoxyphenyl)acrylamide
NMR $^1$H (500 MHz, CDCl$_3$) δ ppm: 7.92 (s, 1H), 7.70 (d, 1H, J=15.5 Hz), 7.28 (dd, 1H, J=5.6 Hz, J=13.6 Hz), 7.11 (d, 1H, J=7.7 Hz), 7.08 (m, 1H), 6.98 (dd, 1H, J=2.6 Hz, J=8.5 Hz), 6.57 (d, 1H, J=15.5 Hz), 4.68 (d, 1H, J=2.4 Hz), 3.82 (s, 3H), 3.80 (s, 6H) 3.30 (s, 1H).

NMR $^{13}$C (500 MHz, CDCl$_3$) δ ppm: 164.24, 158.05, 153.53, 142.21, 136.25, 134.61, 130.16, 121.63, 116.70, 114.43, 97.82, 78.48, 76.14, 61.22, 56.25, 46.79.

Compound 21

(E)-3-(3-(allyloxy)phenyl)-N-(3,4,5-trimethoxyphenyl)acrylamide

NMR $^1$H (500 MHz, CD$_2$OD) δ ppm: 7.60 (d, 1H, J=15.6 Hz), 7.31 (t, 1H, J=7.8 Hz), 7.16 (m, 2H), 7.06 (s, 2H), 6.97 (dd, 1H, J=8.2 Hz, J=2.0 Hz), 6.73 (d, 1H, J=15.6 Hz), 6.07 (m, 1H), 5.42 (dd, 1H, J=1.4 Hz, J=17.3 Hz), 5.27 (dd, 1H, J=1.5 Hz, J=10.5 Hz), 4.58 (d, 2H, J=5.1 Hz), 3.83 (s, 6H), 3.76 (s, 3H)


Compound 22

(E)-3-(3-(benzyloxy)phenyl)-N-(3,4,5-trimethoxyphenyl)acrylamide
NMR $^1$H (500 MHz, CDCl$_3$) $\delta$ ppm: 8.08 (br s, 1H), 7.92 (s, 1H), 7.70 (d, 1H, J=15.5 Hz), 7.36 (s, 1H), 7.08 (m, 1H), 7.00 (m, 1H), 6.57 (d, 1H, J=15.5 Hz), 5.04 (m, 1H), 3.82 (s, 3H), 3.81 (s, 3H), 3.80 (s, 3H).

NMR $^{13}$C (500 MHz, CDCl$_3$) $\delta$ ppm: 169.03, 164.30, 159.31, 153.52, 142.36, 136.84, 136.23, 134.82, 134.65, 134.34, 130.16, 128.88, 128.35, 127.72, 121.44, 120.92, 119.14, 116.69, 114.73, 114.49, 112.90, 97.80, 80.64, 70.29, 61.21, 57.13, 56.23, 46.81.

**Compound 23**

(E)-N-(3,5-dimethoxyphenyl)-3-(3-methoxyphenyl)acrylamide

NMR $^1$H (500 MHz, CD$_3$OD) $\delta$ ppm: 7.60 (d, 1H, J=15.6 Hz), 7.31 (t, 1H, J=7.9 Hz), 7.16 (d, 1H, J=7.6 Hz), 7.12 (s, 1H) ppm 6.95 (dd, 1H, J=2.5 Hz, J=8.2 Hz), 6.91 (d, 1H, J=2.2 Hz), 6.74 (d, 1H, J=15.6 Hz), 6.25 (t, 1H, J=2.2 Hz), 3.82 (s, 3H) 3.76 (s, 6H).

NMR $^{13}$C (500 MHz, CD$_3$OD) $\delta$ ppm: 165.48, 153.61, 141.58, 139.70, 138.82, 130.91, 128.70, 124.11, 120.52, 120.00, 105.16, 60.01, 55.45.

**Compound 24**

(E)-N-(2-methoxyphenyl)-3-(3-methoxyphenyl)acrylamide

NMR $^1$H (500 MHz, CD$_3$OD) $\delta$ ppm: 8.14 (d, 1H, J=7.8 Hz), 7.60 (d, 1H, J=15.6 Hz), 7.31 (t, 1H, 7.8 Hz), 7.17 (m, 2H), 7.11 (t, 1H, J=7.5 Hz), 6.97 (m, 4H), 3.90 (s, 3H), 3.82 (s, 3H).
NMR $^{13}$C (500 MHz, CD$_3$OD) δ ppm: 165.51, 160.36, 150.14, 141.52, 136.50, 129.77, 124.97, 121.88, 121.56, 120.49, 120.31, 115.66, 112.57, 110.56, 55.07, 54.55.

Compound 25

$^{1}$NMR 3-bis(3-methoxyphenyl)acrylamide

NMR $^1$H (500 MHz, CD$_3$OD) δ ppm: 7.61 (d, 1H, J=15.7 Hz), 7.40 (s, 1H), 7.31 (t, 1H, J=7.9 Hz), 7.22 (t, 1H, J=8.1 Hz), 7.15 (m, 3H), 6.95 (dd, 1H, J=10.2 Hz, J=2.0 Hz), 6.76 (d, 1H, J=15.6 Hz), 6.68 (dd, 1H, J=9.9 Hz, J=1.8 Hz), 3.82 (s, 3H), 3.79 (s, 3H).

NMR $^{13}$C (500 MHz, CD$_3$OD) δ ppm: 165.41, 160.37, 141.58, 139.94, 136.38, 129.81, 129.40, 121.36, 121.29, 115.55, 112.79, 112.19, 109.66, 105.82, 54.55, 54.48.

Compound 26

(E)-3-(3-methoxyphenyl)-N-(4-methoxyphenyl)acrylamide

NMR $^1$H (500 MHz, CD$_3$OD) δ ppm: 7.59 (d, 1H, J=15.7 Hz), 7.55 (dd, 2H, J=2.2 Hz, J=9.1 Hz), 7.31 (t, 1H, J=7.9 Hz), 7.17 (d, 1H, J=7.7 Hz), 7.13 (s, 1H), 6.97 (dd, 1H, J=10.3 Hz, J=2.1 Hz), 6.90 (m, 2H), 6.75 (d, 1H, J=15.7 Hz), 3.83 (s, 3H), 3.78 (s, 3H).

NMR $^{13}$C (500 MHz, CD$_3$OD) δ ppm: 165.14, 160.38, 156.82, 141.12, 136.46, 131.79, 129.80, 121.66, 121.38, 120.24, 115.44, 113.83, 112.73, 54.66, 54.55.

Compound 27
(E)-3-(3-methoxyphenyl)-N-phenylacrylamide

NMR $^1$H (500 MHz, CD$_3$OD) δ ppm: 7.65 (d, 2H, J=7.7 Hz), 7.61 (d, 1H, J=15.7 Hz), 7.31 (m, 3H), 7.16 (d, 1H, J=7.6 Hz), 7.11 (m, 2H), 6.94 (dd, 1H, J=10.2 Hz, J=2.1 Hz), 6.77 (s, 1H, 15.7 Hz), 3.81 (s, 3H).

NMR $^{13}$C (500 MHz, CD$_3$OD) δ ppm: 165.41, 160.36, 141.54, 138.79, 136.39, 129.81, 128.69, 124.14, 121.36, 120.29, 120.04, 115.54, 112.79, 54.56.

Compound 28

(E)-N-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-3-(3-methoxyphenyl)acrylamide

NMR $^1$H (500 MHz, CD$_3$OD) δ ppm: 7.58 (d, 1H, J=15.7 Hz), 7.31 (m, 2H), 7.16 (d, 1H, J=7.7 Hz), 7.11 (s, 1H), 7.01 (dd, 1H, J=11.2 Hz, J=2.5 Hz), 6.95 (dd, 1H, J=10.3 Hz, J=2.1 Hz), 6.78 (d, 1H, J=8.7 Hz), 6.72 (d, 1H, J=15.7 Hz), 4.21 (m, 4H), 3.82 (s, 3H).

NMR $^{13}$C (500 MHz, CD$_3$OD) δ ppm: 165.09, 160.37, 143.62, 141.17, 140.73, 136.44, 132.38, 129.79, 121.36, 120.24, 116.84, 115.46, 113.33, 112.73, 109.45, 64.54, 64.36, 54.55.

Compound 29

(E)-N-(3,5-dimethylphenyl)-3-(3-methoxyphenyl)acrylamide
NMR $^1$H (500 MHz, CD$_3$OD) δ ppm: 7.60 (d, 1H, J=15.6 Hz), 7.29 (m, 3H), 7.16 (d, 1H, J=7.5 Hz), 7.12 (s, 1H), 6.95 (d, 1H, J=8.1 Hz), 6.76 (m, 2H), 3.82 (s, 3H), 2.28 (s, 6H).

NMR $^{13}$C (500 MHz, CD$_3$OD) δ ppm: 165.33, 160.36, 141.36, 138.53, 138.42, 136.43, 129.79, 125.75, 121.48, 120.28, 117.81, 115.50, 112.75, 54.547, 20.33.

Compound 30

$(E)$-N-(2,6-dimethylphenyl)-3-(3-methoxyphenyl)acrylamide

NMR $^1$H (500 MHz, CD$_3$OD) δ ppm: 7.62 (d, 1H, J=15.7 Hz), 7.32 (t, 1H, J=7.8 Hz), 7.19 (d, 1H, J=7.6 Hz), 7.13 (m, 4H), 6.97 (dd, 1H, J=8.2 Hz, J=2.5 Hz), 6.87 (d, 1H, J=15.7 Hz), 3.83 (s, 3H), 2.22 (s, 6H).

NMR $^{13}$C (500 MHz, CD$_3$OD) δ ppm: 166.07, 160.41, 141.63, 136.37, 135.61, 134.31, 129.86, 127.91, 127.24, 120.41, 120.30, 115.57, 112.75, 54.55, 17.30, 17.27.

Compound 31

3-(3-methoxyphenyl)-N-(3,4,5-trimethoxyphenyl)propanamide
**NMR** $^1$H (500 MHz, CD$_3$OD) δ ppm: 7.15 (t, 1H, J=8.2 Hz), 6.88 (s, 2H), 6.79 (m, 2H), 6.72 (m, 1H), 3.76 (s, 6H), 3.71 (s, 3H), 3.70 (s, 3H), 2.94 (t, 2H, J=7.5 Hz), 2.61 (t, 2H, J=7.5 Hz).

**NMR** $^{13}$C (500 MHz, CD$_3$OD) δ ppm: 172.27, 160.07, 153.23, 142.51, 135.00, 129.32, 120.52, 113.92, 111.49, 97.82, 60.04, 55.30, 54.58, 54.36, 38.62, 31.63.

**Compound 32**

$N$-(2-methoxyphenyl)-3-(3-methoxyphenyl)propanamide

![Chemical structure of Compound 32](image)

**NMR** $^1$H (500 MHz, CD$_3$OD) δ ppm: 7.91 (dd, 1H, J=7.5 Hz, J=1.6 Hz), 7.16 (t, 1H, J=8.0 Hz), 7.06 (dt, 1H, J=1.6, J=8.2 Hz), 6.94 (dd, 1H, J=1.1Hz, J=8.2 Hz), 6.88 (dt, 1H, J=8.9, J=1.3 Hz), 6.81 (m, 2H), 6.73 (dd, 1H, J=1.6Hz, J=8.2Hz), 3.79 (s, 3H), 3.72 (s, 3H), 2.94 (t, 2H, J=7.4 Hz), 2.69 (t, 2H, J=8.0 Hz).

**NMR** $^{13}$C (500 MHz, CD$_3$OD) δ ppm: 172.48, 160.09, 150.33, 142.51, 129.30, 126.93, 125.01, 122.34, 120.57, 120.23, 113.82, 111.60, 110.61, 55.00, 54.36, 38.41, 31.71.

**Compound 33**

$(E)$-3-(3-methoxyphenyl)-$N$-(3,4,5-trimethoxybenzyl)acrylamide

![Chemical structure of Compound 33](image)

**NMR** $^1$H (500 MHz, (CD$_3$)$_2$O) δ ppm: 7.80 (br s, 1H), 7.58 (d, 1H, J=15.7 Hz), 7.30 (d, 1H, J=7.9 Hz), 7.14 (m, 2H), 6.94 (dd, 1H, J=8.2 Hz, J=2.5 Hz), 6.78 (d, 1H, J=15.7 Hz), 6.67 (s, 2H), 4.47 (d, 2H, J=5.9 Hz), 3.81 (s, 3H), 3.79 (s, 6H), 3.70 (s, 3H).
NMR $^{13}$C (500 MHz, (CD$_3$)$_2$O) $\delta$ ppm: 165.32, 160.36, 153.72, 139.80, 137.59, 136.97, 135.27, 130.07, 122.41, 120.23, 115.39, 112.90, 105.32, 59.86, 55.73, 54.91, 43.41.
NMR Spectra for library compounds
HPLC analysis of library compounds

Compound 8H
Compound 6

RT: 0.00 - 30.00  SM: 9G

RT: 18.12
AA: 32098863

RT: 8.54
AA: 1290567

T: + c ESI Full ms [150.00-1000.00]
Compound 7
Compound 8

RT: 11.98
AA: 23741816

NL:
1.28E6
Total Scan
PDA
Genesis
Lcq_5684

Lcq_5684 #675-810  RT: 11.10-13.05  AV: 136  NL: 7.20E3
T: + c ESI Full ms [ 150.00-1000.00]
Compound 9

RT: 0.00 - 30.00  SM: 9G

RT: 13.44
AA: 4121787

NL:
5.82E5
nm=250.0-
260.0 PDA
Genesis
Lcq_5885

cq_5885 #800-831  RT: 13.17-13.64  AV: 32  NL: 8.47E7

*: + ESI Full ms [150.00-1000.00]
Compound 10
Compound 12
Compound 15
Compound 17

RT: 0.00 - 30.00  SM: 9G

RT: 16.92
AA: 29369539

NL:
3.08E6
Channel A
UV
Genesis
Lcq_5647

Lcq_5647 #1016-1049  RT: 16.64-17.09  AV: 34  NL: 9.03E8
T: + c ESI Full ms [150.00-1000.00]
Compound 18

RT: 0.00 - 30.00  SM: 15G

RT: 11.46  AA: 12615891

RT: 10.22  AA: 755122

NL:
1.88E6
Channel A
UV
Genesis
Lcq_5648
Compound 20

RT: 15.96
AA: 17581489

NL: 1.20E6
Total Scan
PDA
Genesis
Lcq_5687

cq_5687 #947.987 RT: 15.64-16.20 AV: 41 NL: 2.87E9
Γ: + c ESI Full ms [150.00-1000.00]
Compound 21

RT: 0.00 - 30.00  SM: 9G

RT: 17.17
AA: 26235748

RT: 11.44
AA: 1754582

Lcq_5650 #1037-1071  RT: 16.95-17.40  AV: 35  NL: 2.44E9
T: + c ESI Full ms [ 150.00-1000.00]
Compound 22

RT: 19.58
AA: 13822704

NL:
1.13E6
Total Scan
PDA
Genesis
Lcq_5688

Lcq_5688 #1167-1205 RT: 19.28-19.80 AV: 39 NL: 1.76E9
T: + c ESI Full ms [150.00-1000.00]

Relative Abundance

m/z
184.14 278.98 391.24 465.07 560.80 670.16 823.29 860.85 926.93

838.91 420.26
Compound 23
Compound 24

![Graph of Compound 24](image)

- Compound 24 is shown on a graph with mVolts on the x-axis and some unknown units on the y-axis.
- The graph includes a line with points labeled 24.7, 23.815, and a note "Wt=8.0".
Compound 25
Compound 26
Compound 27
Compound 28
Compound 29
Compound 30
Compound 31
Compound 32

RT: 0.00 - 30.00  SM: 9G

RT: 15.23
AA: 28083600

NL:
2.90E6
Channel A
UV
Genesis
Lcq_5660

Lcq_5660 #925-946  RT: 15.07-15.36  AV: 22  NL: 4.01E8
T: + c ESI Full ms [ 150.00-1000.00]
Compound 33
SI References