Electronic Supplementary Information

Fine-tuning thio-pyridazinediones as SMDC scaffolds (with intracellular thiol release via a novel self-immolative linker)

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General Experimental

All reagents were purchased from Sigma Aldrich, Alfa Aesar, Thermo Fisher and Acros. Compounds and solvents were used as received. Petrol refers to petroleum ether (40–60 °C). All reactions were monitored using thin-layer chromatography (TLC) on pre-coated SIL G/UV254 silica gel plates (254 μm). Detection was by UV (254 nm and 365 nm) or chemical stain (KMnO₄). The term in vacuo refers to solvent removal using Büchi rotary evaporation between 15–60 °C, at approximately 10 mmHg. Flash column chromatography was carried out with pre-loaded FlashPure flash cartridges on a Biotage Isolera Spektra One flash chromatography system. ¹H NMR spectra were obtained at 600 or 700 MHz and ¹³C NMR spectra were obtained at 150 MHz on Bruker NMR instrument Avance III 600 or Bruker NMR instrument Avane Neo 700. All samples were run at the default number of scans and at 21 °C. Chemical shifts (δ) for ¹H NMR and ¹³C NMR are quoted relative to residual signals of the solvent on a parts per million (ppm) scale. Coupling constants (J values) are reported in Hertz (Hz) and are reported as J_H-H couplings. The multiplicity of each signal is indicated as s-singlet, d-doublet, t-triplet, q-quartet and m-multiplet (i.e. complex peak obtained due to overlap). App. implies apparent. Infrared spectra were obtained on a Perkin Elmer Spectrum 100 FTIR Spectrometer operating in ATR mode with frequencies given in reciprocal centimetres (cm⁻¹). Optical rotations were determined from an average of five measurements at 21 °C using a 1 mL, 1 dm cell and were measured using a Perkin-Elmer 343 polarimeter. [α]_D values are reported in 10⁻¹ deg cm² g⁻¹, c is concentration (g/100 mL). Mass spectra were obtained for synthetic products, from the UCL mass spectroscopy service on either a Thermo Finnigan MAT900Xp (EI and CI) or Waters LCT Premier XE (ES) mass spectrometer. Melting points and decomposition temperatures (d.t.) were measured with a Gallenkamp apparatus and are uncorrected. All bioconjugation reactions were carried out in duplicate.

Bioconjugation General Remarks

Conjugation experiments were carried out in standard polypropylene Eppendorf® safe-lock tubes (2.0 mL) at atmospheric pressure. All buffer solutions were prepared with doubly deionised water and filter-sterilised. Phosphate-buffered saline (PBS) was 10 mM phosphates, 137 mM NaCl and 2.7 mM KCl at pH 7.4. Ultrafiltration was carried out in Amicon® Ultra-4 Centrifugal Filter Units with a molecular weight cut-off (MWCO) of 5 kDa or in Vivaspin® 500 centrifugal concentrators (5 kDa MWCO). Centrifugation was carried out on an Eppendorf 5415R fixed
angle rotor centrifuge operating at 14000 rcf at 21 °C or in an Eppendorf 5810 swing-bucket rotor centrifuge operating at 3220 rcf at 21 °C. FPLC system (GE Healthcare), equilibrated in PBS. Detection was by absorption at 280 nm.

**Protein LC-MS**

After the 4 h incubations, the samples were diluted to 3 µM (0.2 mg/mL) in ammonium acetate buffer (20 mM, pH 7.4) and submitted to the Chemistry Mass Spectrometry Facility at the Chemistry Department, UCL for analysis of unmodified protein on the Agilent 6510 QTOF LC-MS system (Agilent, UK). 10 µL of each sample were injected onto a PLRP-S, 1000A, 8 µM, 150 mm × 2.1 mm column, which was maintained at 60 °C. The separation was achieved using mobile phase A (95% H₂O, 5% MeCN, 0.1% formic acid) and B (95% MeCN, 5% H₂O, 0.1% formic acid) using a gradient elution. Agilent 6510 QTOF mass spectrometer was operated in a positive polarity mode, coupled with an ESI ion source. The ion source parameters were set up with a VCap of 3500 V, a gas temperature at 350 °C, a dry gas flow rate at 10 L/min and a nebulizer of 30 psig. MS TOF was acquired under conditions of a fragmentor at 350 V, a skimmer at 65 V and an acquisition rate at 0.5 spectra/s in a profile mode, within a scan range between 40,000 and 100,000 m/z in profile mode. The raw data was converted to zero charge mass spectra using maximum entropy deconvolution algorithm over the ca. region 18.5–22.8 min with MassHunter software (version B.07.00).

**Small Molecule LC-MS**

After 0.05, 1, 2, 4 and 24 h incubations, the samples were analysed on a Waters Acquity uPLC connected to Waters Acquity Single Quad Detector (SQD) and a photodiode array. Flow rate was set at 0.600 mL/min. LC-MS was performed on a ThermoScientific MSQ Plus connected to an Accela 1250 pump and Accela UV-Vis detector, with 10 µL of each sample being injected onto an Acquity UPLC BEH C18 (50 × 21 mm) maintained at 50 °C. The separation was achieved using mobile phase A (H₂O, 0.1% formic acid) and B (MeCN, 0.1% formic acid) using a gradient elution. Mobile phase: 95:5 A:B; gradient over 5 minutes to 5:95 A:B. MS mode ES+; scan range: m/z 100–1000; scan time: 0.25 s. The electrospray source of the MS was operated with a capillary voltage of 3.5 kV and a cone voltage of 20 V were employed. All deconvoluted mass spectra were produced using the software provided by the manufacturer.
**UV–Vis Spectroscopy**

UV-Vis spectroscopy was used to determine the maximum UV absorption of a given reaction mixture. Measurements were obtained using a Varian Cary 100 Bio UV-Visible spectrophotometer operating at 21 °C. Sample buffer was used as a blank for baseline correction.

**Fluorescence Emission Spectroscopy**

Fluorescence emission spectroscopy was used to determine the maximum fluorescence emission of a given reaction mixture. Measurements were obtained using a Varian Cary Eclipse Fluorescence spectrophotometer operating at 21 °C. Sample buffer was used as a blank for baseline correction.
Synthesis of compounds

Di-\textit{tert}-butyl 1,2-diethylhydrazine-1,2-dicarboxylate\(^1\)

\[
\begin{align*}
\text{H} \quad \text{O} \\
\text{N} \quad \text{N} \\
\text{O} \quad \text{O}
\end{align*}
\]

To a solution of di-\textit{tert}-butyl hydrazine-1,2-dicarboxylate (3.10 g, 13.4 mmol) and bromoethane (2.34 mL, 31.4 mmol) in DMF (60 mL) was added cesium carbonate (17.4 g, 47.4 mmol), and the reaction mixture was stirred at 21 °C for 21 h. Following this, the reaction mixture was diluted with water (60 mL) and extracted with EtOAc (3 × 35 mL). The organic extracts were combined and subsequently washed with sat. aq. LiCl solution (35 mL). The organic phase was dried over MgSO\(_4\), concentrated \textit{in vacuo} and the crude residue was purified by flash column chromatography (0–20% EtOAc/Pet.). The appropriate fractions were then combined and concentrated \textit{in vacuo} to afford di-\textit{tert}-butyl 1,2-diethylhydrazine-1,2-dicarboxylate (3.70 g, 12.8 mmol, 96%) as a colourless oil. \(^1\)H NMR (600 MHz, CDCl\(_3\), rotamers) \(\delta\) 3.54–3.38 (m, 4H), 1.50–1.43 (m, 18H), 1.18–1.14 (m, 6H); \(^13\)C NMR (150 MHz, CDCl\(_3\), rotamers) \(\delta\) 155.8 (C), 155.1 (C), 154.9 (C), 80.7 (C), 80.6 (C), 80.5 (C), 46.4 (CH\(_2\)), 44.4 (CH\(_2\)), 28.4 (CH\(_3\)), 28.1 (CH\(_3\)), 13.6 (CH\(_3\)), 13.1 (CH\(_3\)), 13.0 (CH\(_3\)); IR (thin film) 2976, 1703 cm\(^{-1}\).
Figure S1. $^1$H and $^{13}$C NMR data for di-tert-butyl 1,2-diethylhydrazine-1,2-dicarboxylate.
To a solution of bromomaleic anhydride (0.16 mL, 1.7 mmol) in AcOH (5 mL) was added di-tert-butyl 1,2-diethylhydrazine-1,2-dicarboxylate (0.50 g, 1.7 mmol), and the reaction mixture was stirred under reflux for 17 h. Following this, the reaction mixture was concentrated in vacuo and the crude residue was purified by flash column chromatography (15–85% EtOAc/Pet.). The appropriate fractions were then combined and concentrated in vacuo to afford 4-bromo-1,2-diethyl-1,2-dihydropyridazine-3,6-dione (0.40 g, 1.6 mmol, 94%) as a brown solid. m.p 73–76 °C; $^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 7.39 (s, 1H), 4.18 (q, $J = 7.1$ Hz, 2H), 4.11 (q, $J = 7.1$ Hz, 2H), 1.29 (t, $J = 7.1$ Hz, 3H), 1.26 (t, $J = 7.1$ Hz, 3H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 156.4 (C), 154.3 (C), 135.9 (CH), 134.0 (C), 42.1 (CH$_2$), 41.0 (CH$_2$), 13.3 (CH$_3$), 13.2 (CH$_3$); IR (solid) 3047, 2982, 1712, 1615, 1591 cm$^{-1}$. 

4-Bromo-1,2-diethyl-1,2-dihydropyridazine-3,6-dione$^2$
Figure S2. $^1$H and $^{13}$C NMR data for 4-bromo-1,2-diethyl-1,2-dihydropyridazine-3,6-dione.
4,5-Dibromo-1,2-diethyl-1,2-dihydropyridazine-3,6-dione¹

To a solution of dibromomaleic acid 19 (1.27 g, 4.64 mmol) in AcOH (6 mL) was added di-tert-butyl 1,2-diethylhydrazine-1,2-dicarboxylate (1.10 g, 3.81 mmol), and the reaction mixture was stirred under reflux for 20 h. Following this, the reaction mixture was concentrated in vacuo and the crude residue was purified by flash column chromatography (15–60% EtOAc/Pet.). The appropriate fractions were then combined and concentrated in vacuo to afford 4,5-dibromo-1,2-diethyl-1,2-dihydropyridazine-3,6-dione (1.00 g, 3.07 mmol, 81%) as an orange solid. m.p. 115–117 °C; ¹H NMR (600 MHz, CDCl₃) δ 4.18 (q, J = 7.1 Hz, 4H), 1.29 (t, J = 7.1 Hz, 6H); ¹³C NMR (150 MHz, CDCl₃) δ 153.3 (C), 136.1 (C), 42.5 (CH₂), 13.2 (CH₃); IR (solid) 2978, 2937, 1655, 1567 cm⁻¹.
Figure S3. $^1$H and $^{13}$C NMR data for 4,5-dibromo-1,2-diethyl-1,2-dihydropyridazine-3,6-dione.
1,2-Diethyl-4-(phenylthio)-1,2-dihydropyridazine-3,6-dione 2

To a solution of thiophenol (0.05 mL, 0.5 mmol) and triethylamine (0.18 mL, 1.3 mmol) in CH₂Cl₂ (6 mL) at 21 °C, was added a solution of 4-bromo-1,2-diethyl-1,2-dihydropyridazine-3,6-dione (0.11 g, 0.45 mmol) in CH₂Cl₂ (6 mL), and the reaction mixture was stirred for 10 mins. Following this, the reaction mixture was diluted with CH₂Cl₂ (20 mL) and washed with water (3 × 15 mL) and brine (15 mL). The organic phase was dried over MgSO₄, concentrated \textit{in vacuo} and the crude residue was purified by flash column chromatography (15–85% EtOAc/Pet.). The appropriate fractions were then combined and concentrated \textit{in vacuo} to afford 1,2-diethyl-4-(phenylthio)-1,2-dihydropyridazine-3,6-dione (0.11 g, 0.40 mmol, 89%) as a green solid. m.p. 104–105 °C; \(^1\)H NMR (600 MHz, CDCl₃) \(\delta\) 7.53–7.46 (m, 5H), 5.96 (s, 1H), 4.17 (q, \(J = 7.0\) Hz, 2H), 4.07 (q, \(J = 7.0\) Hz, 2H), 1.29 (t, \(J = 7.0\) Hz, 3H), 1.21 (t, \(J = 7.0\) Hz, 3H); \(^1^3\)C NMR (150 MHz, CDCl₃) \(\delta\) 157.3 (C), 155.7 (C), 151.9 (C), 135.8 (C), 130.7 (CH), 130.5 (CH), 127.5 (CH), 123.0 (CH), 40.8 (CH₂), 40.1 (CH₂), 13.2 (CH₃), 13.2 (CH₃); IR (solid) 2967, 2926, 2854, 1654, 1616, 1573 cm\(^{-1}\); LRMS (ES+) 277 (100, [M+H]\(^+\)); HRMS (ES+) calcd for C₁₄H₁₇N₂O₂S [M+H]\(^+\) 277.1011, observed 277.1011.
Figure S4. $^1$H and $^{13}$C NMR data for 1,2-diethyl-4-(phenylthio)-1,2-dihydropyridazine-3,6-dione 2.
Methyl \(N\)-(tert-butoxycarbonyl)-\(S\)-(1,2-diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazin-4-yl)cysteinate 3

To a solution of \(N\)-(tert-butoxycarbonyl)-L-cysteine methyl ester (0.24 g, 1.02 mmol) and triethylamine (0.40 mL, 2.9 mmol) in CH\(_2\)Cl\(_2\) (8 mL) at 21 °C, was added a solution of 4-bromo-1,2-diethyl-1,2-dihydropyridazine-3,6-dione (0.24 g, 0.97 mmol) in CH\(_2\)Cl\(_2\) (8 mL), and the reaction mixture was stirred for 10 mins. Following this, the reaction mixture was diluted with CH\(_2\)Cl\(_2\) (20 mL) and washed with water (3 × 15 mL) and brine (15 mL). The organic phase was dried over MgSO\(_4\), concentrated \textit{in vacuo} and the crude residue was purified by flash column chromatography (20–85% EtOAc/Pet.). The appropriate fractions were then combined and concentrated \textit{in vacuo} to afford methyl \(N\)-(tert-butoxycarbonyl)-\(S\)-(1,2-diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazin-4-yl)cysteinate (0.31 g, 0.77 mmol, 80%) as a white solid. \([\alpha]_D^{20.0} +3.0\) (c 1, CHCl\(_3\)); m.p. 86–90 °C; \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 6.56 (s, 1H), 5.37 (d, \(J = 7.6\) Hz, 1H), 4.68–4.65 (m, 1H), 4.17–4.07 (m, 4H), 3.79 (s, 3H), 3.31 (dd, \(J = 13.2, 5.0\) Hz, 1H), 3.20 (dd, \(J = 13.2, 5.0\) Hz, 1H), 1.44 (s, 9H), 1.26 (t, \(J = 7.1\) Hz, 3H), 1.22 (t, \(J = 7.1\) Hz, 3H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)) \(\delta\) 170.5 (C), 156.9 (C), 155.6 (C), 155.1 (C), 148.7 (C), 122.6 (CH), 80.7 (C), 53.1 (CH\(_3\)), 52.2 (CH), 40.9 (CH\(_2\)), 40.2 (CH\(_2\)), 33.0 (CH\(_2\)), 28.4 (CH\(_3\)), 13.2 (CH\(_3\)), 13.1 (CH\(_3\)); IR (solid) 2979, 1746, 1709, 1615 cm\(^{-1}\); LRMS (ES+) 402 (100, [M+H]\(^+\)); HRMS (ES+) calcd for C\(_{17}\)H\(_{28}\)N\(_3\)O\(_6\)S [M+H]\(^+\) 402.1693, observed 402.1694.
Figure S5. $^1$H and $^{13}$C NMR data for methyl $N$-(tert-butoxycarbonyl)-$S$-(1,2-diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazin-4-yl)cysteinate 3.
1,2-Diethyl-4,5-bis(phenylthio)-1,2-dihydropyridazine-3,6-dione 4

To a solution of thiophenol (0.10 mL, 0.97 mmol) and triethylamine (0.39 mL, 2.80 mmol) in CH\textsubscript{2}Cl\textsubscript{2} (6 mL) at 21 °C, was added a solution of 4,5-dibromo-1,2-diethyl-1,2-dihydropyridazine-3,6-dione (0.10 g, 0.31 mmol) in CH\textsubscript{2}Cl\textsubscript{2} (6 mL), and the reaction mixture was stirred for 10 mins. Following this, the reaction mixture was diluted with CH\textsubscript{2}Cl\textsubscript{2} (20 mL) and washed with water (3 × 15 mL) and brine (15 mL). The organic phase was dried over MgSO\textsubscript{4}, concentrated \textit{in vacuo} and the crude residue was purified by flash column chromatography (15–80% EtOAc/Pet.). The appropriate fractions were then combined to afford 1,2-diethyl-4,5-bis(phenylthio)-1,2-dihydropyridazine-3,6-dione (0.09g, 0.23 mmol, 76%) as a yellow solid. m.p. 126–130 °C; \textsuperscript{1}H NMR (600 MHz, CDCl\textsubscript{3}) δ 7.28–7.25 (m, 7H), 7.22–7.20 (m, 3H), 4.05 (q, \textit{J} = 7.1 Hz, 4H), 1.23 (t, \textit{J} = 7.1 Hz, 6H); \textsuperscript{13}C NMR (150 MHz, CDCl\textsubscript{3}) δ 156.0 (C), 141.9 (C), 132.6 (C), 131.0 (CH), 129.1 (CH), 127.9 (CH), 41.2 (CH\textsubscript{2}), 12.8 (CH\textsubscript{3}); IR (solid) 3058, 2967, 2928, 1657, 1574 cm\textsuperscript{-1}; LRMS (ES+) 385 (100, [M+H]\textsuperscript{+}); HRMS (ES+) calcd for C\textsubscript{20}H\textsubscript{21}N\textsubscript{2}O\textsubscript{2}S\textsubscript{2} [M+H]\textsuperscript{+} 385.1039, observed 385.1040.
Figure S6. $^1$H and $^{13}$C NMR data for 1,2-diethyl-4,5-bis(phenylthio)-1,2-dihydropyridazine-3,6-dione 4.
Dimethyl 3,3'-(1,2-diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazine-4,5-diyl)bis(sulfanediyl)bis(2-((tert-butoxycarbonyl)amino)propanoate) 5

To a solution of 4,5-dibromo-1,2-diethyl-1,2-dihydropyridazine-3,6-dione (0.13 g, 0.40 mmol) and N-(tert-butoxycarbonyl)-L-cysteine methyl ester (0.47 g, 2.0 mmol) in CH₂Cl₂ (10 mL) was added triethylamine (0.07 mL, 0.5 mmol), and the reaction mixture was stirred at 21 °C for 65 h. Following this, the reaction mixture was diluted with CH₂Cl₂ (20 mL) and washed with water (3 × 20 mL) and brine (15 mL). The organic phase was dried over MgSO₄, concentrated in vacuo and the crude residue was purified by flash column chromatography (15–60% EtOAc/Pet.). The appropriate fractions were then combined and concentrated in vacuo to afford dimethyl 3,3'-(1,2-diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazine-4,5-diyl)bis(sulfanediyl)bis(2-((tert-butoxycarbonyl)amino)propanoate) (0.15 g, 0.24 mmol, 59%) as a yellow oil. [α]D²⁰.⁰ +60.6 (c 1, CHCl₃); ¹H NMR (600 MHz, CDCl₃) δ 5.76 (d, J = 7.8 Hz, 2H), 4.55–4.53 (m, 2H), 4.09–3.98 (m, 4H), 3.74–3.68 (m, 3H), 3.68 (s, 6H), 3.65–3.60 (m, 1H) 1.38 (s, 18H), 1.21 (t, J = 7.2 Hz, 6H); ¹³C NMR (150 MHz, CDCl₃) δ 171.2 (C), 155.3 (C), 155.3 (C), 141.9 (C), 80.1 (C), 53.9 (CH), 52.6 (CH₃), 41.3 (CH₂), 35.7 (CH₂), 28.4 (CH₃), 13.0 (CH₃); IR (thin film) 2978, 1707, 1617 cm⁻¹; LRMS (ES+) 635 (100, [M+H]⁺); HRMS (ES+) calcd for C₂₆H₄₅N₄O₁₀S₂ [M+H]⁺ 635.2415, observed 635.2411.
Figure S7. $^1$H and $^{13}$C NMR data for dimethyl 3,3'-(1,2-diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazine-4,5-diyl)bis(sulfanediyl))bis(2-((tert-butoxycarbonyl)amino)propanoate)
Methyl S-(5-bromo-1,2-diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazin-4-yl)-N-(tert-butoxycarbonyl)cysteinate

To a solution of 4,5-dibromo-1,2-diethyl-1,2-dihydropyridazine-3,6-dione (0.20 g, 0.61 mmol) in CH₂Cl₂ (6 mL) at 21 °C, was added dropwise over 10 mins a solution of N-(tert-butoxycarbonyl)-L-cysteine methyl ester (0.14 g, 0.59 mmol) and triethylamine (0.13 mL, 0.93 mmol) in CH₂Cl₂ (6 mL). Following this, the reaction mixture was diluted with CH₂Cl₂ (12 mL) and washed with water (3 × 15 mL) and brine (15 mL). The organic phase was dried over MgSO₄, concentrated in vacuo and the crude residue was purified by flash column chromatography (0–30% EtOAc/CHCl₃). The appropriate fractions were then combined and concentrated in vacuo to afford methyl S-(5-bromo-1,2-diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazin-4-yl)-N-(tert-butoxycarbonyl)cysteinate (0.17 g, 0.35 mmol, 60%) as a yellow oil. [α]D²⁰ 0.0 +17.7 (c 1, CHCl₃); ¹H NMR (600 MHz, CDCl₃) δ 5.42 (d, J = 8.1 Hz, 1H), 4.63–4.59 (m, 1H), 4.22–4.03 (m, 4H), 3.85–3.82 (m, 1H), 3.75 (d, J = 7.0 Hz, 1H), 3.73 (s, 3H), 1.42 (s, 9H), 1.30–1.25 (m, 6H); ¹³C NMR (150 MHz, CDCl₃) δ 171.1 (C), 155.2 (C), 154.6 (C), 153.7 (C), 153.7 (C), 145.3 (C), 130.9 (C), 80.4 (C), 53.9 (CH), 52.8 (CH₃), 42.2 (CH₂), 41.1 (CH₂), 35.9 (CH₂), 28.4 (CH₃), 13.2 (CH₃), 12.9 (CH₃); IR (thin film) 2977, 2934, 1743, 1708, 1622 cm⁻¹; LRMS (ES+) 482 (100, [M⁺Br+H]+), 480 (96, [M⁺Br+H]+); HRMS (ES+) calcd for C₁₇H₂₇N₃O₆SBr [M⁺Br+H]⁺ 482.0779, observed 482.0770.
Figure S8. $^1$H and $^{13}$C NMR spectra for methyl S-(5-bromo-1,2-diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazin-4-yl)-N-(tert-butoxycarbonyl)cysteinate.
Methyl N-(tert-butoxycarbonyl)-S-(1,2-diethyl-3,6-dioxo-5-(phenylthio)-1,2,3,6-tetrahydropyridazin-4-yl)cysteinate 6

To a solution of methyl S-(5-bromo-1,2-diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazin-4-yl)-N-(tert-butoxycarbonyl)cysteinate (0.45 g, 0.94 mmol) in CH₂Cl₂ (8 mL) at 21 °C, was added a solution of thiophenol (0.10 mL, 0.98 mmol) and triethylamine (0.20 mL, 1.4 mmol) in CH₂Cl₂ (8 mL), and the reaction was stirred for 10 mins. Following this, the reaction mixture was diluted with CH₂Cl₂ (16 mL) and washed with water (3 × 15 mL) and brine (15 mL). The organic phase was dried over MgSO₄, concentrated in vacuo and the crude residue was purified by flash column chromatography (0–40% EtOAc/CHCl₃). The appropriate fractions were then combined and concentrated in vacuo to afford methyl N-(tert-butoxycarbonyl)-S-(1,2-diethyl-3,6-dioxo-5-(phenylthio)-1,2,3,6-tetrahydropyridazin-4-yl)cysteinate (0.24 g, 0.47 mmol, 50%) as a yellow oil. [α]D²⁰⁺26.9 (c 1, CHCl₃); ¹H NMR (600 MHz, CDCl₃) δ 7.37–7.27 (m, 5H), 5.48 (d, J = 8.1 Hz, 1H), 4.52 (m, 1H), 4.15–3.98 (m, 4H), 3.70 (s, 3H), 3.68 (d, J = 6.3 Hz, 1H), 3.58 (dd, J = 14.0, 6.3 Hz, 1H), 1.41 (s, 9H), 1.27 (t, J = 7.1 Hz, 3H), 1.22 (t, J = 7.1 Hz, 3H); ¹³C NMR (150 MHz, CDCl₃) δ 171.3 (C), 155.8 (C), 155.3 (C), 155.3 (C), 142.6 (C), 142.1 (C), 132.8 (C), 131.1 (CH), 129.3 (CH), 128.0 (CH), 80.3 (C), 53.8 (CH), 52.7 (CH₃), 41.3 (CH₂), 41.3 (CH₂), 35.7 (CH₂), 28.4 (CH₃), 13.0 (CH₃), 12.9 (CH₃); IR (thin film) 2975, 2932, 1743, 1708, 1614 cm⁻¹; LRMS (ES⁺) 510 (100, [M+H]⁺); HRMS (ES⁺) calcd for C₂₃H₉₂N₄O₆S₂ [M+H]⁺ 510.1727, observed 510.1718.
Figure S9. $^1$H and $^{13}$C NMR spectra for methyl $N$-(tert-butoxycarbonyl)-$S$-(1,2-diethyl-3,6-dioxo-5-(phenylthio)-1,2,3,6-tetrahydropyridazin-4-yl)cysteinate 6.
1,2-Diethyl-4,5-bis(p-tolylthio)-1,2-dihydropyridazine-3,6-dione 8

To a solution of 4,5-dibromo-1,2-diethyl-1,2-dihydropyridazine-3,6-dione (1.63 g, 5.00 mmol) in CH₂Cl₂ (10 mL) at 21 °C, was added a solution of 4-methylbenzenethiol 23 (1.55 g, 12.5 mmol) and triethylamine (2.27 mL, 16.3 mmol) in CH₂Cl₂ (10 mL), and the reaction mixture was stirred for 10 mins. Following this, the reaction mixture was diluted with CH₂Cl₂ (20 mL) and washed with water (3 × 30 mL) and brine (30 mL). The organic phase was dried over MgSO₄, concentrated in vacuo and the crude residue was purified by flash column chromatography (10–60% EtOAc/Pet.). The appropriate fractions were then combined and concentrated in vacuo to afford 1,2-diethyl-4,5-bis(p-tolylthio)-1,2-dihydropyridazine-3,6-dione (1.85 g, 4.49 mmol, 90%) as a yellow solid. m.p. 114–116 °C; ¹H NMR (600 MHz, CDCl₃) δ 7.15 (d, J = 8.2 Hz, 4H), 7.09 (d, J = 8.2 Hz, 4H), 4.02 (q, J = 7.1 Hz, 4H), 2.33 (s, 6H), 1.21 (t, J = 7.1 Hz, 6H); ¹³C NMR (150 MHz, CDCl₃) δ 156.1 (C), 142.3 (C), 138.1 (C), 131.3 (CH), 129.9 (CH), 129.3 (C), 41.1 (CH₂), 21.4 (CH₃), 12.8 (CH₃); IR (solid) 2980, 2956, 2923, 2868, 1617, 1567 cm⁻¹; LRMS (ES+) 413 (100, [M+H]⁺); HRMS (ES+) calcd for C₂₂H₂₅N₂O₂S₂ [M+H]⁺ 413.1352, observed 413.1346.
Figure S10. $^1$H and $^{13}$C NMR spectra for 1,2-diethyl-4,5-bis(p-tolylthio)-1,2-dihydropyridazine-3,6-dione 8.
1,2-Diethyl-4,5-bis(4-(((2-oxo-2H-chromen-7-yl)oxy)methyl)phenylthio)-1,2-dihydropyridazine-3,6-dione 13

To a solution of 1,2-diethyl-4,5-bis(p-tolylthio)-1,2-dihydropyridazine-3,6-dione 8 (0.11 g, 0.27 mmol) in fluorobenzene (6 mL) was added NBS 9 (0.13 g, 0.73 mmol) and AIBN 10 (0.03 g, 0.2 mmol), and the reaction mixture was stirred under reflux for 7 h. Following this, the reaction mixture was diluted with EtOAc (20 mL) and washed with water (3 × 20 mL). The organic phase was dried over MgSO$_4$ and concentrated in vacuo to afford the crude 4,5-bis((4-(bromomethyl)phenylthio)-1,2-diethyl-1,2-dihydropyridazine-3,6-dione 11 (0.11 g total). The crude mixture was dissolved in dry THF (4 mL) along with cesium carbonate (0.22 g, 0.68 mmol) and umbelliferone 12 (0.08 g, 0.5 mmol), and the reaction mixture was stirred under reflux for 21 h. Following this, the reaction mixture was diluted with water (10 mL) and extracted with EtOAc (3 × 15 mL). The organic phase was dried over MgSO$_4$, concentrated in vacuo and the crude residue was purified by preparative TLC (50% EtOAc/CHCl$_3$) to afford 1,2-diethyl-4,5-bis((4-(((2-oxo-2H-chromen-7-yl)oxy)methyl)phenylthio)-1,2-dihydropyridazine-3,6-dione (0.02 g, 0.03 mmol, 9%) as a yellow solid. m.p. 179–183 °C; $^1$H NMR (600 MHz, CDCl$_3$) δ 7.62 (d, $J$ = 9.5 Hz, 2H), 7.37 (d, $J$ = 8.6 Hz, 2H), 7.32 (d, $J$ = 8.2 Hz, 4H), 7.22 (d, $J$ = 8.2 Hz, 4H), 6.89 (dd, $J$ = 8.6, 2.5 Hz, 2H), 6.86 (d,$J$ = 2.5 Hz, 2H), 6.26 (d, $J$ = 9.5 Hz, 2H), 5.10 (s, 4H), 4.05 (q, $J$ = 7.0 Hz, 4H), 1.23 (t, $J$ = 7.0 Hz, 6H); $^{13}$C NMR (150 MHz, CDCl$_3$) δ 161.8 (C), 161.2 (C), 156.0 (C), 155.8 (C), 143.5 (CH), 141.9 (C), 135.7 (C), 132.7 (C), 131.3 (CH), 129.0 (CH), 128.2 (CH), 113.5 (CH), 113.3 (CH), 113.0 (C), 102.1 (CH), 70.0 (CH$_2$), 41.4 (CH$_2$), 12.9
(CH$_3$); IR (solid) 2919, 2851, 1726, 1608 cm$^{-1}$; LRMS (ES+) 733 (100, [M+H]$^+$); HRMS (ES+) calcd for C$_{40}$H$_{33}$N$_2$O$_8$S$_2$ [M+H]$^+$ 733.1678, observed 733.1674.
Figure S11. $^1$H and $^{13}$C NMR spectra for 1,2-diethyl-4,5-bis((4-(((2-oxo-2H-chromen-7-yl)oxy)methyl)phenyl)thio)-1,2-dihydropyridazine-3,6-dione 13. *29.8 (H grease), 1.15 (silicon grease).
**Tert-butyl 7-hydroxy-2-oxo-2H-chromene-3-carboxylate**

To a solution of di-tert-butyl malonate (0.69 g, 3.2 mmol) and potassium carbonate (1.11 g, 8.03 mmol) in DMF (16 mL), was added 2,4-dihydroxybenzaldehyde (0.22 g, 1.6 mmol), and the reaction mixture was stirred at 80 °C for 19 h. Following this, the reaction mixture was diluted with water (16 mL), 0.1 M citric acid (16 mL), and extracted with EtOAc (3 × 40 mL). The organic extracts were combined and subsequently washed with sat. aq. LiCl solution (40 mL). The organic phase was dried over MgSO₄, concentrated in vacuo and the crude residue was purified by flash column chromatography (10–60% EtOAc/Pet.). The appropriate fractions were then combined and concentrated in vacuo to afford tert-butyl 7-hydroxy-2-oxo-2H-chromene-3-carboxylate (0.05 g, 0.2 mmol, 12%) as a beige solid. m.p. 249–251 °C; ¹H NMR (700 MHz, CDCl₃) δ 8.39 (s, 1H), 7.47 (d, J = 8.5 Hz, 1H), 6.91 (d, J = 2.2 Hz, 1H), 6.87 (dd, J = 8.5, 2.2 Hz, 1H), 1.59 (s, 9H); ¹³C NMR (150 MHz, CDCl₃) δ 162.5 (C), 162.3 (C), 158.0 (C), 157.3 (C), 148.5 (CH), 131.2 (CH), 115.1 (C) 114.3 (CH), 111.8 (C), 103.2 (CH), 82.6 (C), 28.3 (CH₃); IR (solid) 3314, 2920, 2851, 1743, 1615, 1558 cm⁻¹.
Figure S12. $^1$H and $^{13}$C NMR spectra for tert-butyl 7-hydroxy-2-oxo-2$H$-chromene-3-carboxylate.
Di-\textit{tert}-butyl 7,7'-'-((((1,2-diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazine-4,5-diyl)bis(sulfanediyl))bis(4,1-phenylene))bis(methylene))bis(oxy))bis(2-oxo-2\textit{H}-chromene-3-carboxylate)

To a solution of 1,2-diethyl-4,5-bis(\textit{p}-tolylthio)-1,2-dihydropyridazine-3,6-dione 8 (0.10 g, 0.24 mmol) in fluorobenzene (7 mL) was added NBS 9 (0.09 g, 0.5 mmol) and AIBN 10 (0.02 g, 0.1 mmol), and the reaction mixture was stirred at 60 °C for 21 h. Following this, the reaction mixture was diluted with fluorobenzene (7 mL) and washed with water (3 × 6 mL) and brine (7 mL). The organic phase was dried over MgSO\textsubscript{4} and concentrated \textit{in vacuo} to afford the crude 4,5-bis((4-(bromomethyl)phenyl)thio)-1,2-diethyl-1,2-dihydropyridazine-3,6-dione 11 (0.11 g total). The crude mixture (0.04 g) was dissolved in dry THF (3 mL) along with cesium carbonate (0.03 g, 0.09 mmol) and \textit{tert}-butyl 7-hydroxy-2-oxo-2\textit{H}-chromene-3-carboxylate (0.02 g, 0.08 mmol), and the reaction mixture was stirred under reflux for 21 h. Following this, the reaction mixture was diluted with water (7 mL) and extracted with EtOAc (3 × 8 mL). The organic extracts were combined and subsequently washed with brine (8 mL). The organic phase was dried over MgSO\textsubscript{4}, concentrated \textit{in vacuo} and the crude residue was purified by flash column
chromatography (20–80% EtOAc/Pet.). The appropriate fractions were then combined and concentrated *in vacuo* to afford di-tert-butyl 7,7′-(((1,2-diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazine-4,5-diyl)bis(sulfanediyl))bis(4,1-phenylene))bis(methylene))bis(2-oxo-2H-chromene-3-carboxylate) (0.02 g, 0.02 mmol, 23%) as a yellow solid. m.p. 83–86 °C; \(^1\)H NMR (700 MHz, CDCl\(_3\)) \(\delta\) 8.37 (s, 2H), 7.49 (d, \(J = 8.7\) Hz, 2H), 7.33 (d, \(J = 8.4\) Hz, 4H), 7.24 (d, \(J = 8.4\) Hz, 4H), 6.93 (dd, \(J = 8.7, 2.4\) Hz, 2H), 6.84 (d, \(J = 2.4\) Hz, 2H), 5.12 (s, 4H), 4.05 (q, \(J = 7.0\) Hz, 4H), 1.59 (s, 18H), 1.23 (t, \(J = 7.0\) Hz, 6H); \(^1^3\)C NMR (150 MHz, CDCl\(_3\)) \(\delta\) 163.7 (C), 162.3 (C), 157.4 (C), 157.3 (C), 155.7 (C), 148.0 (CH), 141.9 (C), 135.3 (C), 132.9 (C), 131.3 (CH), 130.7 (CH), 128.2 (CH), 116.0 (C), 114.1 (CH), 112.1 (C), 101.5 (CH), 82.6 (C), 70.2 (CH\(_2\)), 41.4 (CH\(_2\)), 28.3 (CH\(_3\)), 12.9 (CH\(_3\)); IR (solid) 2924, 2854, 1748, 1606 cm\(^{-1}\); LRMS (ES+) 933 (100, [M+H]\(^+\)); HRMS (ES+) calcd for C\(_{50}\)H\(_{49}\)N\(_2\)O\(_{12}\)S\(_2\) [M+H]\(^+\) 933.2727, observed 933.2778.
Figure S13. $^1$H and $^{13}$C NMR spectra for di-tert-butyl 7,7'-((((1,2-diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazine-4,5-diyl)bis(sulfanediyl))bis(4,1-phenylene))bis(methylene))bis(oxy))bis(2-oxo-2$H$-chromene-3-carboxylate). *29.8 (H grease), 1.15 (silicon grease).
7,7’-(((1,2-Diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazine-4,5-diyl)bis(sulfanediyl))bis(4,1-phenylene))bis(methylene)bis(oxy))bis(2-oxo-2H-chromene-3-carboxylic acid) 16

Di-tert-butyl 7,7’-(((1,2-diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazine-4,5-diyl)bis(sulfanediyl))bis(4,1-phenylene))bis(methylene)bis(2-oxo-2H-chromene-3-carboxylate) (11 mg, 0.010 mmol) was dissolved in TFA (0.25 mL) and CH$_2$Cl$_2$ (0.75 mL), and stirred at 21 °C for 4 h. Following this, the reaction mixture was concentrated in vacuo to afford 7,7’-(((1,2-diethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazine-4,5-diyl)bis(sulfanediyl))bis(4,1-phenylene))bis(methylene)bis(2-oxo-2H-chromene-3-carboxylic acid) (10 mg, 0.010 mmol, quant.) as a yellow solid. d.t. 195–198 °C; $^1$H NMR (700 MHz, CDCl$_3$) δ 8.86 (s, 2H), 7.66 (d, $J$ = 8.8 Hz, 2H), 7.35 (d, $J$ = 8.5 Hz, 4H), 7.28 (d, $J$ = 8.5 Hz, 4H), 7.08 (dd, $J$ = 8.8, 2.4 Hz, 2H), 6.97 (d, $J$ = 2.4 Hz, 2H), 5.18 (s, 4H), 4.05 (q, $J$ = 7.0 Hz, 4H), 4.05 (q, $J$ = 7.0 Hz, 4H), 1.24 (t, $J$ = 7.0 Hz, 6H); $^{13}$C NMR (150 MHz, CDCl$_3$) δ 165.1 (C), 164.6 (C), 163.1 (C), 157.0 (C), 155.7 (C), 151.3 (CH), 142.1 (C), 134.8 (C), 133.4 (C), 131.9 (CH), 131.4 (CH), 128.2 (CH), 115.8 (CH), 112.7 (C), 111.4 (C), 102.0 (CH), 70.6 (CH$_2$), 41.4 (CH$_2$), 12.9 (CH$_3$); IR (solid) 3056, 2926, 2853, 1787, 1717, 1596 cm$^{-1}$; LRMS (ES+) 821 (100, [M+H]$^+$); HRMS (ES+) calcd for C$_{42}$H$_{33}$N$_2$O$_{12}$S$_2$ [M+H]$^+$ 821.1450, observed 821.1475.
Figure S14. $^1$H and $^{13}$C NMR spectra for 7,7'-$(((1,2$-dithyl-3,6-dioxo-1,2,3,6-tetrahydropyridazine-4,5-diyl)bis(sulfanediyl))bis(4,1-phenylene))bis(methylene))bis(oxy))bis(2-oxo-$2H$-chromene-3-carboxylic acid) 16.
Di-tert-butyl 1-(3-(tert-butoxy)-3-oxopropyl)hydrazine-1,2-dicarboxylate

To a solution of di-tert-butyl hydrazine-1,2-dicarboxylate (1.22 g, 5.25 mmol) in EtOH (10 mL), was added fifteen drops of 2 M NaOH, and the reaction mixture was stirred at 21 °C for 10 mins. Following this, tert-butyl acrylate (0.91 mL, 6.3 mmol) was added to the solution and the reaction mixture was stirred under reflux for 48 h. Following this, the reaction mixture was concentrated in vacuo and the crude residue was purified by flash column chromatography (0–20% EtOAc/Pet.). The appropriate fractions were then combined and concentrated in vacuo to afford di-tert-butyl 1-(3-(tert-butoxy)-3-oxopropyl)hydrazine-1,2-dicarboxylate (1.11 g, 3.08 mmol, 59%) as a colourless oil. $^1$H NMR (700 MHz, CDCl$_3$, rotamers) δ 6.39 (s, 0.70H), 6.08 (s, 0.20H), 3.71 (app. s, 2H), 2.52 (t, $J = 6.6$ Hz, 2H), 1.46–1.43 (m, 27H); $^{13}$C NMR (150 MHz, CDCl$_3$) δ 168.9 (C), 168.6 (C), 152.4 (C), 79.0 (C), 78.6 (C), 78.1 (C), 44.3 (CH$_2$), 43.1 (CH$_2$), 31.8 (CH$_2$), 31.6 (CH$_2$), 25.6 (CH$_3$), 25.5 (CH$_3$); IR (thin film) 2975, 2931, 1707 cm$^{-1}$; LRMS (ES+) 361 (100, [M+H]$^+$); HRMS (ES+) calcd for C$_{17}$H$_{33}$N$_2$O$_6$ [M+H]$^+$ 361.2333, observed 361.2337.
Figure S15. $^1$H and $^{13}$C NMR spectra for di-tert-butyl 1-(3-(tert-butoxy)-3-oxopropyl)hydrazine-1,2-dicarboxylate.
2-(2-(2-Methoxyethoxy)ethoxy)ethyl 4-methylbenzenesulfonate

To a solution of triethylene glycol monomethyl ether (2.00 g, 12.2 mmol) and triethylamine (2.55 mL, 18.3 mmol) in dry THF (15 mL), was added 4-methylbenzenesulfonyl chloride (2.79 g, 14.6 mmol), and the reaction mixture was stirred for 21 h at 21 °C. Following this, the reaction mixture was diluted with water (15 mL) and extracted with EtOAc (3 × 15 mL). The organic extracts were combined and subsequently washed with brine (25 mL). The organic phase was dried over MgSO₄, concentrated in vacuo and the crude residue was purified by flash column chromatography (20–80% EtOAc/Pet.). The appropriate fractions were then combined and concentrated in vacuo to afford 2-(2-(2-methoxyethoxy)ethoxy)ethyl 4-methylbenzenesulfonate (3.74 g, 11.8 mmol, 96%) as a clear yellow oil. ¹H NMR (700 MHz, CDCl₃) δ 7.76 (d, $J = 8.3$ Hz, 2H), 7.31 (d, $J = 8.3$ Hz, 2H), 4.13–4.12 (m, 2H), 3.66–3.65 (m, 2H), 3.58–3.56 (m, 6H), 3.49 (m, 2H), 3.33 (s, 3H), 2.41 (s, 3H); ¹³C NMR (150 MHz, CDCl₃) δ 144.9 (C), 133.1 (C), 130.0 (CH), 128.1 (CH), 72.0 (CH₂), 70.8 (CH₂), 70.7 (CH₂), 70.6 (CH₂), 69.4 (CH₂), 68.8 (CH₂), 59.1 (CH₃), 21.8 (CH₃); IR (thin film) 2877, 1598, 1452 cm⁻¹.
Figure S16. $^1$H and $^{13}$C NMR spectra for 2-(2-(2-methoxyethoxy)ethoxy)ethyl 4-methylbenzenesulfonate.
Tri-tert-butyl 2,5,8-trioxa-11,12-diazatetradecane-11,12,14-tricarboxylate 18

To a solution of di-tert-butyl 1-(3-(tert-butoxy)-3-oxopropyl)hydrazine-1,2-dicarboxylate (0.77 g, 2.1 mmol) and cesium carbonate (1.04 g, 3.19 mmol) in DMF (8 mL), was added 2-(2-(2-methoxyethoxy)ethoxy)ethyl 4-methylbenzenesulfonate (1.02 g, 3.21 mmol), and the reaction mixture was stirred at 21 °C for 72 h. Following this, the reaction mixture was diluted with water (8 mL) and extracted with EtOAc (3 × 15 mL). The organic extracts were combined and subsequently washed with sat. aq. LiCl solution (15 mL). The organic phase was dried over MgSO₄, concentrated in vacuo and the crude residue was purified by flash column chromatography (20–50% EtOAc/Pet.). The appropriate fractions were then combined and concentrated in vacuo to afford tri-tert-butyl 2,5,8-trioxa-11,12-diazatetradecane-11,12,14-tricarboxylate (0.92 g, 1.8 mmol, 85%) as a colourless oil. ¹H NMR (600 MHz, CDCl₃, rotamers) δ 3.78–3.59 (m, 12H), 3.56–3.53 (m, 2H), 3.37 (s, 3H), 2.61 (t, J = 7.8 Hz, 2H), 1.48–1.42 (m, 27H); ¹³C NMR (150 MHz, CDCl₃) δ 171.4 (C), 171.2 (C), 171.1 (C), 155.8 (C), 155.2 (C), 155.0 (C), 154.6 (C), 154.5 (C), 81.6 (C), 81.5 (C), 81.4 (C), 81.4 (C), 81.2 (C), 81.2 (C), 81.1 (C), 80.7 (C), 80.6 (C), 80.4 (C), 72.0 (CH₂), 70.7 (CH₂), 70.7 (CH₂), 70.7 (CH₂), 70.6 (CH₂), 70.5 (CH₂), 70.4 (CH₂), 68.7 (CH₂), 68.5 (CH₂), 59.1 (CH₃), 51.2 (CH₂), 50.5 (CH₂), 50.3 (CH₂), 47.2 (CH₂), 46.1 (CH₂), 46.0 (CH₂), 34.4 (CH₂), 33.9 (CH₂), 33.9 (CH₂), 28.4 (CH₃), 28.4 (CH₃), 28.3 (CH₃), 28.2 (CH₃), 28.2 (CH₃); IR (thin film) 2973, 2928, 2872, 1705 cm⁻¹; LRMS (ES+) 507 (100, [M+H]+); HRMS (ES+) calcd for C₂₅H₄₆N₂O₉ [M+H]+ 507.3282, observed 507.3272.
Figure S17. $^1$H and $^{13}$C NMR spectra for tri-tert-butyl 2,5,8-trioxa-11,12-diazatetradecane-11,12,14-tricarboxylate 18.
3-(4,5-Dibromo-2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-3,6-dihydropyridazin-1(2H)-yl)propanoic acid 20

To a solution of tri-tert-butyl 2,5,8-trioxa-11,12-diazatetradecane-11,12,14-tricarboxylate 18 (1.54 g, 3.04 mmol) in AcOH (10 mL), was added dibromomaleic acid 19 (1.67 g, 6.10 mmol), and the reaction mixture was stirred under reflux for 24 h. Following this, the reaction mixture was concentrated in vacuo and the crude residue was purified by flash column chromatography (0–10% MeOH/CH₂Cl₂). The appropriate fractions were then combined and concentrated in vacuo to afford 3-(4,5-dibromo-2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-3,6-dihydropyridazin-1(2H)-yl)propanoic acid (1.09 g, 2.24 mmol, 74%) as a brown oil. ¹H NMR (700 MHz, CDCl₃) δ 4.49–4.47 (m, 2H), 4.28–4.27 (m, 2H), 3.77–3.76 (m, 2H), 3.61–3.56 (m, 8H), 3.41 (s, 3H), 2.82–2.80 (m, 2H); ¹³C NMR (150 MHz, CDCl₃) δ 173.0 (C), 154.1 (C), 153.4 (C), 136.4 (C), 136.0 (C), 72.1 (CH₂), 70.9 (CH₂), 70.5 (CH₂), 70.3 (CH₂), 68.3 (CH₂), 59.0 (CH₃), 49.8 (CH₂), 44.6 (CH₂), 31.7 (CH₂); IR (thin film) 3452, 2918, 1723, 1628, 1574 cm⁻¹; LRMS (ES) 487 (100, [M⁺²Br⁺H⁺]) ; HRMS (ES) caled for C₁₄H₂₁N₂O₇Br₂ [M⁺²Br⁺H⁺] 486.9545, observed 486.9545.
Figure S18. $^1$H and $^{13}$C NMR spectra for 3-(4,5-dibromo-2-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-3,6-dihydropyridazin-1(2H)-yl)propanoic acid 20.
$N$-(3-Azidopropyl)-3-(4,5-dibromo-2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-3,6-dihydropyridazin-1(2H)-yl)propanamide 21

To a solution of 3-(4,5-dibromo-2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-3,6-dihydropyridazin-1(2H)-yl)propanoic acid 20 (0.15 g, 0.31 mmol) in THF (4 mL) stirring at 0 °C was added DCC (0.08 g, 0.4 mmol), and the reaction mixture was stirred at 0 °C for 30 mins. After this time, 3-azido-1-propanamine (0.04 g, 0.4 mmol) was added, and the reaction mixture was stirred at 21 °C for a further 23 h. Following this, the reaction mixture was filtered to remove insolubles and underwent 3 rounds of successive cooling on acetone/dry ice and filtrations before being concentrated in vacuo. The crude residue was purified by flash column chromatography (0–5% MeOH/CH$_2$Cl$_2$). The appropriate fractions were then combined and concentrated in vacuo to afford $N$-(3-azidopropyl)-3-(4,5-dibromo-2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-3,6-dihydropyridazin-1(2H)-yl)propanamide (0.09 g, 0.2 mmol, 51%) as a clear brown oil. $^1$H NMR (700 MHz, CDCl$_3$) δ 6.40 (app. s, 1H), 4.46 (t, $J$ = 7.0 Hz, 2H), 4.36 (t, $J$ = 4.9 Hz, 2H), 3.74 (t, $J$ = 4.9 Hz, 2H), 3.58–3.56 (m, 6H), 3.53–3.51 (m, 2H), 3.36 (s, 3H), 3.35 (app. d, 2H), 3.31 (q, $J$ = 6.7 Hz, 2H), 2.66 (t, $J$ = 7.0 Hz, 2H), 1.76 (p, $J$ = 6.7 Hz, 2H); $^{13}$C NMR (150 MHz, CDCl$_3$) δ 170.0 (C), 153.8 (C), 153.4 (C), 136.1 (C), 136.0 (C), 72.0 (CH$_2$), 70.6 (CH$_2$), 70.5 (CH$_2$), 70.5 (CH$_2$), 67.9 (CH$_2$), 59.1 (CH$_3$), 49.4 (CH$_2$), 48.8 (CH$_2$), 45.1 (CH$_2$), 37.4 (CH$_2$), 33.9 (CH$_2$), 28.9 (CH$_2$); IR (thin film) 2923, 2874, 2094, 1631 cm$^{-1}$; LRMS (ES+) 571 (100, [M$^{81}$Br$^{79}$Br]$^+$H$^+$); HRMS (ES+) calcd for C$_{17}$H$_{37}$N$_6$O$_8$Br$_2$ [M$^{81}$Br$^{79}$Br]$^+$ 571.0333, observed 571.0337.
Figure S19. $^1$H and $^{13}$C NMR spectra for $N$-(3-azidopropyl)-3-(4,5-dibromo-2-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-3,6-dihydropyridazin-1(2H)-yl)propanamide 21.
To a solution of 3-(4,5-dibromo-2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-3,6-dihydropyridazin-1(2H)-yl)propanoic acid 20 (0.10 g, 0.21 mmol) in THF (4 mL) stirring at 0 °C was added DCC (0.05 g, 0.2 mmol), and the reaction mixture was stirred at 0 °C for 30 mins. After this time, propargylamine (15 µL, 0.23 mmol) was added, and the reaction mixture was stirred at 21 °C for a further 20 h. Following this, the reaction mixture was filtered to remove insolubles and underwent 3 rounds of successive cooling on acetone/dry ice and filtrations before being concentrated in vacuo. The crude residue was purified by flash column chromatography (0–15% MeOH/CH₂Cl₂). The appropriate fractions were then combined and concentrated in vacuo to afford 3-(4,5-dibromo-2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-3,6-dihydropyridazin-1(2H)-yl)-N-(prop-2-yn-1-yl)propanamide (0.06 g, 0.1 mmol, 55%) as a green oil. ¹H NMR (700 MHz, CDCl₃) δ 6.78 (app. s, 1H), 4.46 (t, J = 7.1 Hz, 2H), 4.33 (t, J = 4.8 Hz, 2H), 4.00 (dd, J = 5.4, 2.5 Hz, 2H), 3.74 (t, J = 4.8 Hz, 2H), 3.59–3.56 (m, 6H), 3.53–3.52 (m, 2H), 3.36 (s, 3H), 2.71 (t, J = 7.1 Hz, 2H), 2.20 (t, J = 2.5 Hz, 1H); ¹³C NMR (150 MHz, CDCl₃) δ 169.8 (C), 153.8 (C), 153.3 (C), 136.2 (C), 136.0 (C), 79.7 (C), 72.0 (CH₂), 71.5 (CH), 70.6 (CH₂), 70.5 (CH₂), 70.5 (CH₂), 68.0 (CH₂), 59.0 (CH₃), 49.1 (CH₂), 45.1 (CH₂), 33.3 (CH₂), 29.2 (CH₂); IR (thin film) 2873, 1629 cm⁻¹; LRMS (ES+) 526 (100, [M⁺81Br⁻79Br⁺H⁺]); HRMS (ES+) calcd for C₁₇H₂₄N₃O₆Br₂ [M⁺81Br⁻79Br⁺H⁺] 526.0006, observed 526.0007.
Figure S20. $^1$H and $^{13}$C NMR spectra for 3-(4,5-dibromo-2-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-3,6-dihydropyridazin-1(2H)-yl)-N-(prop-2-yn-1-yl)propanamide 22.
**N-(3-Azidopropyl)-3-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-4,5-bis(p-tolylthio)-3,6-dihydropyridazin-1(2H)-yl)propanamide 24**

To a solution of 4-methylbenzenethiol 23 (0.03 g, 0.2 mmol) and triethylamine (75 µL, 0.54 mmol) in CH₂Cl₂ (2 mL) at 21 °C, was added N-(3-azidopropyl)-3-(4,5-dibromo-2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-3,6-dihydropyridazin-1(2H)-yl)propanamide 21 (0.05 g, 0.09 mmol), and the reaction mixture was stirred for 10 mins. Following this, the reaction mixture was diluted with CH₂Cl₂ (8 mL) and washed with water (3 × 8 mL) and brine (8 mL). The organic phase was then dried over MgSO₄, concentrated in vacuo and the crude residue was purified by flash column chromatography (0–5% MeOH/CH₂Cl₂). The appropriate fractions were then combined and concentrated in vacuo to afford N-(3-azidopropyl)-3-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-4,5-bis(p-tolylthio)-3,6-dihydropyridazin-1(2H)-yl)propanamide (0.05 g, 0.08 mmol, 85%) as a yellow oil. ¹H NMR (700 MHz, CDCl₃) δ 7.17–7.14 (m, 4H), 7.08–7.06 (m, 4H), 6.48 (app. s, 1H), 4.29 (t, J = 6.9 Hz, 2H), 4.16 (t, J = 5.0 Hz, 2H), 3.67 (t, J = 5.0 Hz, 2H), 3.59–3.56 (m, 6H), 3.52–3.51 (m, 2H), 3.34 (s, 3H), 3.26 (q, J = 6.6 Hz, 2H), 2.59 (t, J = 6.9 Hz, 2H), 2.32 (s, 6H), 1.73 (p, J = 6.6 Hz, 2H); ¹³C NMR (150 MHz, CDCl₃) δ 170.3 (C), 156.9 (C-), 156.4 (C), 142.3 (C), 142.1 (C), 138.1 (C), 138.1 (C), 131.3 (CH), 131.2 (CH), 129.9 (CH), 129.3 (C), 129.1 (C), 72.0 (CH₂), 70.6 (CH₂), 70.6 (CH₂), 70.5 (CH₂), 68.1 (CH₂), 59.0 (CH₃), 49.3 (CH₂), 47.8 (CH₂), 43.9 (CH₂), 37.3 (CH₂), 34.0 (CH₂), 28.8 (CH₂), 21.4 (CH₃); IR (thin film) 2921, 2869, 2094, 1621 cm⁻¹; LRMS (ES+) 657 (100, [M+H]+); HRMS (ES+) calcd for C₃₁H₄₁N₆O₇S₂ [M+H]+ 657.2524, observed 657.2527.
Figure S21. $^1$H and $^{13}$C NMR spectra for $N$-(3-azidopropyl)-3-(2-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-4,5-bis($p$-tolylthio)-3,6-dihydropyridazin-1(2H)-yl)propanamide 24.
3-(2-(2-(2-Methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-4,5-bis(p-tolylthio)-3,6-dihydropyridazin-1(2H)-yl)-N-(prop-2-yn-1-yl)propanamide 25

To a solution of 4-methylbenzenethiol 23 (0.01 g, 0.08 mmol) and triethylamine (17 µL, 0.12 mmol) in CH₂Cl₂ (3 mL) at 21 °C, was added 3-(4,5-dibromo-2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-3,6-dihydropyridazin-1(2H)-yl)-N-(prop-2-yn-1-yl)propanamide 22 (0.01 g, 0.02 mmol), and the reaction mixture was stirred for 10 mins. Following this, the reaction mixture was diluted with CH₂Cl₂ (8 mL) and washed with water (3 × 8 mL) and brine (8 mL). The organic phase was then dried over MgSO₄, concentrated in vacuo and the crude residue was purified by flash column chromatography (0–5% MeOH/CH₂Cl₂). The appropriate fractions were then combined and concentrated in vacuo to afford 3-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-4,5-bis(p-tolylthio)-3,6-dihydropyridazin-1(2H)-yl)-N-(prop-2-yn-1-yl)propanamide (0.01 g, 0.02 mmol, 82%) as a yellow oil.

¹H NMR (700 MHz, CDCl₃)* δ 7.18–7.15 (m, 4H), 7.08–7.06 (m, 4H), 6.64 (app. s, 1H), 4.29 (t, J = 7.0 Hz, 2H), 4.13 (t, J = 4.9 Hz, 2H), 3.96 (dd, J = 5.3, 2.5 Hz, 2H), 3.68 (t, J = 4.9 Hz, 2H), 3.60–3.57 (m, 6H), 3.53–3.52 (m, 2H), 3.34 (s, 3H), 2.61 (t, J = 7.0 Hz, 2H), 2.32 (s, 6H), 2.18 (t, J = 2.5 Hz, 1H); ¹³C NMR (150 MHz, CDCl₃) δ 169.9 (C), 156.9 (C), 156.3 (C), 142.4 (C), 142.3 (C), 138.1 (C), 138.0 (C), 131.3 (CH), 131.1 (CH), 129.9 (CH), 129.9 (CH), 129.4 (C), 129.3 (C), 79.8 (C), 72.0 (CH₂), 71.5 (CH), 70.5 (CH₂), 70.5 (CH₂), 68.2 (CH₂), 59.0 (CH₃), 48.4 (CH₂), 44.1 (CH₂), 33.5 (CH₂), 29.2 (CH₂), 21.4 (CH₃); IR (thin film) 2921, 2869, 1621 cm⁻¹; LRMS (ES+) 612 (100, [M+H]⁺); HRMS (ES+) calcd for C₃₁H₃₈N₅O₆S₂ [M+H]⁺ 612.2197, observed 612.2198.
Figure S22. $^1$H and $^{13}$C NMR spectra for 3-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3,6-dioxo-4,5-bis(p-tolylthio)-3,6-dihydropyridazin-1(2H)-yl)-N-(prop-2-yn-1-yl)propanamide 25. *Mixture of impurities at 1.48–1.25 ppm.
Incubations involving human serum albumin, maleimide and PDs 2–6

Human serum albumin control

Human serum albumin (20 µL, 3.8 mg/mL, 57 µM) in PBS (10 mM phosphate, 137 mM NaCl, 2.7 mM KCl, pH 7.4) was incubated at 37 °C for 4 h. The PBS was exchanged with ammonium acetate buffer (20 mM, pH 7.4) by repeated diafiltration (× 3) into VivaSpin sample concentrators (GE Healthcare, 10,000 MWCO). The sample was then analysed by LC-MS. Expected mass: 66,439 Da. Observed mass: 66,438 Da.
Figure S23. (a) TIC, (b) non-deconvoluted and (c) deconvoluted MS data for untreated human serum albumin used in the incubations with PDs 2–6 and maleimide.
Incubation of human serum albumin with mono-bromo PD (10 eq.)

Mono-bromo PD (1.1 µL, 10 mM in MeCN, 10 eq.) was added to human serum albumin (20 µL, 3.8 mg/mL, 57 µM) in PBS (10 mM phosphate, 137 mM NaCl, 2.7 mM KCl, pH 7.4). The mixture was incubated at 37 °C for 4 h. Excess reagents were then removed by repeated diafiltration (× 3) into ammonium acetate buffer (20 mM, pH 7.4) using VivaSpin sample concentrators (GE Healthcare, 10,000 MWCO). The sample was then analysed by LC-MS. Expected mass: 66,605 Da. Observed masses: 66,606 and 66,440 Da.
Figure S24. (a) TIC, (b) non-deconvoluted, (c) deconvoluted and (d) zoomed in of deconvolution MS data for human serum albumin incubated with mono-bromo PD (10 eq.).
Incubation of human serum albumin with di-bromo PD (10 eq.)

Di-bromo PD (1.1 µL, 10 mM in MeCN, 10 eq.) was added to human serum albumin (20 µL, 3.8 mg/mL, 57 µM) in PBS (10 mM phosphate, 137 mM NaCl, 2.7 mM KCl, pH 7.4). The mixture was incubated at 37 °C for 4 h. Excess reagents were then removed by repeated diafiltration (×3) into ammonium acetate buffer (20 mM, pH 7.4) using VivaSpin sample concentrators (GE Healthcare, 10,000 MWCO). The sample was then analysed by LC-MS. Expected mass: 66,685 Da. Observed masses: 66,685 and 66,605 Da.

(a)

(b)
Figure S25. (a) TIC, (b) non-deconvoluted, (c) deconvoluted and (d) zoomed in of deconvolution MS data for human serum albumin incubated with di-bromo PD (10 eq.).
Incubation of human serum albumin with maleimide (10 eq.)

Maleimide (1.1 μL, 10 mM in MeCN, 10 eq.) was added to human serum albumin (20 μL, 3.8 mg/mL, 57 μM) in PBS (10 mM phosphate, 137 mM NaCl, 2.7 mM KCl, pH 7.4). The reaction was incubated at 37 °C for 4 h. Excess reagents were then removed by repeated diafiltration (× 3) into ammonium acetate buffer (20 mM, pH 7.4) using VivaSpin sample concentrators (GE Healthcare, 10,000 MWCO). The sample was then analysed by LC-MS. Expected mass: 66,536 Da. Observed mass: 66,536 Da.
Figure S26. (a) TIC, (b) non-deconvoluted and (c) deconvoluted MS data for human serum albumin reacted with maleimide (10 eq.).
Incubation of human serum albumin with PD 2 (10 eq.)

PD 2 (1.1 µL, 10 mM in MeCN, 10 eq.) was added to human serum albumin (20 µL, 3.8 mg/mL, 57 µM) in PBS (10 mM phosphate, 137 mM NaCl, 2.7 mM KCl, pH 7.4). The mixture was incubated at 37 °C for 4 h. Excess reagents were then removed by repeated diafiltration (× 3) into ammonium acetate buffer (20 mM, pH 7.4) using VivaSpin sample concentrators (GE Healthcare, 10,000 MWCO). The sample was then analysed by LC-MS. Expected mass: 66,438 Da. Observed mass: 66,439 Da.
Figure S27. TIC, (b) non-deconvoluted and (c) deconvoluted MS data for human serum albumin incubated with PD 2 (10 eq.).
Incubation of human serum albumin with PD 3 (10 eq.)

PD 3 (1.1 µL, 10 mM in MeCN, 10 eq.) was added to human serum albumin (20 µL, 3.8 mg/mL, 57 µM) in PBS (10 mM phosphate, 137 mM NaCl, 2.7 mM KCl, pH 7.4). The mixture was incubated at 37 °C for 4 h. Excess reagents were then removed by repeated diafiltration (× 3) into ammonium acetate buffer (20 mM, pH 7.4) using VivaSpin sample concentrators (GE Healthcare, 10,000 MWCO). The sample was then analysed by LC-MS. Expected mass: 66,438 Da. Observed mass: 66,438 Da.

(a)

(b)
Figure S28. (a) TIC, (b) non-deconvoluted and (c) deconvoluted MS data for human serum albumin incubated with PD 3 (10 eq.).
Incubation of human serum albumin with PD 4 (10 eq.)

PD 4 (1.1 µL, 10 mM in MeCN, 10 eq.) was added to human serum albumin (20 µL, 3.8 mg/mL, 57 µM) in PBS (10 mM phosphate, 137 mM NaCl, 2.7 mM KCl, pH 7.4). The mixture was incubated at 37 °C for 4 h. Excess reagents were then removed by repeated diafiltration (× 3) into ammonium acetate buffer (20 mM, pH 7.4) using VivaSpin sample concentrators (GE Healthcare, 10,000 MWCO). The sample was then analysed by LC-MS. Expected mass: 66,438 Da. Observed mass: 66,440 Da.
Figure S29. (a) TIC, (b) non-deconvoluted and (c) deconvoluted MS data for human serum albumin incubated with PD 4 (10 eq.).
Incubation of human serum albumin with PD 5 (10 eq.)

PD 5 (1.1 µL, 10 mM in MeCN, 10 eq.) was added to human serum albumin (20 µL, 3.8 mg/mL, 57 µM) in PBS (10 mM phosphate, 137 mM NaCl, 2.7 mM KCl, pH 7.4). The mixture was incubated at 37 °C for 4 h. Excess reagents were then removed by repeated diafiltration (× 3) into ammonium acetate buffer (20 mM, pH 7.4) using VivaSpin sample concentrators (GE Healthcare, 10,000 MWCO). The sample was then analysed by LC-MS. Expected mass: 66,438 Da. Observed mass: 66,440 Da.
Figure S30. (a) TIC, (b) non-deconvoluted and (c) deconvoluted MS data for human serum albumin incubated with PD 5 (10 eq.).
Incubation of human serum albumin with PD 6 (10 eq.)

PD 6 (1.1 µL, 10 mM in MeCN, 10 eq.) was added to human serum albumin (20 µL, 3.8 mg/mL, 57 µM) in PBS (10 mM phosphate, 137 mM NaCl, 2.7 mM KCl, pH 7.4). The mixture was incubated at 37 °C for 4 h. Excess reagents were then removed by repeated diafiltration (∗3) into ammonium acetate buffer (20 mM, pH 7.4) using VivaSpin sample concentrators (GE Healthcare, 10,000 MWCO). The sample was then analysed by LC-MS. Expected mass: 66,438 Da. Observed mass: 66,439 Da.

(a) [Graph]

(b) [Graph]
Figure S31. (a) TIC, (b) non-deconvoluted and (c) deconvoluted MS data for human serum albumin incubated with PD 6 (10 eq.).
Incubations involving GSH and PDs 2–6 at pH 6.5

Incubation of PD 2 with GSH (10 eq.)

PD 2 (10 µL, 10 mM in MeCN, 1 eq.) was added to GSH 1 (190 µL, 5.3 mM, 10 eq.) in ammonium acetate buffer (50 mM, pH 6.5). The mixture was incubated at 37 °C for 24 h. The samples were analysed by LC-MS at t = 0.05, 1, 2, 4 and 24 h.

LC-MS data for t = 0.05 h

(a)
Figure S32. (a) TIC and UV trace at $t = 0.05$ h, (b) MS data at 0.36 mins in the TIC and (c) MS data at 1.77 mins in the UV for PD 2 incubated with GSH 1 (10 eq.) at pH 6.5.
LC-MS data for $t = 1 \text{ h}$

(a) [Image of LC-MS diagram]

(b) [Image of LC-MS diagram]
Figure S33. (a) TIC and UV trace at $t = 1$ h, (b) MS data at 0.31 mins in the TIC, (c) MS data at 0.64 mins in the UV and (d) at 1.77 mins in the UV for PD 2 incubated with GSH 1 (10 eq.) at pH 6.5.
LC-MS data for $t = 2 \text{ h}$

(a)

(b)
Figure S34. (a) TIC and UV trace at $t = 2$ h, (b) MS data at 0.36 mins in the TIC, (c) MS data at 0.64 mins in the UV and (d) at 1.77 mins in the UV for PD 2 incubated with GSH 1 (10 eq.) at pH 6.5.
LC-MS data for $t = 4$ h

(a)

(b)
Figure S35. (a) TIC and UV trace at t = 4 h, (b) MS data at 0.35 mins in the TIC, (c) MS data at 0.64 mins in the UV and (d) at 1.77 mins in the UV for PD 2 incubated with GSH 1 (10 eq.) at pH 6.5.
LC-MS data for $t = 24 \text{ h}$

(a)

(b)
Figure S36. (a) TIC and UV trace at $t = 24$ h, (b) MS data at 0.42 mins in the TIC, (c) MS data at 0.78 mins in the UV and (d) at 1.97 mins in the UV for PD 2 incubated with GSH 1 (10 eq.) at pH 6.5.
Incubation of PD 3 with GSH (10 eq.)

PD 3 (10 µL, 10 mM in MeCN, 1 eq.) was added to GSH 1 (190 µL, 5.3 mM, 10 eq.) in ammonium acetate buffer (50 mM, pH 6.5). The mixture was incubated at 37 °C for 24 h. The samples were analysed by LC-MS at t = 0.05, 1, 2, 4 and 24 h.

LC-MS data for t = 0.05 h

(a)
Figure S37. (a) TIC and UV trace at $t = 0.05$ h, (b) MS data at 0.42 mins in the UV and (c) MS data at 1.75 mins in the UV for PD 3 incubated with GSH 1 (10 eq.) at pH 6.5.

LC-MS data for $t = 1$ h
Figure S38. (a) TIC and UV trace at t = 1 h, (b) MS data at 0.42 mins in the UV and (c) MS data at 1.75 mins in the UV for PD 3 incubated with GSH 1 (10 eq.) at pH 6.5.

LC-MS data for t = 2 h

(a)
Figure S39. (a) TIC and UV trace at $t = 2\ h$, (b) MS data at 0.26–0.44 mins in the UV and (c) MS data at 1.79 mins in the UV for PD 3 incubated with GSH 1 (10 eq.) at pH 6.5.

LC-MS data for $t = 4\ h$
Figure S40. (a) TIC and UV trace at t = 4 h, (b) MS data at 0.26–0.42 mins in the UV, (c) MS data at 0.68 mins in the UV and (d) at 1.75 mins in the UV for PD 3 incubated with GSH 1 (10 eq.) at pH 6.5.
Figure S41. (a) TIC and UV trace at $t = 24$ h, (b) MS data at 0.26–0.43 mins in the UV, (c) MS data at 0.69 mins in the UV, (d) at 1.51 mins in the UV and (e) at 1.77 mins in the UV for PD 3 incubated with GSH 1 (10 eq.) at pH 6.5.

Incubation of PD 4 with GSH (10 eq.)
PD 4 (10 µL, 10 mM in MeCN, 1 eq.) was added to GSH 1 (190 µL, 5.3 mM, 10 eq.) in ammonium acetate buffer (50 mM, pH 6.5). The mixture was incubated at 37 °C for 24 h. The samples were analysed by LC-MS at t = 0.05, 1, 2, 4 and 24 h.

**LC-MS data for t = 0.05 h**

(a)

(b)
Figure S42. (a) TIC and UV trace at $t = 0.05$ h, (b) MS data at 0.36 mins in the TIC, (c) MS data at 0.54 mins in the UV, (d) at 1.14 mins in the UV and (e) at 2.49 mins in the UV for PD 4 incubated with GSH 1 (10 eq.) at pH 6.5.

LC-MS data for $t = 1$ h
Figure S43. (a) TIC and UV trace at $t = 1$ h, (b) MS data at 0.36 mins in the TIC, (c) MS data at 0.53 mins in the UV and (d) at 1.14 mins in the UV for PD 4 incubated with GSH 1 (10 eq.) at pH 6.5.

LC-MS data for $t = 2$ h
Figure S44. (a) TIC and UV trace at \( t = 2 \) h, (b) MS data at 0.36 mins in the TIC, (c) MS data at 0.52 mins in the UV and (d) at 1.14 mins in the UV for PD 4 incubated with GSH 1 (10 eq.) at pH 6.5.

LC-MS data for \( t = 4 \) h
Figure S45. (a) TIC and UV trace at $t = 4$ h, (b) MS data at 0.35 mins in the TIC and (c) MS data at 0.55 mins in the UV for PD 4 incubated with GSH 1 (10 eq.) at pH 6.5.

LC-MS data for $t = 24$ h

(a)

(b)
Figure S46. (a) TIC and UV trace at t = 24 h, (b) MS data at 0.42 mins in the TIC and (c) MS data at 0.65 mins in the UV for PD 4 incubated with GSH 1 (10 eq.) at pH 6.5.

Incubation of PD 5 with GSH (10 eq.)
PD 5 (10 µL, 10 mM in MeCN, 1 eq.) was added to GSH 1 (190 µL, 5.3 mM, 10 eq.) in ammonium acetate buffer (50 mM, pH 6.5). The mixture was incubated at 37 °C for 24 h. The samples were analysed by LC-MS at t = 0.05, 1, 2, 4 and 24 h.

**LC-MS data for t = 0.05 h**

(a)
Figure S47. (a) TIC and UV trace at $t = 0.05$ h, (b) MS data at 0.43 mins in the TIC, (c) MS data at 1.35 mins in the UV and (d) at 2.53 mins in the UV for PD 5 incubated with GSH 1 (10 eq.) at pH 6.5.
Figure S48. (a) TIC and UV trace at $t = 1\, \text{h}$, (b) MS data at 0.43 mins in the TIC, (c) MS data at 0.59 mins in the UV, (d) at 1.35 mins in the UV and (e) at 2.53 mins in the UV for PD 5 incubated with GSH 1 (10 eq.) at pH 6.5.

LC-MS data for $t = 2\, \text{h}$
Figure S49. (a) TIC and UV trace at t = 2 h, (b) MS data at 0.25–0.44 mins in the UV, (c) MS data at 0.58 mins in the UV, (d) at 1.34 mins in the UV and (e) at 2.52 mins in the UV for PD 5 incubated with GSH 1 (10 eq.) at pH 6.5.

LC-MS data for t = 4 h
Figure S50. (a) TIC and UV trace at t = 4 h, (b) MS data at 0.25–0.44 mins in the UV, (c) MS data at 0.58 mins in the UV, (d) at 1.34 mins in the UV and (e) at 2.52 mins in the UV for PD 5 incubated with GSH 1 (10 eq.) at pH 6.5.

LC-MS data for t = 24 h
Figure S51. (a) TIC and UV trace at $t = 24$ h, (b) MS data at 0.24–0.44 mins in the UV, (c) MS data at 0.59 mins in the UV and (d) at 1.34 mins in the UV for PD 5 incubated with GSH 1 (10 eq.) at pH 6.5.

Incubation of PD 6 with GSH (10 eq.)
PD 6 (10 µL, 10 mM in MeCN, 1 eq.) was added to GSH 1 (190 µL, 5.3 mM, 10 eq.) in ammonium acetate buffer (50 mM, pH 6.5). The mixture was incubated at 37 °C for 24 h. The samples were analysed by LC-MS at t = 0.05, 1, 2, 4 and 24 h.

**LC-MS data for t = 0.05 h**

(a)

(b)
Figure S52. (a) TIC and UV trace at $t = 0.05$ h, (b) MS data at 0.24–0.44 mins in the UV, (c) MS data at 0.61 mins in the UV, (d) at 1.20 mins in the UV, (e) at 1.36 mins in the UV and (f) at 2.50 mins in the UV for PD 6 incubated with GSH 1 (10 eq.) at pH 6.5.

LC-MS data for $t = 1$ h
Figure S53. (a) TIC and UV trace at t = 1 h, (b) MS data at 0.24–0.43 mins in the UV, (c) MS data at 0.59 mins in the UV and (d) at 1.35 mins in the UV for PD 6 incubated with GSH 1 (10 eq.) at pH 6.5.

LC-MS data for t = 2 h
Figure S54. (a) TIC and UV trace at t = 2 h, (b) MS data at 0.24–0.44 mins in the UV, (c) MS data at 0.60 mins in the UV and (d) at 1.36 mins in the UV for PD 6 incubated with GSH 1 (10 eq.) at pH 6.5.

LC-MS data for t = 4 h
Figure S55. (a) TIC and UV trace at \( t = 4 \) h, (b) MS data at 0.28–0.44 mins in the UV, (c) MS data at 0.64 mins in the UV and (d) at 1.41 mins in the UV for PD 6 incubated with GSH 1 (10 eq.) at pH 6.5.

LC-MS data for \( t = 24 \) h
Figure S56. (a) TIC and UV trace at t = 24 h, (b) MS data at 0.25–0.44 mins in the UV, (c) MS data at 0.61–0.72 mins in the UV, (d) at 0.87 mins in the UV and (e) at 1.38 mins in the UV for PD 6 incubated with GSH 1 (10 eq.) at pH 6.5.

Incubations involving GSH and PDs 2–6 at pH 5.0
Incubation of PD 2 with GSH (10 eq.)

PD 2 (10 µL, 10 mM in MeCN, 1 eq.) was added to GSH 1 (190 µL, 5.3 mM, 10 eq.) in ammonium acetate buffer (50 mM, pH 5.0). The mixture was incubated at 37 °C for 24 h. The samples were analysed by LC-MS at t = 0.05, 1, 2, 4 and 24 h.

LC-MS data for t = 0.05 h

(a)
Figure S57. (a) TIC and UV trace at t = 0.05 h, (b) MS data at 0.35 mins in the TIC and (c) MS data at 1.80 mins in the UV for PD 2 incubated with GlSH 1 (10 eq.) at pH 5.0.

LC-MS data for t = 1 h
Figure S58. (a) TIC and UV trace at $t = 1$ h, (b) MS data at 0.36 mins in the TIC and (c) MS data at 1.80 mins in the UV for PD 2 incubated with GSH 1 (10 eq.) at pH 5.0.
Figure S59. (a) TIC and UV trace at $t = 2$ h, (b) MS data at 0.44 mins in the TIC and (c) MS data at 1.97 mins in the UV for PD 2 incubated with GSH 1 (10 eq.) at pH 5.0.

LC-MS data for $t = 4$ h

(a)

(b)
Figure S60. (a) TIC and UV trace at t = 4 h, (b) MS data at 0.40 mins in the TIC and (c) MS data at 1.88 mins in the UV for PD 2 incubated with GSH 1 (10 eq.) at pH 5.0.

LC-MS data for t = 24 h
Figure S61. (a) TIC and UV trace at $t = 24$ h, (b) MS data at 0.44 mins in the TIC, (c) MS data at 0.69 mins in the UV and (d) at 1.82 mins in the UV for PD 2 incubated with GSH 1 (10 eq.) at pH 5.0.

Incubation of PD 3 with GSH (10 eq.)
PD 3 (10 µL, 10 mM in MeCN, 1 eq.) was added to GSH 1 (190 µL, 5.3 mM, 10 eq.) in ammonium acetate buffer (50 mM, pH 5.0). The mixture was incubated at 37 °C for 24 h. The samples were analysed by LC-MS at t = 0.05, 1, 2, 4 and 24 h.

**LC-MS data for t = 0.05 h**

(a)
Figure S62. (a) TIC and UV trace at $t = 0.05$ h, (b) MS data at 0.24–0.42 mins in the UV, and (c) MS data at 1.75 mins in the UV for PD 3 incubated with GSH 1 (10 eq.) at pH 5.0.
Figure S63. (a) TIC and UV trace at $t = 1$ h, (b) MS data at 0.24–0.42 mins in the UV, and (c) MS data at 1.75 mins in the UV for PD 3 incubated with GSH 1 (10 eq.) at pH 5.0.

LC-MS data for $t = 2$ h
Figure S64. (a) TIC and UV trace at $t = 2$ h, (b) MS data at 0.24–0.42 mins in the UV, and (c) MS data at 1.75 mins in the UV for PD 3 incubated with GSH 1 (10 eq.) at pH 5.0.

**LC-MS data for $t = 4$ h**

(a)
Figure S65. (a) TIC and UV trace at t = 4 h, (b) MS data at 0.29–0.42 mins in the UV and (c) MS data at 1.86 mins in the UV for PD 3 incubated with GSH 1 (10 eq.) at pH 5.0.
Figure S66. (a) TIC and UV trace at $t = 24$ h, (b) MS data at 0.25–0.42 mins in the UV, (c) MS data at 0.67 mins in the UV and (d) at 1.75 mins in the UV for PD 3 incubated with GSH 1 (10 eq.) at pH 5.0.

Incubation of PD 4 with GSH (10 eq.)
PD 4 (10 µL, 10 mM in MeCN, 1 eq.) was added to GSH 1 (190 µL, 5.3 mM, 10 eq.) in ammonium acetate buffer (50 mM, pH 5.0). The mixture was incubated at 37 °C for 24 h. The samples were analysed by LC-MS at t = 0.05, 1, 2, 4 and 24 h.

**LC-MS data for t = 0.05 h**

(a)

(b)
Figure S67. (a) TIC and UV trace at t = 0.05 h, (b) MS data at 0.24–0.42 mins in the UV, (c) MS data at 1.17 mins in the UV and (d) at 2.52 mins in the UV for PD 4 incubated with GSH 1 (10 eq.) at pH 5.0.

LC-MS data for t = 1 h

(a)
Figure S68. (a) TIC and UV trace at t = 1 h, (b) MS data at 0.25–0.42 mins in the UV, (c) MS data at 0.57 mins in the UV, (d) at 1.17 mins in the UV and (e) at 2.52 mins in the UV for PD 4 incubated with GSH 1 (10 eq.) at pH 5.0.

LC-MS data for t = 2 h
Figure S69. (a) TIC and UV trace at t = 2 h, (b) MS data at 0.25–0.42 mins in the UV, (c) MS data at 0.57 mins in the UV, (d) at 1.17 mins in the UV and (e) at 2.52 mins in the UV for PD 4 incubated with GSH 1 (10 eq.) at pH 5.0.
Figure S70. (a) TIC and UV trace at t = 4 h, (b) MS data at 0.26–0.42 mins in the UV, (c) MS data at 0.60 mins in the UV and (d) at 1.20 mins in the UV for PD 4 incubated with GSH 1 (10 eq.) at pH 5.0.

LC-MS data for t = 24 h
Figure S71. (a) TIC and UV trace at t = 24 h, (b) MS data at 0.24–0.42 mins in the UV, (c) MS data at 0.56 mins in the UV and (d) at 1.17 mins in the UV for PD 4 incubated with GSH 1 (10 eq.) at pH 5.0.

Incubation of PD 5 with GSH (10 eq.)
PD 5 (10 µL, 10 mM in MeCN, 1 eq.) was added to GSH 1 (190 µL, 5.3 mM, 10 eq.) in ammonium acetate buffer (50 mM, pH 5.0). The mixture was incubated at 37 °C for 24 h. The samples were analysed by LC-MS at t = 0.05, 1, 2, 4 and 24 h.

**LC-MS data for t = 0.05 h**

(a)
Figure S72. (a) TIC and UV trace at $t = 0.05 \text{ h}$, (b) MS data at 0.25–0.42 mins in the UV and (c) MS data at 2.53 mins in the UV for PD 5 incubated with GSH 1 (10 eq.) at pH 5.0.
Figure S73. (a) TIC and UV trace at t = 1 h, (b) MS data at 0.25–0.42 mins in the UV, (c) MS data at 1.34 mins in the UV and (d) at 2.52 mins in the UV for PD 5 incubated with GSH 1 (10 eq.) at pH 5.0.

LC-MS data for t = 2 h
Figure S74. (a) TIC and UV trace at $t = 2$ h, (b) MS data at 0.26–0.42 mins in the UV, (c) MS data at 1.34 mins in the UV and (d) at 2.52 mins in the UV for PD 5 incubated with GSH 1 (10 eq.) at pH 5.0.

LC-MS data for $t = 4$ h
Figure S75. (a) TIC and UV trace at t = 4 h, (b) MS data at 0.26–0.42 mins in the UV, (c) MS data at 1.34 mins in the UV and (d) at 2.52 mins in the UV for PD 5 incubated with GSH 1 (10 eq.) at pH 5.0.

LC-MS data for t = 24 h
Figure S76. (a) TIC and UV trace at t = 24 h, (b) MS data at 0.24–0.42 mins in the UV, (c) MS data at 0.58 mins in the UV, (d) at 1.34 mins in the UV and (e) at 2.52 mins in the UV for PD 5 incubated with GSH 1 (10 eq.) at pH 5.0.

Incubation of PD 6 with GSH (10 eq.)
PD 6 (10 µL, 10 mM in MeCN, 1 eq.) was added to GSH 1 (190 µL, 5.3 mM, 10 eq.) in ammonium acetate buffer (50 mM, pH 5.0). The mixture was incubated at 37 °C for 24 h. The samples were analysed by LC-MS at t = 0.05, 1, 2, 4 and 24 h.

**LC-MS data for t = 0.05 h**

(a)

(b)
Figure S77. (a) TIC and UV trace at $t = 0.05$ h, (b) MS data at 0.24–0.43 mins in the UV and (c) MS data at 2.49 mins in the UV for PD 6 incubated with GSH 1 (10 eq.) at pH 5.0.

LC-MS data for $t = 1$ h
Figure S78. (a) TIC and UV trace at $t = 1$ h, (b) MS data at 0.25–0.43 mins in the UV, (c) MS data at 1.19 mins in the UV, (d) at 1.35 mins in the UV and (e) at 2.48 mins in the UV for PD 6 incubated with GSH 1 (10 eq.) at pH 5.0.

LC-MS data for $t = 2$ h

(a)

(b)
Figure S79. (a) TIC and UV trace at t = 2 h, (b) MS data at 0.26–0.43 mins in the UV, (c) MS data at 0.60 mins in the UV, (d) at 1.20 mins in the UV, (e) at 1.36 mins in the UV and (f) at 2.50 mins in the UV for PD 6 incubated with GSH 1 (10 eq.) at pH 5.0.

LC-MS data for t = 4 h

(a)
Figure S80. (a) TIC and UV trace at t = 4 h, (b) MS data at 0.28–0.43 mins in the UV, (c) MS data at 0.63 mins in the UV, (d) at 1.25 mins in the UV, (e) at 1.40 mins in the UV and (f) at 2.55 mins in the UV for PD 6 incubated with GSH 1 (10 eq.) at pH 5.0.

LC-MS data for t = 24 h

(a)

(b)
Figure S81. (a) TIC and UV trace at t = 24 h, (b) MS data at 0.26–0.43 mins in the UV, (c) MS data at 0.61 mins in the UV and (d) at 1.38 mins in the UV for PD 6 incubated with GSH 1 (10 eq.) at pH 5.0.

Incubation of PD 13 with GSH (10 eq.) at pH 6.5
Pyridazinedione 13 (10 µL, 10 mM in THF, 1 eq.) was added to GSH 1 (190 µL, 5 mM, 10 eq.) in ammonium acetate buffer (50 mM, pH 6.5). The mixture was incubated at 37 °C for 24 h. The samples were analysed by LCMS at t = 4 and 24 h.

LC-MS data for t = 4 h
Figure S82. (a) TIC and UV trace at t = 4 h, (b) MS data at 0.23 mins in the UV, (c) at 0.50 mins in the UV, (d) at 0.99 mins in the UV and (e) at 2.82 mins in the UV for PD 13 incubated with GSH 1 (10 eq.) at pH 6.5.

LC-MS data for t = 24 h

(a)
Figure S83. (a) TIC and UV trace at $t = 24$ h, (b) MS data at 0.23 mins in the UV, (c) at 0.50 mins in the UV, (d) at 1.00 mins in the UV and (e) at 2.82 mins in the UV for PD 13 incubated with GSH 1 (10 eq.) at pH 6.5.

Incubation of PD 16 with GSH (10 eq.) at pH 6.5
PD 16 (15 µL, 10 mM in DMSO, 1 eq.) was added to GSH 1 (285 µL, 5.3 mM, 10 eq.) in ammonium acetate buffer (50 mM, pH 6.5). The mixture was incubated at 37 °C for 24 h. The samples were analysed by LC-MS at t = 0.05, 4 and 24 h.

**LC-MS data for t = 0.05 h**
Figure S84. (a) TIC and UV trace at t = 0.05 h, (b) MS data at 0.32 mins in the UV, (c) at 1.50 mins in the UV, (d) at 1.73 mins in the TIC, (e) at 2.03 mins in the TIC, (f) at 2.36 mins in the UV and (g) at 2.52 mins in the UV for PD 16 incubated with GSH 1 (10 eq.) at pH 6.5. Please note that peaks at 1.73 and 2.03 mins in the TIC are minor impurities on the column that could be removed; they are consistently present.

LC-MS data for t = 4 h
Figure S85. (a) TIC and UV trace at t = 4 h, (b) MS data at 0.25 mins in the UV, (c) at 0.53 mins in the UV, (d) at 0.70 mins in the UV, (e) at 0.97 mins in the UV, (f) at 1.49 mins in the TIC, (g) at 1.67 mins in the TIC, (h) at 1.96 mins in the TIC, (i) at 2.60 mins in the UV and (j) at 3.78 mins in the UV for PD 16 incubated with GSH 1 (10 eq.) at pH 6.5. Please note that peaks at 1.67 and 1.96 mins in the TIC, and at 3.78 mins in the UV are minor impurities on the column that could be removed; they are consistently present.
Figure S86. (a) TIC and UV trace at $t = 24$ h, (b) MS data at 0.28 mins in the UV, (c) at 0.57 mins in the UV, (d) at 0.80 mins in the UV, (e) at 1.04 mins in the UV, (f) at 1.74 mins in the TIC, (g) at 2.03 mins in the TIC and (h) at 3.79 mins in the TIC for PD 16 incubated with GSH 1 (10 eq.) at pH 6.5. Please note that peaks at 1.74 and 2.03 mins in the TIC, and at 3.79 mins in the UV are minor impurities on the column that could be removed; they are consistently present.
Fluorescence emission spectroscopy of the reaction between PD 16 and GSH (10 eq.) at pH 6.5

UV absorption of 7-hydroxy-2-oxo-2H-chromene-3-carboxylic acid 17

[Chemical structure of 17]

7-Hydroxy-2-oxo-2H-chromene-3-carboxylic acid 17 (100 µL, 10 mM in DMSO) was added to ammonium acetate buffer (1900 µL, 50 mM, pH 6.5). The solution was then scanned in the 200–800 nm range using a UV–Vis spectrophotometer in order to obtain 7-hydroxy-2-oxo-2H-chromene-3-carboxylic acid 17’s maximum UV absorption in the DMSO/buffer mixture.

Figure S87. UV absorbance spectrum of 7-hydroxy-2-oxo-2H-chromene-3-carboxylic acid 17 in a 5:95 mixture of DMSO/NH₄OAc buffer (50 mM, pH 6.5). When scanned in the 200–800 nm range, 7-hydroxy-2-oxo-2H-chromene-3-carboxylic acid 17’s maximum UV absorption occurred at 335 nm and ε₃₃₅ = 5462 M⁻¹cm⁻¹.
Fluorescence emission of 7-hydroxy-2-oxo-2H-chromene-3-carboxylic acid 17

7-Hydroxy-2-oxo-2H-chromene-3-carboxylic acid 17 (100 µL, 10 mM in DMSO) was added to ammonium acetate buffer (1900 µL, 50 mM, pH 6.5). The solution was then excited at 335 nm using a fluorescence spectrophotometer in order to obtain 7-hydroxy-2-oxo-2H-chromene-3-carboxylic acid 17’s maximum fluorescence intensity in the DMSO/buffer mixture.

Figure S88. Fluorescence emission spectrum of 7-hydroxy-2-oxo-2H-chromene-3-carboxylic acid 17 in a 5:95 mixture of DMSO/NH₄OAc buffer (50 mM, pH 6.5). When excited at 335 nm, 7-hydroxy-2-oxo-2H-chromene-3-carboxylic acid 17’s maximum fluorescence emission occurred at 447 nm with a maximum intensity of 110.6 a.u.
Fluorescence emission of PD 16

PD 16 (100 µL, 10 mM in DMSO) was added to ammonium acetate buffer (1900 µL, 50 mM, pH 6.5). The solution was incubated at 37 °C for 48 h. The solution was then excited at 335 nm using a fluorescence spectrophotometer in order to obtain PD 16’s maximum fluorescence intensity in the DMSO/buffer mixture.
Figure S89. Fluorescence emission spectrum of PD 16 in a 5:95 mixture of DMSO/NH$_4$OAc buffer (50 mM, pH 6.5). When excited at 335 nm (and performed in triplicate), PD 16’s maximum fluorescence emission occurred at 445 nm with a maximum intensity of (a) 14.4 a.u., (b) 18.5 a.u. and (c) 20.0 a.u.
Fluorescence emission spectroscopy of the reaction between PD 16 and GSH (10 eq.) at pH 6.5

PD 16 (40 µL, 10 mM in DMSO, 1 eq.) was added to GSH 1 (760 µL, 5.3 mM, 10 eq.) in ammonium acetate buffer (50 mM, pH 6.5). The mixture was incubated at 37 °C for 48 h. The reaction was excited at 335 nm at t = 0.05, 4, 24 and 48 h and the maximum fluorescence absorption was recorded at each time point.
Fluorescence emission at $t = 0.05$ h

(a)

(b)
Figure S90. Fluorescence emission spectrum of the reaction between PD 16 and GSH 1 to release 7-hydroxy-2-oxo-2H-chromene-3-carboxylic acid 17 at t = 0.05 h. When excited at 335 nm (and performed in triplicate), maximum fluorescence emission occurred at 446 nm with a maximum intensity of (a) 25.8 a.u., (b) 39.1 a.u. and (c) 31.1 a.u.
Fluorescence emission at $t = 4\text{ h}$

(a)

(b)
Figure S91. Fluorescence emission spectrum of the reaction between PD 16 and GSH 1 to release 7-hydroxy-2-oxo-2H-chromene-3-carboxylic acid 17 at t = 4 h. When excited at 335 nm (and performed in triplicate), maximum fluorescence emission occurred at 448 nm with a maximum intensity of (a) 165.1 a.u., (b) 158.5 a.u. and (c) 170.7 a.u.

Fluorescence emission at t = 24 h
Figure S92. Fluorescence emission spectrum of the reaction between PD 16 and GSH 1 to release 7-hydroxy-2-oxo-2H-chromene-3-carboxylic acid 17 at t = 24 h. When excited at 335 nm (and performed in triplicate), maximum fluorescence emission occurred at 446 nm with a maximum intensity of (a) 199.6 a.u., (b) 205.3 a.u. and (c) 197.8 a.u.
Fluorescence emission at $t = 48$ h

(a)

(b)

(c)
Figure S93. Fluorescence emission spectrum of the reaction between PD 16 and GSH 1 to release 7-hydroxy-2-oxo-2H-chromene-3-carboxylic acid 17 at \( t = 48 \) h. When excited at 335 nm (and performed in triplicate), maximum fluorescence emission occurred at 446 nm with a maximum intensity of (a) 201.7 a.u., (b) 222.1 a.u. and (c) 196.6 a.u.
Figure S94. Summary of fluorescence emission data for the reaction between PD 16 and GSH 1 at 37 °C and pH 6.5.
References