Predicting the hydrolytic breakdown rates of organophosphorus chemical warfare agent simulants using association constants derived from hydrogen bonded complex formation events

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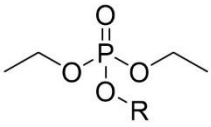
Chemical structures



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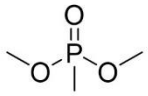

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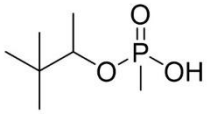

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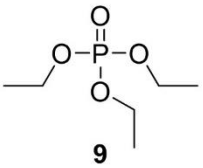

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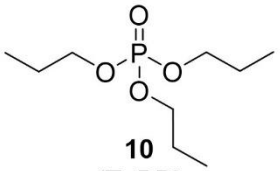

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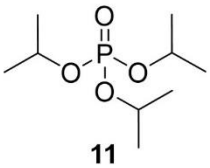

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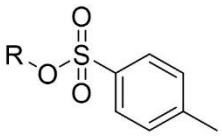

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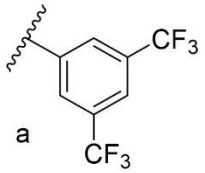

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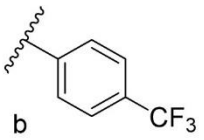

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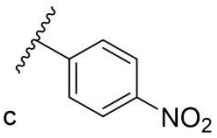

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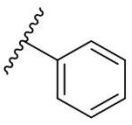

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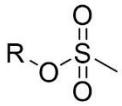

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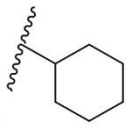

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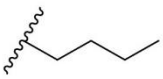

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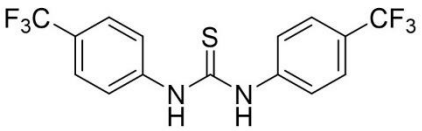

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Experimental

General remarks: All reactions were performed under slight positive pressure of nitrogen using oven dried glassware. NMR spectra were determined using a Bruker AV II or NEO 400 MHz spectrometer with chemical shifts reported in parts per million (ppm) and calibrated to the centre of the solvent peak set. Herein: br = broad; s = singlet; d = doublet; t = triplet; q = quartet, sept = septet and m = multiplet. All solvents and starting materials were purchased from commercial sources or chemical stores where available and, used as purchased unless stated otherwise. Tensiometry measurements were undertaken using the Biolin Scientific Theta Attension optical tensiometer. Viscosity measurements were recorded on an Anton Par modular compact rheometer (MCR302) using a cone plate CP60-1. Density measurements were conducted using an OHAUS Explorer analytical balance.

Hydrolytic stability studies (to asses simulant stability in DMSO-d_6:D_2O (70:30)): Stock solutions of simulants **1**-**22** (10 mM) were prepared in DMSO-d_6:D_2O (70:30) at 291 K. T = 0 was defined as the point at which the simulant came into contact with D_2O. A ^1H NMR experiment was then conducted every 2 hours thereafter. The mono hydrolysis product was the sole species observed as the result of simulant breakdown under these conditions.

Reactivity studies using sodium hydroxide (to assess simulant reactivity towards those reagents representative of certain commercially available kits): For the reactivity studies stock solutions of simulants **1**-**22** (10mM) were prepared in MeOD-d_4:D_2O (70:30) at 291 K, one equivalent of NaOH (10 mM) or five equivalents of NaOH (50 mM) was then added as appropriate (T = 0). A ^1H NMR experiment was then conducted for each sample every 2 hours thereafter. The mono hydrolysis product was the sole species observed as the result of simulant breakdown under these conditions.

Viscosity method: Only simulants that are liquid at 298 K were studied. Each simulant was loaded onto the base plate and trimmed to the CP60-1 plate. Each experiment was run in triplicate, with three intervals within each run, at a d(gamma)/dt = 0-100 1/s logarithmic (sheer rate). The plateau of each viscosity measurement was used to calculate the average viscosity for each sample.

Surface tension method: A succession of 3 droplets were measured for each sample and an average for these measurements reported.

Syntheses for compounds 1-23

Compound 1: Diethyl chlorophosphate (0.45 mL, 3.08 mmol) was added to a stirring solution of 3,5-(trifluoromethyl)phenol (0.47 mL, 3.08 mmol) and triethylamine (0.43 mL, 3.08 mmol) in chloroform (10 mL). The mixture was then allowed to stir at room temperature overnight. The organic phase was then washed with an aqueous 0.3 M NaOH solution (30 mL). The organic layer was then taken to dryness to give this final product as a colourless oil (0.73 g, 2.00 mmol) with a yield of 64.9 %. $^{1}H\{^{31}P\}$ NMR: (400 MHz, 298 K, $CDCl_3$): δ: 1.32 (t, J= 7.08 Hz, 6H), 4.22 (q, J = 7.12 Hz, 4H), 7.64 (br s, 3H).

This compound has been previously synthesised by Hiscock and co-workers. The ^{1}H NMR data provided was found to match these previously published data.[1]

Compound 2: Diethyl chlorophosphate (0.59 g, 3.08 mmol) was added to a stirring solution of 4-(trifluoromethyl)phenol (0.50 g, 3.08 mmol) and triethylamine (0.43 mL, 3.08 mmol) in chloroform (10 mL). The mixture was then allowed to stir at room temperature overnight. The organic phase was then washed with an aqueous 0.3 M NaOH solution (30 mL). The organic layer was then taken to dryness to give the final product as a colourless oil (0.83 g, 2.78 mmol) in a yield of 90.3 %. $^{1}H\{^{31}P\}$ NMR: (400 MHz, 298 K, $CDCl_3$): δ: 1.39 (t, J= 7.08 Hz, 6H), 4.26 (q, J = 7.08 Hz, 4H), 7.36 (d, J = 8.56 Hz, 2H), 7.64 (d, J = 8.64 Hz, 2H).

This compound has been previously synthesised by Hiscock and co-workers. The ^{1}H NMR data provided was found to match these previously published data.[1]

Compound 3: Diethyl chlorophosphate (0.52 mL, 3.59 mmol) was added to a stirring solution of 4-nitrophenol (0.50 g, 3.59 mmol) and triethylamine (0.50 mL, 3.59 mmol) in chloroform (10 mL). This mixture was then allowed to stir at room temperature overnight. The organic phase was then washed with an aqueous 0.3 M NaOH solution (30 mL). The organic layer was then taken to dryness to give the pure product as a clear yellow oil (0.86 g, 2.86 mmol) in a yield of 79.7 %. ^{1}H NMR: (400 MHz, 298 K, $CDCl_3$): δ: 1.31 (t, J = 7.08 Hz, 6H), 4.19 (q, J = 7.08, 4H), 7.31 (d, J = 9.20 Hz, 2H), 8.18 (d, J = 9.16, 2H).

This compound has been previously synthesised by Kuei and co-workers.[2] The ^{1}H NMR data provided was found to match previously these published data.

Compound 4: Diethyl chlorophosphate (0.77 mL, 5.31 mmol) was added to a stirring solution of phenol (0.5 g, 5.31 mmol) and triethylamine (0.74 mL, 5.31 mmol) in chloroform (10 mL). The mixture was then allowed to stir at room temperature overnight. The mixture was then allowed to stir at room temperature overnight. The organic phase was then washed with an aqueous 0.3 M NaOH solution (30 mL). The organic layer was then taken to dryness to give the pure product as a colourless oil (0.77 g, 3.37 mmol) with a yield of 63.5 %. $^{1}H\{^{31}P\}$ NMR: (400 MHz, 298 K, $CDCl_3$): δ: 1.34 (t, J = 7.08 Hz, 6H), 4.20 (q, J = 7.08 Hz, 4H), 7.14 – 7.22 (m, 3H), 7.33 (t, J = 8.58 Hz, 2H).

This compound has been previously synthesised by Katritzky and co-workers.[3] The ^{1}H NMR data provided was found to match previously these published data.

Compound 5: Diethyl chlorophosphate (2.20 mL, 15.0 mmol) in pyridine (1.20 mL, 15.0 mmol) was added to a stirring solution of cyclohexanol (1.00 g, 9.98 mmol) in dichloromethane (10

mL).The solution was stirred at 0 °C then allowed to warm up to room temperature overnight. The reaction was then quenched with methanol (50 mL) and concentrated in vaccu. The resulting white solid was then dissolved in ethyl acetate (50 mL) and washed with 1M HCl (50 mL), saturated $NaHCO_3$ solution (50 mL). The organic layer was then taken to dryness to give a colourless oil (1.93 g, 8.17 mmol) with a yield of 81.7 %. $^1H\{^{31}P\}$ NMR (298 K, $CDCl_3$, 400 MHz): δ; 1.24-1.99 (m, 18H), 4.11 (q, J = 7.08, 4H), 4.34-4.41 (m, 1H).

This compound has been previously synthesised by Kang et al.[4] The ^1H NMR data provided was found to match previously these published data.

Compound 6: Diethyl chlorophosphate (0.97 mL, 6.74 mmol) was added to a stirring solution of butanol (0.50 g, 6.74 mmol) and triethylamine (0.94 mL, 6.74 mmol) in chloroform (10 mL). The mixture was then allowed to stir at room temperature overnight. The organic phase was then washed with an aqueous 0.3 M NaOH solution (30 mL). The organic layer was then taken to dryness to give the pure product as a colourless oil (1.21 g, 5.74 mmol) in a yield of 85.2 %. $^1H\{^{31}P\}$ NMR: (400 MHz, 298 K, $CDCl_3$): δ: 0.93 (t, J = 7.36 Hz, 3H), 1.32 – 1.46 (m, 8H), 1.63 – 1.70 (m, 2H), 4.02 – 4.13 (m, 6H).

This compound has been previously synthesised by Hiscock and co-workers. The ^1H NMR data provided was found to match these previously published data.[1]

Compound 12: *p*-Toluene sulfonylchloride (0.588 g, 3.08 mmol) was added to a stirring solution of 4-(trifluoromethyl)phenol (0.75 g, 4.62 mmol) and triethylamine (0.43 mL, 4.62 mmol) in chloroform (10 mL). The mixture was then allowed to stir at room temperature overnight and then washed with an aqueous 0.3 M NaOH solution (30 mL). The organic layer was then taken to dryness under reduced pressure to give the pure product as a white solid (0.58 g, 1.82 mmol) in a yield of 59.1 %. ^1H NMR: (400 MHz, 298 K, $CDCl_3$): δ: 2.44 (s, 3H), 7.10 (d, J = 8.36 Hz, 2H), 7.32 (d, J = 8.00 Hz, 2H), 7.55 (d, J = 8.52 Hz, 2H), 7.70 (d, J = 8.40 Hz, 2H).

This compound has been previously synthesised by Hiscock and co-workers. The ^1H NMR data provided was found to match these previously published data.[1]

Compound 13: *p*-Toluene sulfonylchloride (0.69 g, 3.59 mmol) was added to a stirring solution of 4-nitrophenol (0.50 g, 3.59 mmol) and triethylamine (0.50 mL, 3.59 mmol) in chloroform (10 mL). This mixture was allowed to stir at room temperature overnight, then washed with an aqueous 0.3 M NaOH solution (30 mL), and the organic layer was then taken to dryness to give the pure product as a pale yellow solid (0.84 g, 2.88 mmol) in a yield of 80.2 %. ^1H NMR: (400 MHz, 298 K, $CDCl_3$): δ: 2.50 (s, 3H), 7.21 (d, J = 9.20 Hz, 2H), 7.38 (d, J = 8.04 Hz, 2H), 7.76 (d, J = 8.40 Hz, 2H), 8.22 (d, J = 9.20 Hz, 2H).

This compound has been previously synthesised by Wei and co-workers.[5] The ^1H NMR data provided was found to match these previously published data.

Compound 14: *p*-Toluene sulfonylchloride (1.01 g, 5.31 mmol) was added to a stirring solution of phenol (0.50 g, 5.31 mmol) and triethylamine (0.74 mL, 5.31 mmol) in chloroform (10 mL) and, stirred at room temperature overnight. The solution was then washed with an aqueous 0.3 M NaOH solution (30 mL), and the organic layer was then taken to dryness to give the pure product as a white solid (1.27 g, 5.10 mmol) in a yield of 96.0 %. ^1H NMR: (400 MHz, 298

K, $CDCl_3$): δ: 2.42 (s, 3H), 7.00 (d, J = 8.16 Hz, 2H), 7.31 (t, J = 7.36 Hz, 1H), 7.38 (t, J = 7.12 Hz, 2H), 7.46 (d, J = 7.96 Hz, 2H), 7.72 (d, J = 8.32 Hz, 2H).

This compound has been previously synthesised by Gibson and co-workers.[6] The ^{1}H NMR data provided was found to match these previously published data.

Compound 15: *p*-Toluenesulfonyl chloride (2.85 g, 15.00 mmol) in pyridine (1.20 mL, 15.00 mmol) was added to a stirring solution of cyclohexanol (1.00 g, 9.98 mmol) in dichloromethane (10 mL). The solution was stirred at 0 °C and allowed to warm to room temperature overnight. The reaction was then quenched with methanol (50 mL) and concentrated in vaccu. The resulting white solid was then dissolved in ethyl acetate (50 mL) and washed with 1 M HCl (50 mL), saturated $NaHCO_3$ solution (50 mL). The organic layer was taken to dryness to give a colourless oil (1.82 g, 7.16 mmol) with a yield 71.6 %. ^{1}H NMR (298 K, $CDCl_3$, 400 MHz): δ; 0.85-1.81 (m, 12H), 2.46 (s, 3H), 4.49 – 4.55 (m, 1H), 7.34 (d, J = 7.96 Hz, 2H), 7.34 (d, J = 8.32 Hz, 2H).

This compound has been previously synthesised by Wei and co-workers.[7] The ^{1}H NMR data provided was found to match those previously published data.

Compound 16: *p*-Toluene sulfonylchloride (1.29 g, 6.74 mmol) was added to a stirring solution of butanol (0.62 mL, 6.74 mmol) and triethylamine (0.94 mL, 6.74 mmol) in chloroform (10 mL). This mixture was allowed to stir at room temperature overnight, then washed with an aqueous 0.3 M NaOH solution (30 mL), and the organic layer was then taken to dryness to give the pure product as a colourless oil (1.32 g, 5.78 mmol) in a yield of 85.8 %. ^{1}H NMR: (400 MHz, 298 K, $CDCl_3$): δ: 0.85 (t, J = 7.40 Hz, 3H), 1.29-1.39 (m, 2H), 1.59-1.66 (m, 2H), 2.45 (s, CH_3), 4.03 (t, J = 6.74 Hz, 2H), 7.35 (d, J = 8.00 Hz, 2H), 7.79 (d, J = 7.79 Hz, 2H).

This compound has been previously synthesised by Wei and co-workers.[5] The ^{1}H NMR data provided was found to match these previously published data.

Compound 17: To a stirring solution of 3,5-bis(trifluoromethyl) phenol (1.00 g, 4.34 mmol) in chloroform (10 mL) and trimethylamine (0.86 ml, 6.17 mmol), was added methylsulfonyl chloride (0.34 mL, 4.34 mmol). The solution was stirred at room temperature for three hours, washed with an aqueous 0.3 M NaOH solution (30 mL), and the organic layer taken to dryness to give a white solid (1.31 g, 4.25 mmol) with a yield of 98.5 % . ^{1}H NMR (298 K, $CDCl_3$, 400 MHz): δ; 3.31 (s, 3H), 7.79 (s, 2H), 7.89 (s, 2H).

This compound has been previously synthesised by Seayad and co-workers.[7] The ^{1}H NMR data provided was found to match previously these published data.

Compound 18: Methylsulfonyl chloride (0.13 mL, 1.58 mmol) was added to a stirring solution of 4-trifluoromethyl phenol (0.26 g, 1.58 mmol) in chloroform (10 mL) and trimethylamine (0.22 ml, 1.58 mmol). The solution was stirred at room temperature for three hours, washed with an aqueous 0.3M NaOH solution (30 mL), and the organic layer taken to dryness to give a pale yellow solid (0.35 g, 1.44 mmol) with a yield of 91.2 %, mp 49-51 °C. ^{1}H NMR (298 K, $CDCl_3$, 400 MHz): δ; 3.23 (s, 3H), 7.44 (d, J = 8.52 Hz, 2H), 7.73 (d, J = 8.52 Hz, 2H).

This compound has been previously synthesised by Hiscock and co-workers. The ^{1}H NMR data provided was found to match these previously published data.[1]

Compound 19: Methylsulfonyl chloride (0.56 mL, 7.19 mmol) was added to a stirring solution of 4-nitrophenol (1.00 g, 7.19 mmol) in chloroform (10 mL) and trimethylamine (0.50 ml, 3.56 mmol). The solution was stirred at room temperature for three hours, washed with an aqueous 0.3 M NaOH solution (30 mL), and the organic layer taken to dryness to give a white solid (0.94 g, 4.35 mmol) with a yield of 60.5 %**.** ^{1}H NMR (298 K, $CDCl_3$, 400 MHz): δ; 3.23 (s, 3H), 7.50 (d, J = 9.20 Hz, 2H), 8.34 (d, J = 9.16 Hz, 2H).

This compound has been previously synthesised by Tokuyama and co-workers.[8] The ^{1}H NMR data provided was found to match previously these published data.

Compound 20: Methylsulfonyl chloride (0.82 mL, 10.63 mmol) was added to a stirring solution of phenol (1.00 g, 10.63 mmol) in chloroform (10 mL) and trimethylamine (0.50 ml, 3.56 mmol). The solution was stirred at room temperature for three hours, washed with an aqueous 0.3 M NaOH solution (30 mL), and the organic layer taken to dryness to give a white solid (0.96 g, 5.56 mmol) with a yield of 52.3 %**.** ^{1}H NMR (298 K, $CDCl_3$, 400 MHz): δ; 3.16 (s, 3H), 7.31 – 7.38 (m, 3H), 7.45 (t, J = 7.28 Hz, 2H).

This compound has been previously synthesised by Seayad and co-workers.[7] The ^{1}H NMR data provided was found to match previously these published data.

Compound 21: Methylsulfonyl chloride (0.78 mL, 10.10 mmol) in pyridine (0.82 mL, 10.10 mmol) was added to a stirring solution of cyclohexanol (1.00 g, 9.98 mmol) in dichloromethane (10 mL). The solution was stirred at 0 ℃ and allowed to warm to room temperature. The reaction was then quenched with methanol (50 mL) and concentrated in vaccu. The resulting white solid was then dissolved in ethyl acetate (50 mL) and washed with 1 M HCl (50 mL), saturated $NaHCO_3$ solution (50 mL). The organic layer was then taken to dryness to give a yellow oil (1.68 g, 9.42 mmol) with a yield of 94.4 %. ^{1}H NMR (298 K, $CDCl_3$, 400 MHz): δ; 1.29-2.03 (m, 10H), 3.02 (s, 3H), 4.72 (m, 1H).

This compound has been previously synthesised by Martín and co-workers.[9] The ^{1}H NMR data provided was found to match previously these published data.

Compound 22: Methylsulfonyl chloride (1.56 mL, 20.20 mmol) in pyridine (1.64 mL, 20.20 mmol) was added to a stirring solution of butanol (1.00 g, 13.4 mmol) in dichloromethane (10 mL). The solution was stirred at 0 ℃ and allowed to warm to room temperature. The reaction was then quenched with methanol (50 mL) and concentrated in vaccu. The resulting white solid was then dissolved in ethyl acetate (50 mL) and washed with 1M HCl (50 mL), saturated $NaHCO_3$ solution (50 mL) organic layer taken to dryness to give a yellow oil (1.43 g, 9.39 mmol) with a yield of 70.1 %. ^{1}H NMR (298 K, $CDCl_3$, 400 MHz): δ; 0.89 (t, J = 7.36 Hz, 3H), 1.37 (m, 2H), 1.67 (m, 2H), 2.93 (s, 3H), 4.17 (t, J = 6.56 Hz, 2H).

This compound has been previously synthesised by Li and co-workers.[10] The ^{1}H NMR data provided was found to match previously these published data.

Compound 23: A solution of 4-(trifluoromethyl)phenyl isothiocyanate (1.57 g, 7.16 mmol) and 4-(trifluoromethyl)aniline (0.90 mL, 7.16 mmol) in pyridine (4 mL) was stirred at room temperature overnight. The pyridine solution was then added to water (30 mL) to precipitate a white solid. This solid was collected by filtration and washed with water and then dried to

give the final product as a white solid (1.92 g, 5.26 mmol) in a yield of 73.5 %. ^{1}H NMR: (400 MHz, 298 K, DMSO-d_6): δ: 7.72 (dd, J_1= 8.80 Hz, J_2 = 16.40 Hz, 8H), 10.37 (s, 2NH).

This compound has been previously synthesised by Gale and co-workers.[11] The ^{1}H NMR data provided was found to match these previously published data.

NMR characterisation

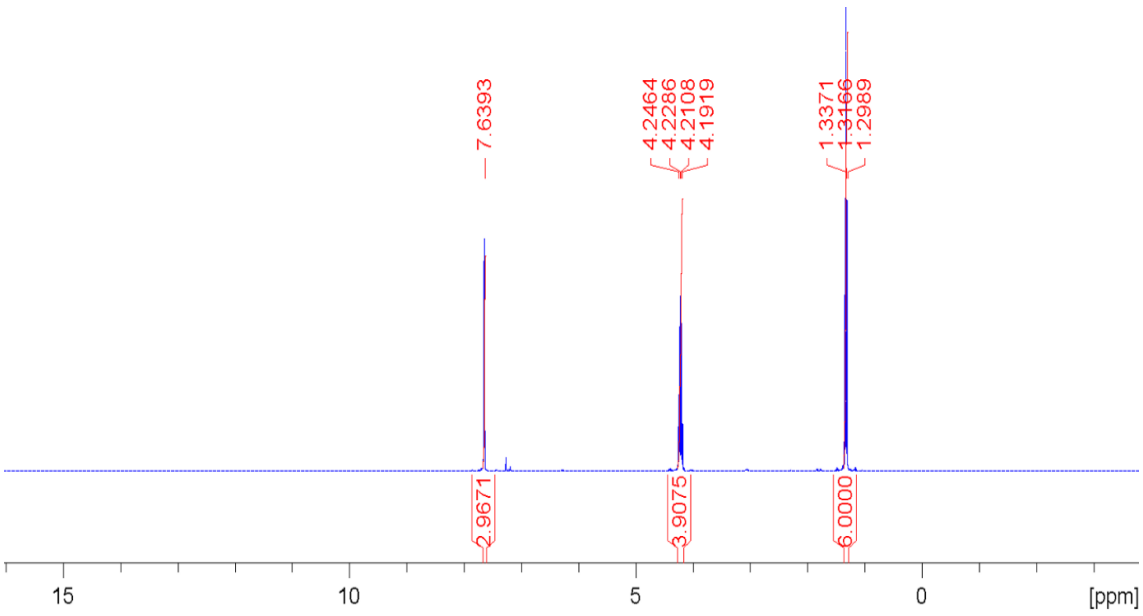

Figure S1: ^{1}H{^{31}P} NMR spectra of compound **1** in $CDCl_3$ conducted at 298 K.

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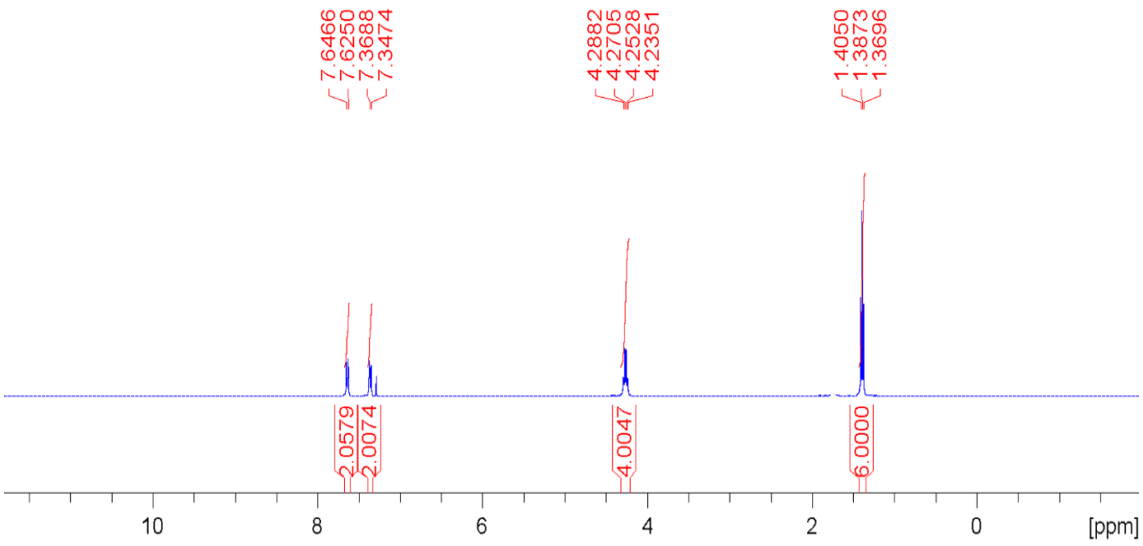

Figure S2: ^{1}H{^{31}P} NMR spectra of compound **2** in $CDCl_3$ conducted at 298 K.

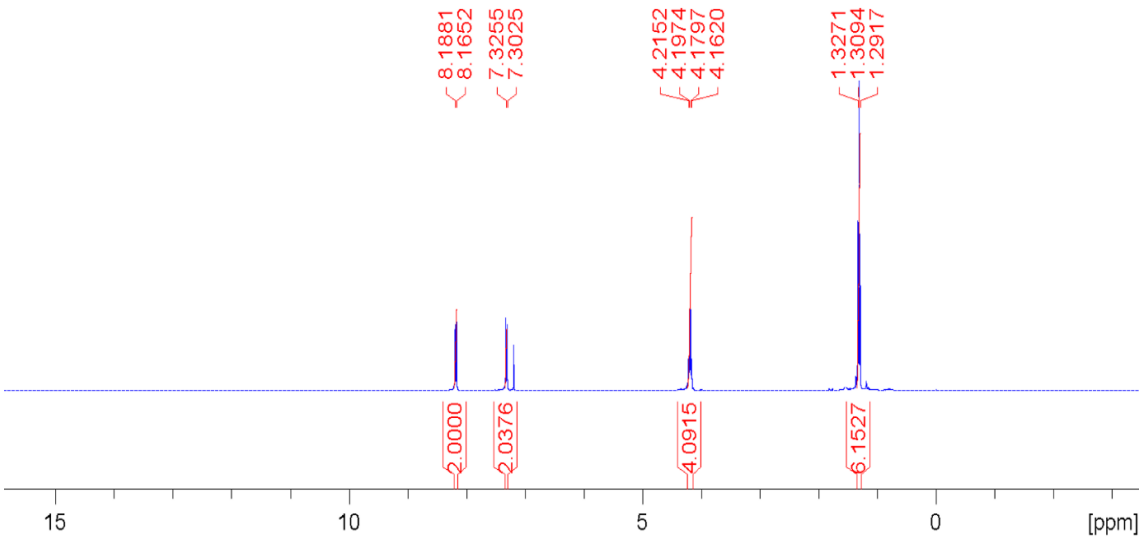

Figure S3: $^{1}H\{^{31}P\}$ NMR spectra of compound **3** in $CDCl_3$ conducted at 298 K.

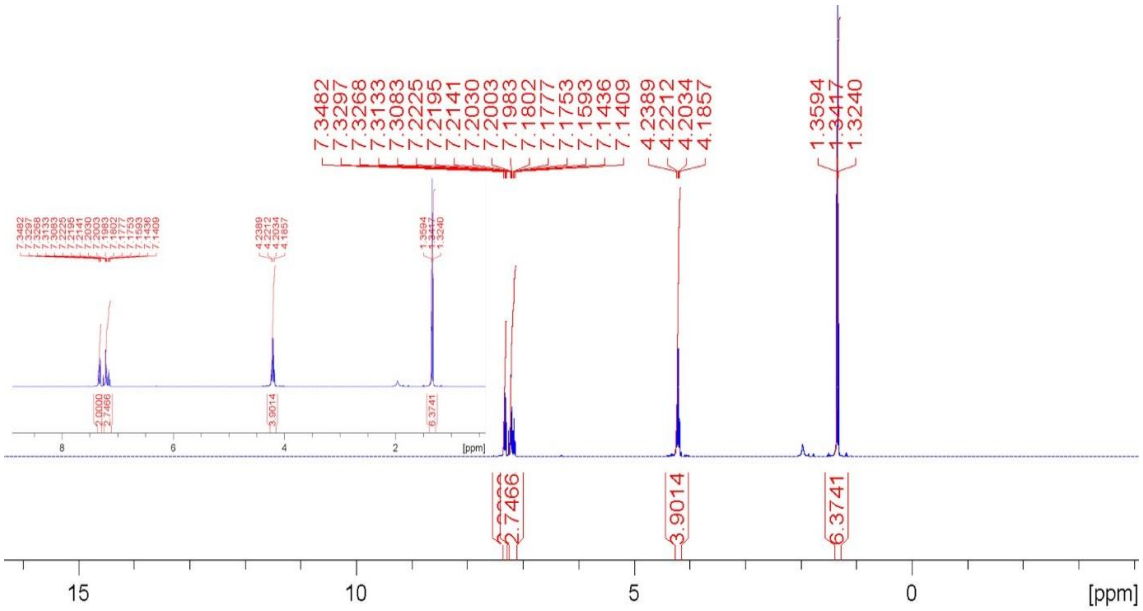

Figure S4: $^{1}H\{^{31}P\}$ NMR spectra of compound **4** in $CDCl_3$ conducted at 298 K.

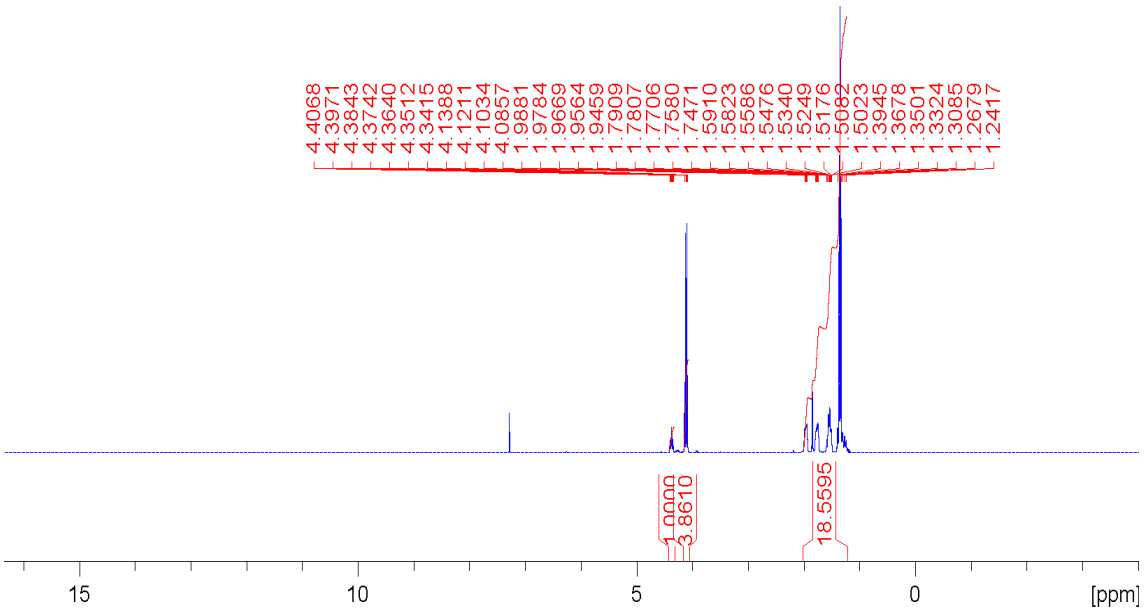

Figure S5: ^{1}H NMR spectra of **5** in $CDCl_3$ at 298 K. Residual H_2O present within the aliphatic region increasing the expected integration by two.

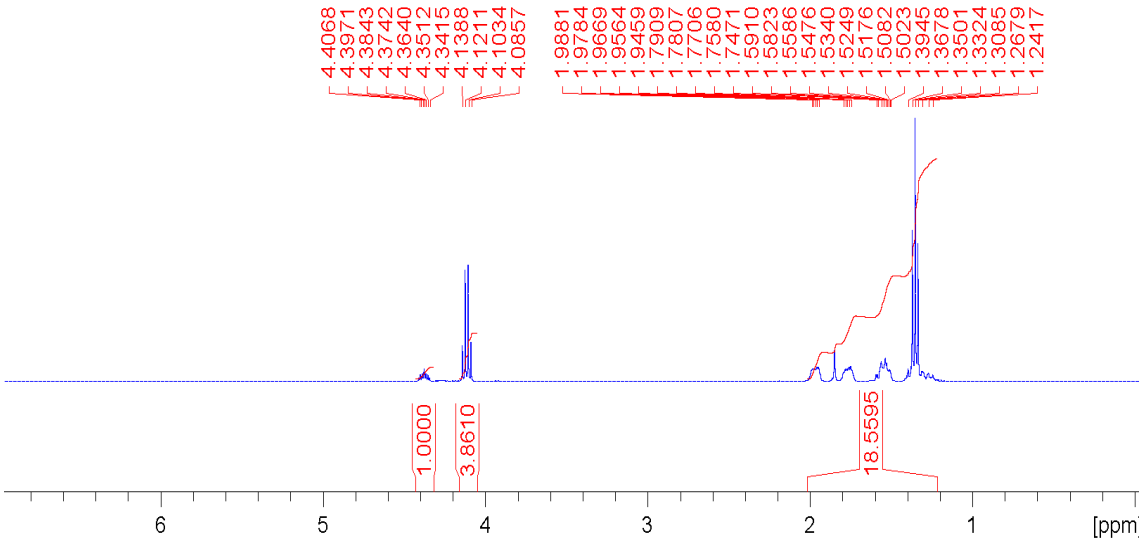

Figure S6: Zoomed in ^{1}H NMR spectra of **5** in $CDCl_3$ at 298 K. Residual H_2O present within the aliphatic region increasing the expected integration by two.

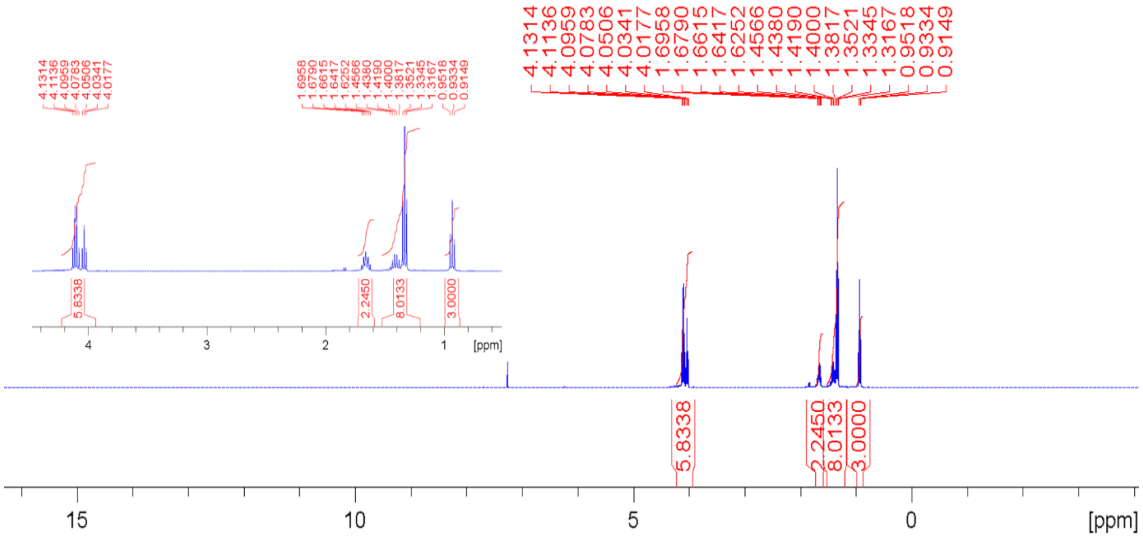

Figure S7: $^{1}H\{^{31}P\}$ NMR spectra of compound **6** in $CDCl_3$ conducted at 298 K.

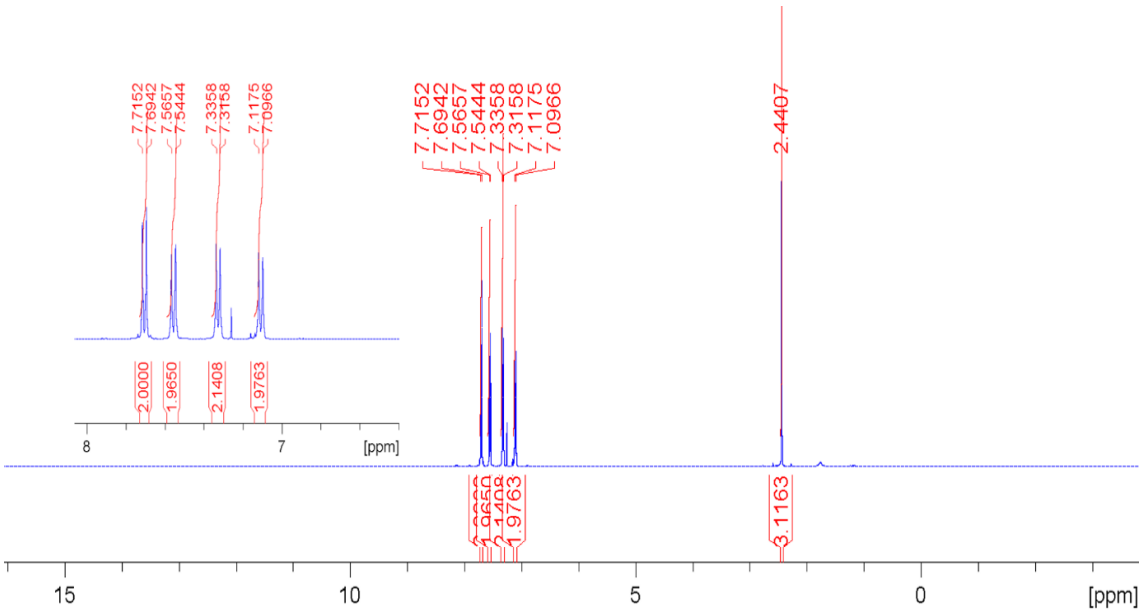

Figure S8: ^{1}H NMR spectra of compound **12** in $CDCl_3$ conducted at 298 K.

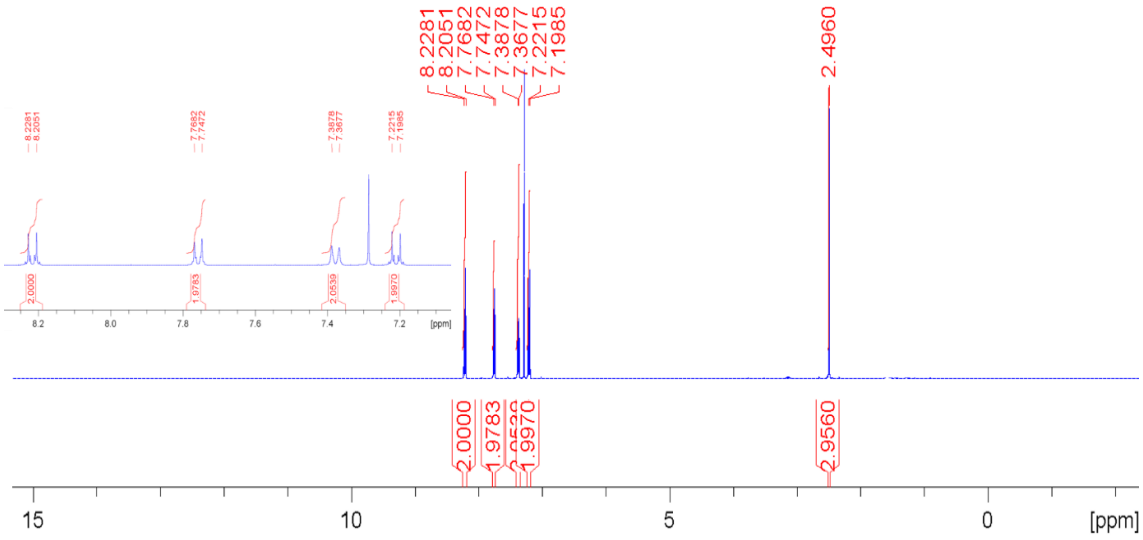

Figure S9*:* ^{1}H NMR spectra of compound **13** in $CDCl_3$ conducted at 298 K.

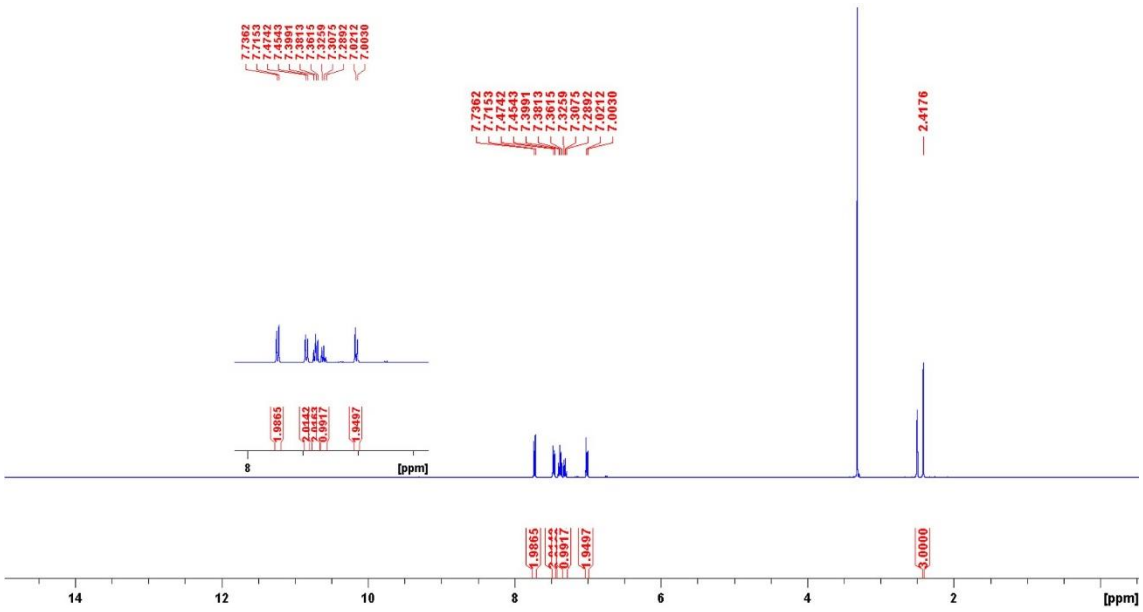

Figure S10: ^{1}H NMR spectra of compound **14** in DMSO-d_6 conducted at 298 K.

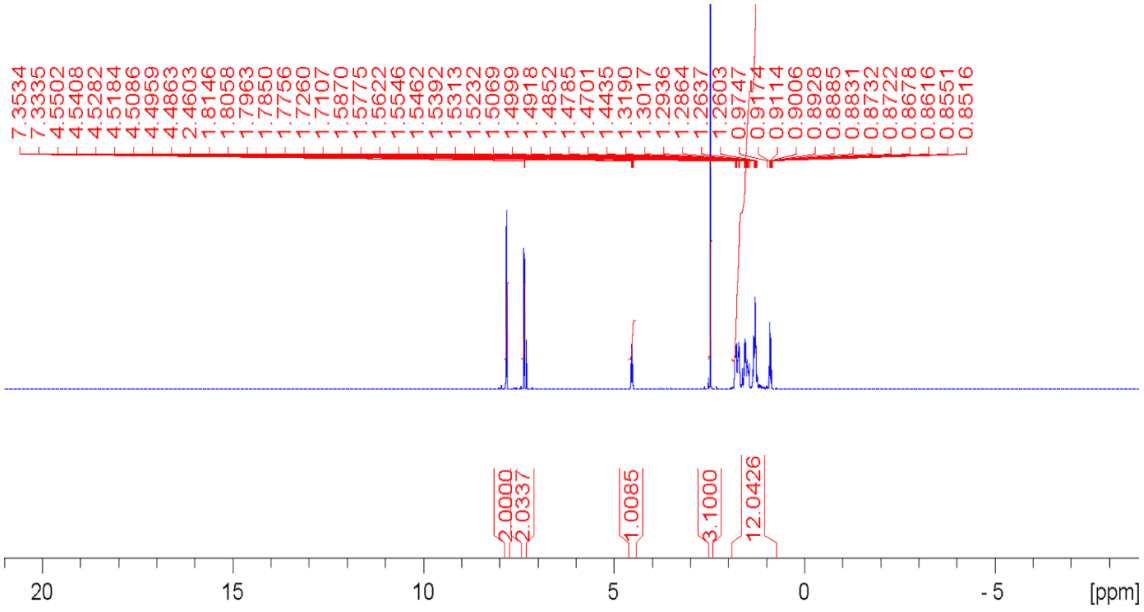

Figure S11: ^{1}H NMR spectra of **15** in $CDCl_3$ at 298 K.

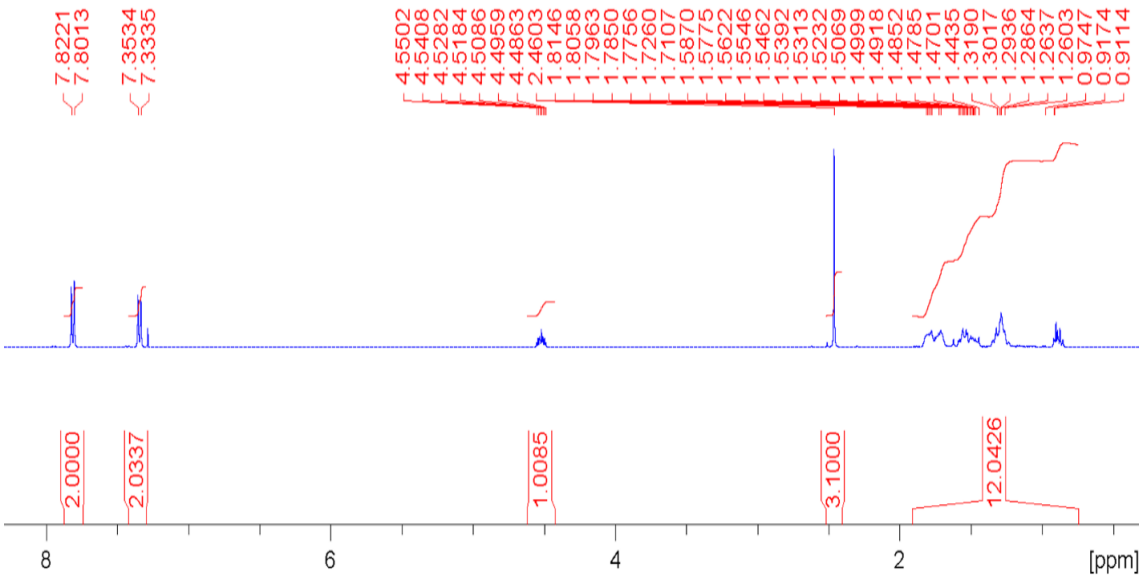

Figure S12: Zoomed in ^{1}H NMR spectra of **15** in $CDCl_3$ at 298 K. Residual H_2O present within the aliphatic region increasing the expected integration by two.

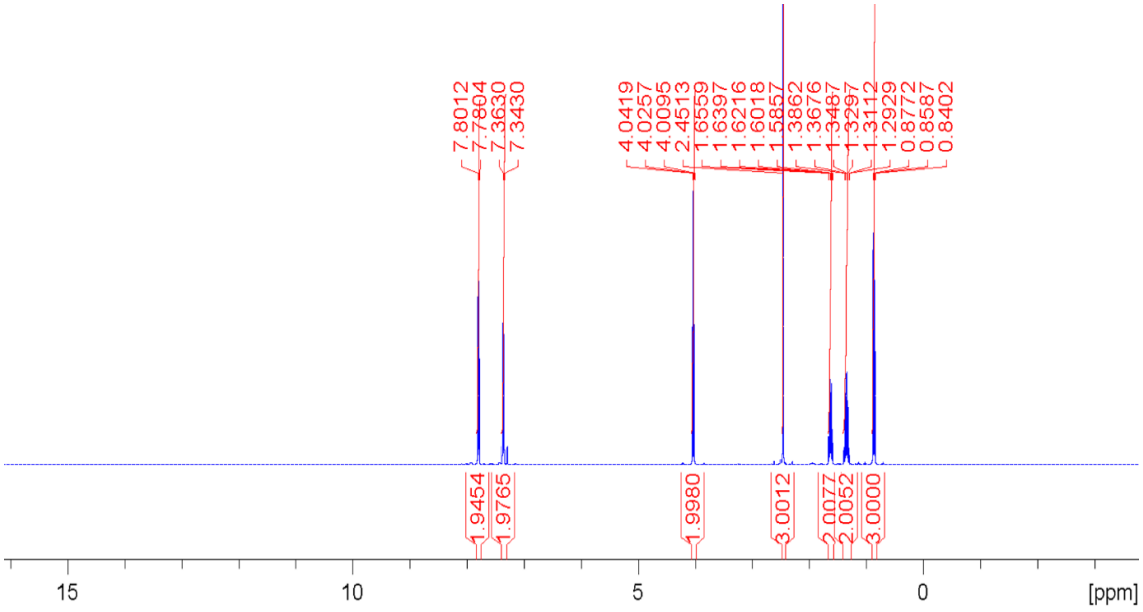

Figure S13: ^{1}H NMR spectra of compound **16** in $CDCl_3$ conducted at 298 K.

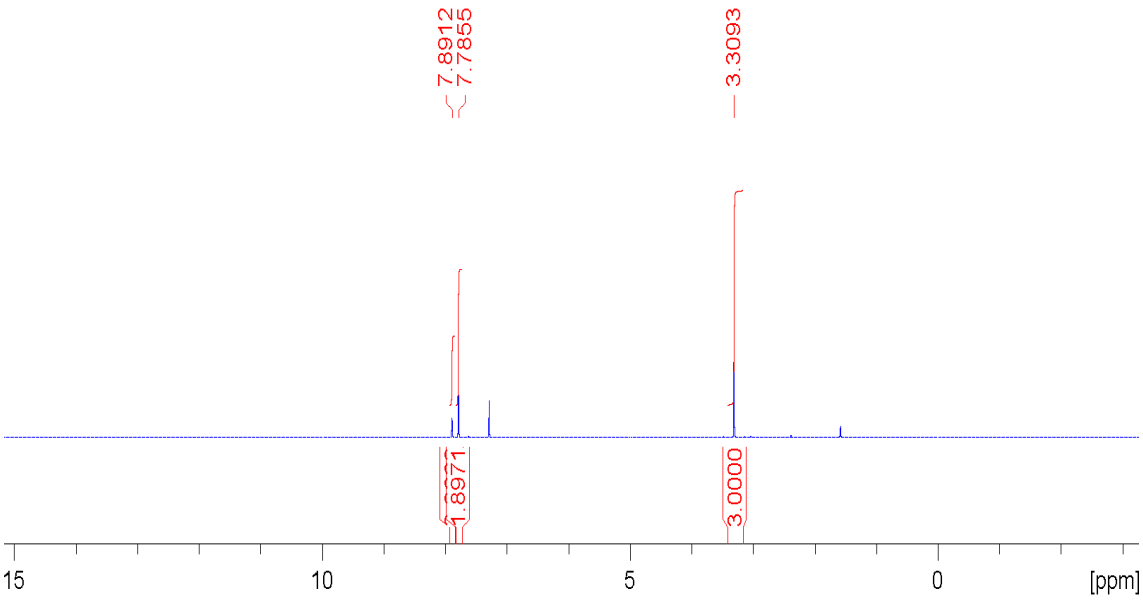

Figure S14: ^{1}H NMR spectra of compound **16** in $CDCl_3$ at 298 K.

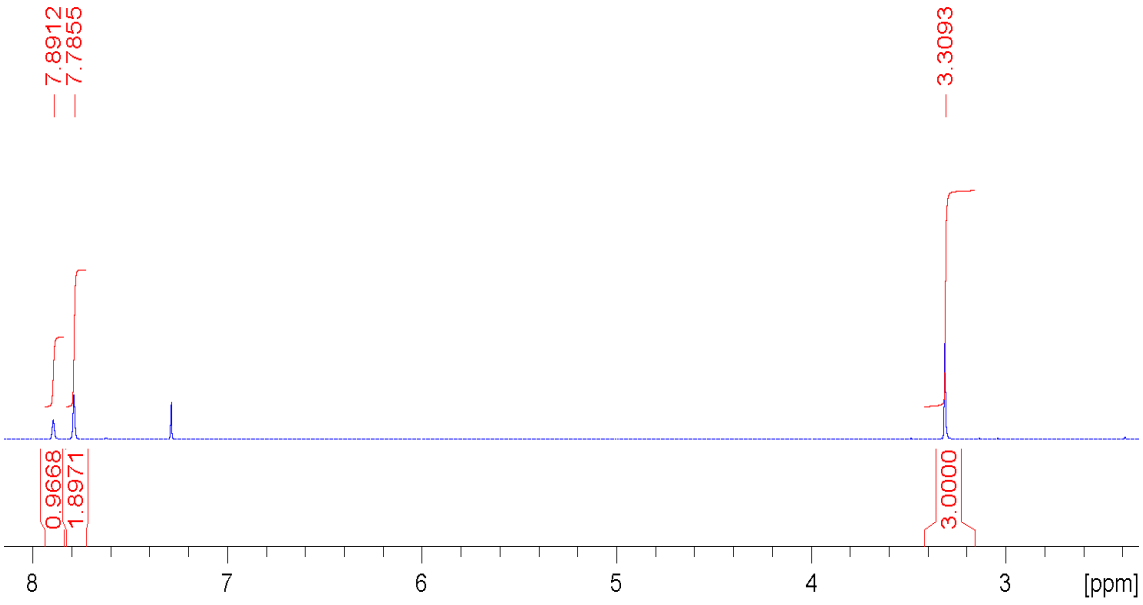

Figure S15: Zoomed in ^{1}H NMR spectra of **17** in $CDCl_3$ at 298 K.

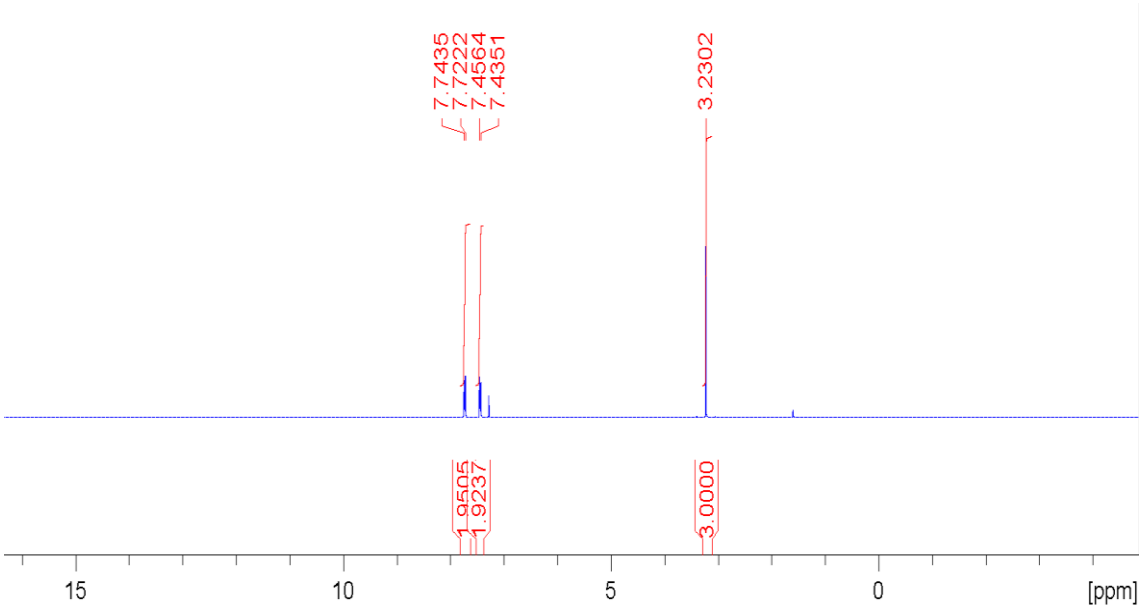

Figure S16: ^{1}H NMR spectra of **18** in $CDCl_3$ at 298 K.

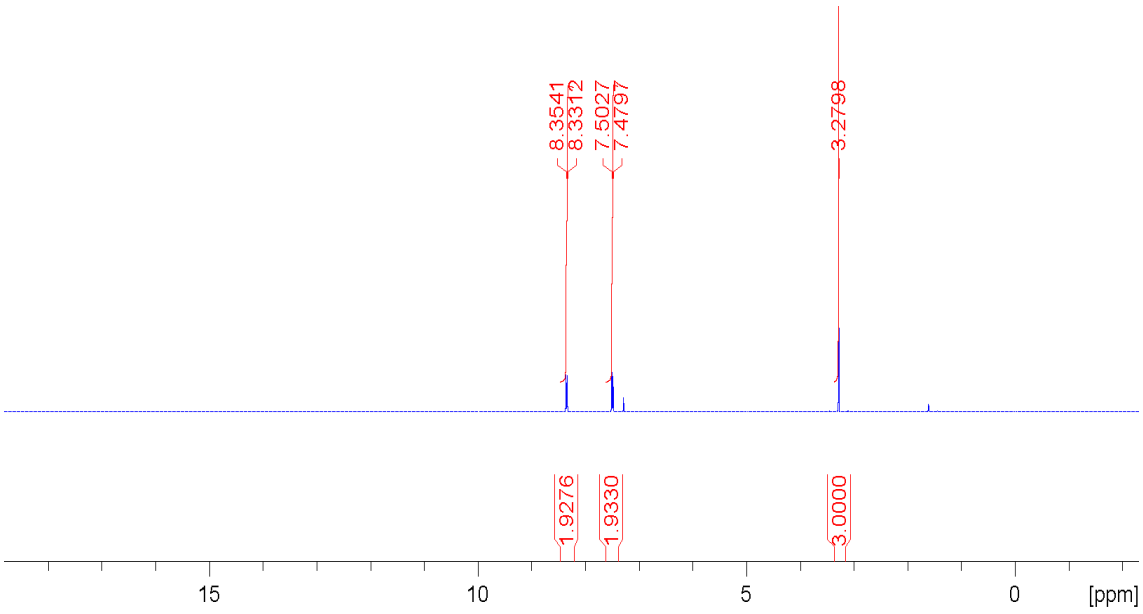

Figure S17: ^{1}H NMR spectra of **19** in $CDCl_3$ at 298 K.

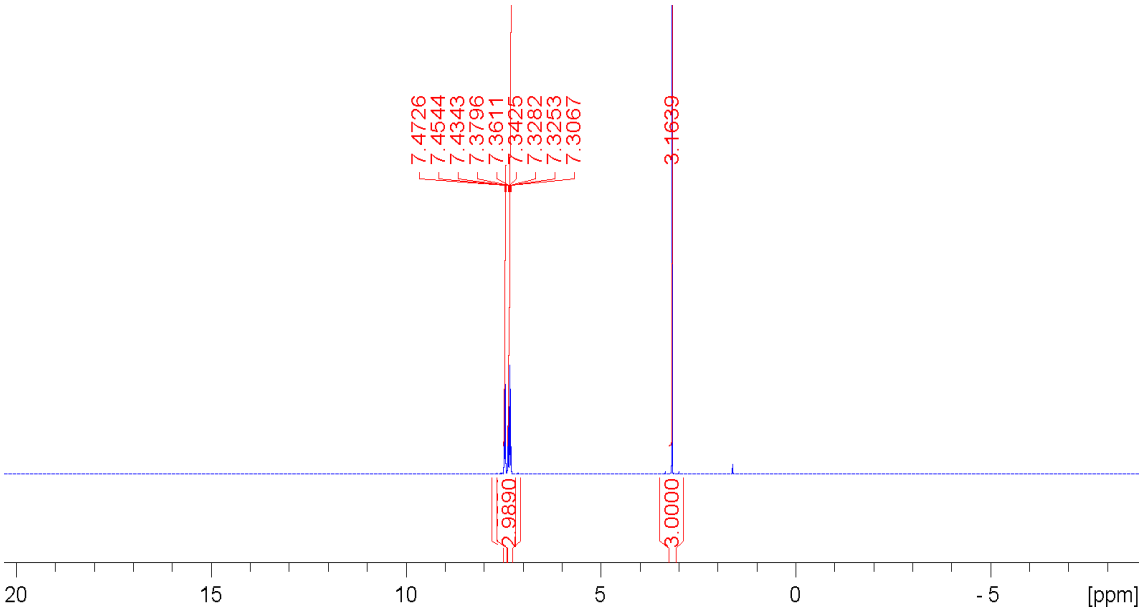

Figure S18: ^{1}H NMR spectra of **20** in $CDCl_3$ at 298 K.

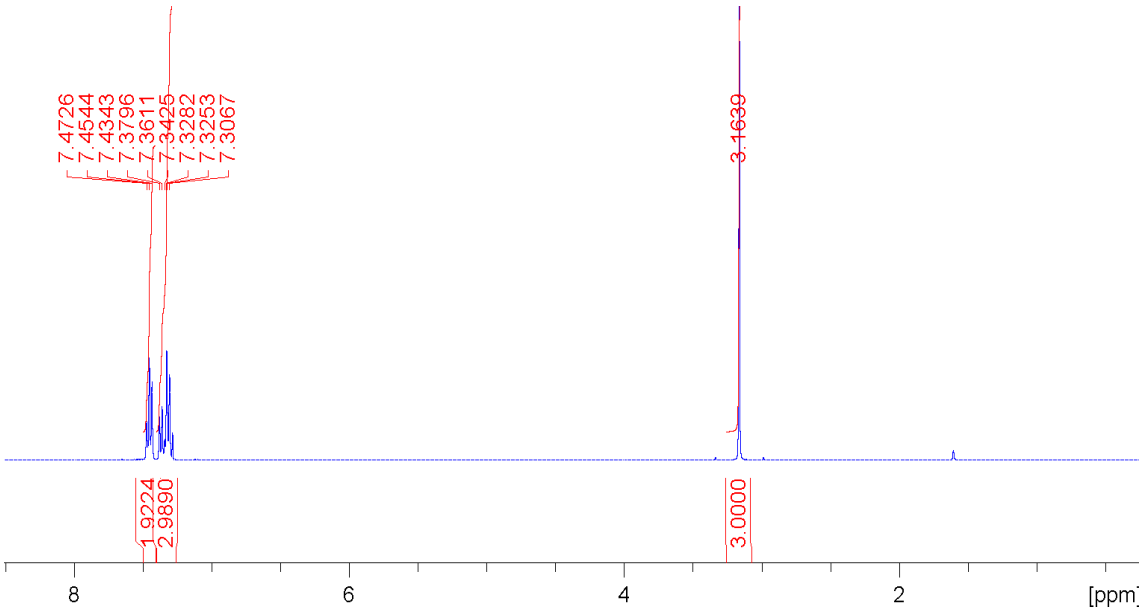

Figure S19: Zoomed in ^{1}H NMR spectra of **20** in $CDCl_3$ at 298 K.

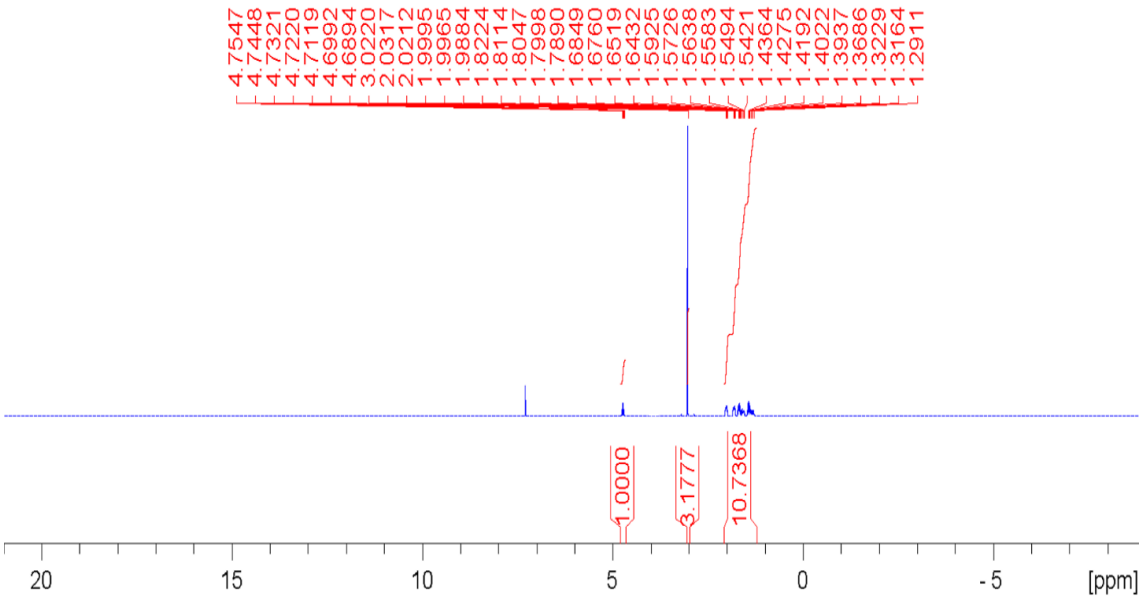

Figure S20: ^{1}H NMR spectra of **21** in $CDCl_3$ at 298 K.

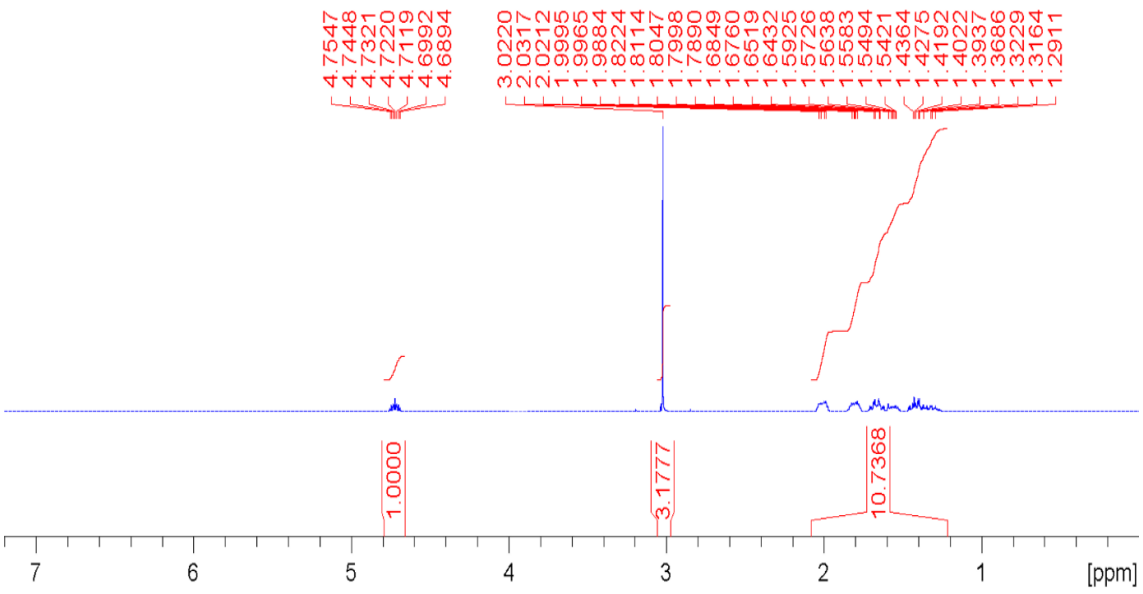

Figure S21: Zoomed in ^{1}H NMR spectra of **21** in $CDCl_3$ at 298 K.

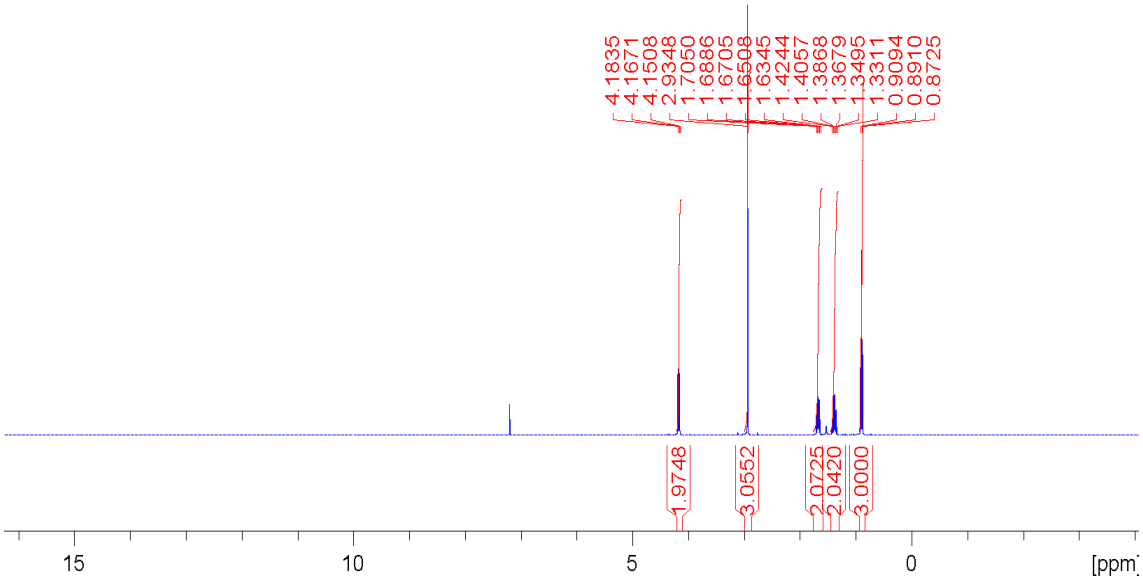

Figure S22: ^{1}H NMR spectra of **22** in $CDCl_3$ at 298 K.

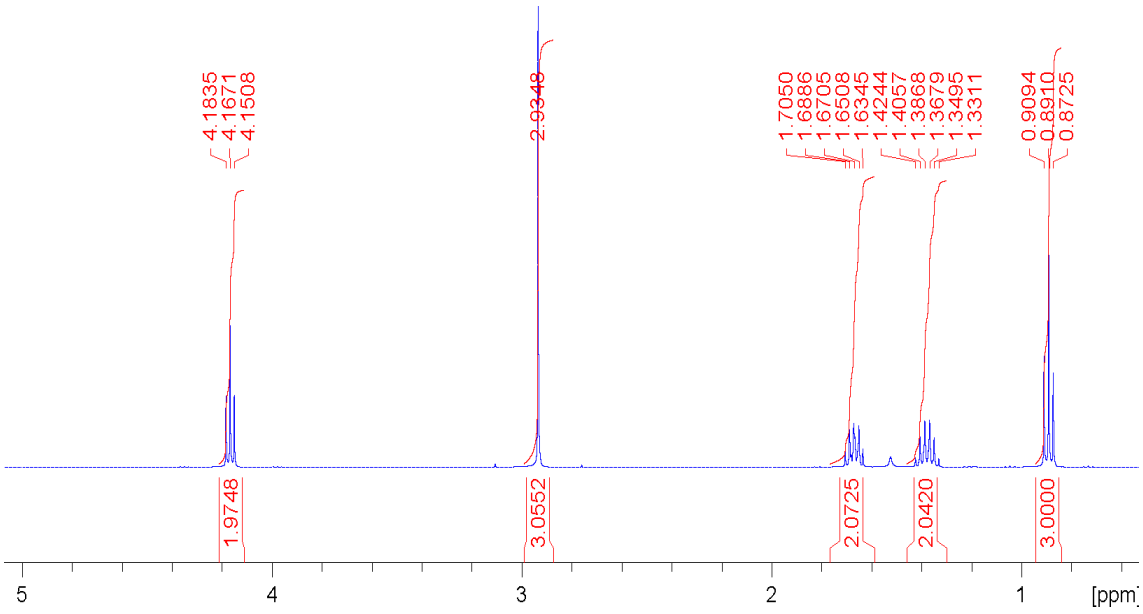

Figure S23: Zoomed in ^{1}H NMR spectra of **22** in $CDCl_3$ at 298 K.

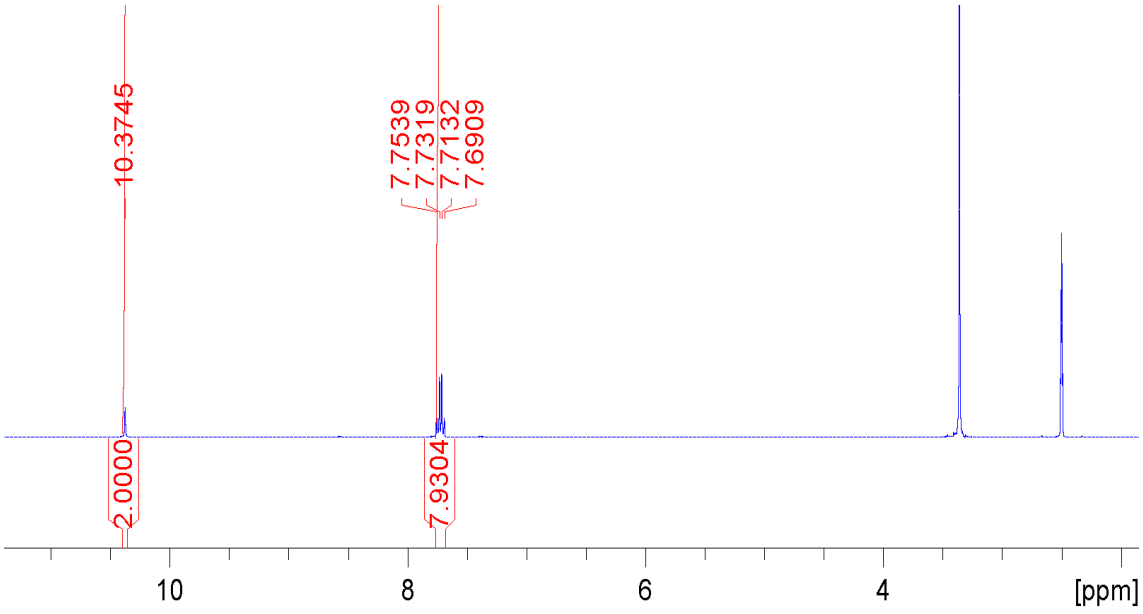

Figure S24: ^{1}H NMR spectra of compound **23** in DMSO-d_6 conducted at 298 K.

^{1}H NMR titration results

The ^{1}H NMR titration results used have been previously published by Hiscock and co-workers.[1]

Hydrolytic stability results

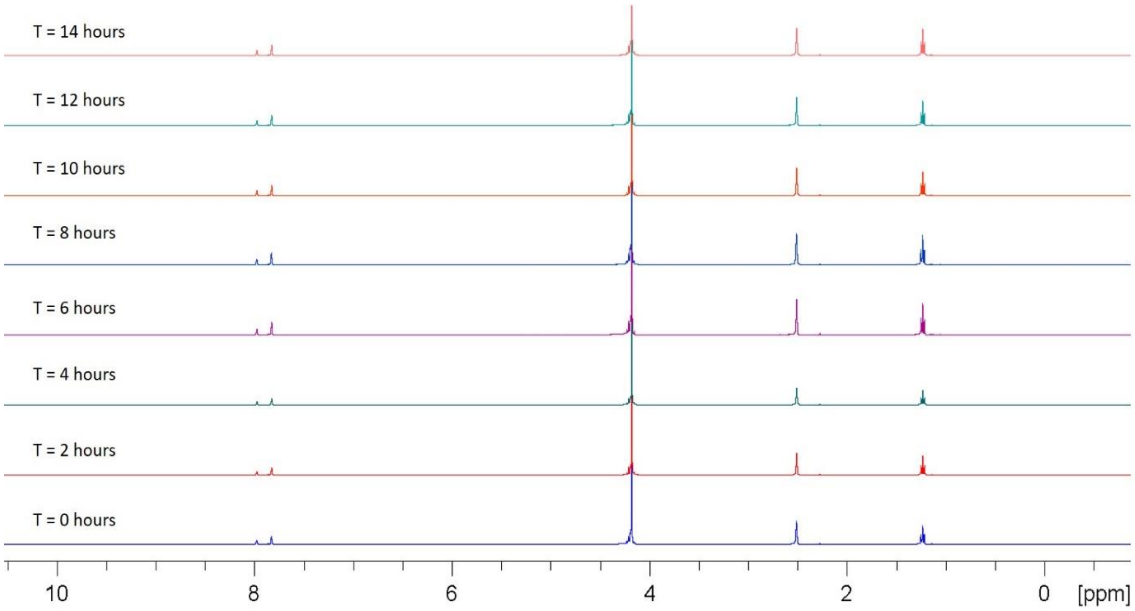

Figure S25: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **1** hydrolysis over 14 hours. Results indicate 0 % breakdown.

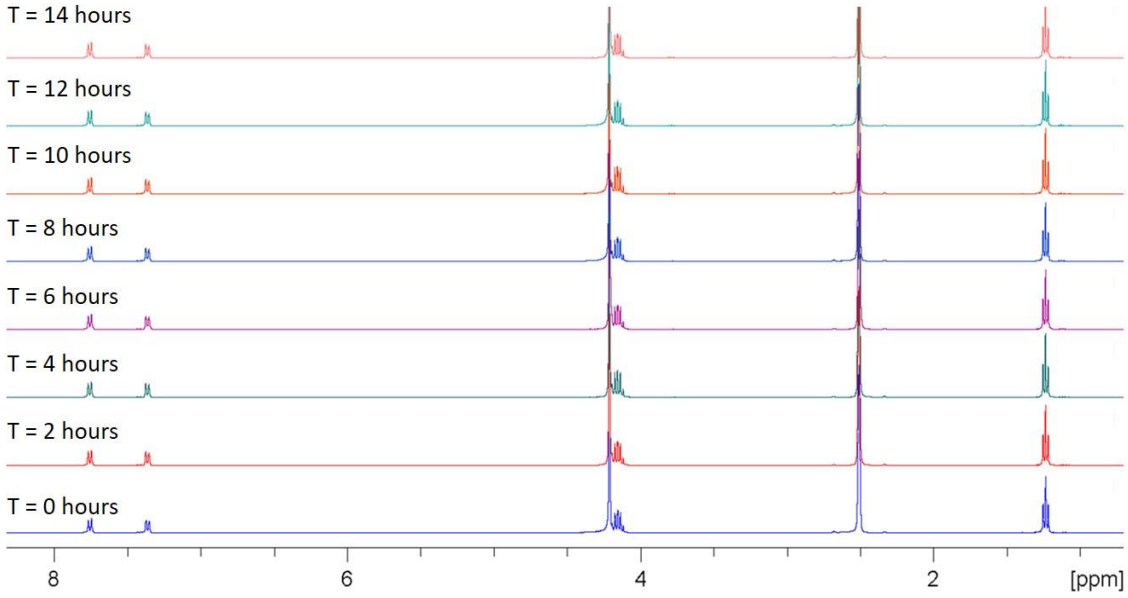

Figure S26: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **2** hydrolysis over 14 hours. Results indicate 0 % breakdown.

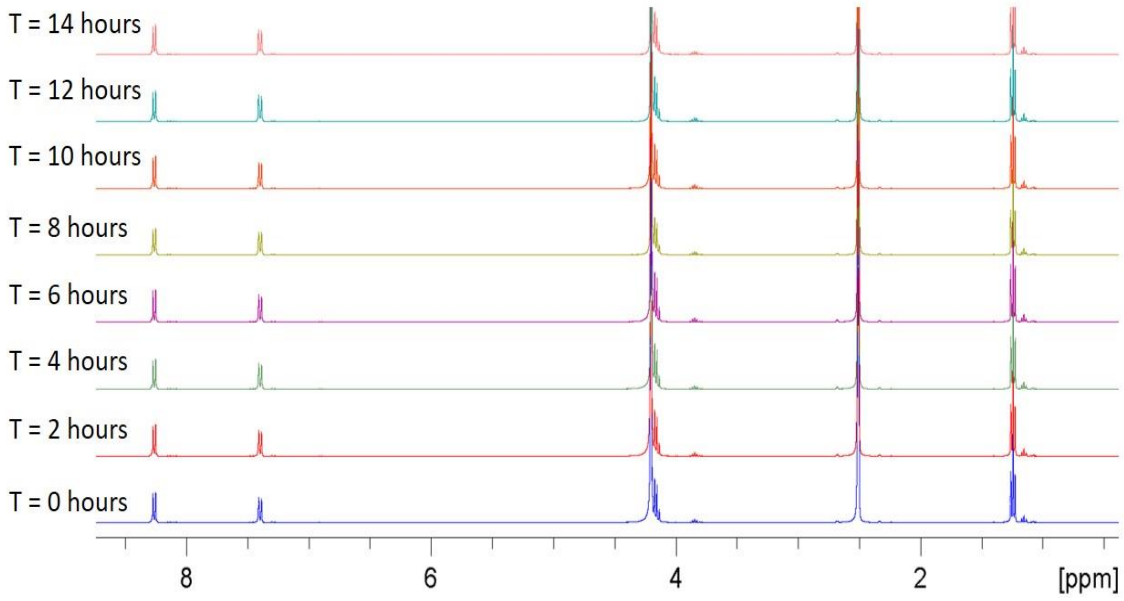

Figure S27: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **3** hydrolysis over 14 hours. Results indicate 0 % breakdown.

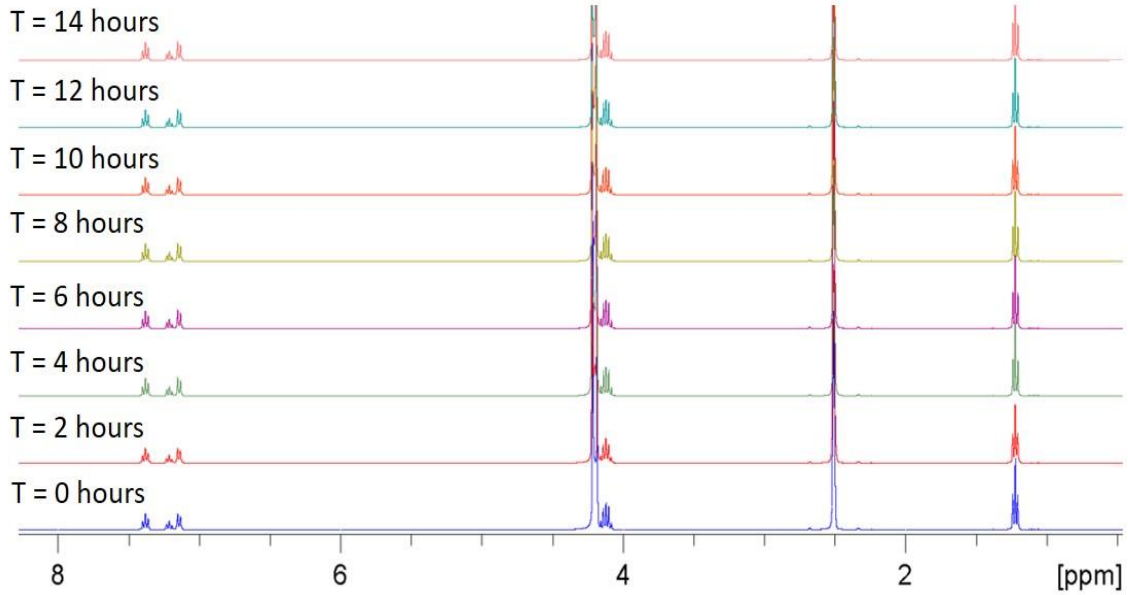

Figure S28: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **4** hydrolysis over 14 hours. Results indicate 0 % breakdown.

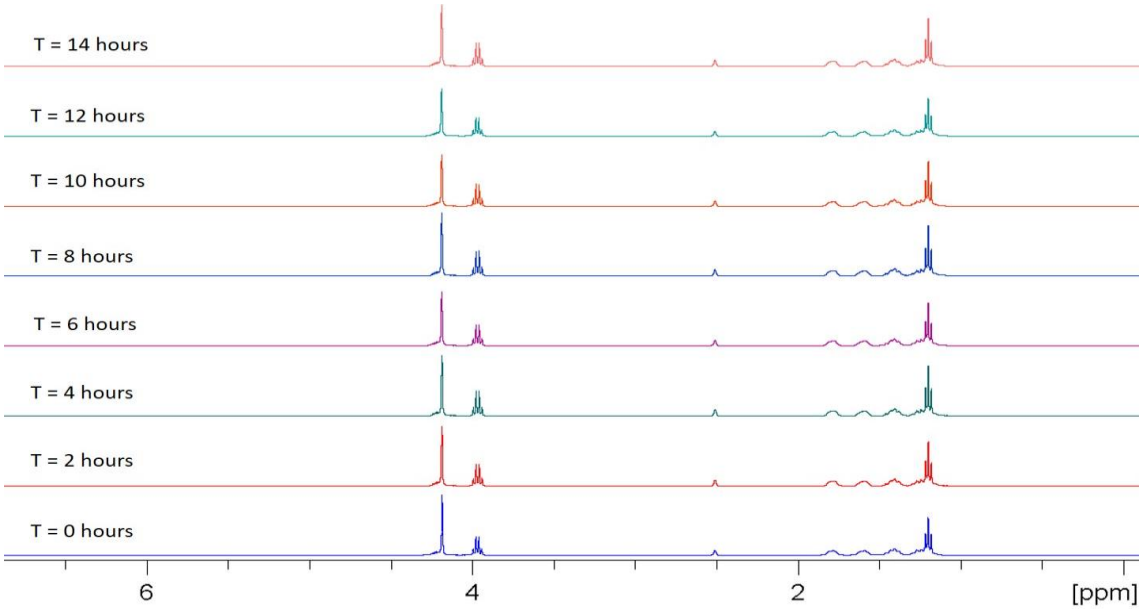

Figure S29: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **5** hydrolysis over 14 hours. Results indicate 0 % breakdown.

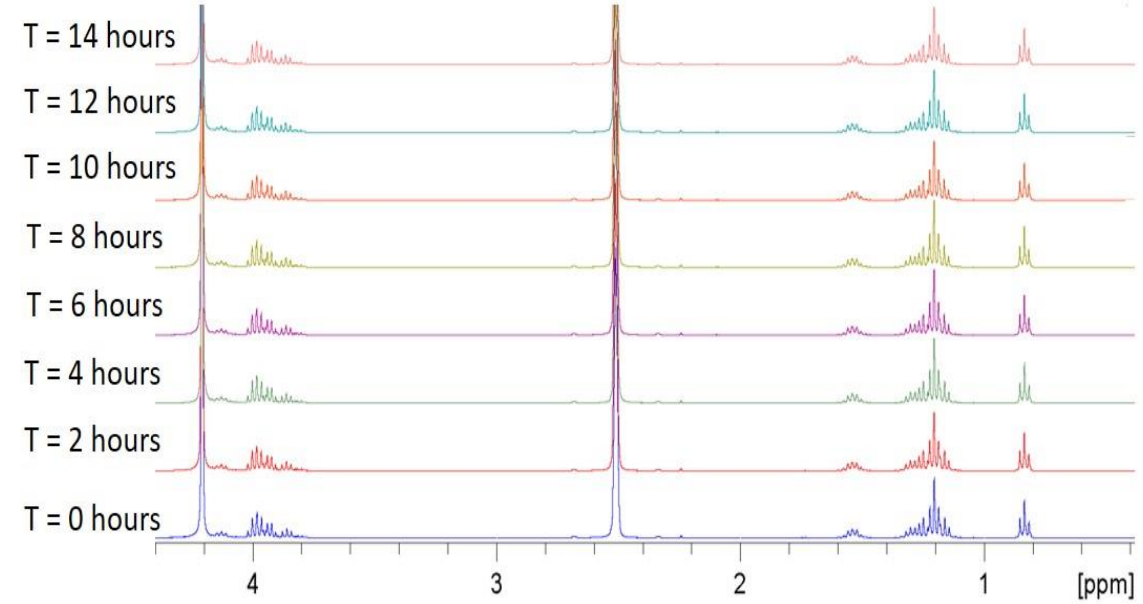

Figure S30: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **6** hydrolysis over 14 hours. Results indicate 0 % breakdown.

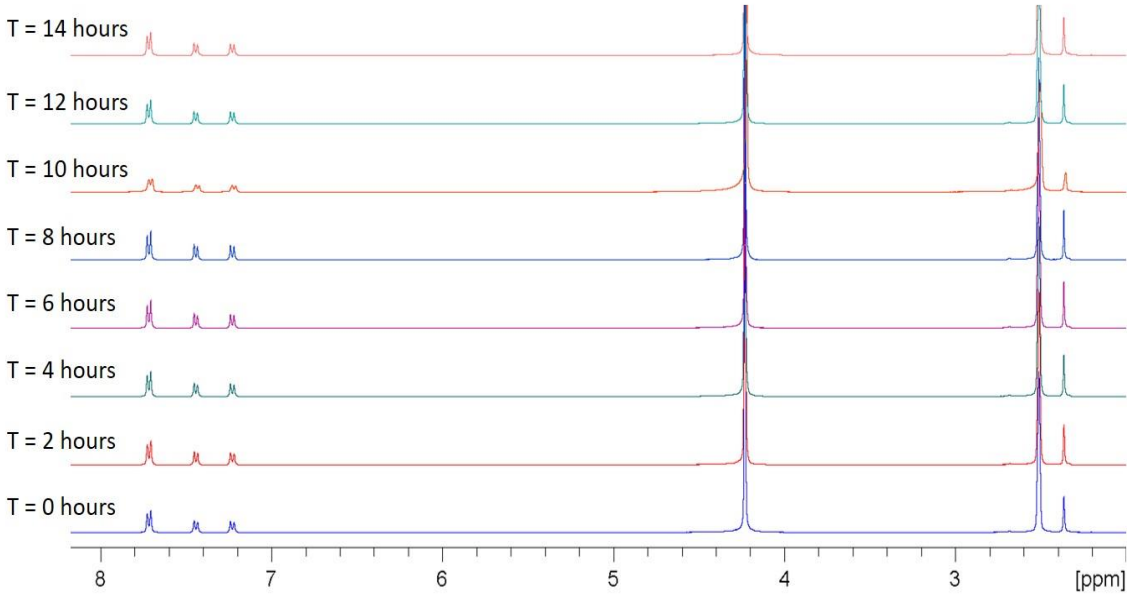

Figure S31: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **12** hydrolysis over 14 hours. Results indicate 0 % breakdown.

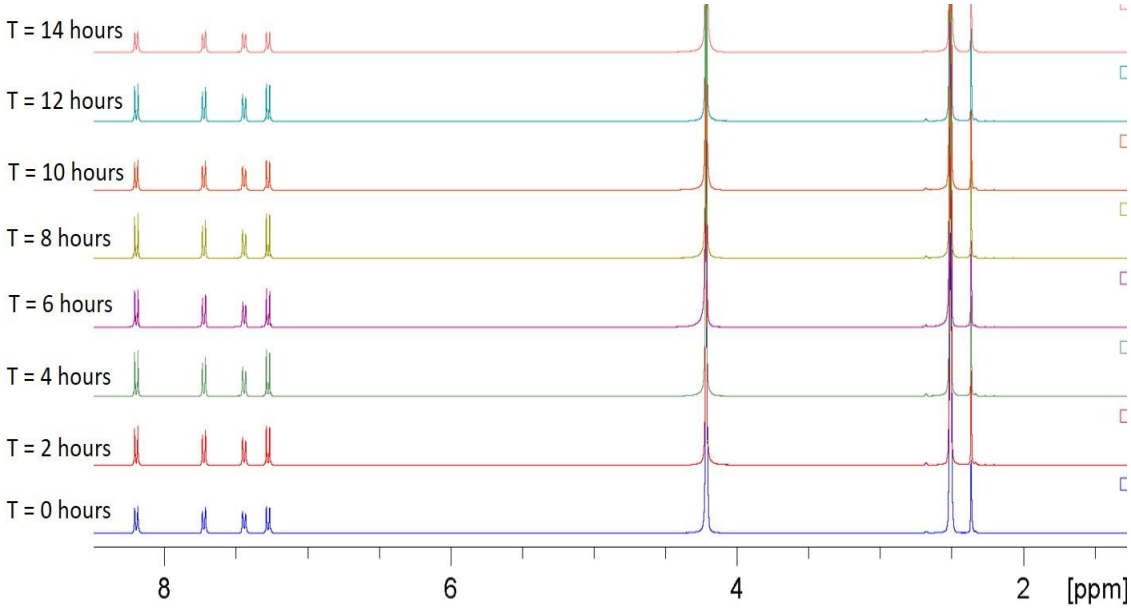

Figure S32: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **13** hydrolysis over 14 hours. Results indicate 0 % breakdown.

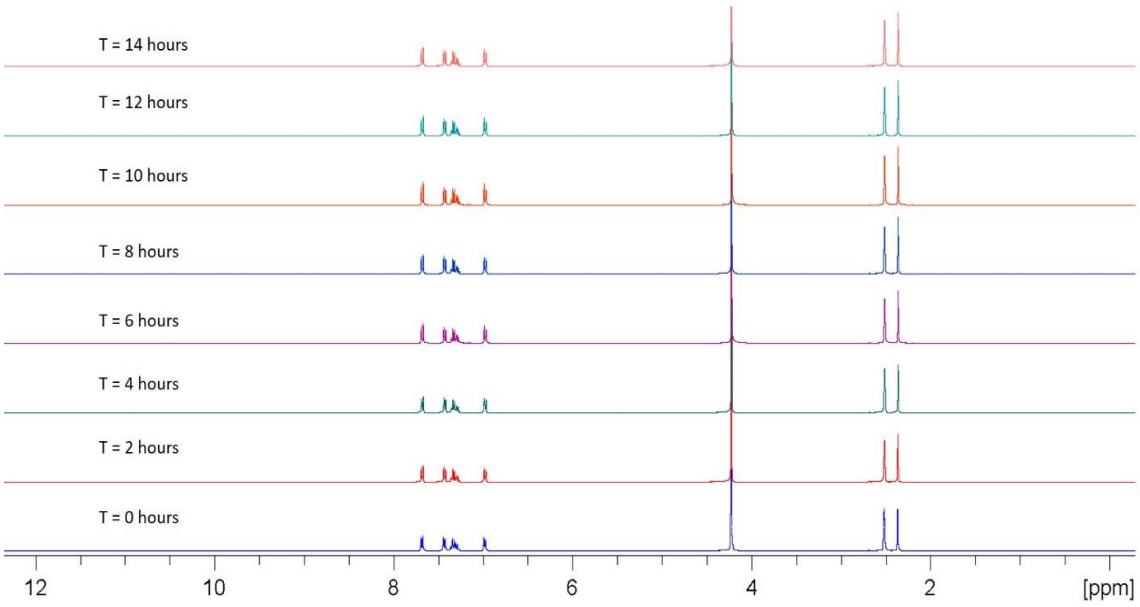

Figure S33: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **14** hydrolysis over 14 hours. Results indicate 0 % breakdown.

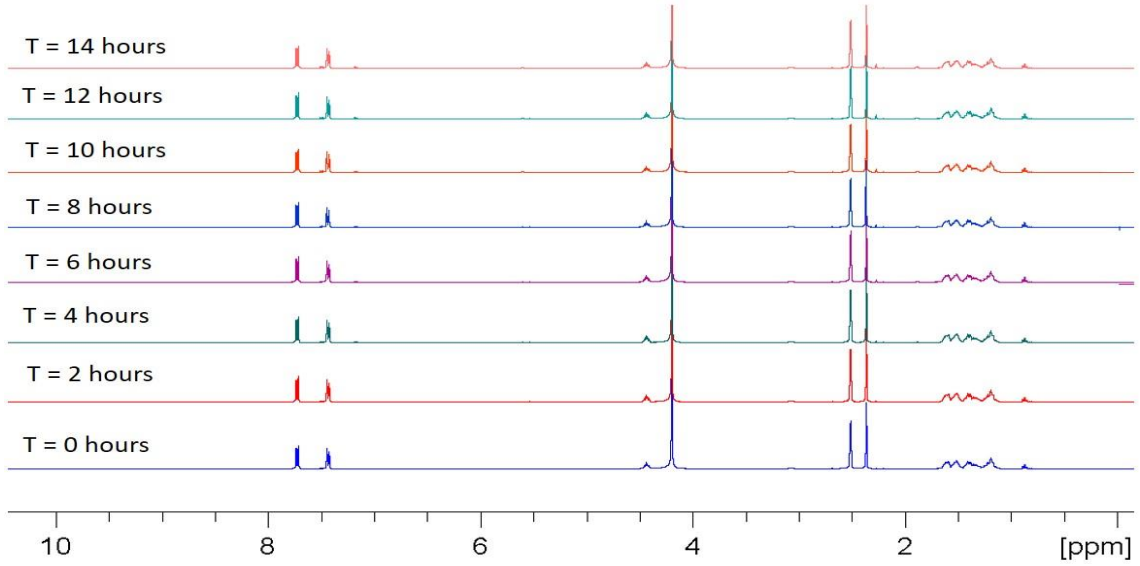

Figure S34: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **15** hydrolysis over 14 hours. Results indicate 2.0 % breakdown.

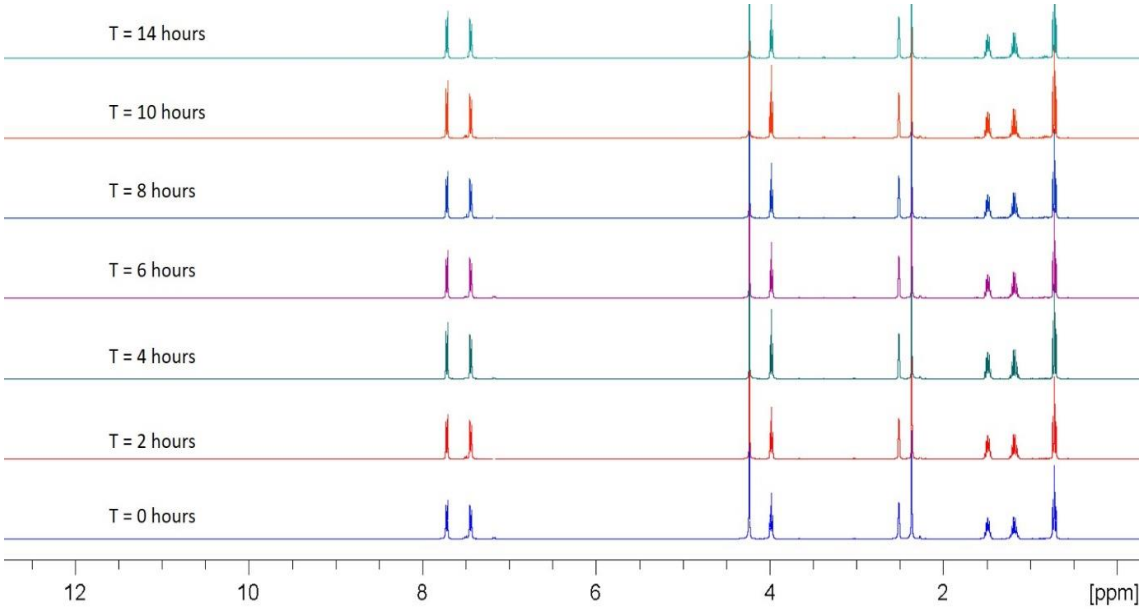

Figure S35: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **16** hydrolysis over 14 hours. Results indicate 0 % breakdown. The 12 hour time slot was removed due to shimming issues.

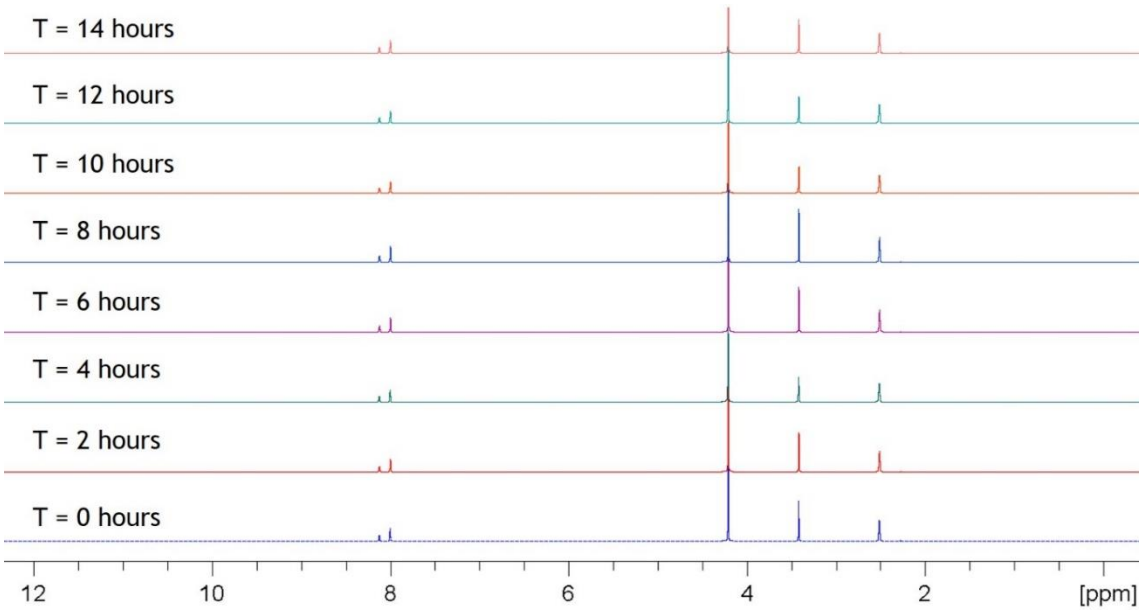

Figure S36: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **17** hydrolysis over 14 hours. Results indicate 0 % breakdown.

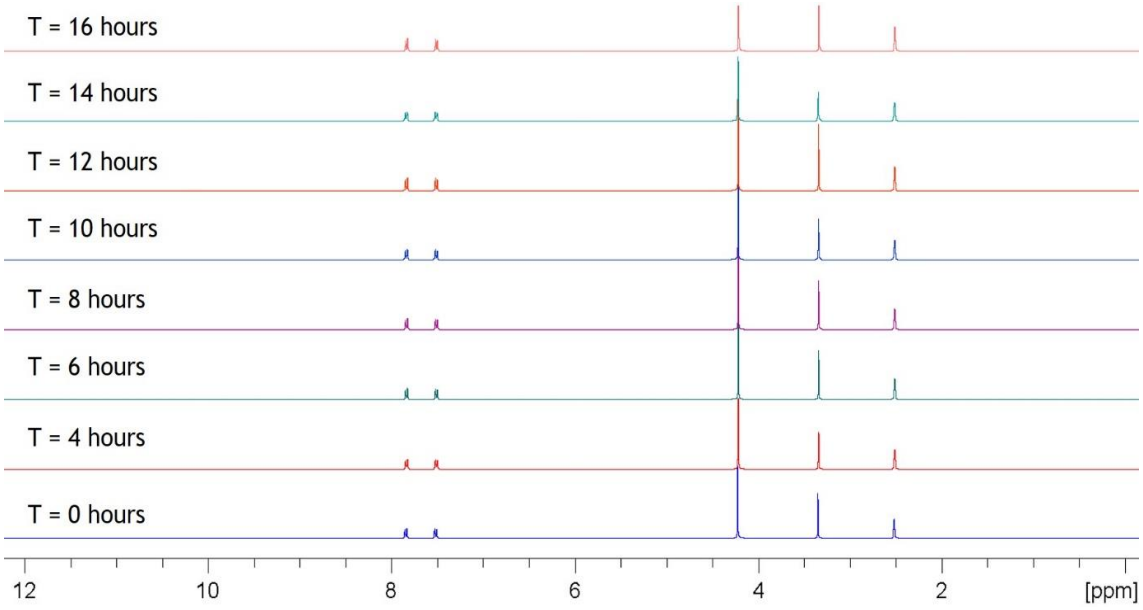

Figure S37: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **18** hydrolysis over 14 hours. Results indicate 0 % breakdown.

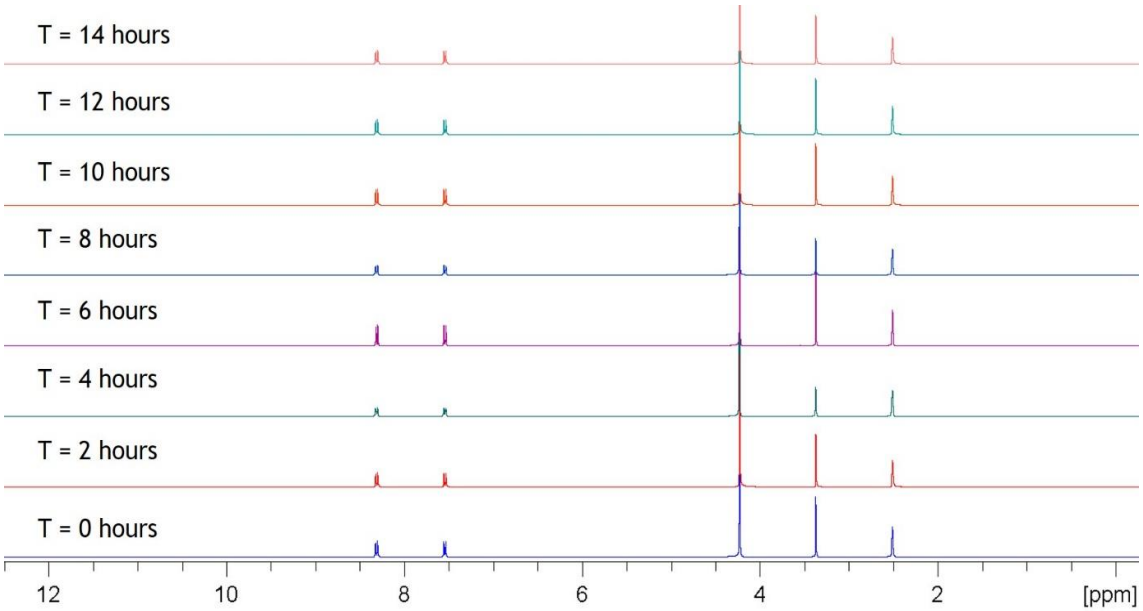

Figure S38: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **19** hydrolysis over 14 hours. Results indicate 0 % breakdown.

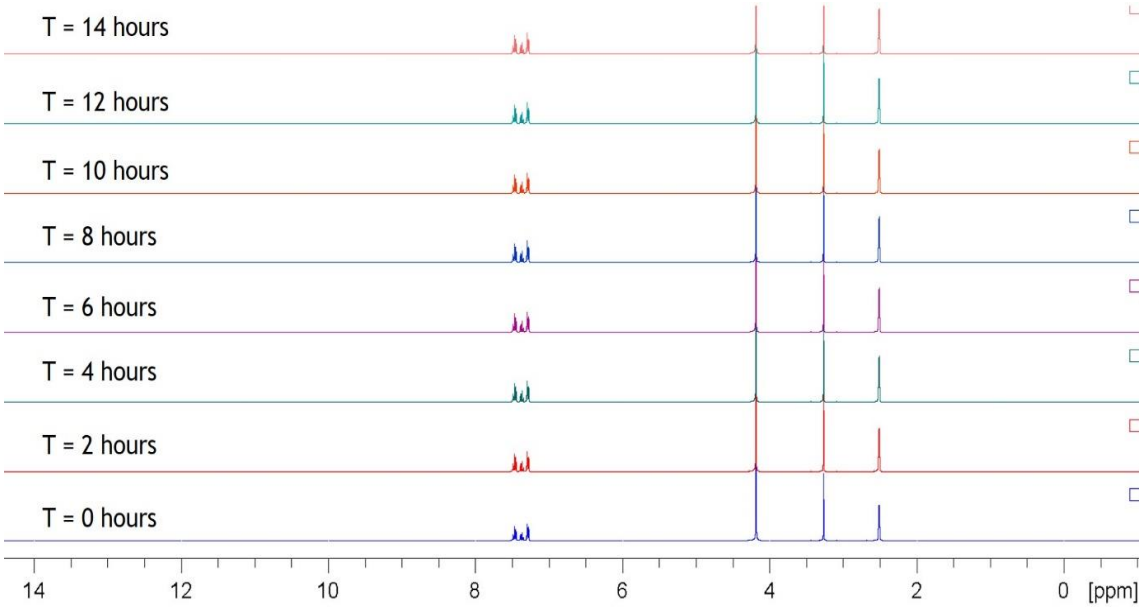

Figure S39: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **20** hydrolysis over 14 hours. Results indicate 0 % breakdown.

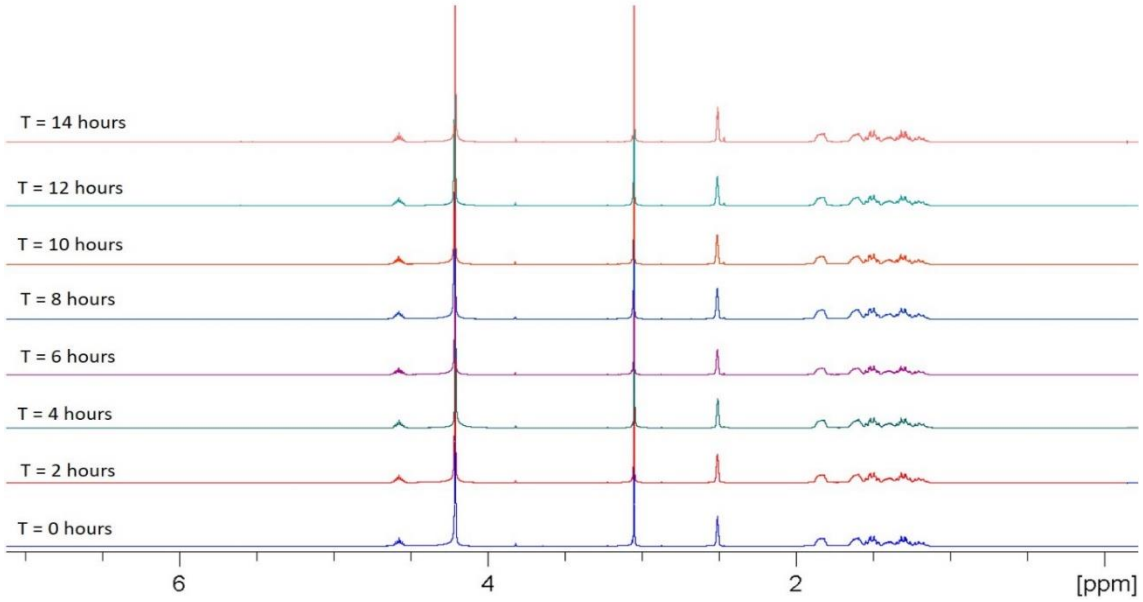

Figure S40: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **21** hydrolysis over 14 hours. Results indicate 0 % breakdown.

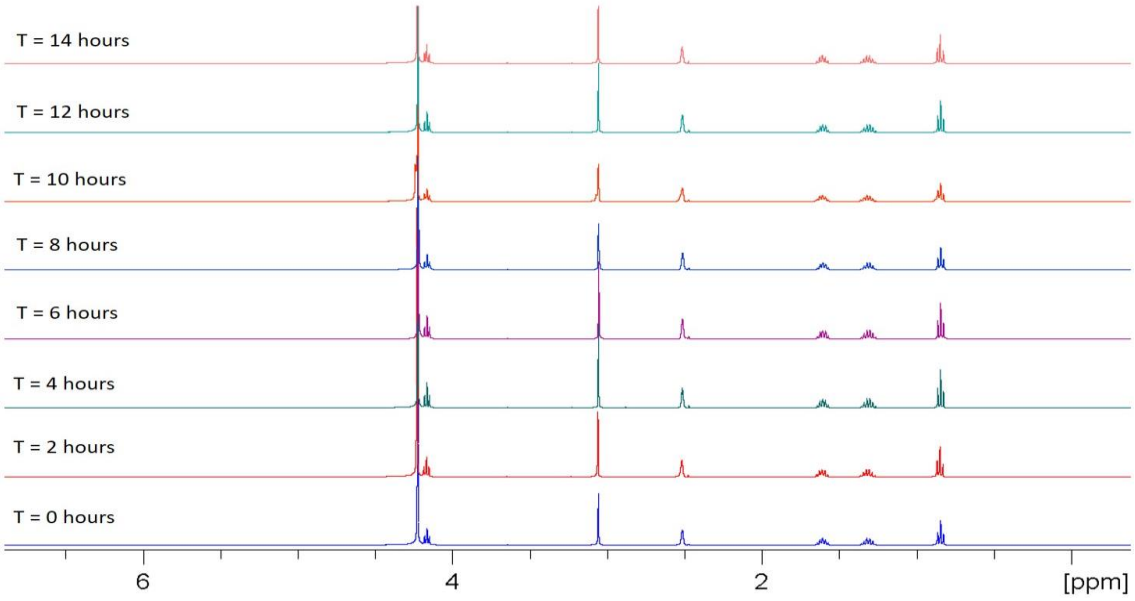

Figure S41: Stacked ^{1}H NMR spectra (DMSO-d_6:D_2O (70:30)), showing the results of compound **22** hydrolysis over 14 hours. Results indicate 0 % breakdown.

Reactivity studies of potential simulants using NaOH

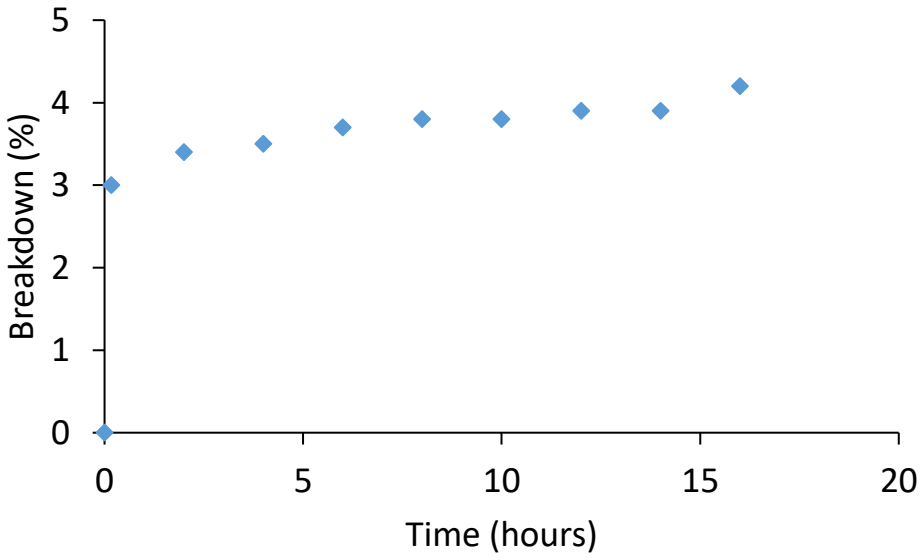

Figure S42: Percentage breakdown of **1** upon the addition of 1 equivalent of NaOH (10 mM) in MeOD-d_4:D_2O (70:30) at 291 K.

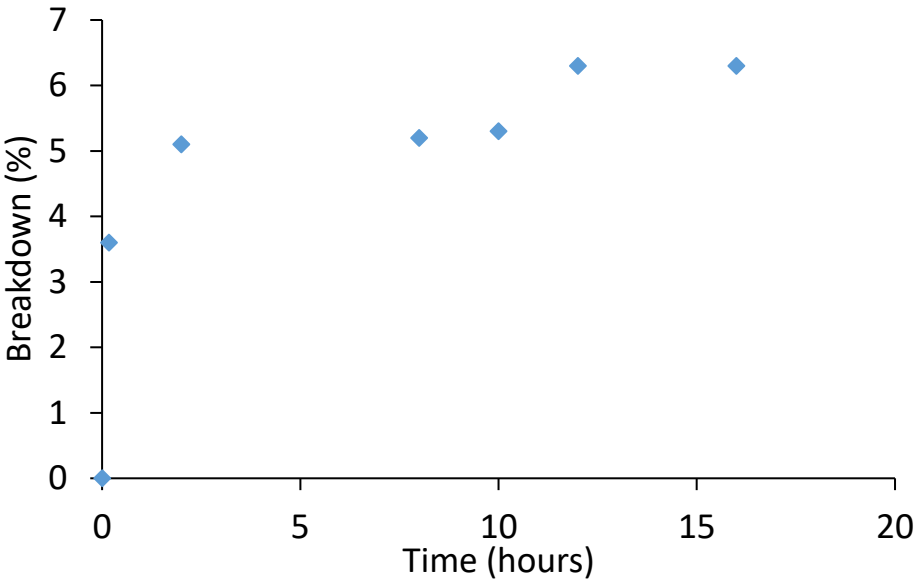

Figure S43: Percentage breakdown of **2** upon the addition of 1 equivalent of NaOH (10 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Time points 4, 6 and 14 hours have been removed due to shimming error.

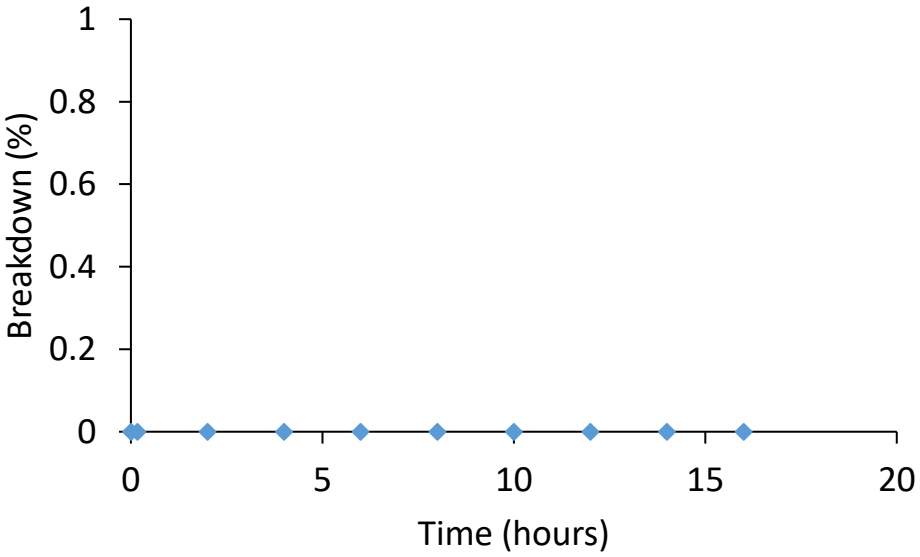

Figure S44: Percentage breakdown of **8** upon the addition of 1 equivalent of NaOH (10 mM) in MeOD-d_4:D_2O (70:30) at 291 K.

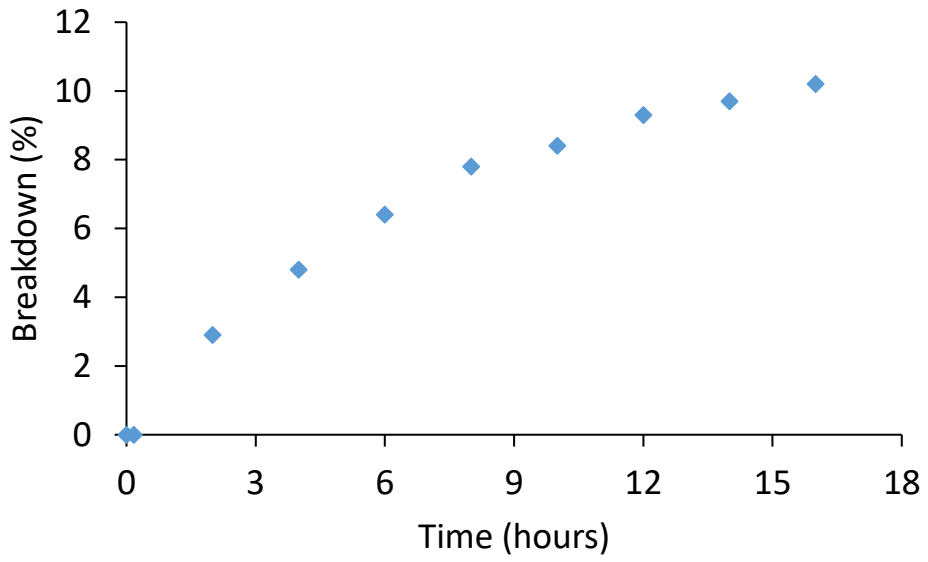

Figure S45: Percentage breakdown of **12** upon the addition of 1 equivalence of NaOH (0.2 mg, 10 mM) in MeOD-d_4:D_2O (70:30) at 291 K.

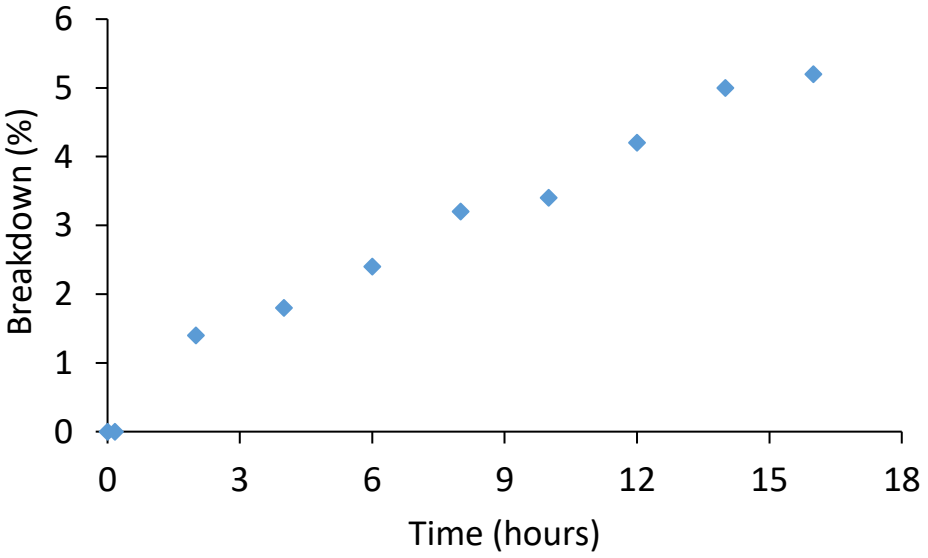

Figure S46: Percentage breakdown of **15** upon the addition of 1 equivalent of NaOH (10 mM) in MeOD-d_4:D_2O (70:30) at 291 K.

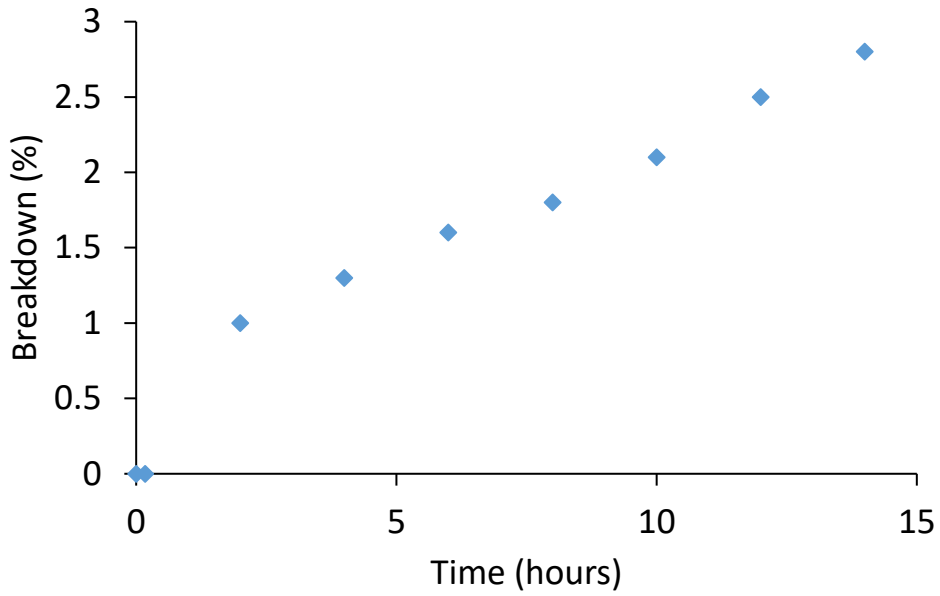

Figure S47: Percentage breakdown of **16** upon the addition of 1 equivalent of NaOH (10 mM) in MeOD-d_4:D_2O (70:30) at 291 K.

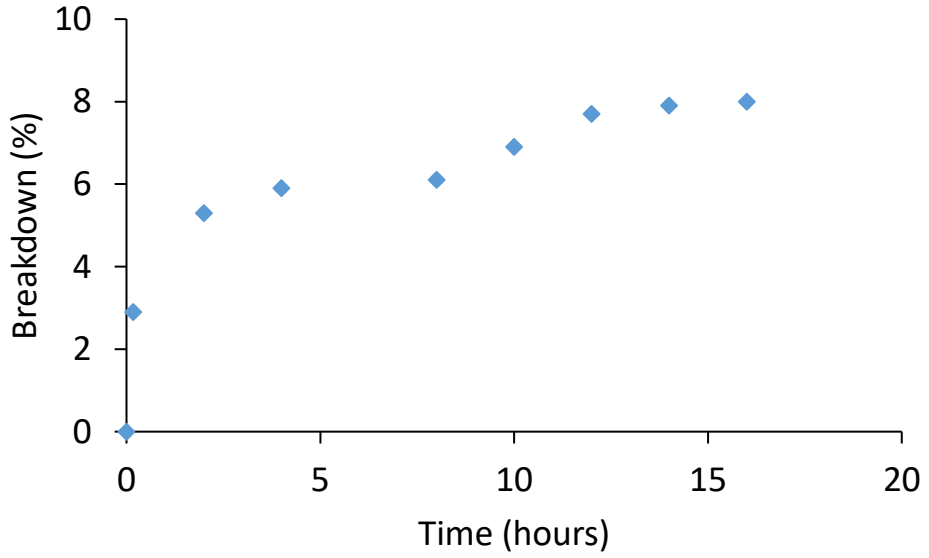

Figure S48: Percentage breakdown of **17** upon the addition of 1 equivalent of NaOH (10 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Time point at 6 hours have been removed due to shimming error.

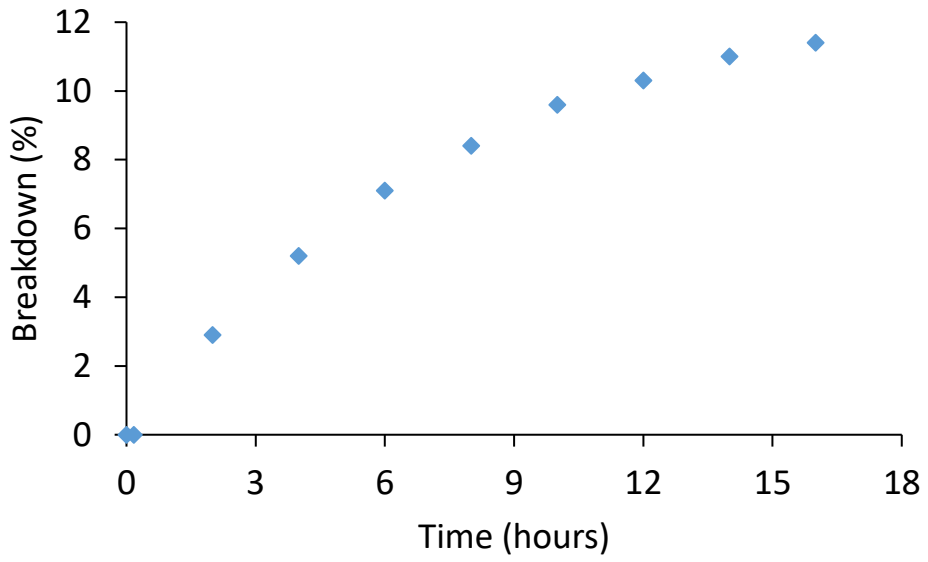

Figure S49: Percentage breakdown of **18** upon the addition of 1 equivalent of NaOH (10 mM) in MeOD-d_4:D_2O (70:30) at 291 K.

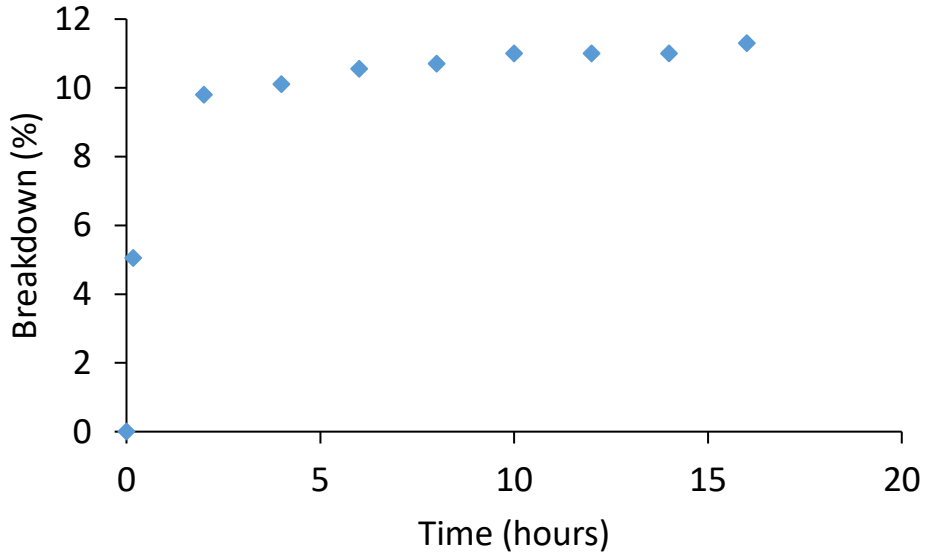

Figure S50: Percentage breakdown of **19** upon the addition of 1 equivalent of NaOH (10 mM) in MeOD-d_4:D_2O (70:30) at 291 K.

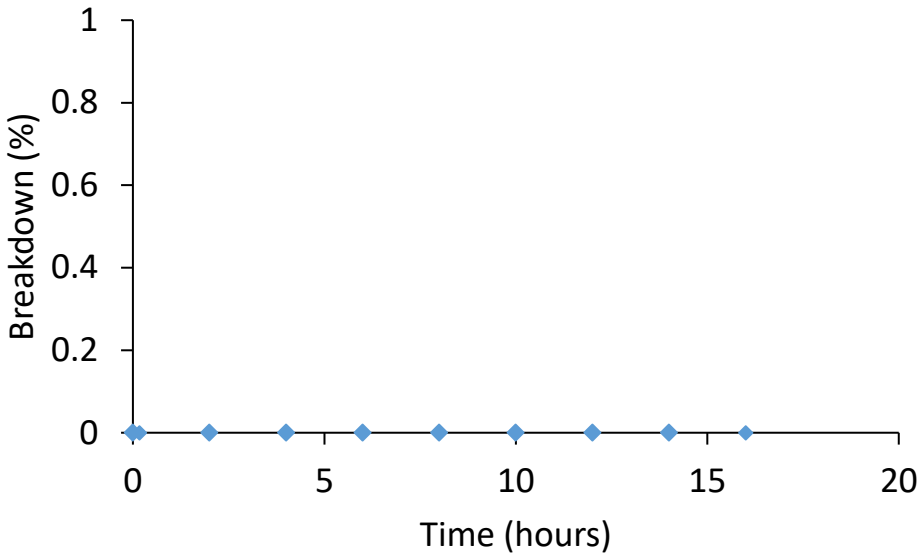

Figure S51: Percentage breakdown of **20** upon the addition of 1 equivalent of NaOH (10 mM) in MeOD-d_4:D_2O (70:30) at 291 K.

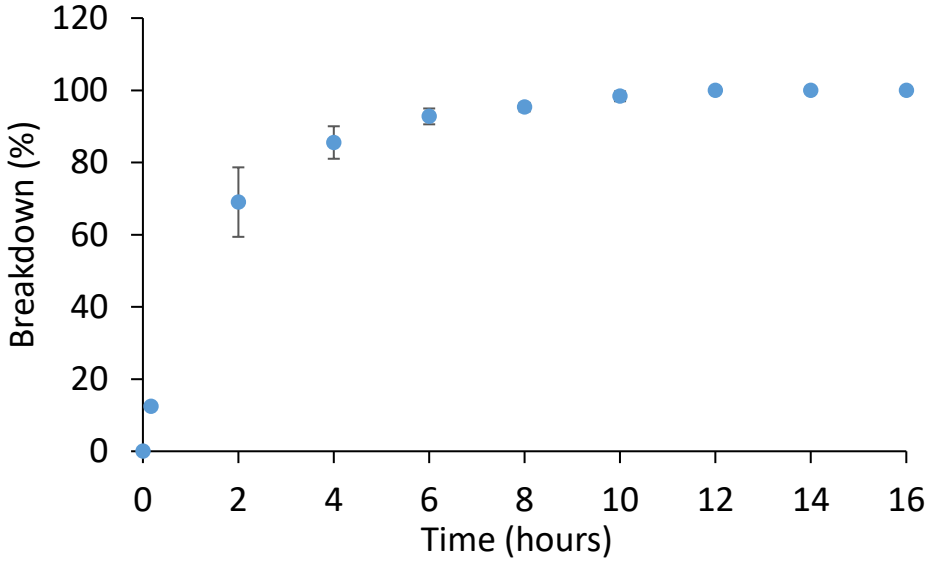

Figure S52: Percentage breakdown of **1** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

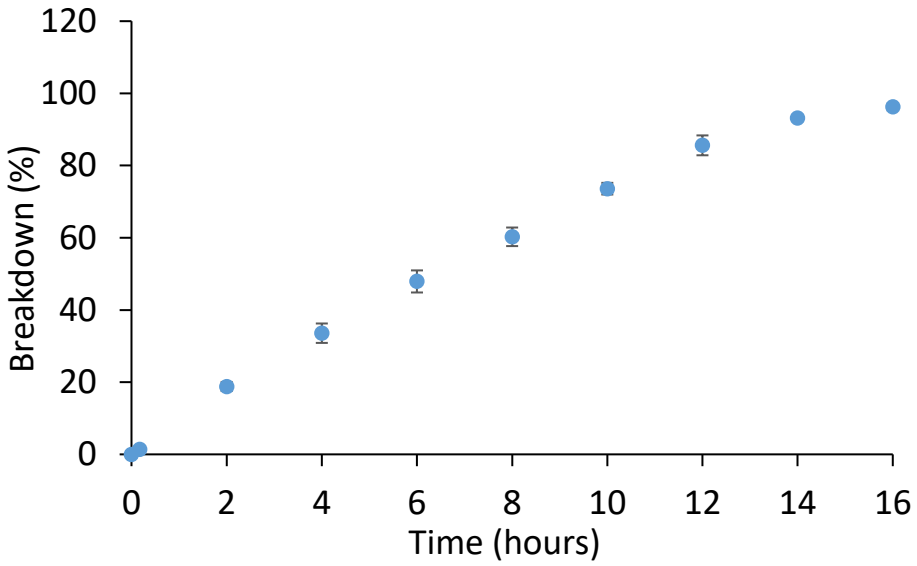

Figure S53: Percentage breakdown of **2** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

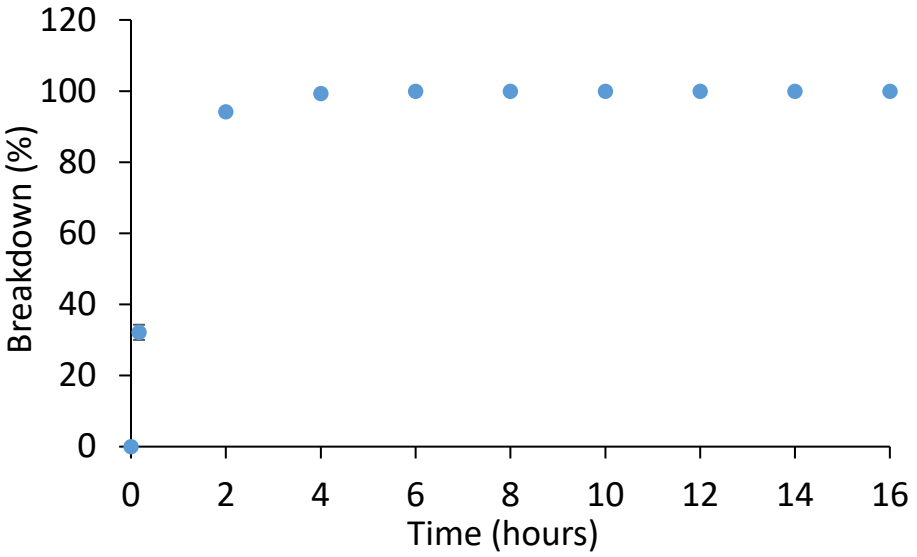

Figure S54: Percentage breakdown of **3** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

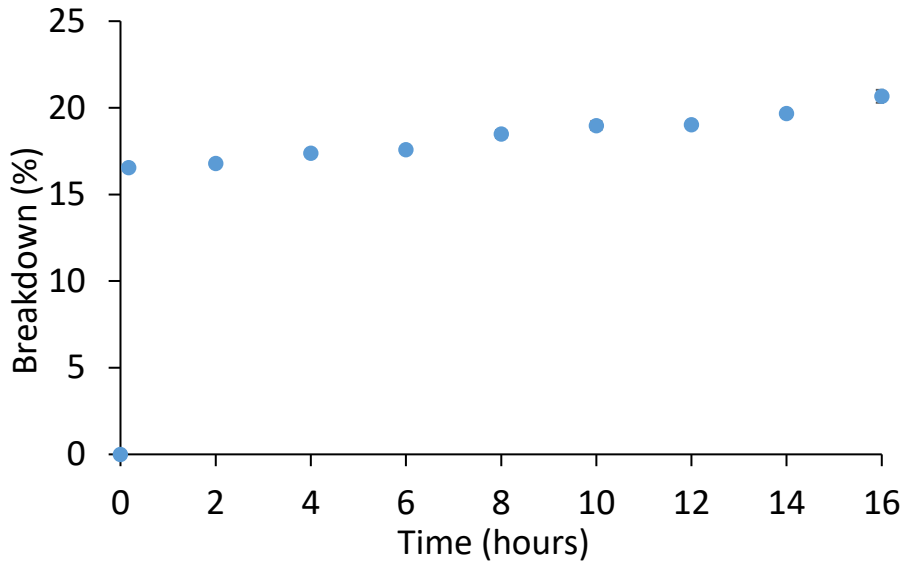

Figure S55: Percentage breakdown of **4** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

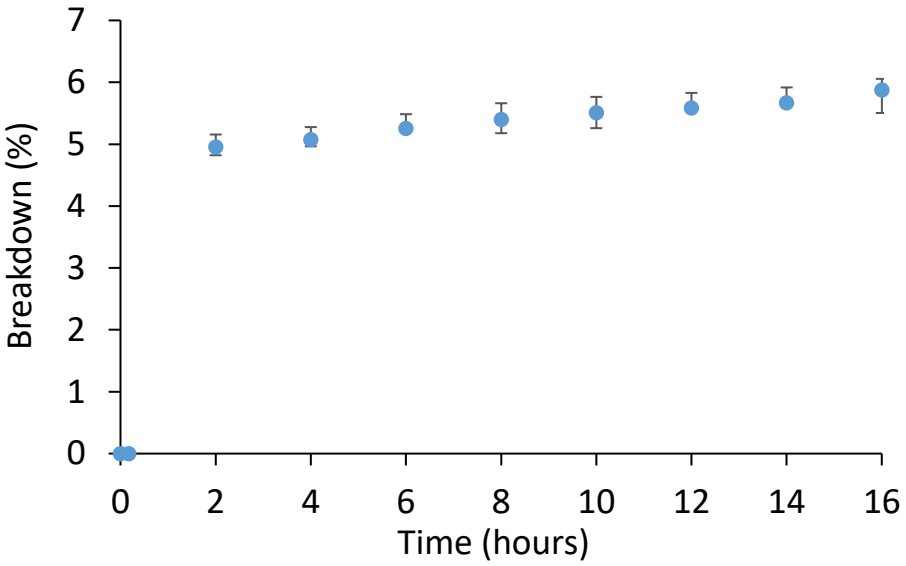

Figure S56: Percentage breakdown of **5** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

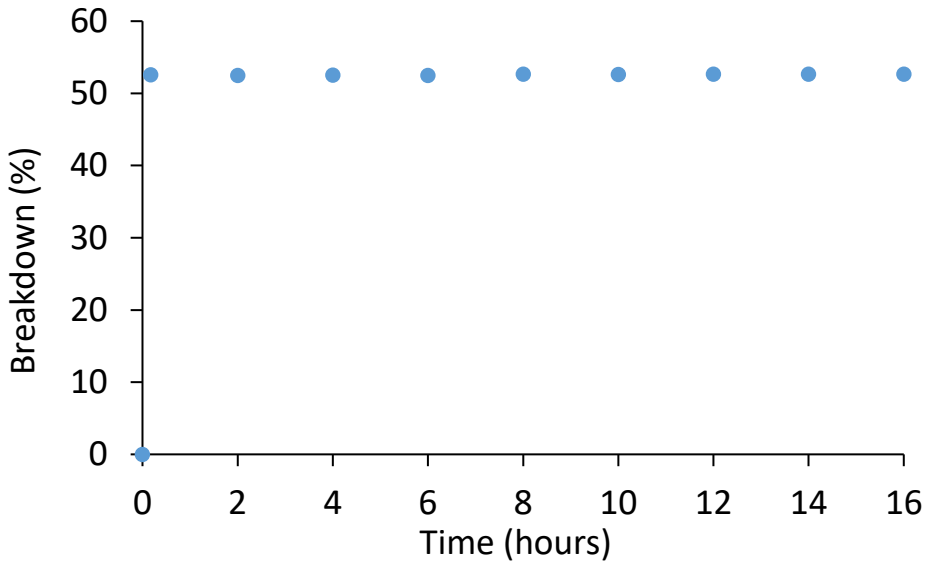

Figure S57: Percentage breakdown of **6** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

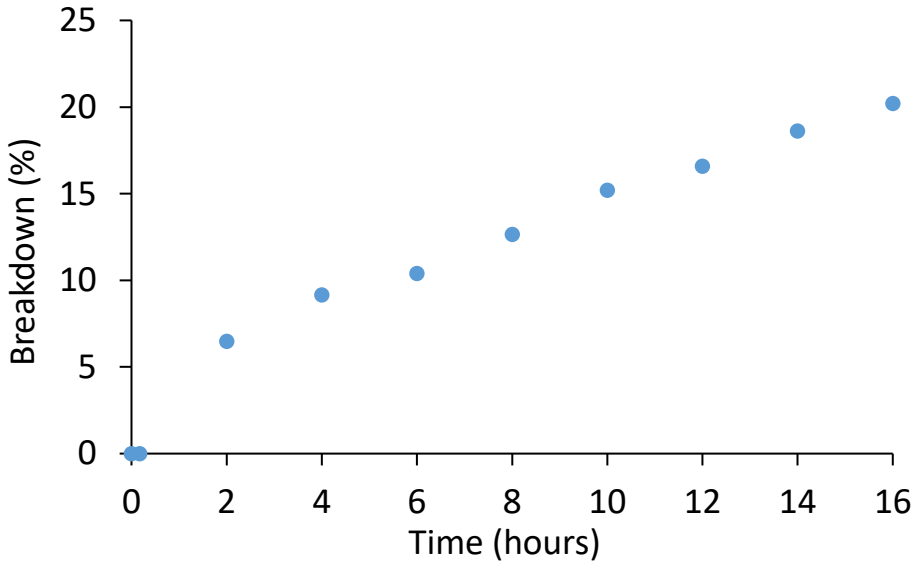

Figure S58: Percentage breakdown of **7** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

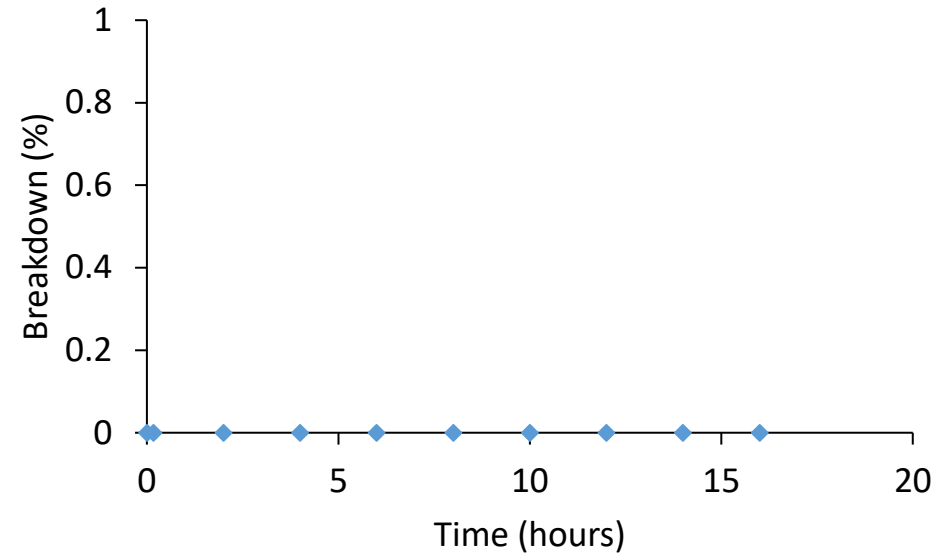

Figure S59: Percentage breakdown of **8** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

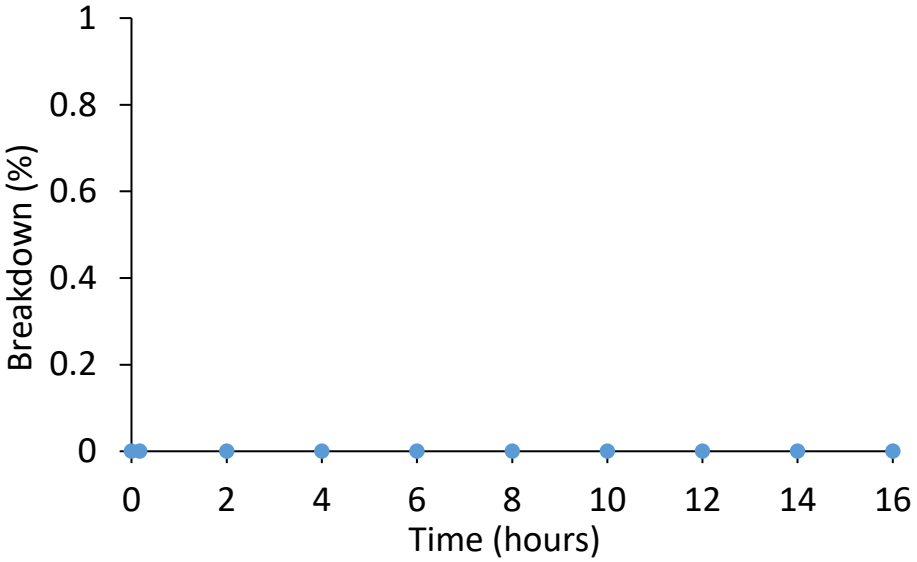

Figure S60: Percentage breakdown of **9** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

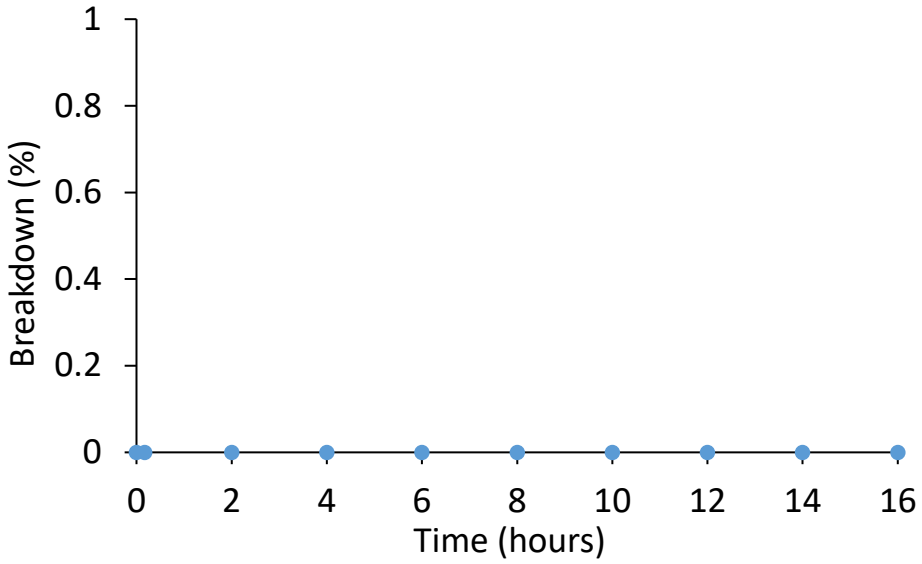

Figure S61: Percentage breakdown of **10** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

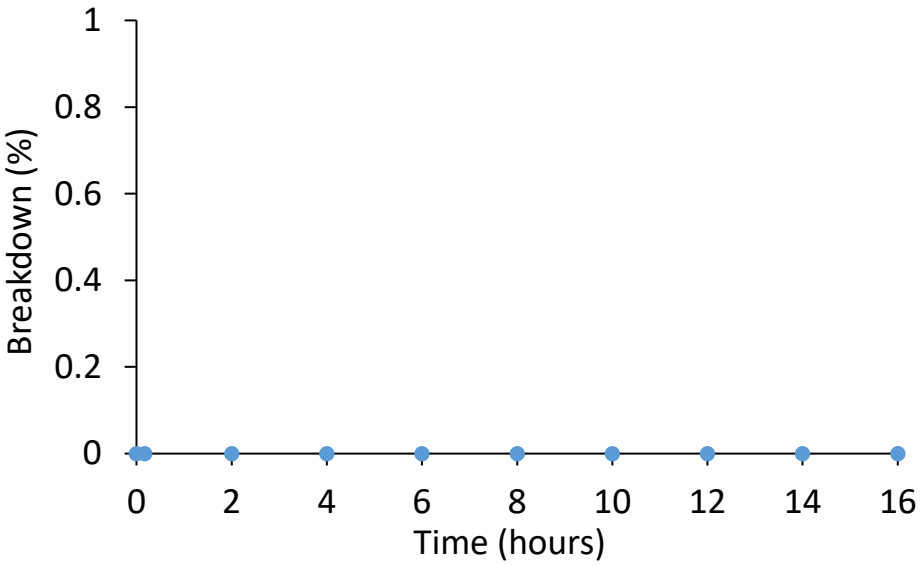

Figure S62: Percentage breakdown of **11** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

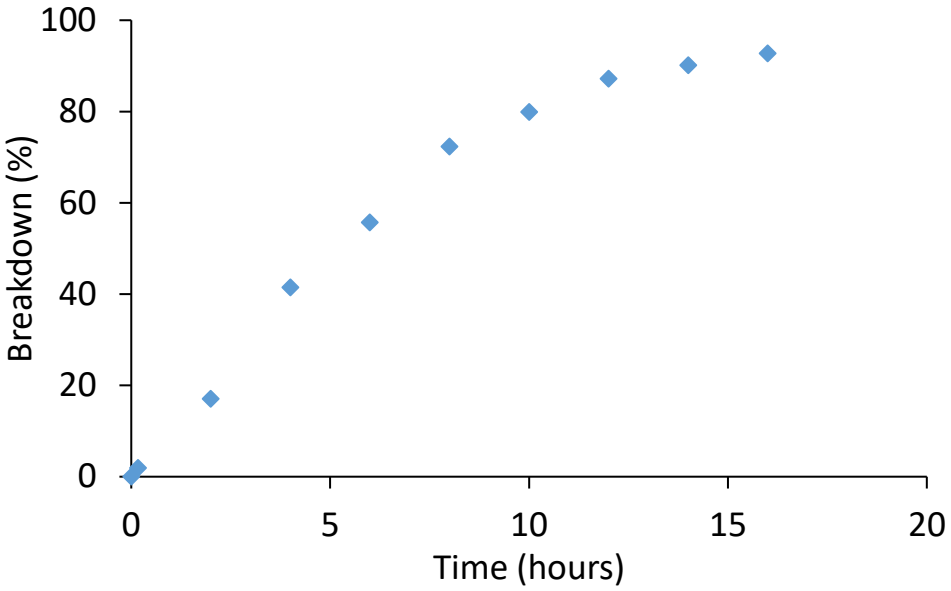

Figure S63: Percentage breakdown of **12** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

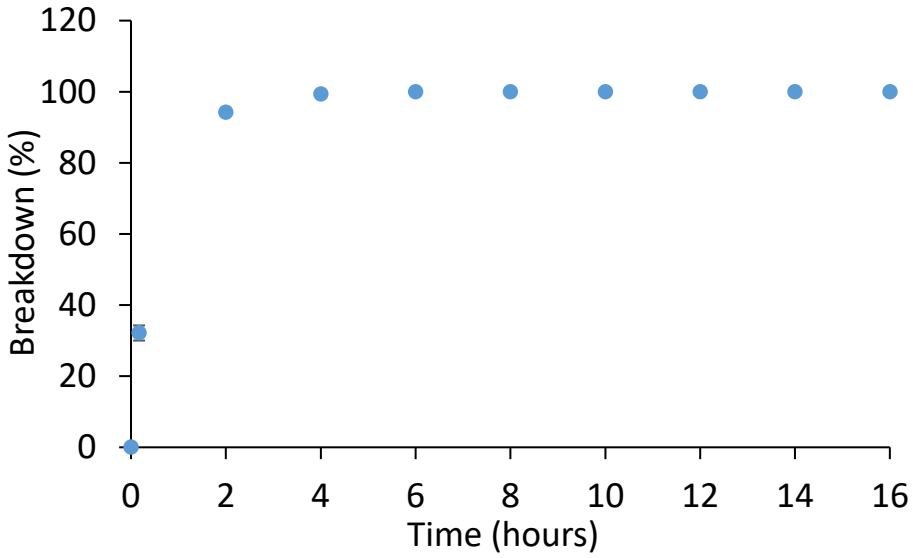

Figure S64: Percentage breakdown of **13** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

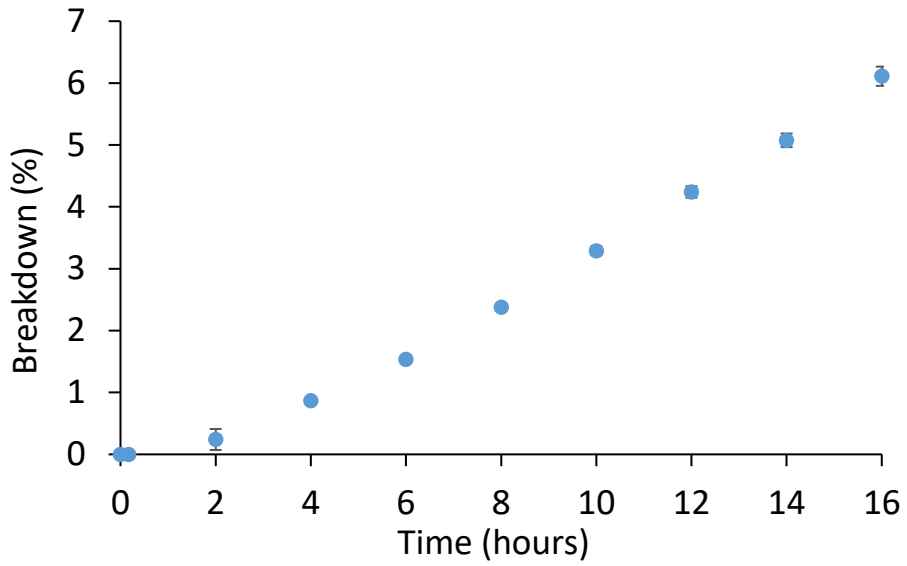

Figure S65: Percentage breakdown of **14** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

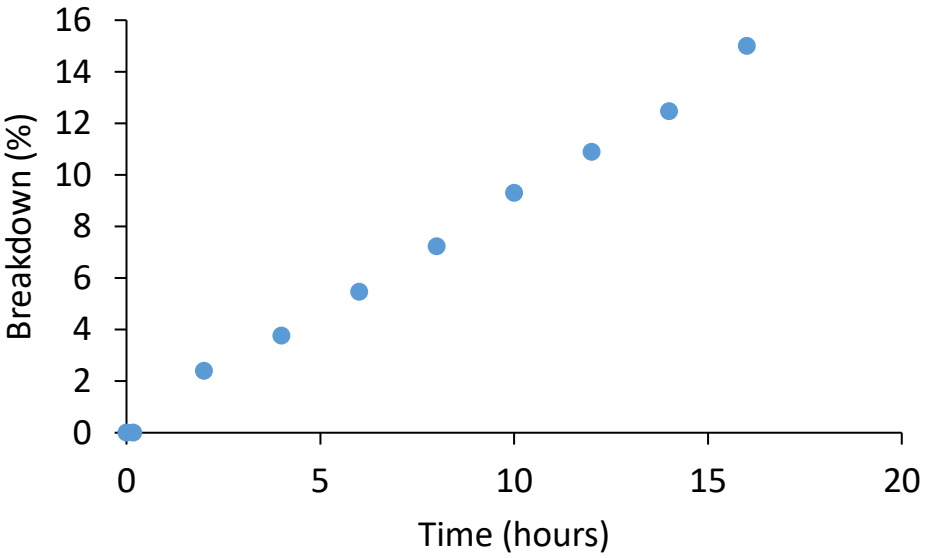

Figure S66: Percentage breakdown of **15** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

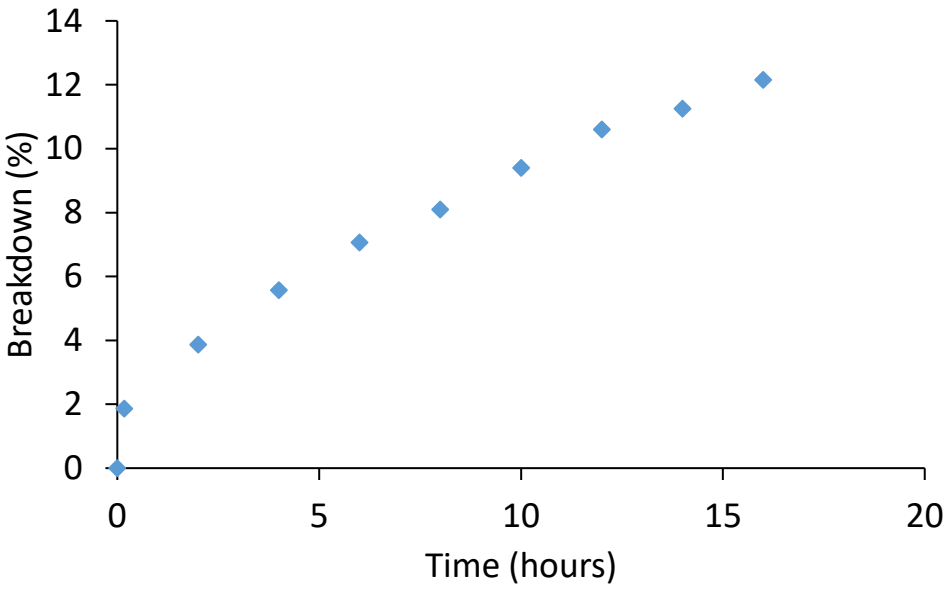

Figure S67: Percentage breakdown of **16** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

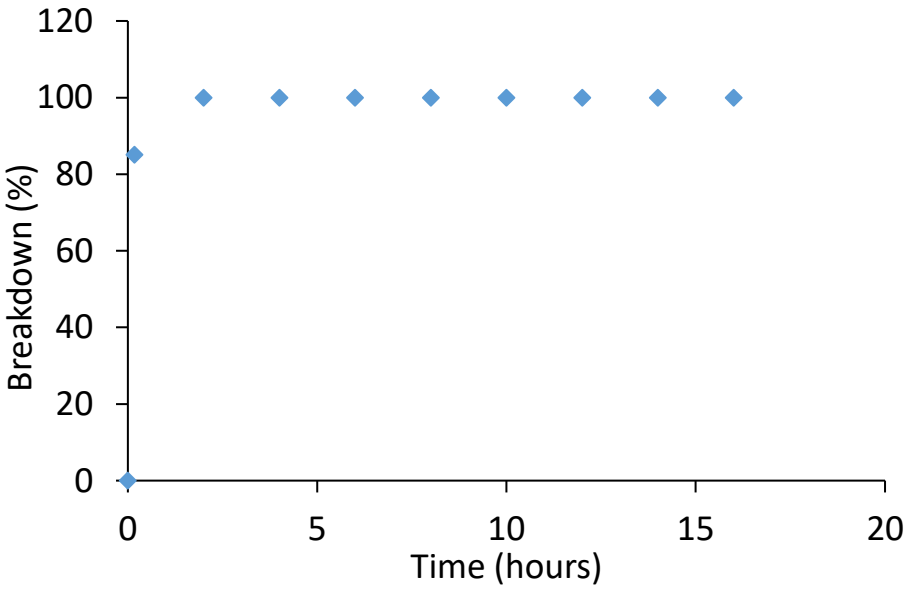

Figure S68: Percentage breakdown of **17** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

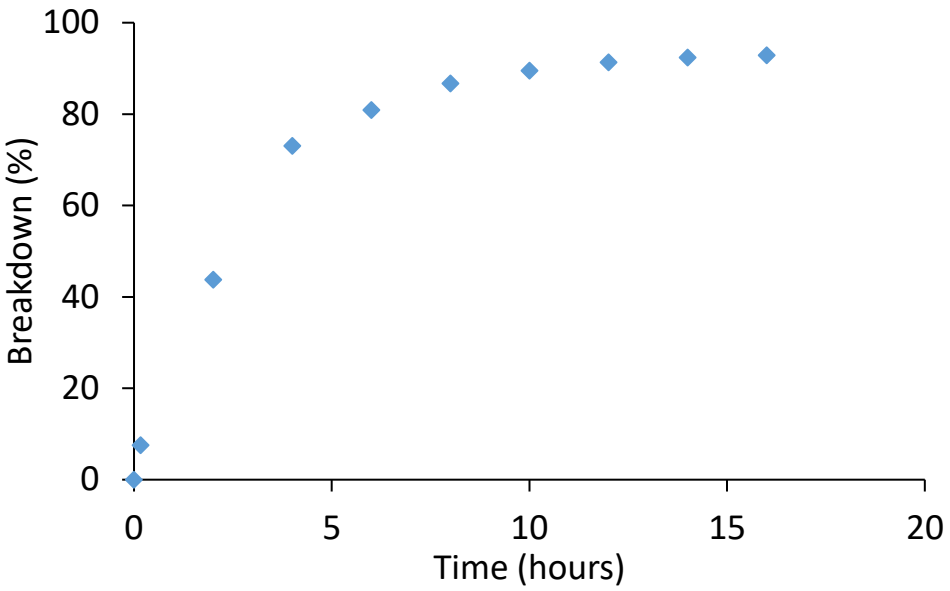

Figure S69: Percentage breakdown of **18** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

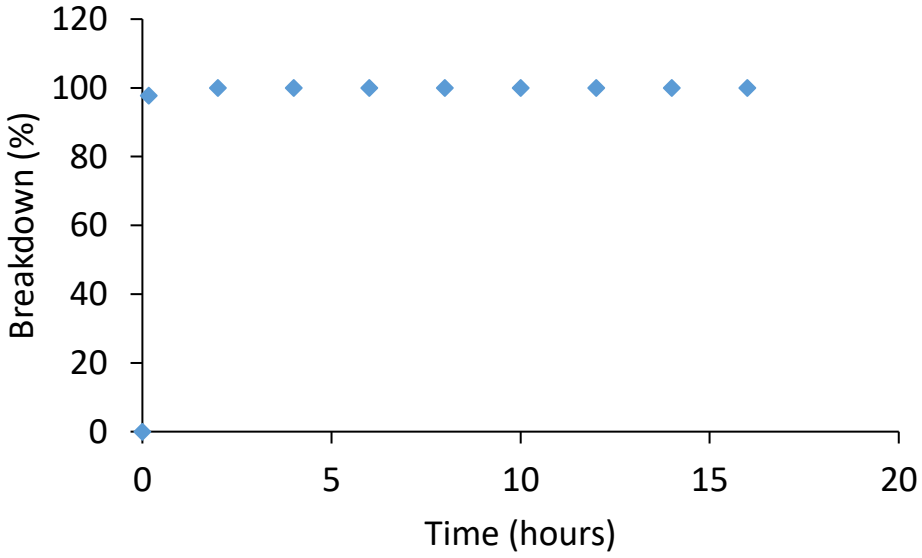

Figure S70: Percentage breakdown of **19** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

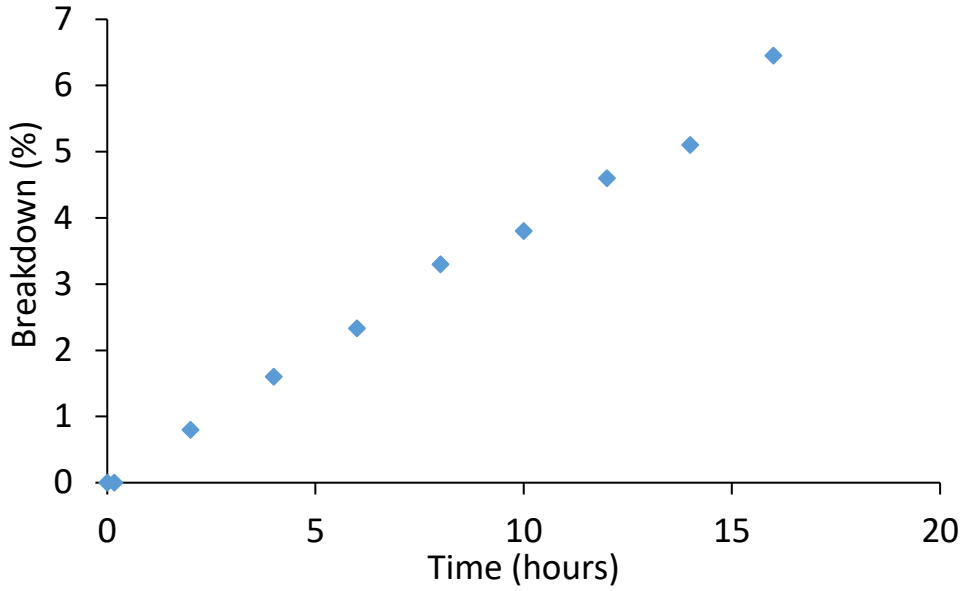

Figure S71: Percentage breakdown of **20** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

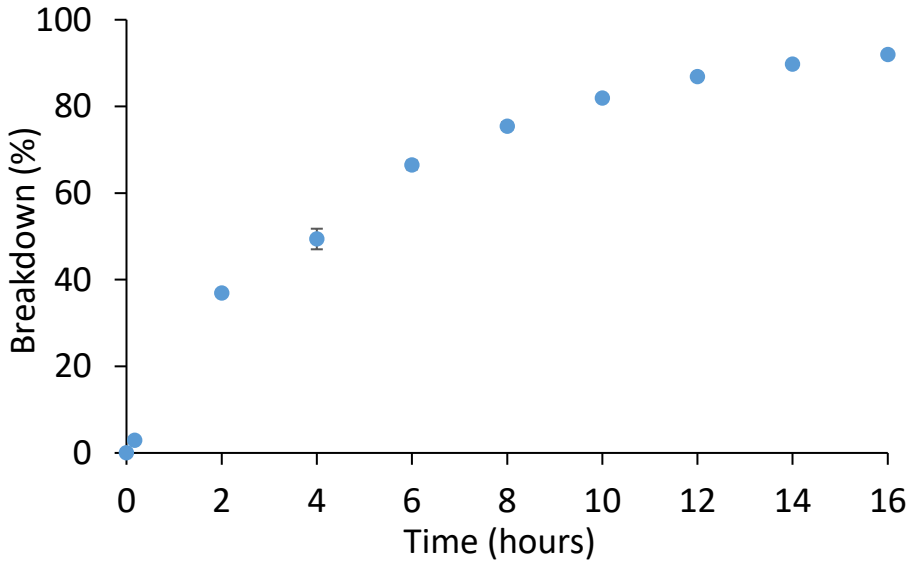

Figure S72: Percentage breakdown of **21** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

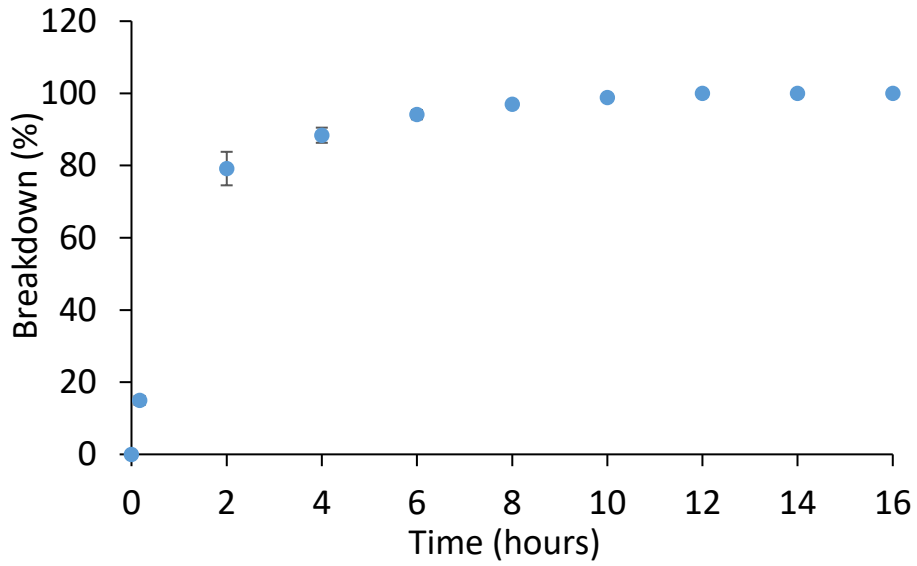

Figure S73: Percentage breakdown of **22** upon the addition of 5 equivalents of NaOH (50 mM) in MeOD-d_4:D_2O (70:30) at 291 K. Data shown is an average of three repeats.

Table S1: Average results of reactivity studies (n = 3) with 5 equivalents of NaOH (50 mM), indicating percentage breakdown after 6 hours.

OP CWA simulant	Simulant breakdown after 6 hours (%)	Rate order	Experimental rate constant (s^{-1})
1	92.8 (± 2.19)	1^{st}	0.42
2	47.9 (± 3.06)	1^{st}	0.22
3	100 (± ≤ 0.01)	1^{st}	0.46
4	17.6 (± 0.01)	1^{st}	0.08
5	5.3 (± 0.23)	*a*	n/a
6	52.5 (± 0.01)	*a*	n/a
7	10.4 (± 0.01)	1^{st}	0.05
8	0 (± ≤ 0.01)	-	-
9	0 (± ≤ 0.01)	-	-
10	0 (± ≤ 0.01)	-	-
11	0 (± ≤ 0.01)	-	-
12	55.7 (± 2.24)	1^{st}	0.26
13	57.4 (± 0.06)	1^{st}	0.27
14	1.5 (± 0.05)	1^{st}	0.01
15	5.0 (± 0.36)	1^{st}	0.02
16	8.2 (± 0.52)	1^{st}	0.04
17	100 (± ≤ 0.01)	*b*	n/a
18	80.9 (± 0.16)	2^{nd}	0.37[c]
19	100 (± ≤ 0.01)	*b*	n/a
20	2.1 (± 0.16)	*a*	n/a
21	66.5 (± 1.00)	1^{st}	0.31
22	94.1 (± 1.28)	1^{st}	0.44

a – Rate order could not be definitively assigned when fitting reaction data to either 1^{st} order or 2^{nd} order curves, b – Rate of reaction could not be obtained due to speed of reaction being too fast to track using the NMR method and c – Reaction rate units = $M^{-1}s^{-1}$.

Viscosity study results

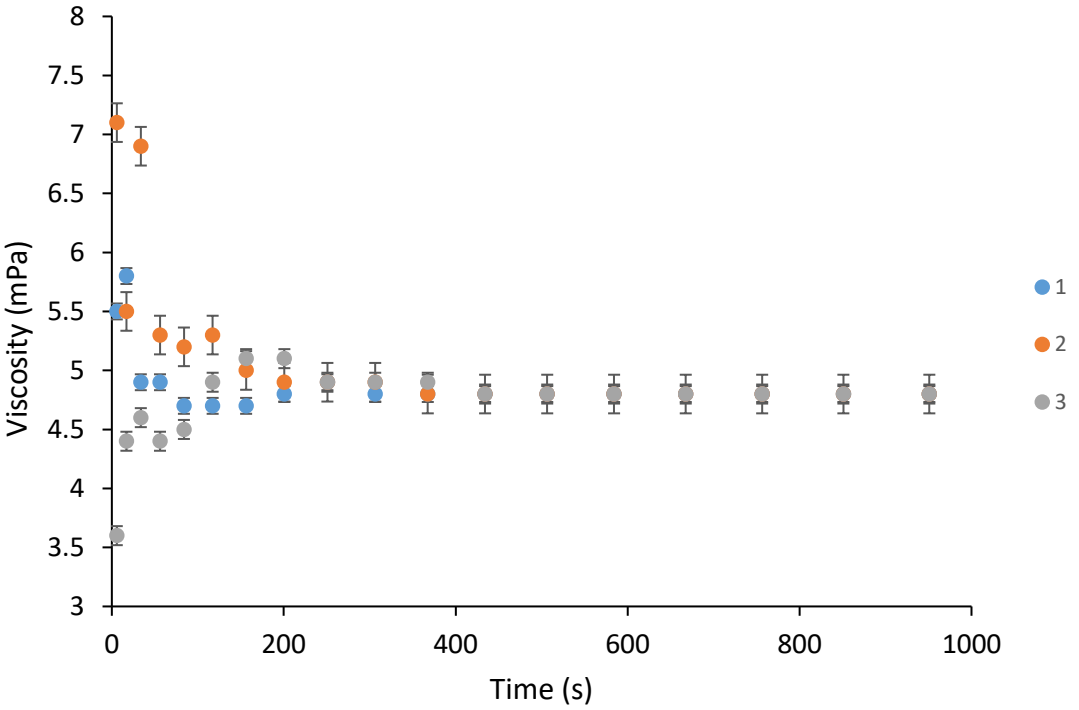

Figure S74: Viscosity run 1 for **1** at 298 K. Viscosity = 4.80 mPa ± < 0.01.

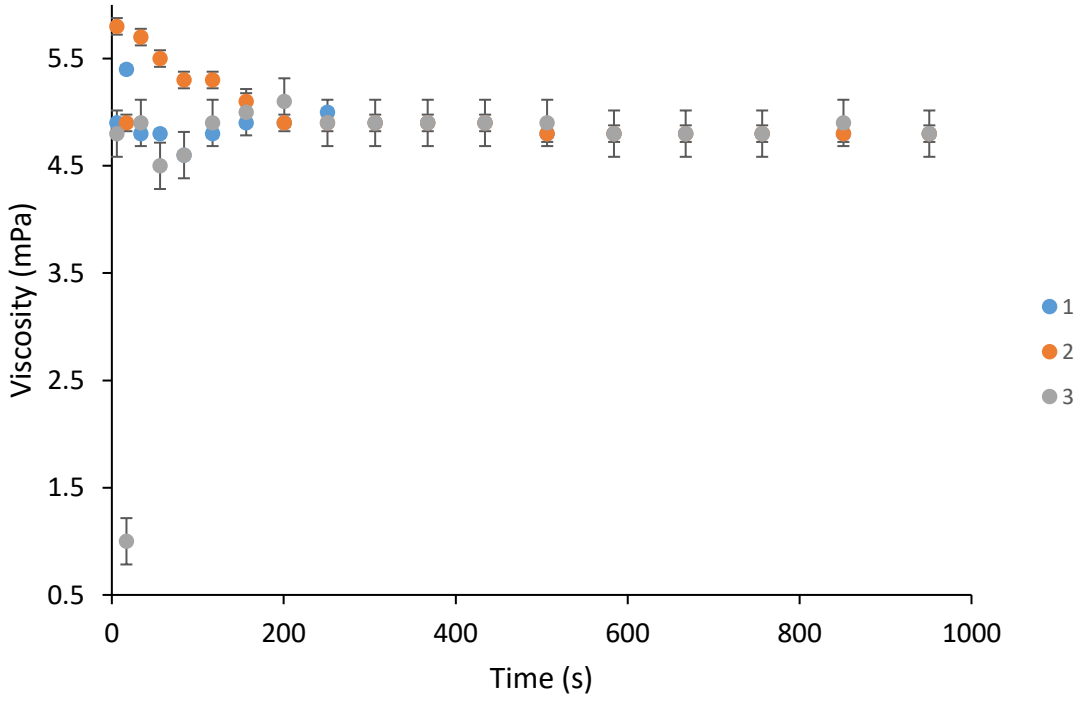

Figure S75: Viscosity run 2 for **1** at 298 K. Viscosity = 4.80 mPa ± < 0.01.

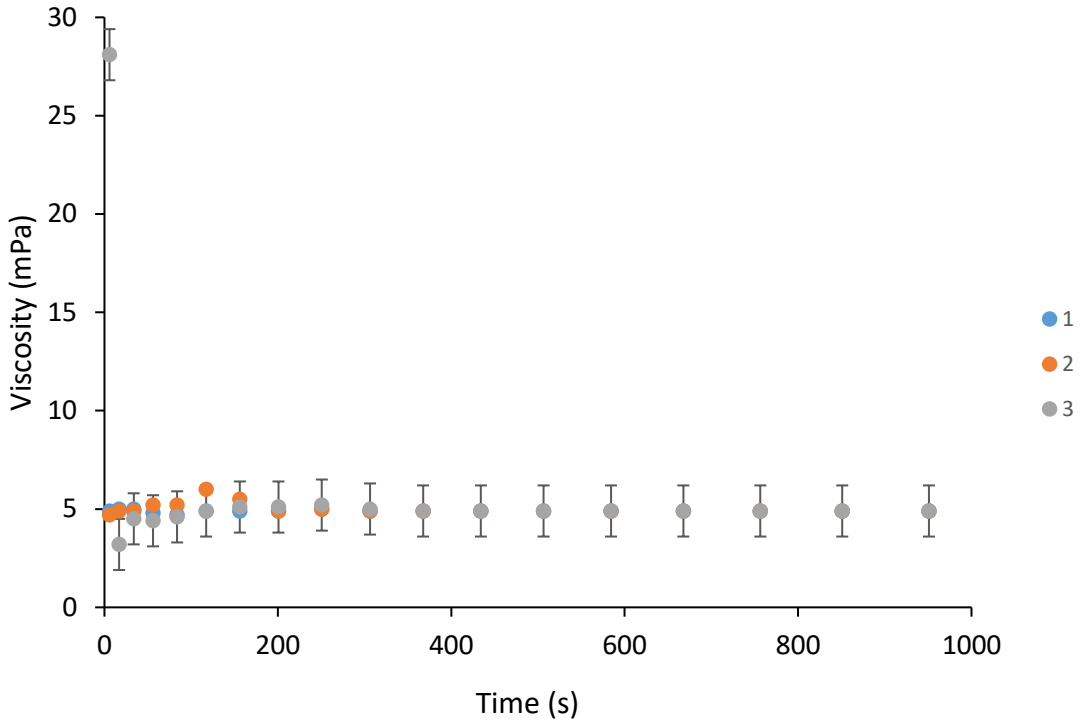

Figure S76: Viscosity run 3 for **1** at 298 K. Viscosity = 4.90 mPa ± < 0.01.

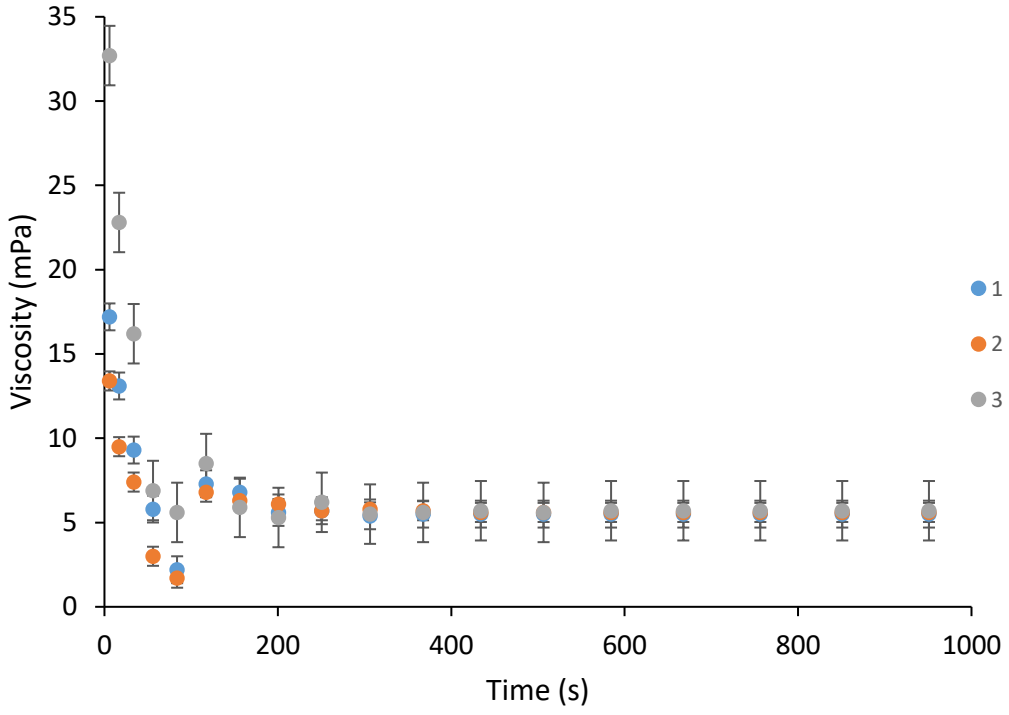

Figure S77: Viscosity run 1 for **2** at 298 K. Viscosity = 5.60 mPa ± 0.06.

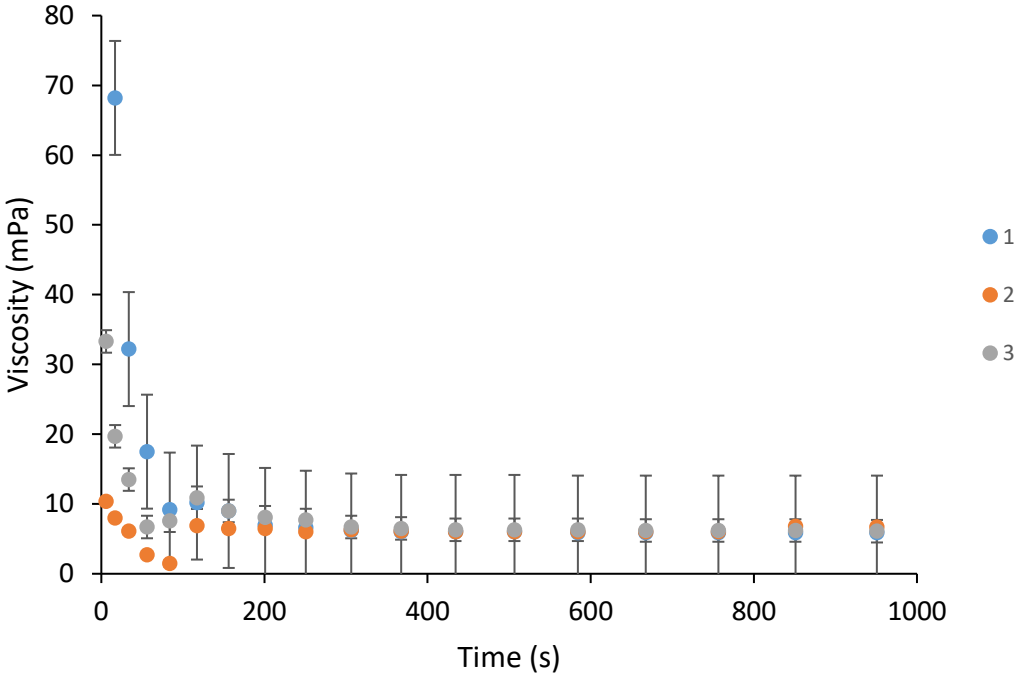

Figure S78: Viscosity run 2 for **2** at 298 K. Viscosity = 6.00 mPa ± 0.06.

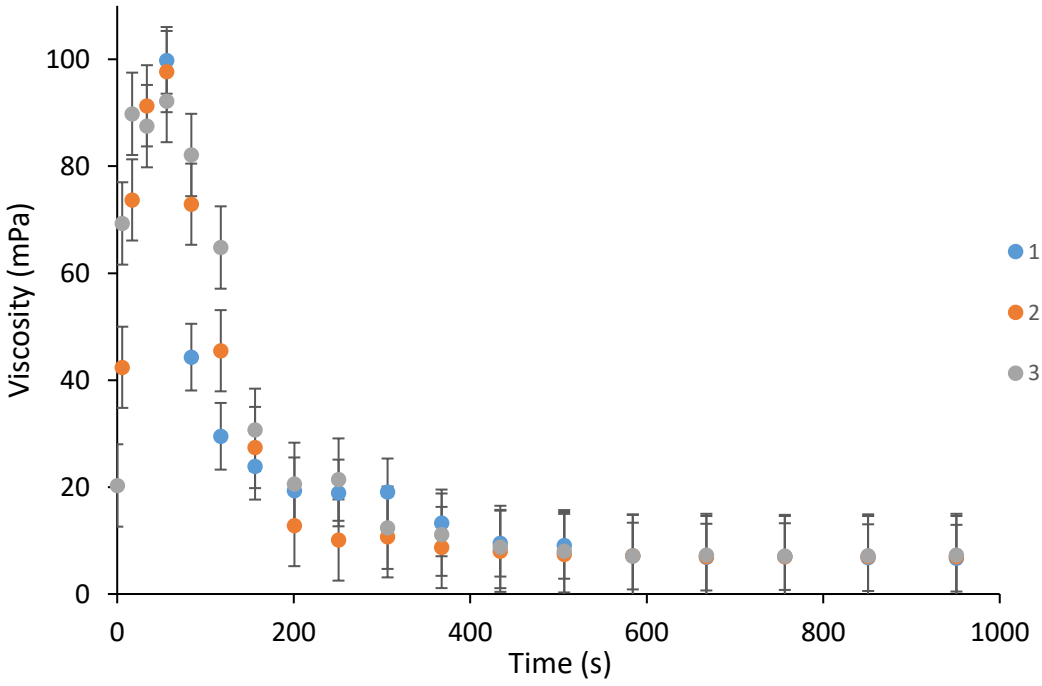

Figure S79: Viscosity run 3 for **2** at 298 K. Viscosity = 7.00 mPa ± 0.17.

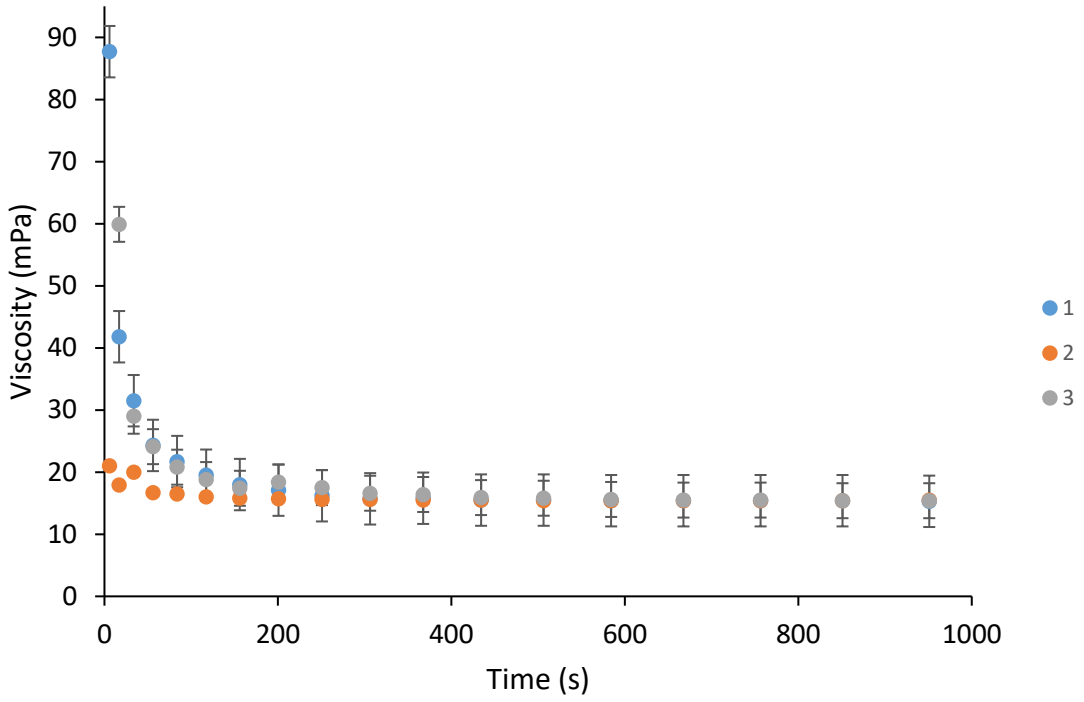

Figure S80: Viscosity run 1 for **3** at 298 K. Viscosity = 15.40 mPa ± < 0.01.

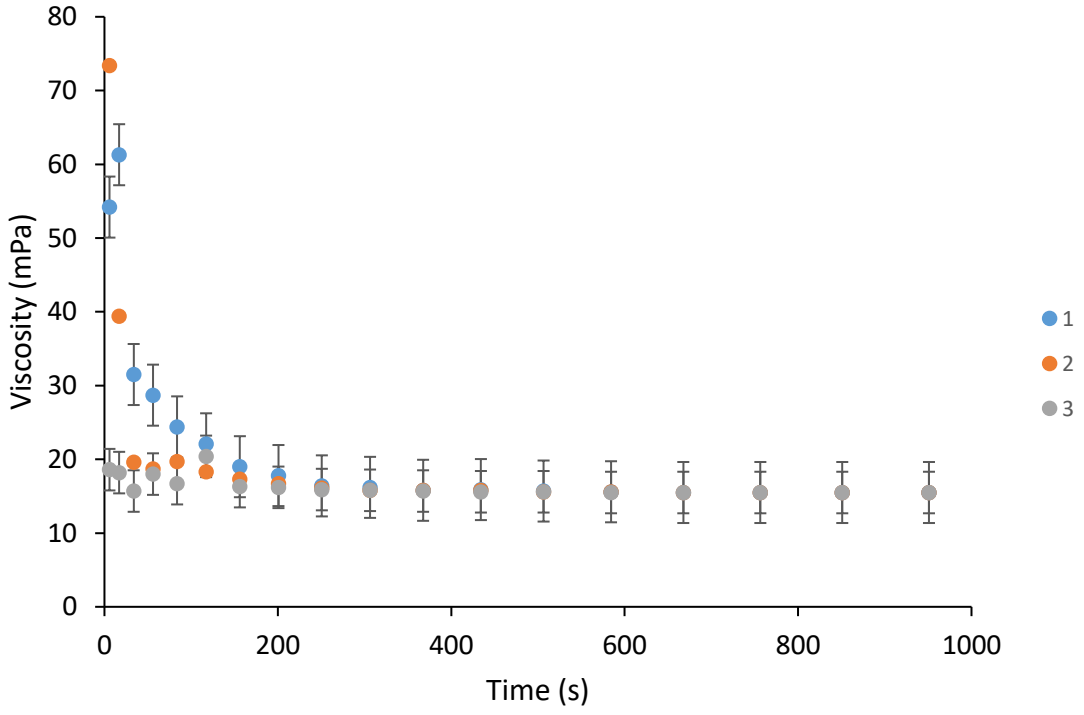

Figure S81: Viscosity run 2 for **3** at 298 K. Viscosity = 15.50 mPa ± < 0.01.

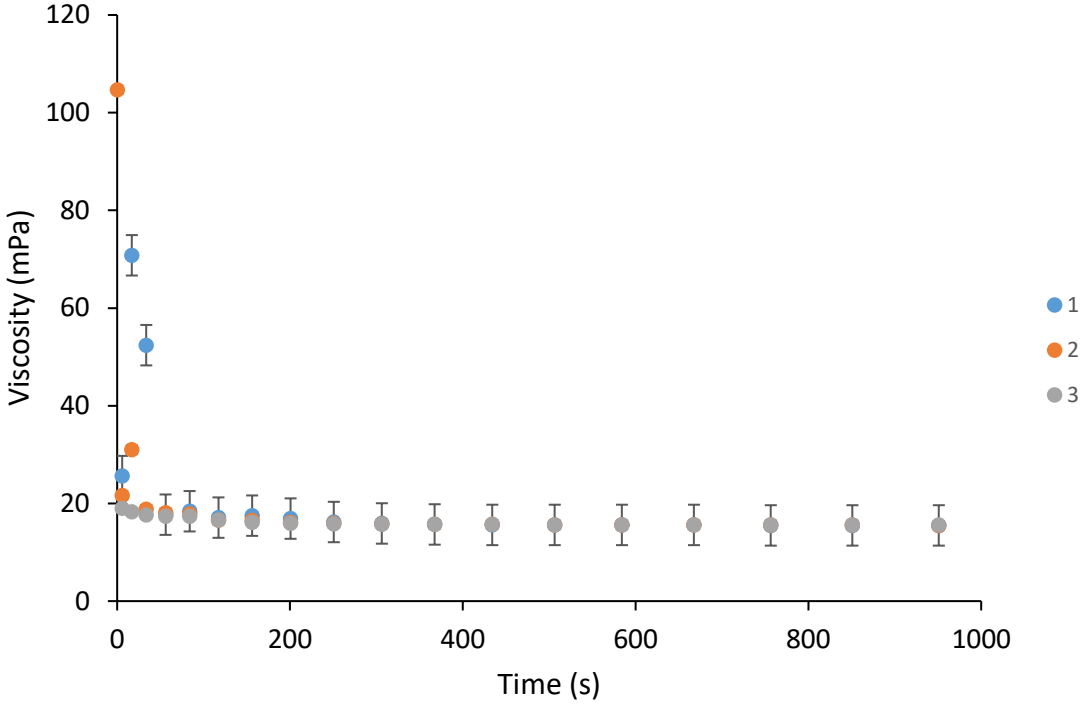

Figure S82: Viscosity run 3 for **3** at 298 K. Viscosity = 15.50 mPa ± 0.03.

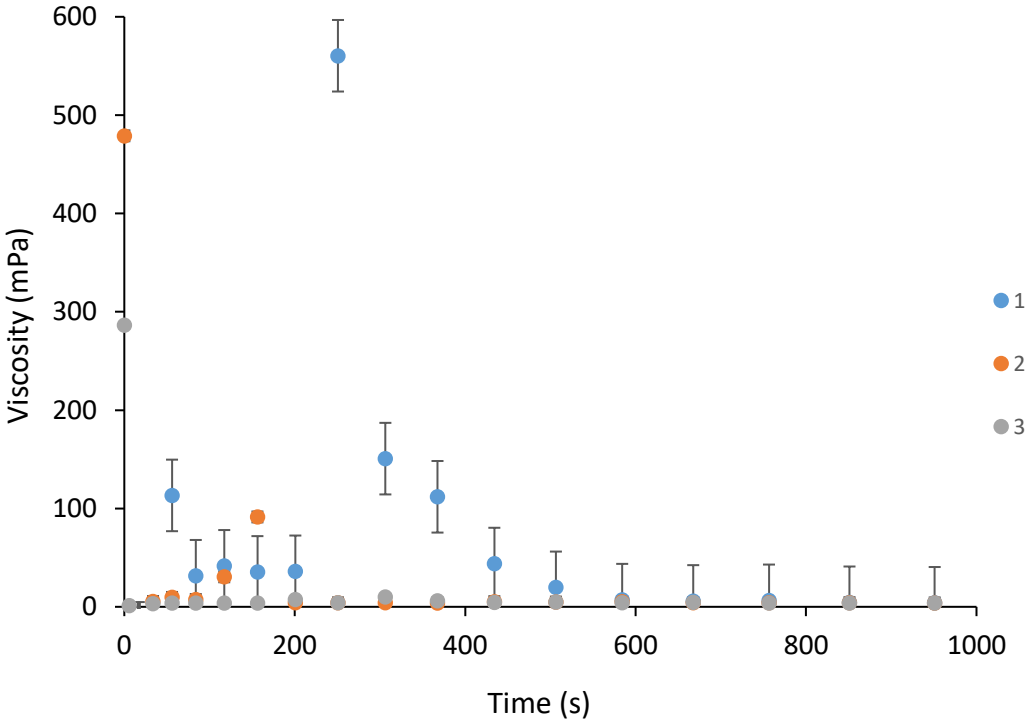

Figure S83: Viscosity run 1 for **4** at 298 K. Viscosity = 4.00 mPa ± 0.06.

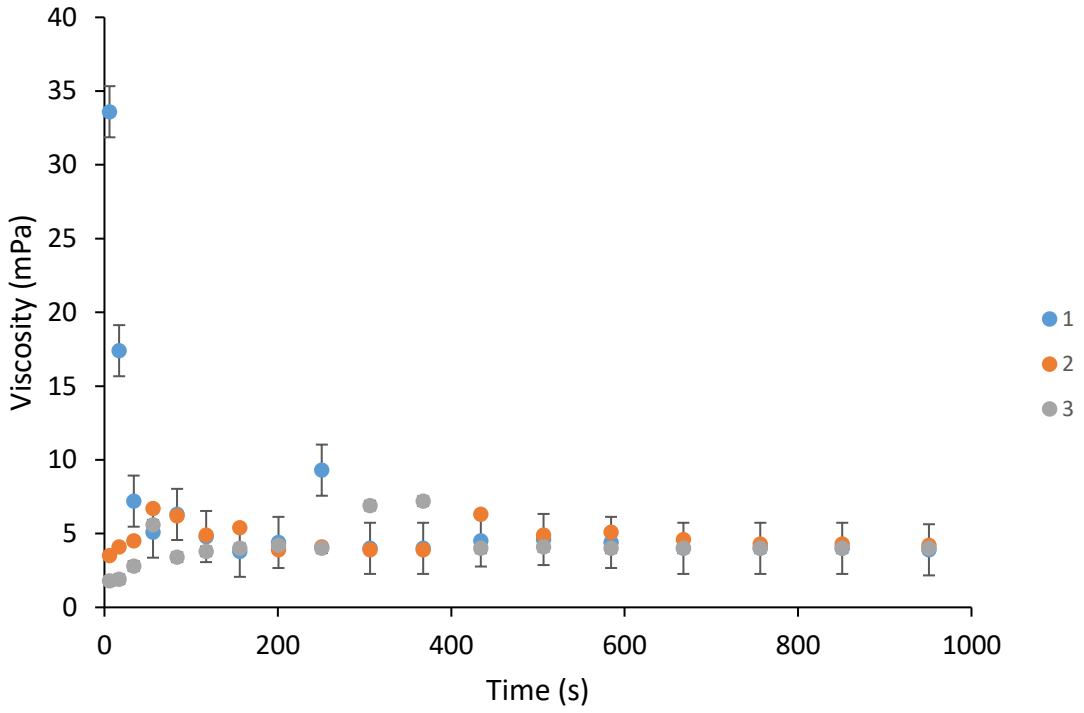

Figure S84: Viscosity run 2 for **4** at 298 K. Viscosity = 4.00 mPa ± 0.09.

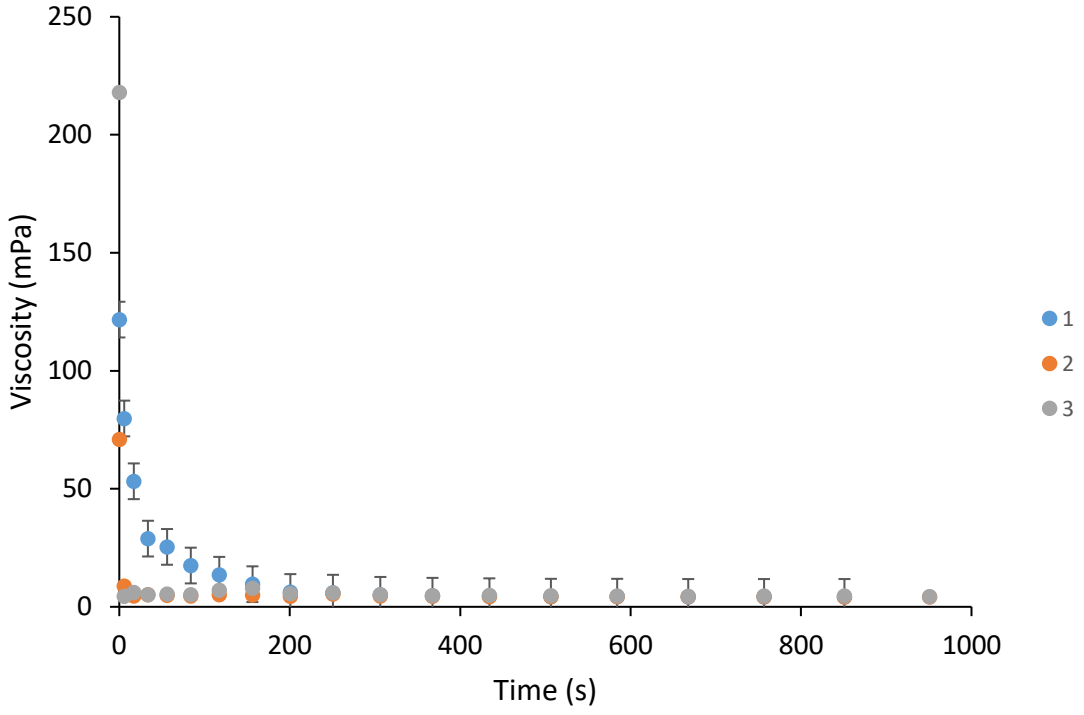

Figure S85: Viscosity run 3 for **4** at 298 K. Viscosity = 4.30 mPa ± 0.08.

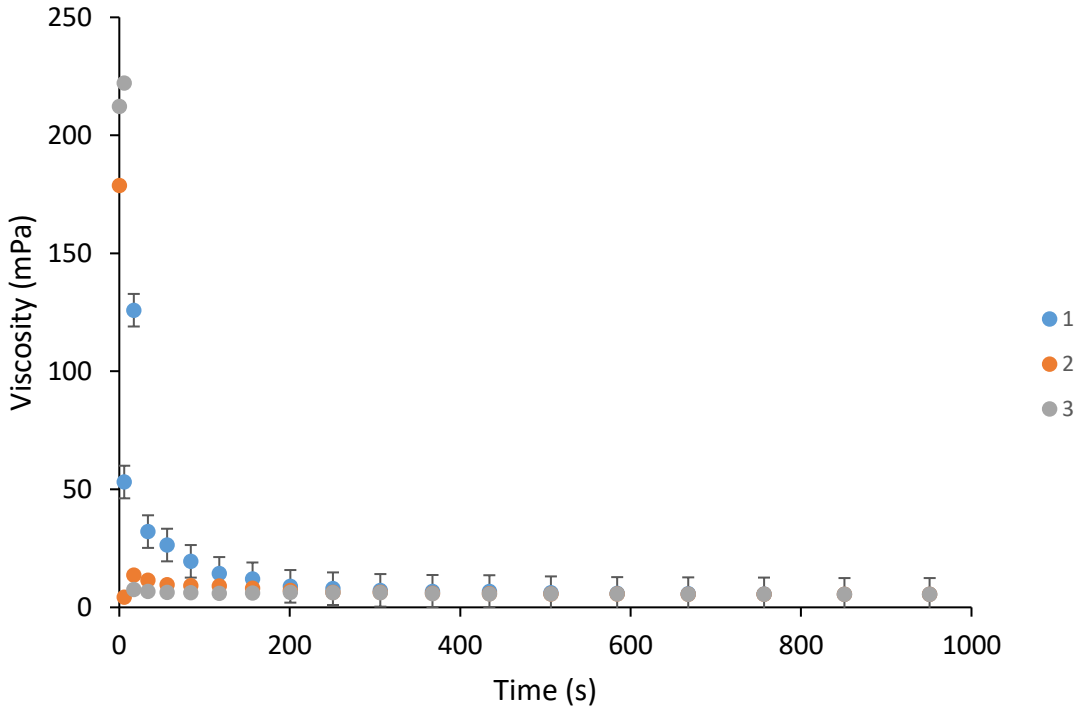

Figure S86: Viscosity run 1 for **5** at 298 K. Viscosity = 5.50 mPa ± < 0.01.

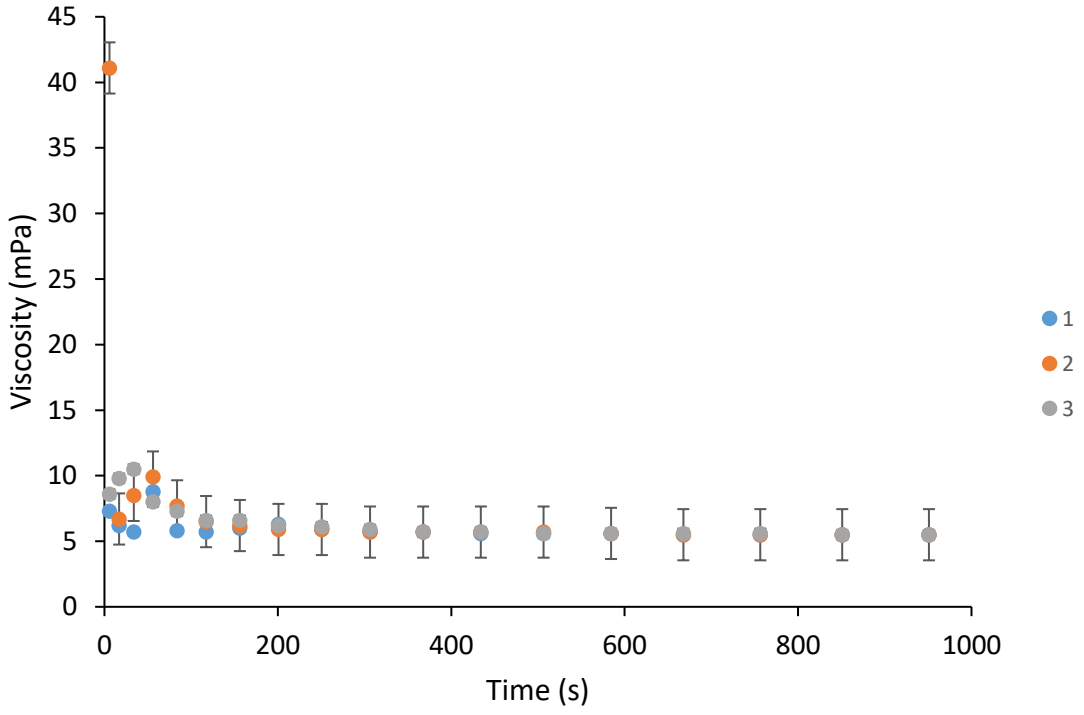

Figure S87: Viscosity run 2 for **5** at 298 K. Viscosity = 5.50 mPa ± < 0.01.

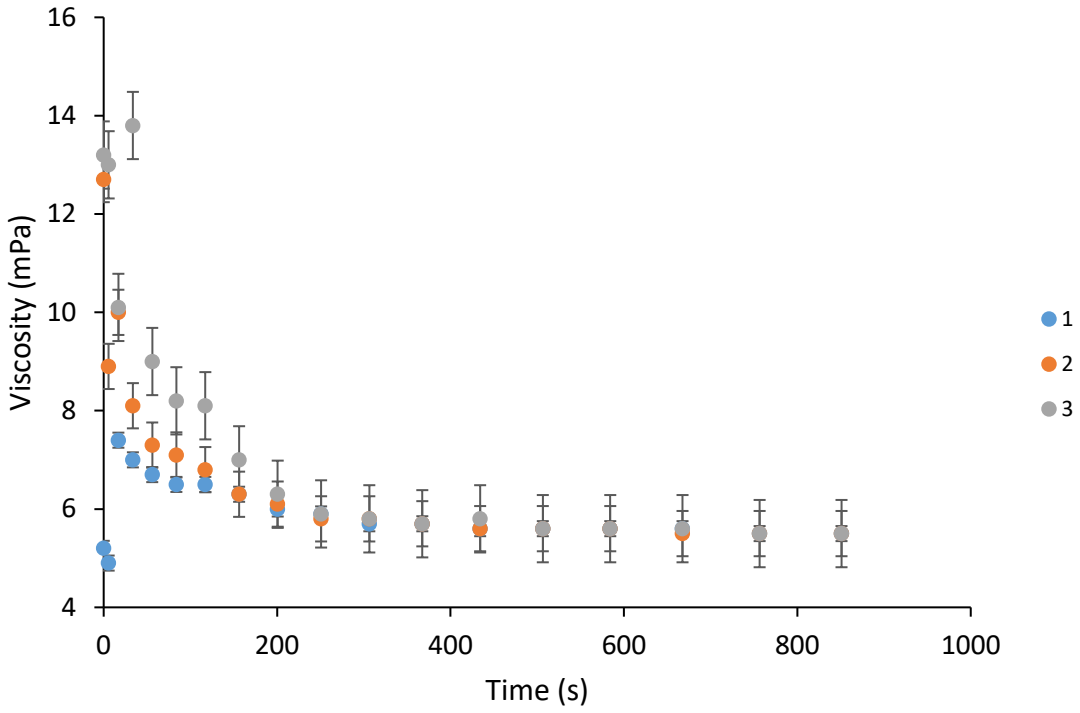

Figure S88: Viscosity run 3 for **5** at 298 K. Viscosity = 5.50 mPa ± < 0.01.

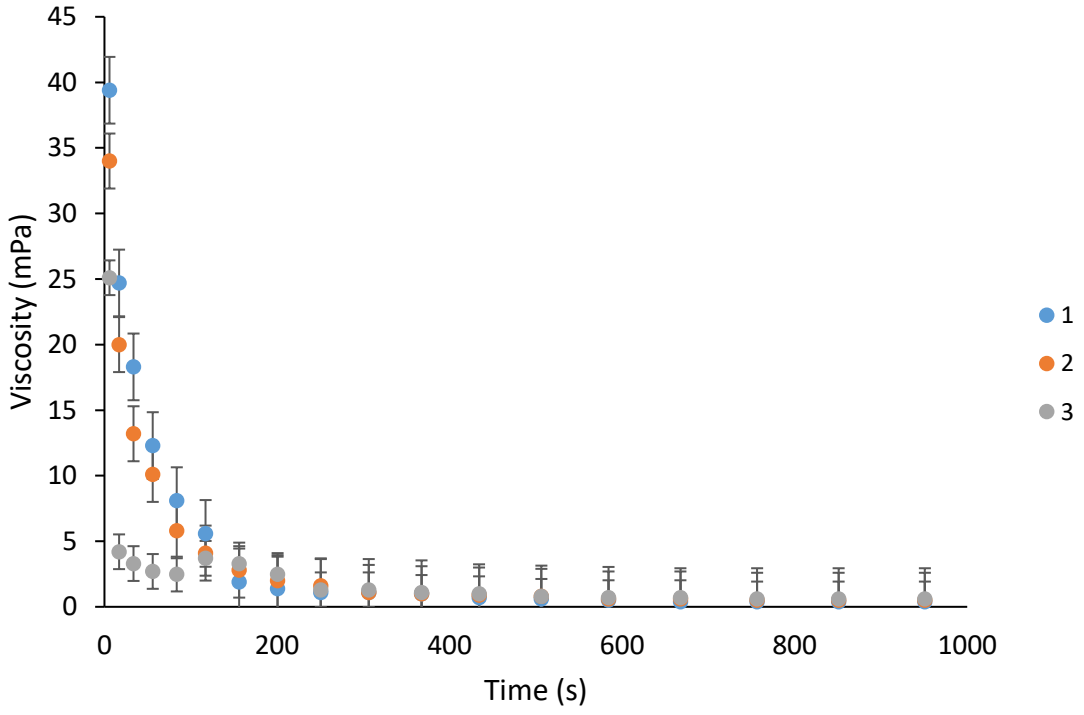

Figure S89: Viscosity run 1 for **6** at 298 K. Viscosity = 0.50 mPa ± 0.06.

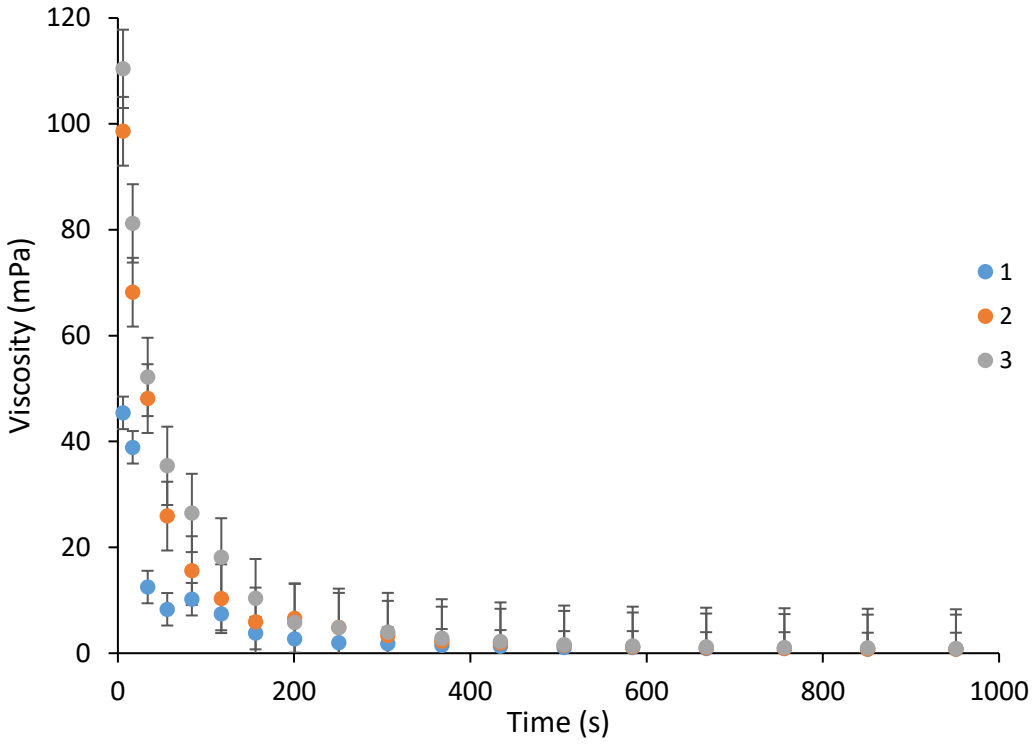

Figure S90: Viscosity run 2 for **6** at 298 K. Viscosity = 0.83 mPa ± 0.03.

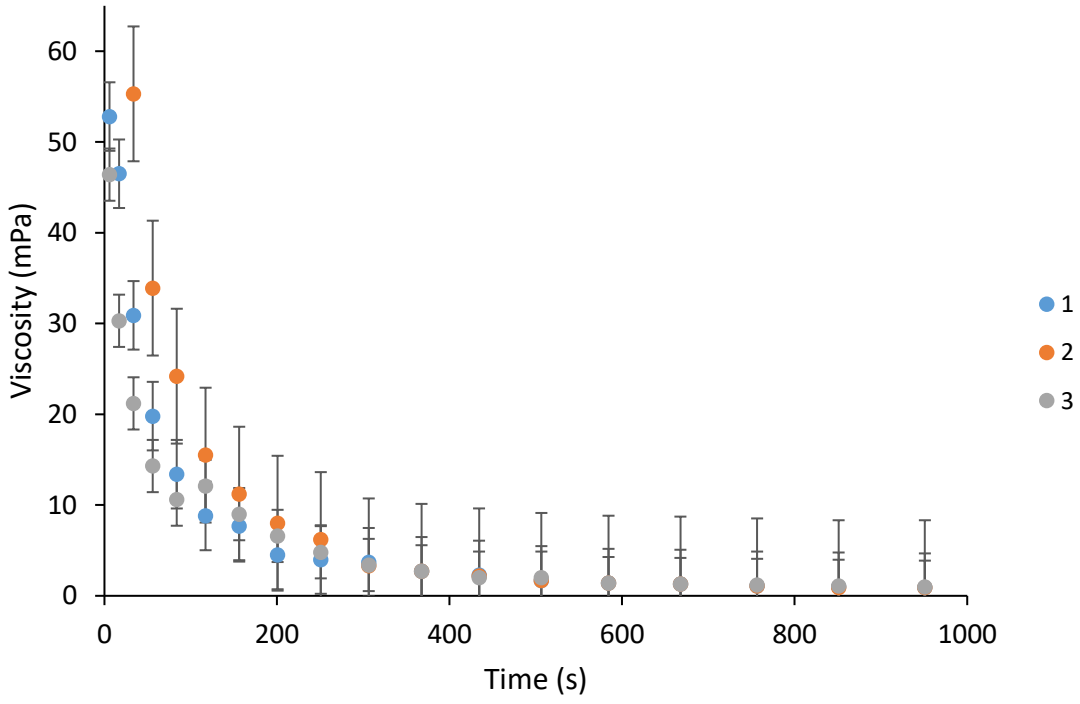

Figure S91: Viscosity run 3 for **6** at 298 K. Viscosity = 0.93 mPa ± 0.03.

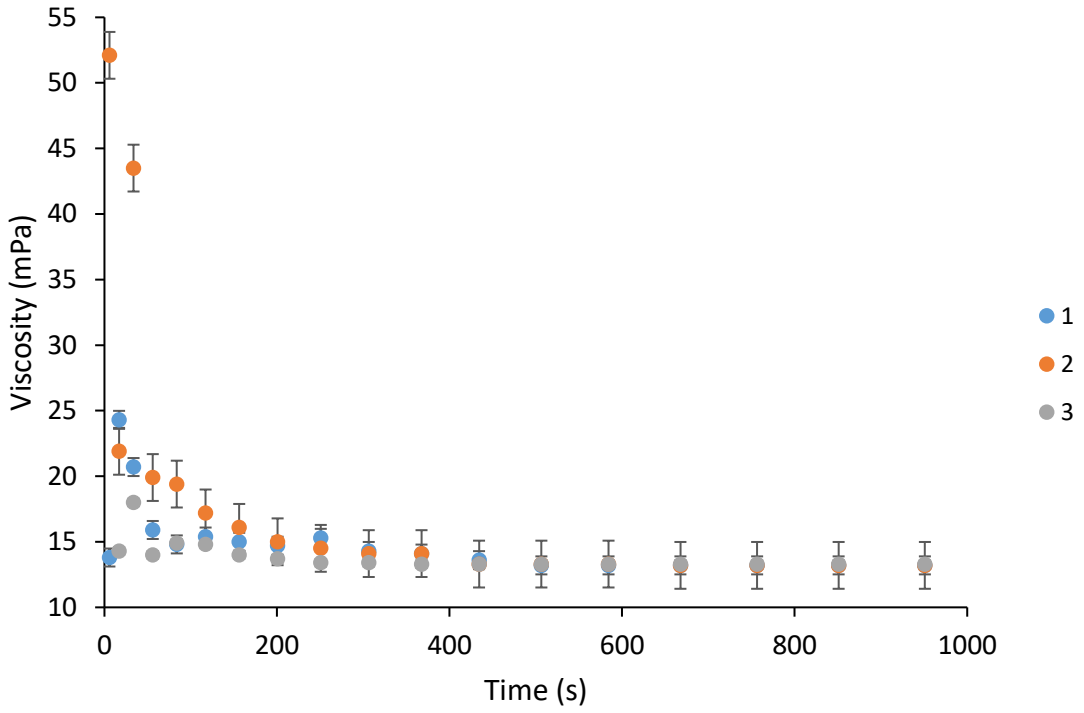

Figure S92: Viscosity run 1 for **21** at 298 K. Viscosity = 13.20 mPa ± 0.03.

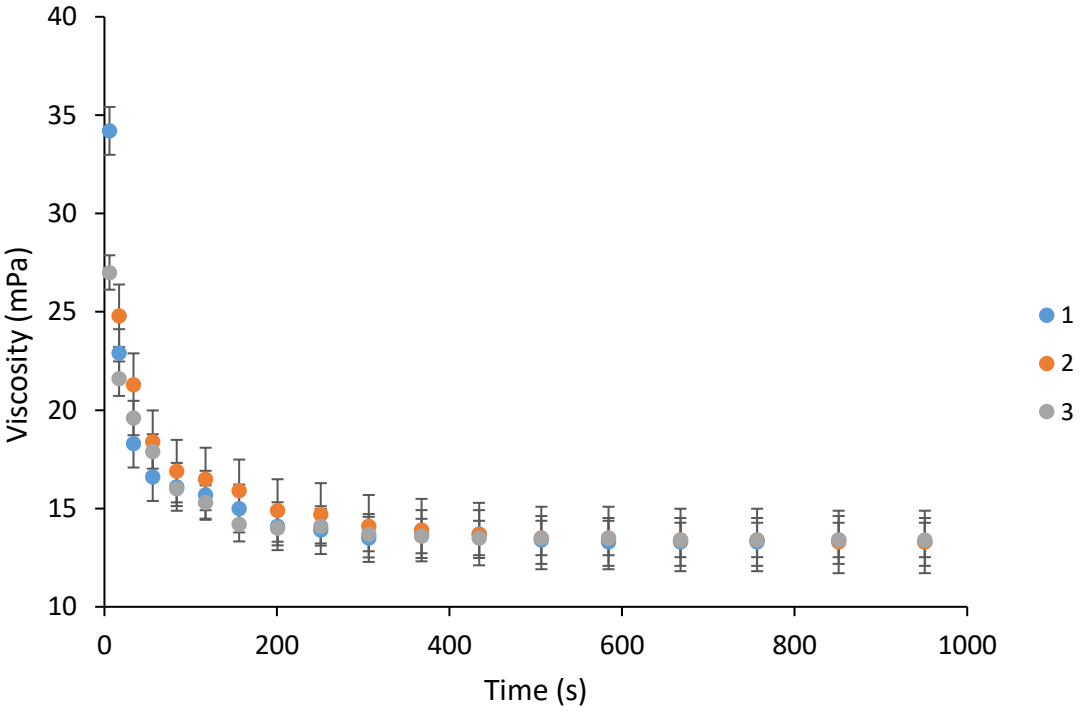

Figure S93: Viscosity run 2 for **21** at 298 K. Viscosity = 13.30 mPa ± 0.03.

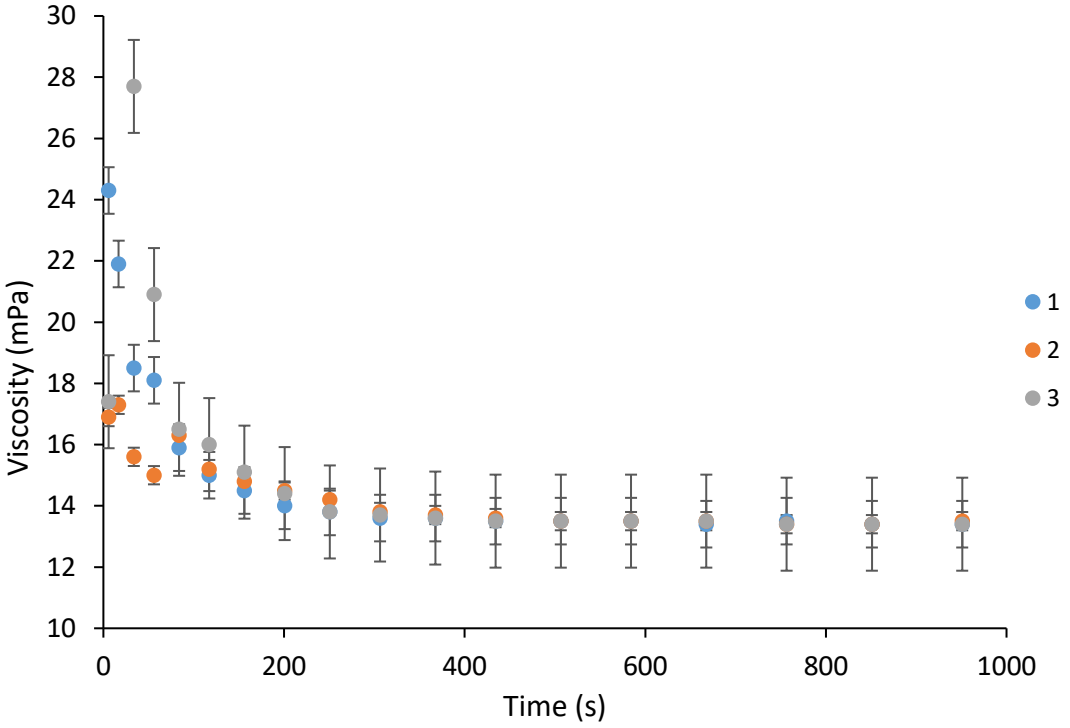

Figure S94: Viscosity run 3 for **21** at 298 K. Viscosity = 13.40 mPa ± < 0.01.

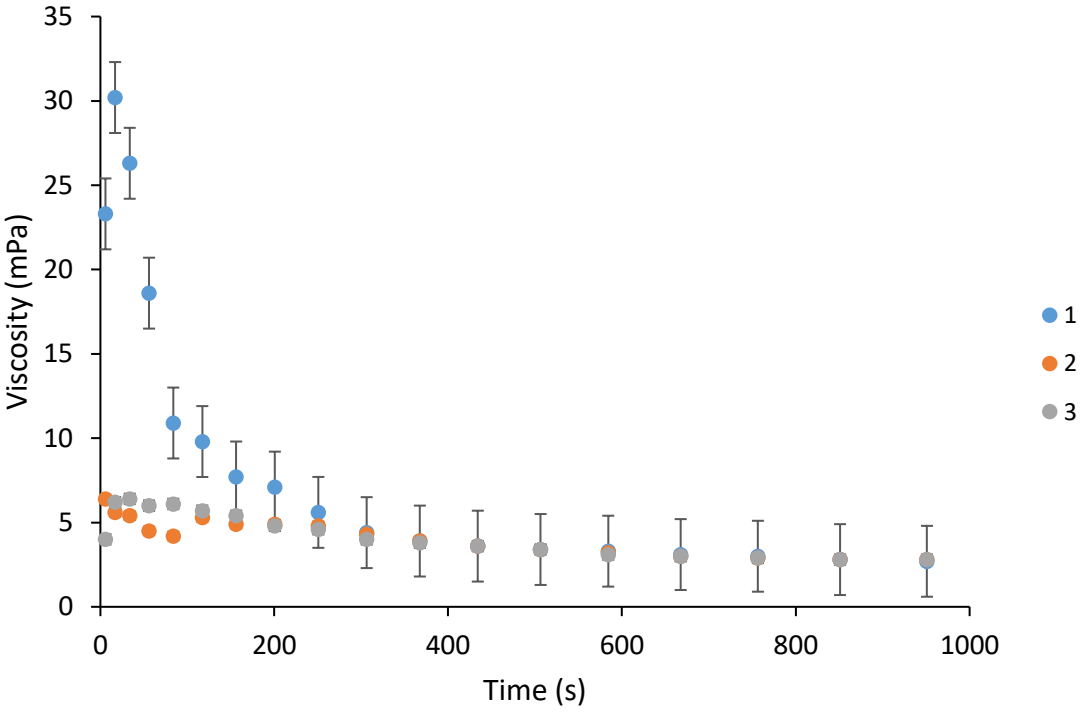

Figure S95: Viscosity run 1 for **22** at 298 K. Viscosity = 2.80 mPa ± 0.03.

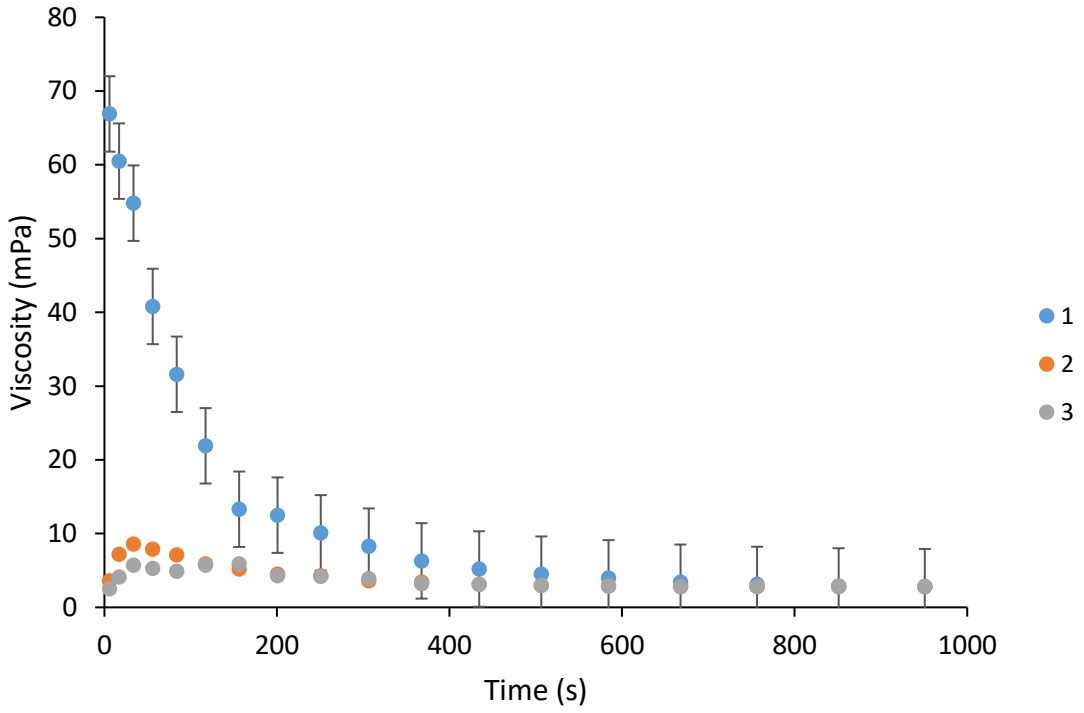

Figure S96: Viscosity run 2 for **22** at 298 K. Viscosity = 2.80 mPa ± < 0.01.

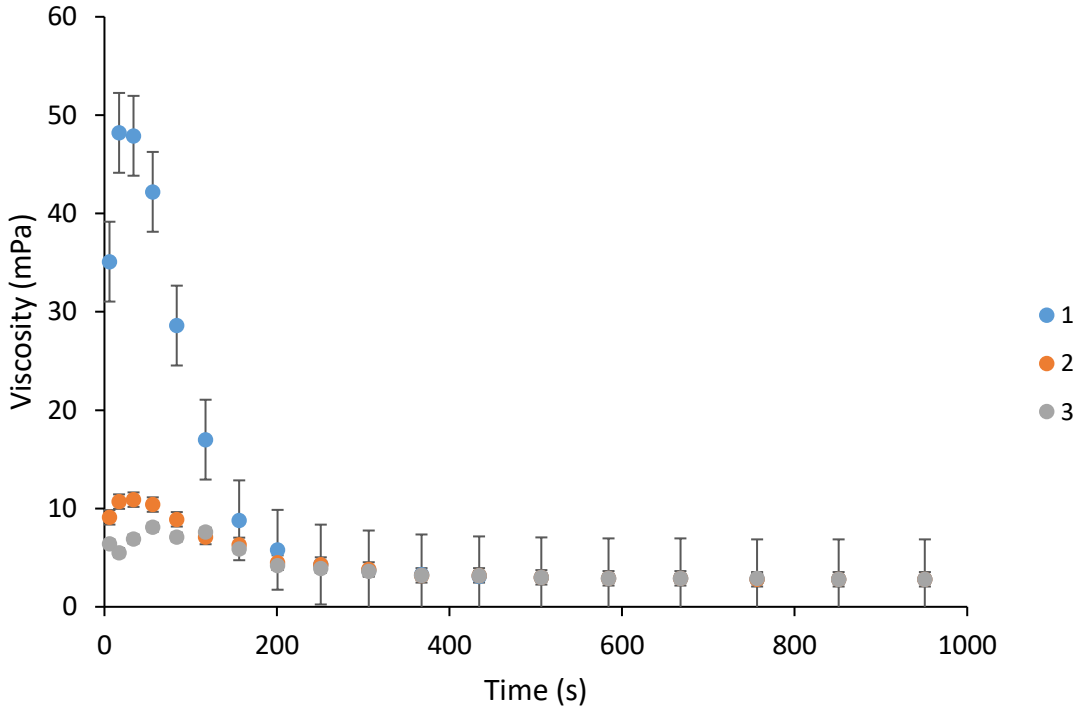

Figure S97: Viscosity run 3 for **22** at 298 K. Viscosity = 2.80 mPa ± < 0.01.

Table S2**:** Summary of viscosity results at 298 K. Results shown are an average of three repeats.

Compound	Viscosity (mPa)	Error (±)
1	4.80	0.02
2	6.20	0.22
3	15.50	0.02
4	4.10	0.06
5	5.50	< 0.01
6	0.80	0.07
16	6.80	0.08
21	2.80	0.01
22	13.20	0.03

Surface tension results

Table S3**:** Surface tension results at 298 K. Results shown are an average of three repeats.

Compound	Surface tension (mN/m)	Error (±)
1	18.0	0.0007
2	23.2	0.0013
3	26.1	0.0008
4	25.9	0.0027
5	27.2	0.0001
6	24.4	0.0008
16	28.6	0.0019
21	32.0	0.0715
22	22.7	0.0021

Density measurements

Table S4: Density measurements for compounds at 298 K.

Compound	Density (g/mL)
1	1.39
2	1.17
3	1.83
4	1.30
5	1.06
6	1.19
7	1.15
8	1.03
9	1.07
10	1.01
11	0.97
12	Solid
13	Solid
14	Solid
15	Solid
16	1.31
17	Solid
18	Solid
19	Solid
20	Solid
21	1.45
22	1.12

Vapour density

Vapour density for compounds 1-**22** were calculated using the following formula:

$$\text{Vapour density} = \frac{MW}{29}$$

Where MW is the molecular weight and, 29 is the average molecular weight of air.

Table S5: Vapour density values calculated for compounds **1**-**22**.

Compound	Vapour density (relative to air)
1	10.3
2	12.6
3	8.2
4	9.5
5	7.5
6	7.9
7	7.2
8	4.3
9	6.3
10	7.7
11	7.7
12	6.2
13	8.6
14	10.9
15	5.9
16	10.1
17	8.6
18	10.9
19	6.2
20	5.2
21	6.2
22	5.2

Low level *in-silico* modelling

Computational calculations to identify primary hydrogen bond donating and accepting sites were conducted in line with studies reported by Hunter using Spartan 16'.[12] Calculations were performed using semi-empirical PM6 methods, after energy minimisation calculations, to identify E_{min} and polarizability values. PM6 was used over AM1 in line with research conducted by Stewart.[13] These data has previously been published by Hiscock and co-workers.[1]

High-level DFT modelling

Each individual compound was pre-optimised in the gas phase at the PM6 level[14] using Spartan '16[18] before further geometry optimisation at the M06-2X level[15] and the 6-311g(d,p) basis set[14] using Gaussian16[16] with a PCM solvent model for acetonitrile. These data have previously been reported by Hiscock and co-workers.[1]

Exhaustive parameter search

R Studio was used to compile all possible parameter combinations for both direct and inverse linear models using Equations 1 and 2 and the following data sets (1) all data generated for all parameters and potential simulants listed in Table S7 and

Table S8; (2) exclusion of association constant (P_1) from the complete data set (1); (3) exclusion of association constant values less than 10 M^{-1} from the P_1 data set, (4) exclusion of percentage breakdown data from P_0, where potential simulant breakdown was found to be < 10 % over 6 hours; (5) and the exclusion of both association constant (P_1) < 10 M^{-1} and percentage breakdown values (P_0) < 10 %.

$$P_0 = P_x^a \times P_y^b \qquad |a| + |b| = 2 \qquad (1)$$

$$P_0 = P_x^a \times P_y^b \times P_z^c \qquad |a| + |b| + |c| = 3 \qquad (2)$$

- Models 1-10 are Equation 1 data set 1.
- Models 11-20 are Equation 2 data set 1.
- Models 21-30 are Equation 1 data set 2.
- Models 31-40 are Equation 2 data set 2.
- Models 41-50 are Equation 1 data set 3.
- Models 51-60 are Equation 2 data set 3.
- Models 61-70 are Equation 1 data set 4.
- Models 71-80 are Equation 2 data set 4.
- Models 81-90 are Equation 1 data set 5.
- Models 91-100 are Equation 2 data set 5.

These parameter combinations are shown in Figure S98 - Figure S197 and summarised in Table S9 -

Table S18.

Table S6: Table of all the parameters used within this study. [a] SWF is determined by the area that is within 1/8th of the E_{min}, [b] SAF is determined by the area that is within 1/8th of the E_{max} at the electrophilic centre, [c] the positive surface area is the area within 2/8th of the E_{max} across the whole molecule.

Parameter	Parameter description	Parameter definition
P0	Breakdown after 6 hours (%)	Percentage breakdown after 6 hours determined via ^{1}H NMR experiments.
P1	Association constant (M^{-1})	Association constant derived using a 1:1 binding isotherm.
P2	E_{min} (kJ/mol)	Electrostatic surface energy minimum
P3	E_{max} (kJ/mol)	Electrostatic surface energy maximum
P4	Molecular Volume (Å^3)	Total volume the molecule occupies
P5	Molecular Area (Å^2)	Total molecular area of the molecule.
P6	Solvent accessible area (Å^2)	Area accessible with a 1.4 Å radius probe.
P7	Polar surface area (Å^2)	The area due to nitrogen and oxygen and any attached hydrogens.
P8	% Polar surface area (Å^2)	The percentage polar surface area of the total surface area.
P9	Polarizability	How easily an electron cloud is distorted by an electric field
P10	Steric weighting factor (SWF) (Å^2)	Area within 1/8th of the E_{min}
P11	Steric accessibility factor (SAF) (Å^2)	Area within 1/8th of the E_{max}
P12	HOMO (eV)	Highest occupied molecular orbital
P13	LUMO (eV)	Lowest unoccupied molecular orbital
P14	Energy (kJ)	Total energy
P15	Electrostatic charge	The electrostatic charge of the HBA oxygen atom of the simulant.
P16	Additive N..O Bond length (Å)	The N..O bond lengths from both N atoms of the receptor added together.
P17	Log P	Octanol water partition coefficient
P18	Dipole moment (D)	Separation of charge across the molecule.
P19	Additive NH..O bond length	Sum of both NH..O bond lengths between receptor and simulant.
P20	Additive angle difference from 180°	Sum of the N.H..O angles difference from 180° between receptor and simulant.

Table S7: A summary of the data used for parameters P_0-P_{10} for compounds **1**-**22**.

Compound No.	P_0	P_1	P_2	P_3	P_4	P_5	P_6	P_7	P_8	P_9	P_{10}
1	92.77	36.23	-165.35	102.84	148.72	295.21	335.54	192.44	39.71	20.63	63.19

2	47.90	17.05	-171.16	88.99	124.91	263.00	299.22	186.99	39.45	21.10	60.52
3	100	7.65	-163.76	106.07	198.23	252.74	290.74	192.33	77.84	40.47	59.80
4	17.59	9.01	-188.83	73.35	131.47	230.88	261.59	180.57	38.48	21.31	57.87
5	5.26	8.06	-204.75	66.59	81.05	244.17	276.91	166.89	37.68	22.58	58.45
6	52.50	9.40	-206.16	68.24	77.02	220.54	260.41	163.62	39.51	24.15	56.51
7	10.41	10.99	-210.78	97.04	110.25	120.22	152.22	112.36	33.26	29.60	48.33
8	0	51.82	-209.93	273.78	173.99	190.08	220.96	136.88	44.41	32.45	54.00
9	0	3.42	-149.90	148.71	304.57	159.52	183.03	138.17	40.53	29.34	52.19
10	0	5.52	-166.68	124.63	272.44	173.28	200.22	129.64	41.20	31.78	52.86
11	0	6.42	-166.25	122.61	267.26	149.75	185.44	124.59	43.04	34.54	50.89
12	55.70	11.73	-174.75	84.88	183.73	219.8	147.63	39.34	26.65	53.54	3.48
13	57.35	25.48	-178.83	100.74	237.99	273.99	160.48	35.24	21.96	57.93	3.43
14	1.54	6.62	-189.35	72.83	239.17	281.93	177.93	39.73	22.33	58.06	4.17
15	4.97	6.68	-154.57	115.91	316.38	275.91	302.35	202.24	39.84	19.70	61.74
16	8.15	48.16	-167.05	128.22	329.31	265.90	293.17	206.83	79.61	38.49	60.92
17	100	106.25	-154.27	107.07	262.12	244.12	267.24	197.37	40.91	20.73	59.25
18	80.90	40.71	-174.34	96.91	223.55	257.30	281.72	186.59	40.07	21.48	59.97
19	100	63.85	-175.68	99.08	235.86	233.8	267.08	182.95	41.98	22.95	58.07
20	2.10	45.92	-131.70	161.79	371.31	223.99	256.69	149.34	40.71	27.26	57.43
21	66.46	75.61	-143.62	151.76	355.94	191.88	220.72	145.64	40.86	28.06	54.79
22	94.12	7.00	-157.62	169.89	386.40	181.83	211.57	147.57	80.73	54.70	54.04

Table S8: A summary of the data for parameters P_{11}-P_{20} for compounds **1**-**22**.

Compound No.	P_{11}	P_{12}	P_{13}	P_{14}	P_{15}	P_{16}	P_{18}	P_{19}	P_{20}
1	3.93	-7.22	-1.30	-1706.50	-0.59	5.94	4.05	4.03	49.34
2	3.50	-6.91	-0.61	-1369.47	-0.60	5.97	3.98	4.05	47.61
3	4.12	-7.19	-2.34	-1236.93	-0.61	5.98	6.33	4.05	44.31
4	3.47	-6.46	-0.06	-1032.43	-0.61	5.95	1.23	4.00	42.67
5	4.24	-7.34	1.79	-1036.06	-0.63	5.89	1.03	3.94	40.96
6	3.92	-7.57	1.79	-958.64	-0.62	5.89	1.09	3.95	44.29
7	4.06	-7.56	1.88	-686.82	-0.64	5.91	2.07	3.96	42.23
8	4.77	-9.74	3.66	-848.93	-0.68	5.87	1.90	3.98	53.20
9	8.25	-8.61	1.69	-8958.17	-0.50	3.08	2.92	4.24	16.32
10	9.31	-7.60	1.27	-898.99	-0.51	6.06	3.18	4.17	24.91
11	9.46	-7.80	1.29	-821.56	-0.50	6.25	3.29	4.17	49.46
12	2.13	-10.82	0.83	-1115.05	-0.96	5.75	0.50	3.61	47.10
13	0.54	-10.63	1.08	-1240.27	-0.96	5.89	2.74	4.33	45.48
14	2.32	-10.82	0.72	-1168.96	-0.97	5.91	0.92	3.87	41.21
15	8.26	-7.17	-1.44	-1463.44	-0.47	6.08	6.30	4.25	54.00
16	9.05	-7.13	-2.29	-1330.91	-0.46	6.12	9.00	4.33	62.63
17	9.00	-6.37	-1.23	-1126.40	-0.47	6.12	4.30	4.23	57.99
18	8.74	-7.15	-1.01	-1130.04	-0.49	6.06	3.96	4.12	50.38
19	9.11	-7.18	-1.04	-1052.61	-0.48	6.02	4.17	4.09	42.00
20	8.48	-7.70	-1.49	-1569.42	-0.47	6.03	4.28	4.31	18.11
21	8.68	-7.35	-1.08	-1232.39	-0.48	6.31	4.28	4.36	46.91
22	9.34	-7.33	-2.43	-1099.85	-0.47	6.27	6.62	4.20	19.44

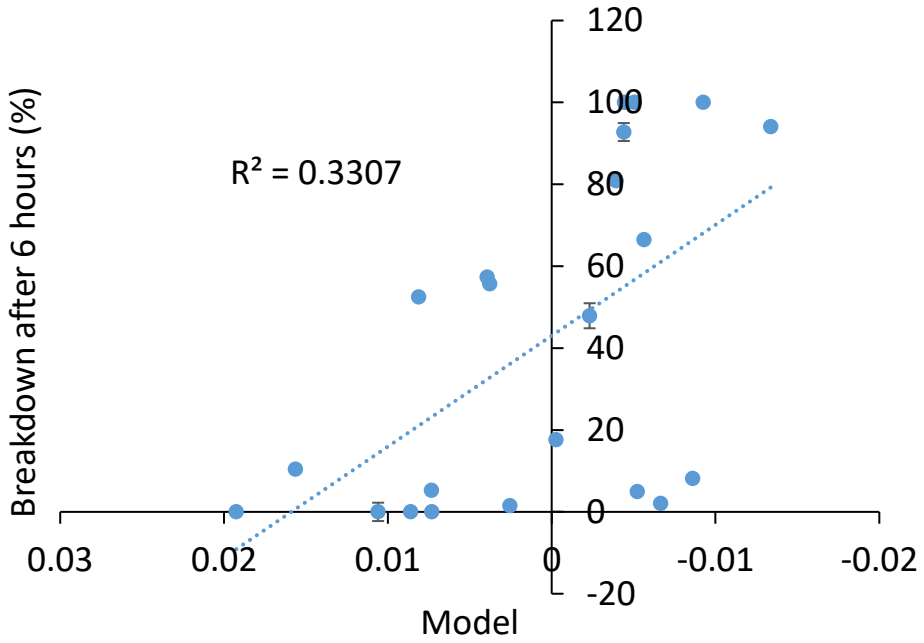

Figure S98: Model 1 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P5)^{-1}$. R^2 = 0.3307.

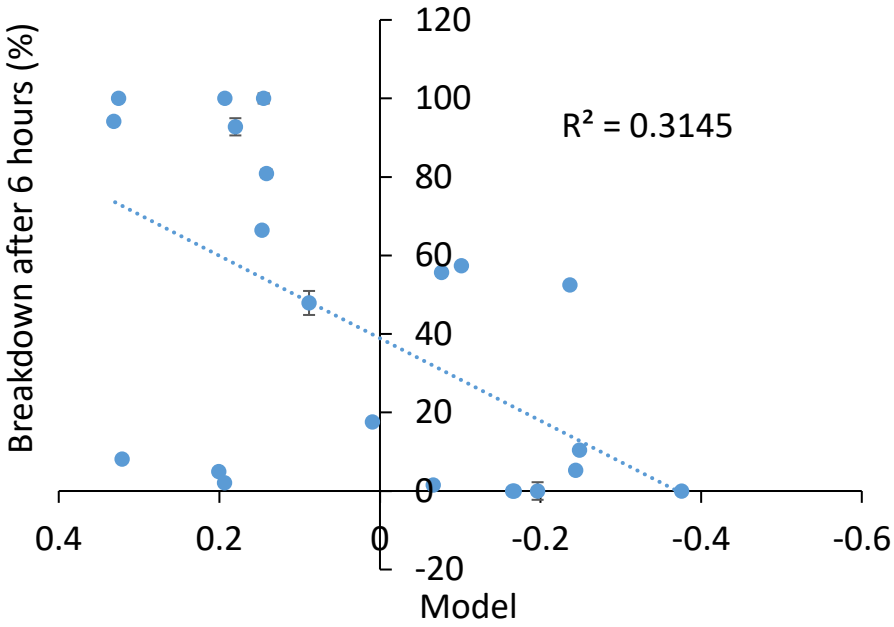

Figure S99: Model 2 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P12)^{-1}$. R^2 = 0.3145.

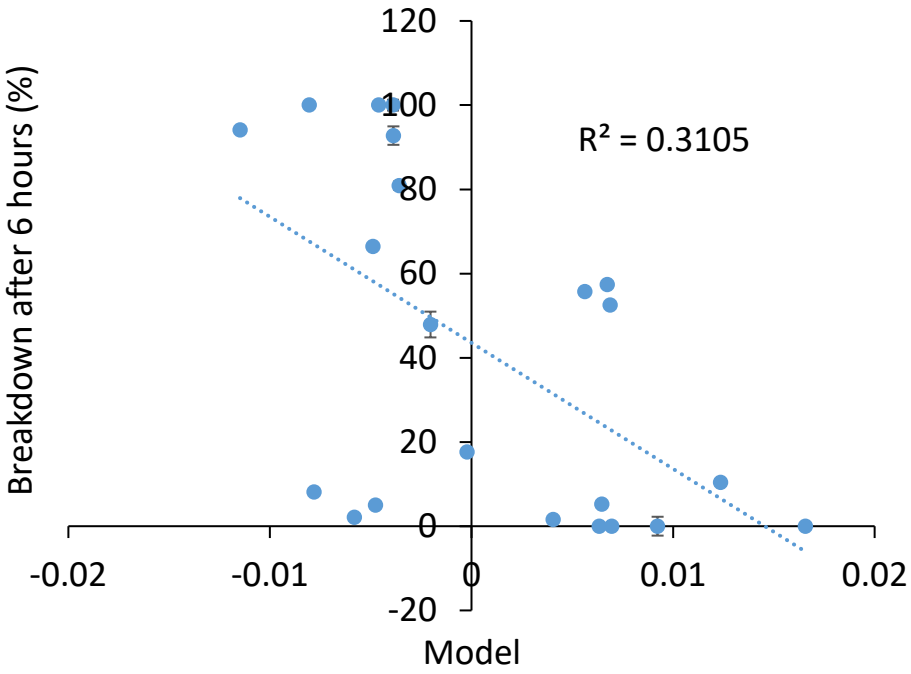

Figure S100: Model 3 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P6)^{-1}$. R^2 = 0.3105.

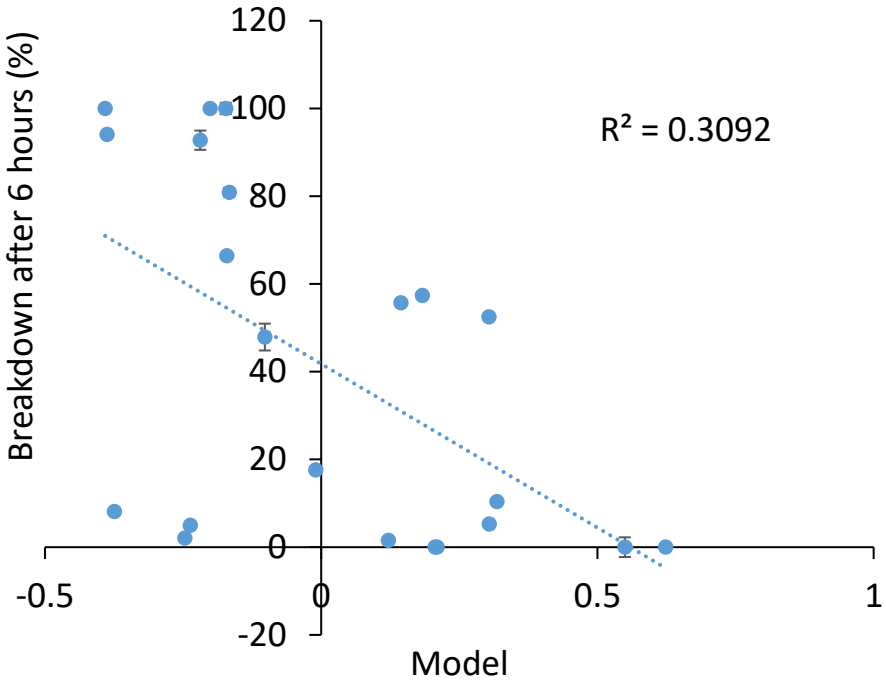

Figure S101: Model 4 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P16)^{-1}$. R^2 = 0.3092.

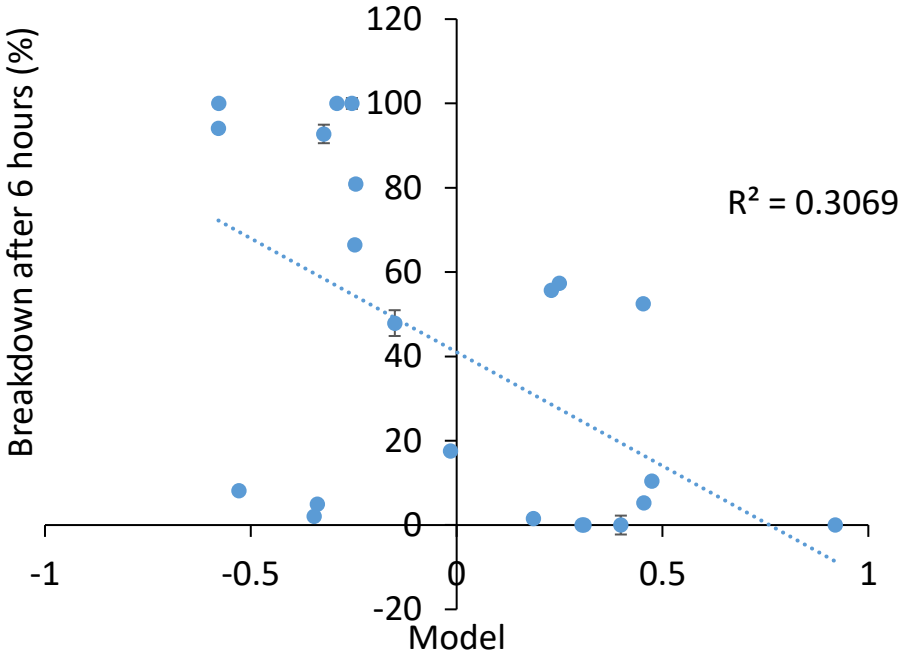

Figure S102: Model 5 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P19)^{-1}$. R^2 = 0.3069.

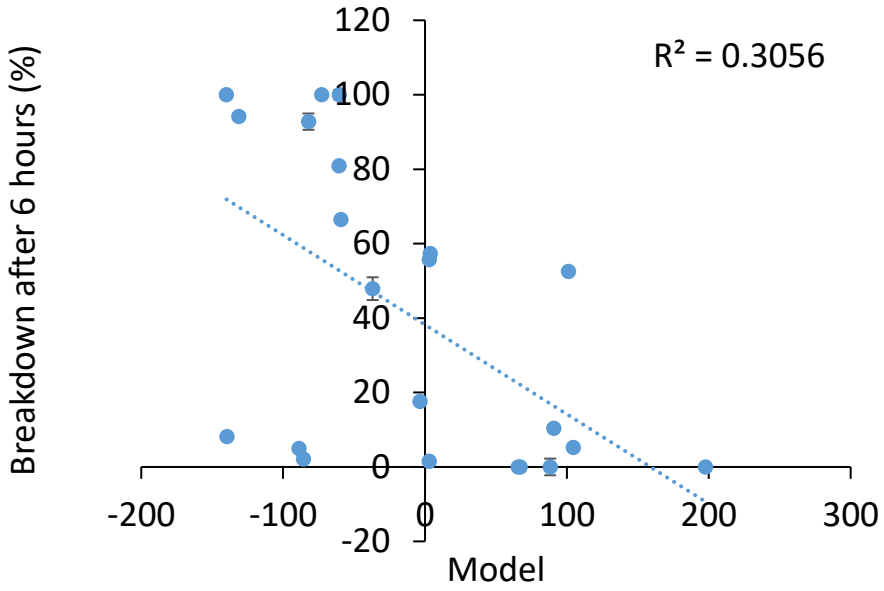

Figure S103: Model 6 vs breakdown after 6 hours (%). Model parameters are P0 = P10 * P13. R^2 = 0.3056.

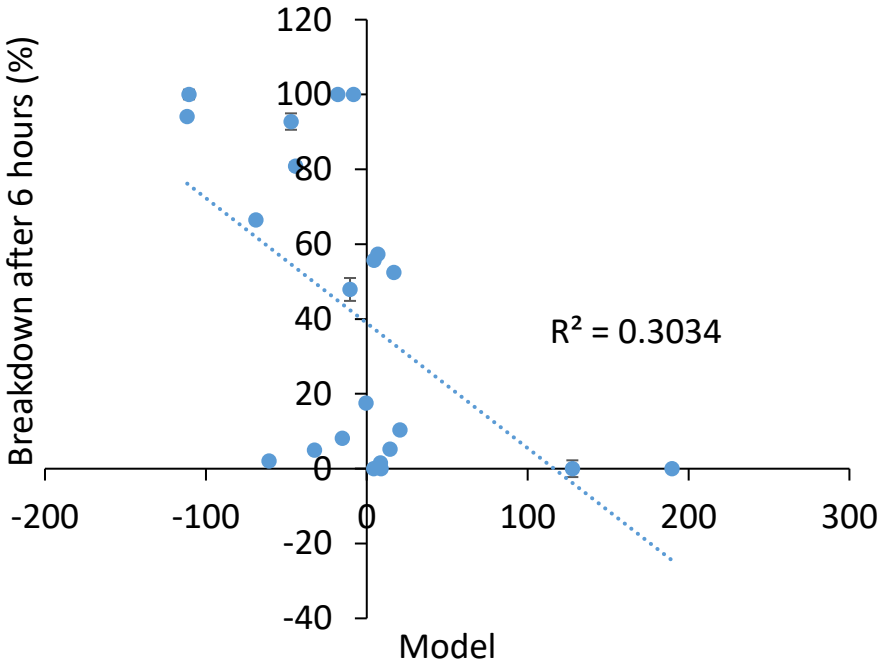

Figure S104: Model 7 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * P13. R^2 = 0.3034.

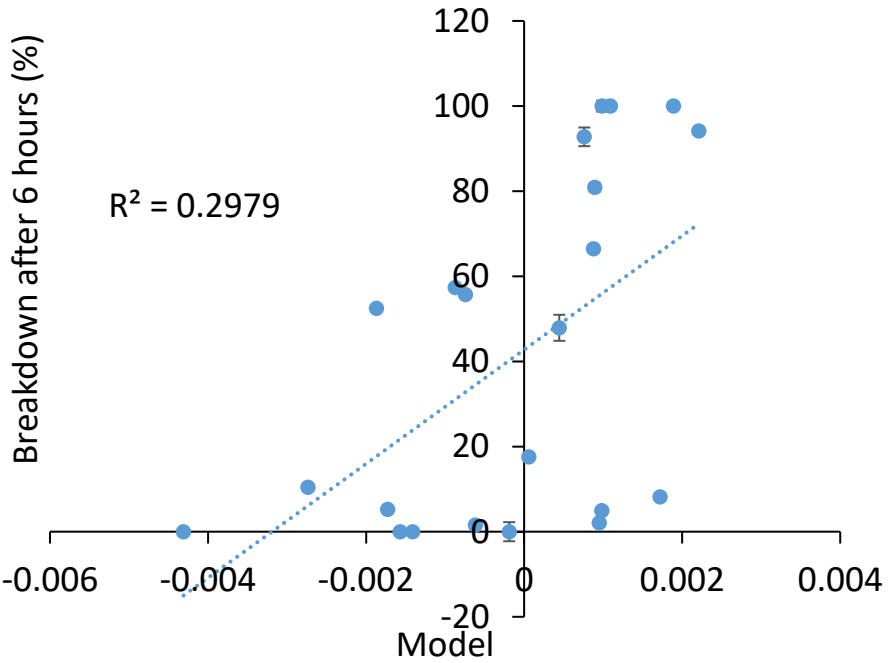

Figure S105: Model 8 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P14)^{-1}$. R^2 = 0.2979.

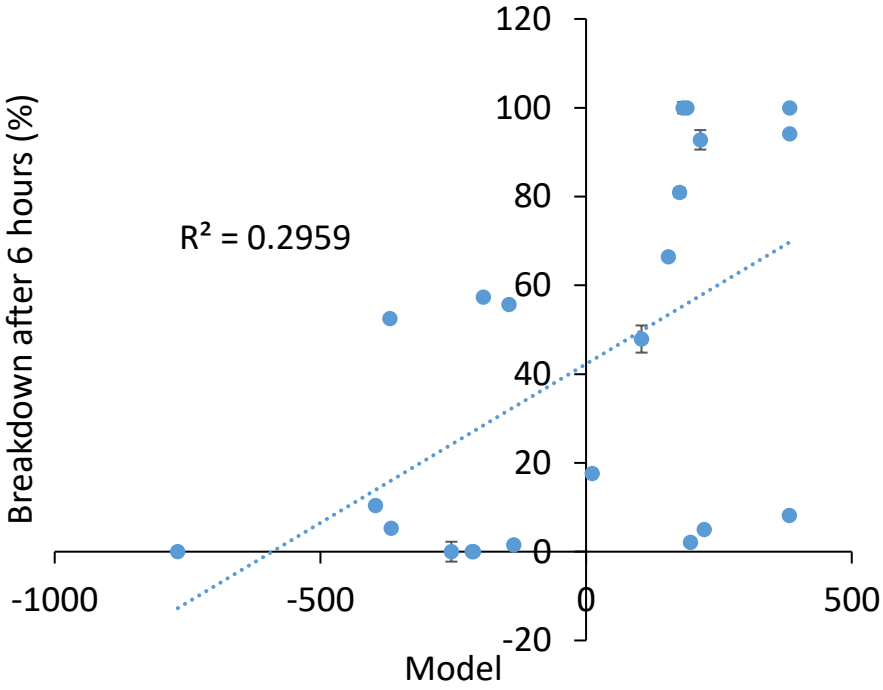

Figure S106: Model 9 vs breakdown after 6 hours (%). Model parameters are P0 = P2 * P13. R^2 = 0.2959.

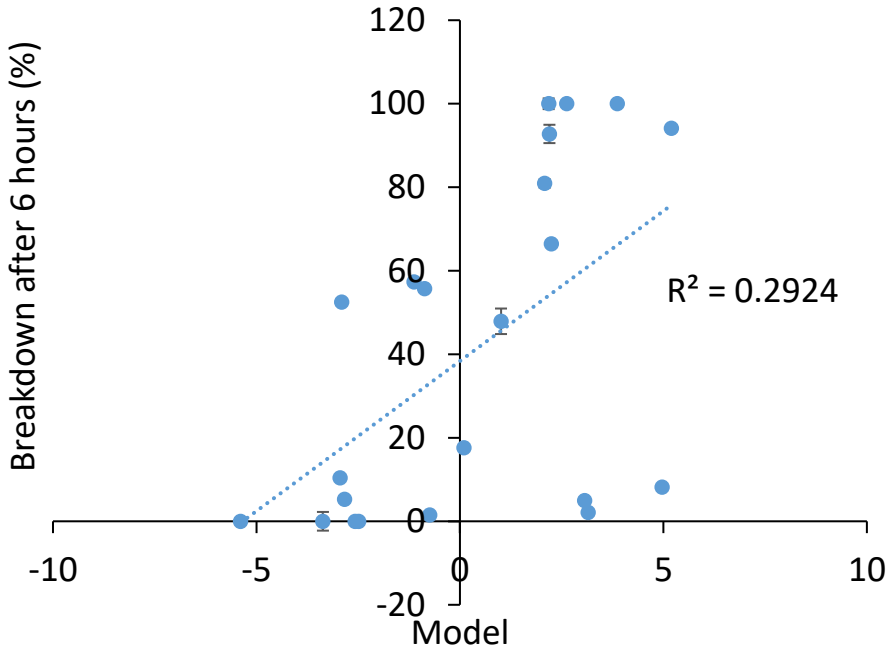

Figure S107: Model 10 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * P19. R^2 = 0.2924.

Table S9 – Summary of the parameters used within models 1-10.

Parameter	Model Number										Total
	1	2	3	4	5	6	7	8	9	10	
R^2	0.3307	0.3145	0.3105	0.3092	0.3069	0.3056	0.3034	0.2979	0.2959	0.2924	
Equation	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * P_y$	$P0 = P_x * P_y$	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * P_y$	$P0 = P_x * (P_y)^{-1}$	
P_1							×				1
P_2									×		1
P_3											0
P_4											0
P_5	×										1
P_6			×								1
P_7											0
P_8											0
P_9											0
P_{10}						×					1
P_{11}											0
P_{12}		×									1
P_{13}	×	×	×	×	×	×	×	×	×	×	10
P_{14}								×			1
P_{15}										×	1
P_{16}				×							1
P_{17}											0
P_{18}											0
P_{19}					×						1
P_{20}											0

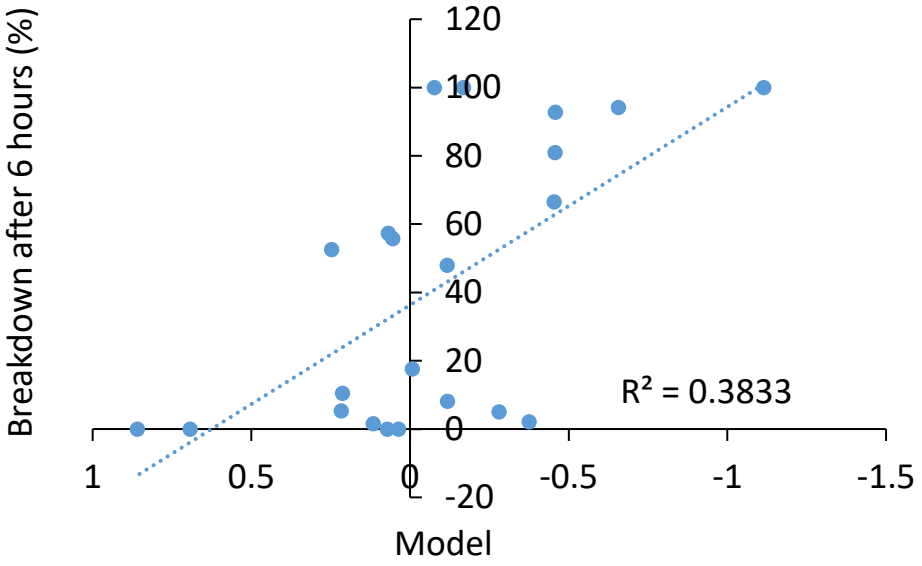

Figure S108: Model 11 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * P13 * $(P3)^{-1}$. R^2 = 0.3833.

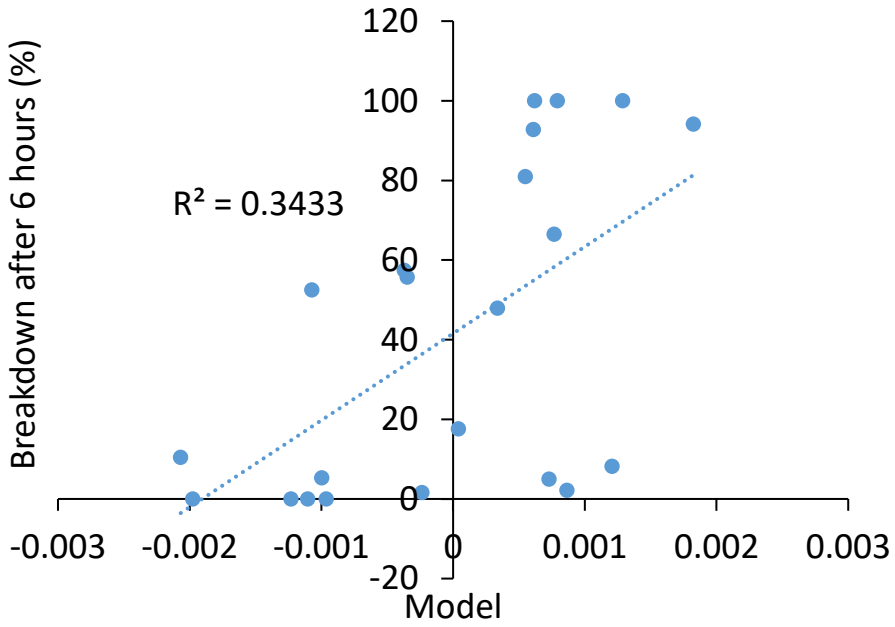

Figure S109: Model 12 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P12 * P5)^{-1}$. R^2 = 0.3433.

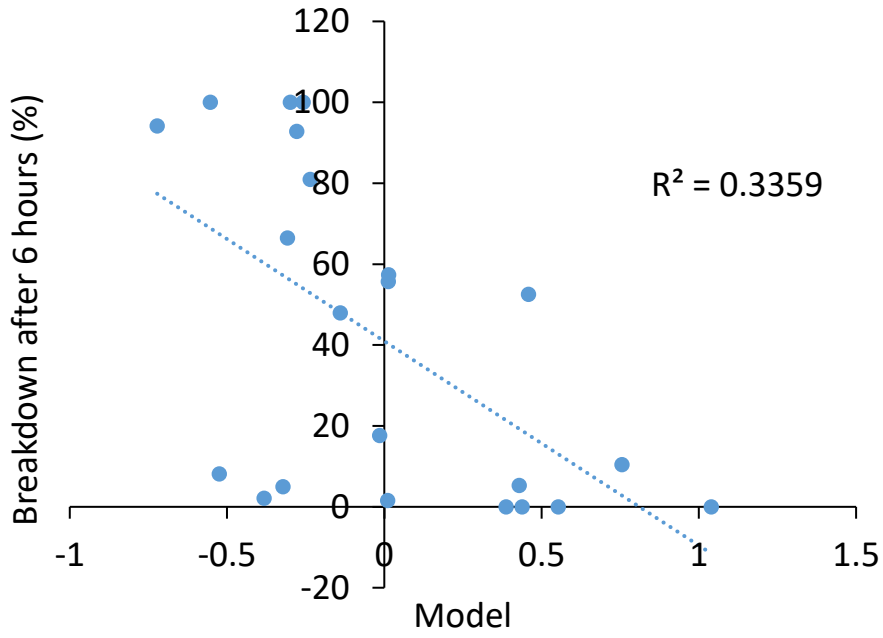

Figure S110: Model 13 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * P10 * $(P5)^{-1}$. R^2 = 0.3359.

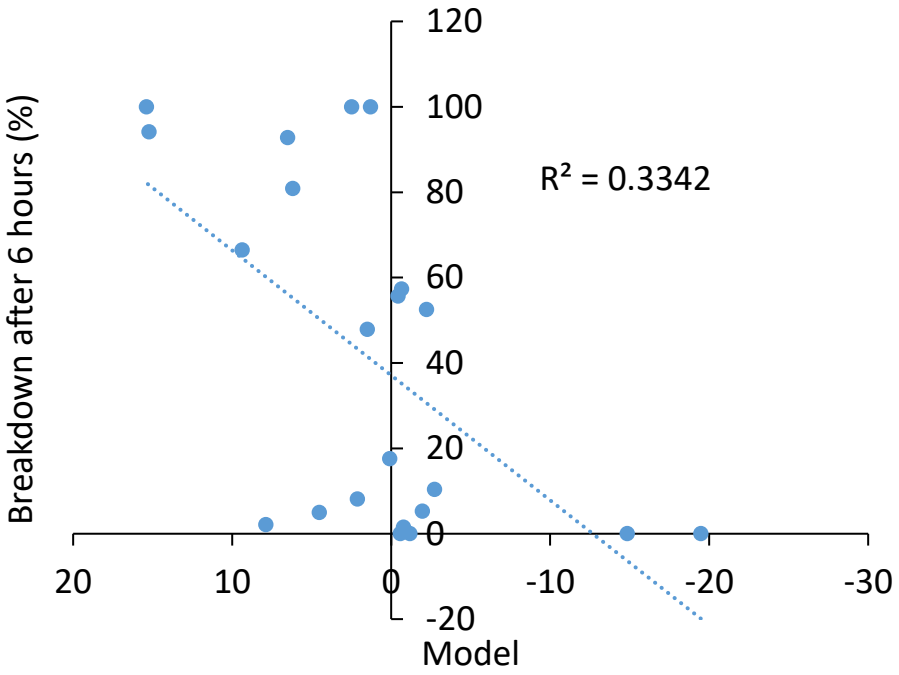

Figure S111: Model 14 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * P13 * $(P12)^{-1}$. R^2 = 0.3342.

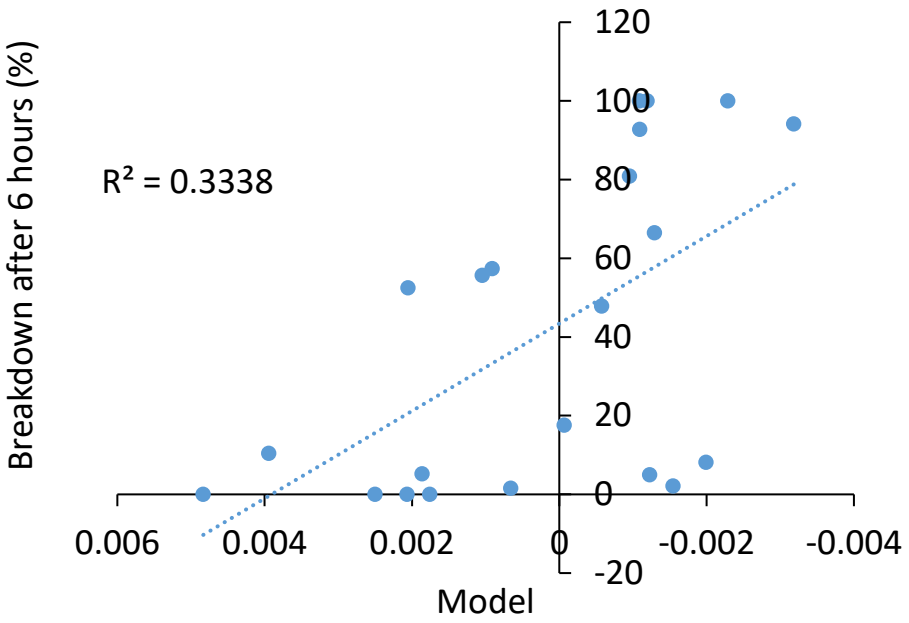

Figure S112: Model 15 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * (P5 * P19)$^{-1}$. R^2 = 0.3338.

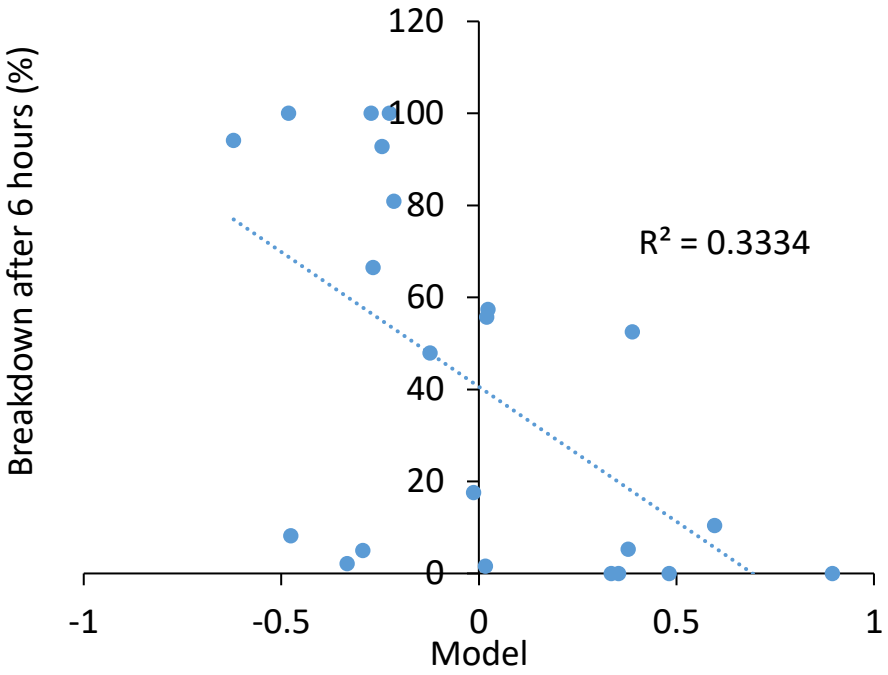

Figure S113: Model 16 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * P10 * (P6)$^{-1}$. R^2 = 0.3334.

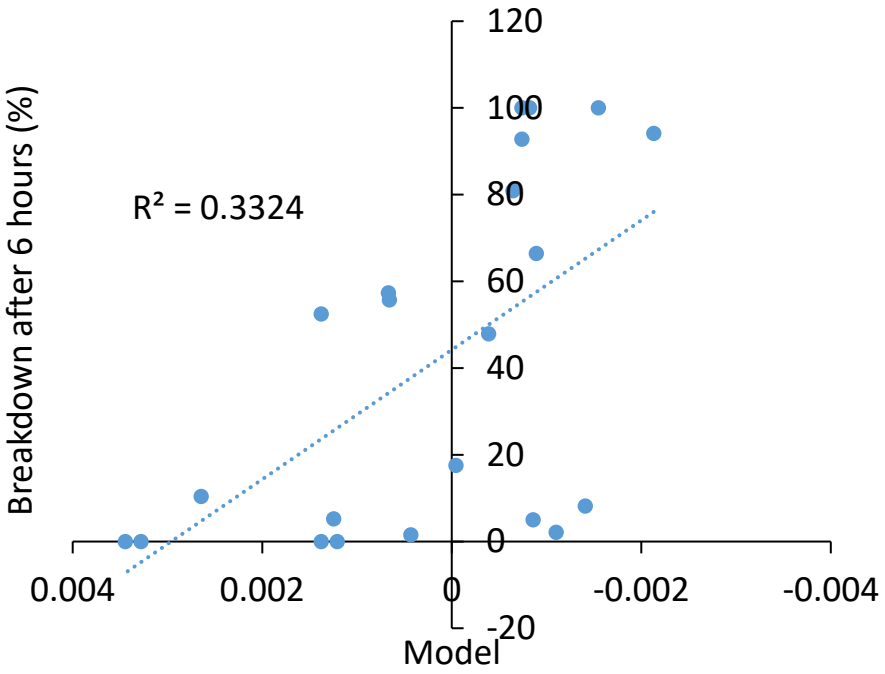

Figure S114: Model 17 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * (P5 * P16)$^{-1}$. R^2 = 0.3324.

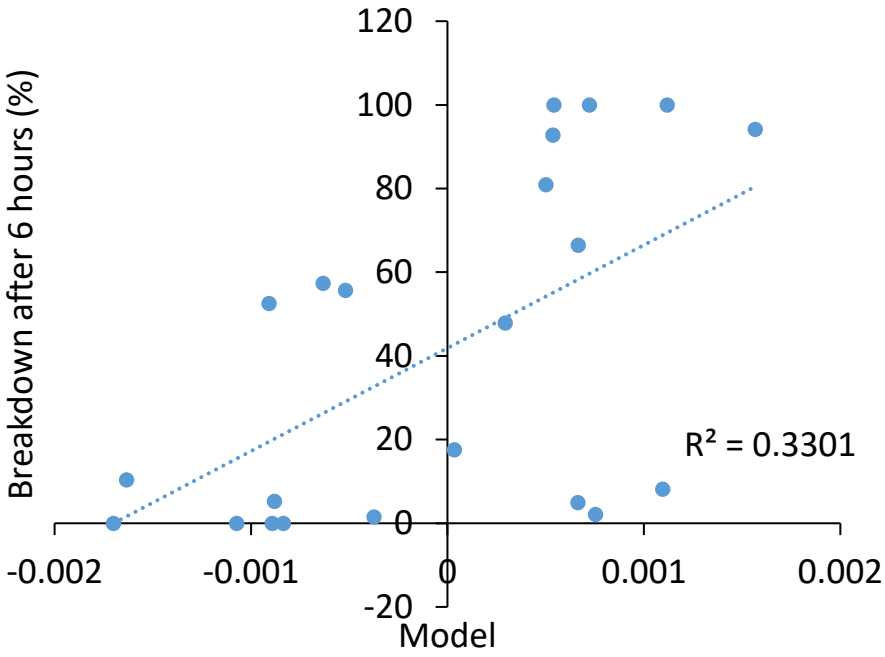

Figure S115: Model 18 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * (P12 * P6)$^{-1}$. R^2 = 0.3301.

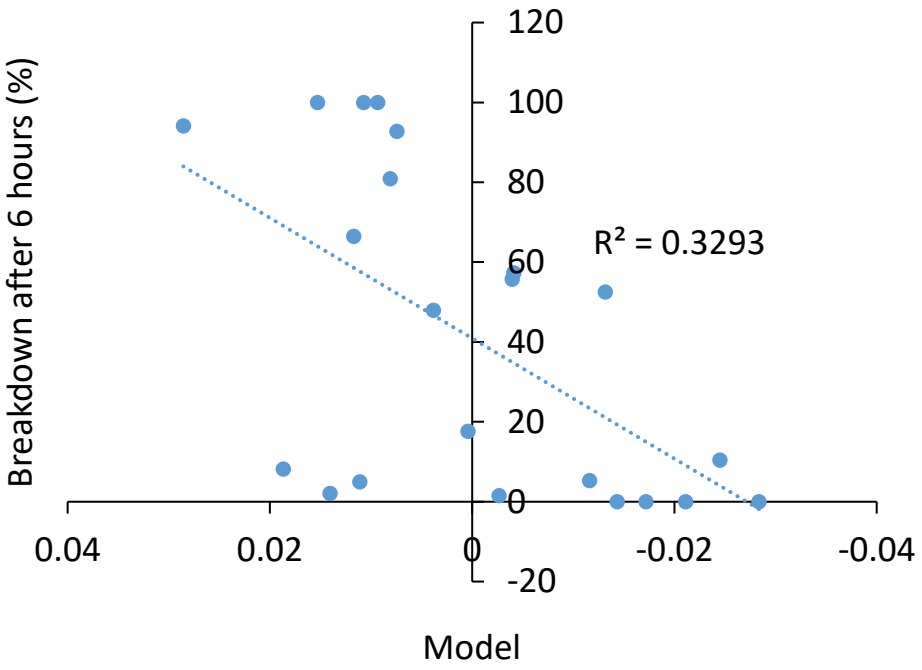

Figure S116: Model 19 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * (P5 * P15)$^{-1}$. R^2 = 0.3293.

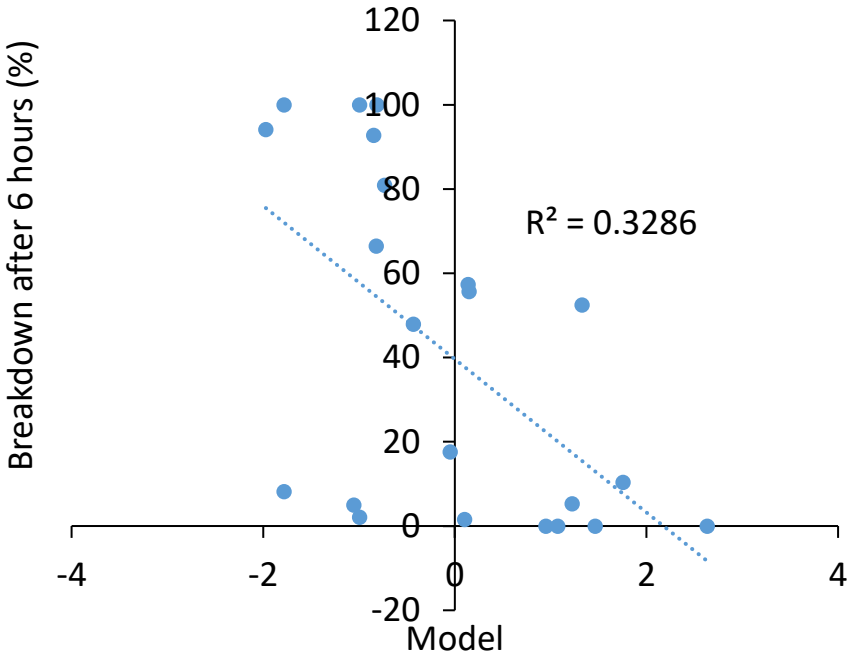

Figure S117: Model 20 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * P7 * (P5)$^{-1}$. R^2 = 0.3286.

Table S10: Summary of the parameters used within models 11-20.

Parameter	Model Number										Total
	11	12	13	14	15	16	17	18	19	20	
R^2	0.3833	0.3433	0.3359	0.3342	0.3338	0.3334	0.3324	0.3301	0.3293	0.3286	
Equation	$P0 = P_x * P_y * (P_z)^{-1}$	$P0 = P_x * (P_y * P_z)^{-1}$	$P0 = P_x * P_y * (P_z)^{-1}$	$P0 = P_x * P_y * (P_z)^{-1}$	$P0 = P_x * (P_y * P_z)^{-1}$	$P0 = P_x * P_y * (P_z)^{-1}$	$P0 = P_x * (P_y * P_z)^{-1}$	$P0 = P_x * (P_y * P_z)^{-1}$	$P0 = P_x * (P_y * P_z)^{-1}$	$P0 = P_x * P_y * (P_z)^{-1}$	
P_1	×			×							2
P_2											0
P_3	×										1
P_4											0
P_5		×	×		×		×		×	×	6
P_6						×		×			2
P_7										×	1
P_8											0
P_9											0
P_{10}			×			×					2
P_{11}											0
P_{12}		×		×				×			3
P_{13}	×	×	×	×	×	×	×	×	×	×	10
P_{14}											0
P_{15}									×		1
P_{16}							×				1
P_{17}											0
P_{18}											0
P_{19}					×						1
P_{20}											0

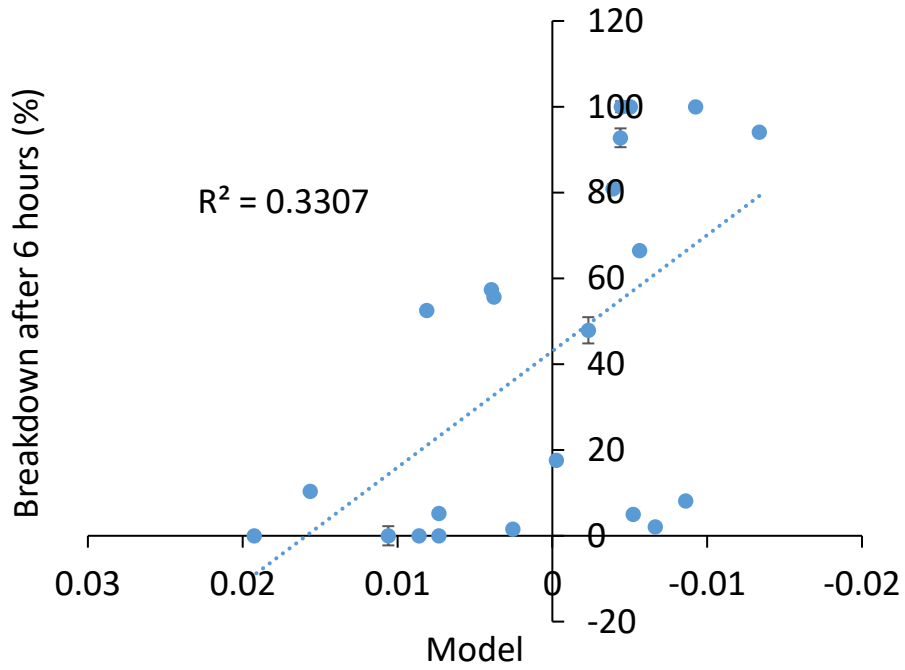

Figure S118: Model 21 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P5)^{-1}$. R^2 = 0.3307.

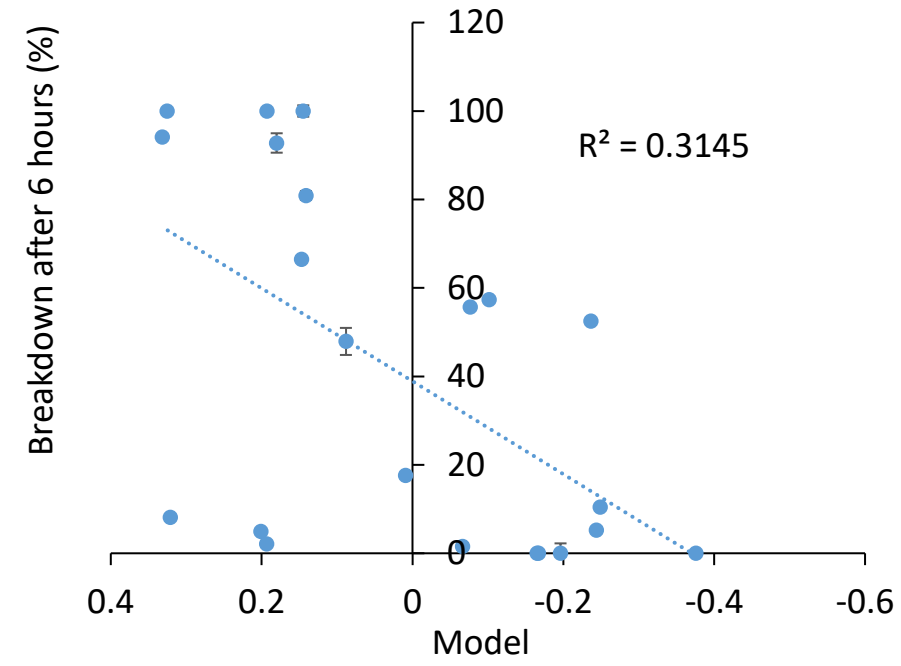

Figure S119: Model 22 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P12)^{-1}$. R^2 = 0.3145.

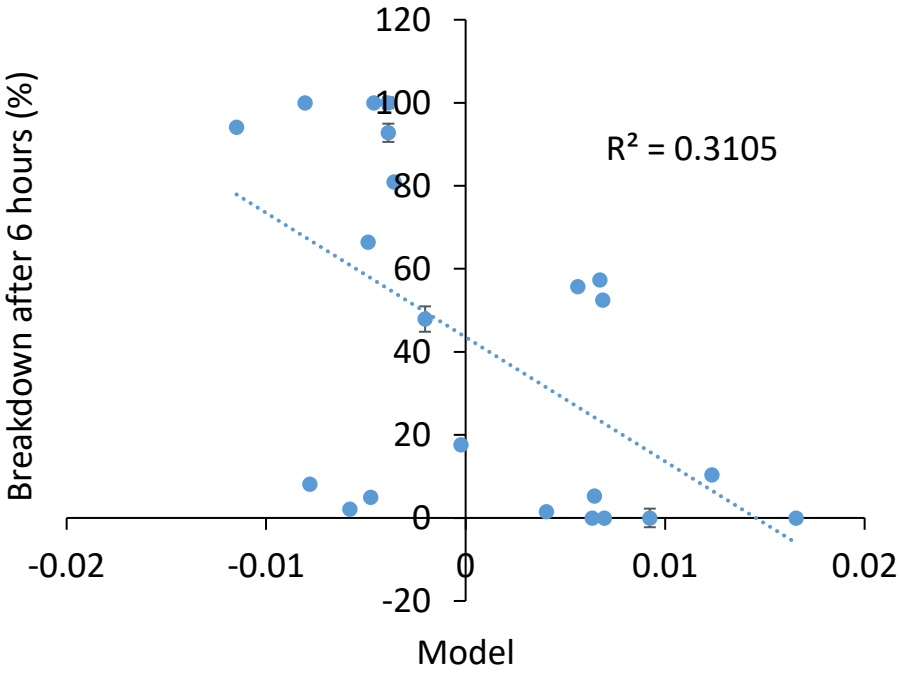

Figure S120: Model 23 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P6)^{-1}$. R^2 = 0.3105.

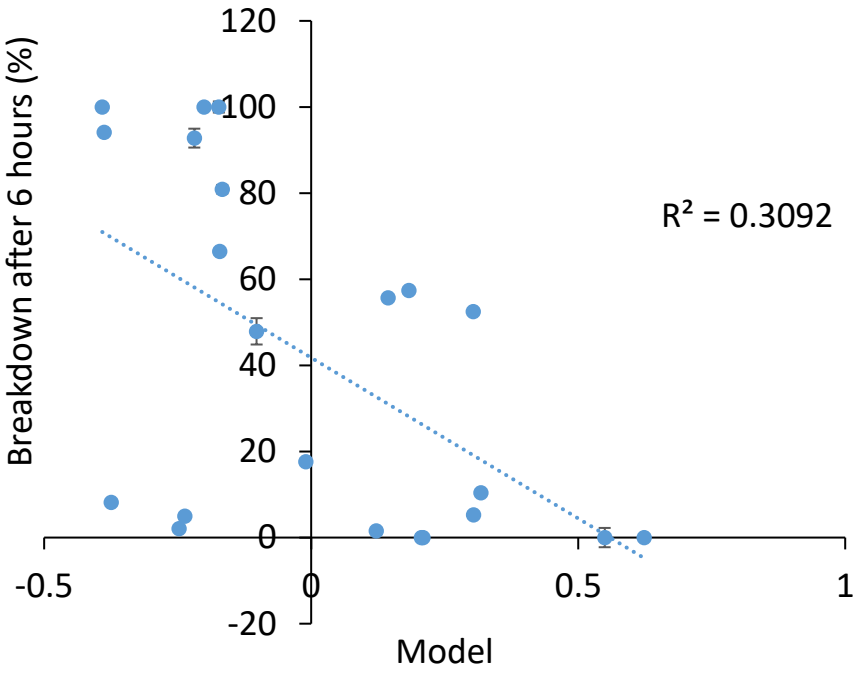

Figure S121: Model 24 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P16)^{-1}$. R^2 = 0.3092.

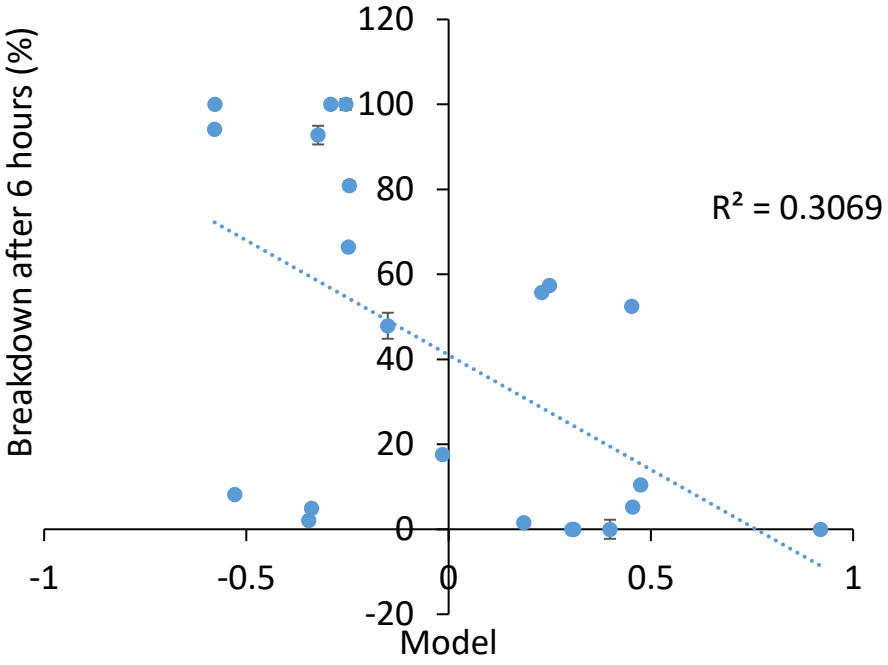

Figure S122: Model 25 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P19)^{-1}$. R^2 = 0.3069.

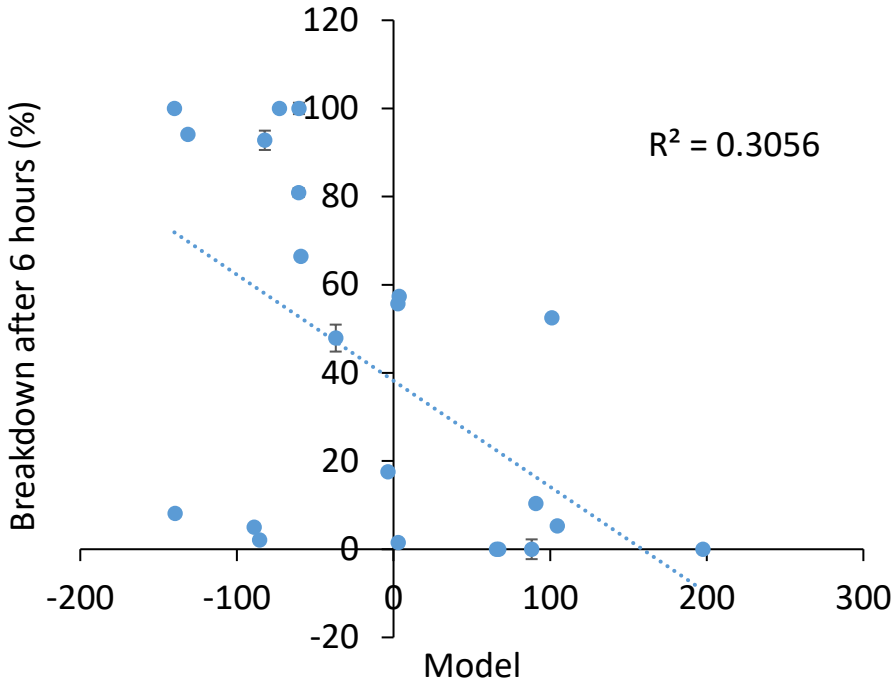

Figure S123: Model 26 vs breakdown after 6 hours (%). Model parameters are P0 = P10 * P13. R^2 = 0.3056.

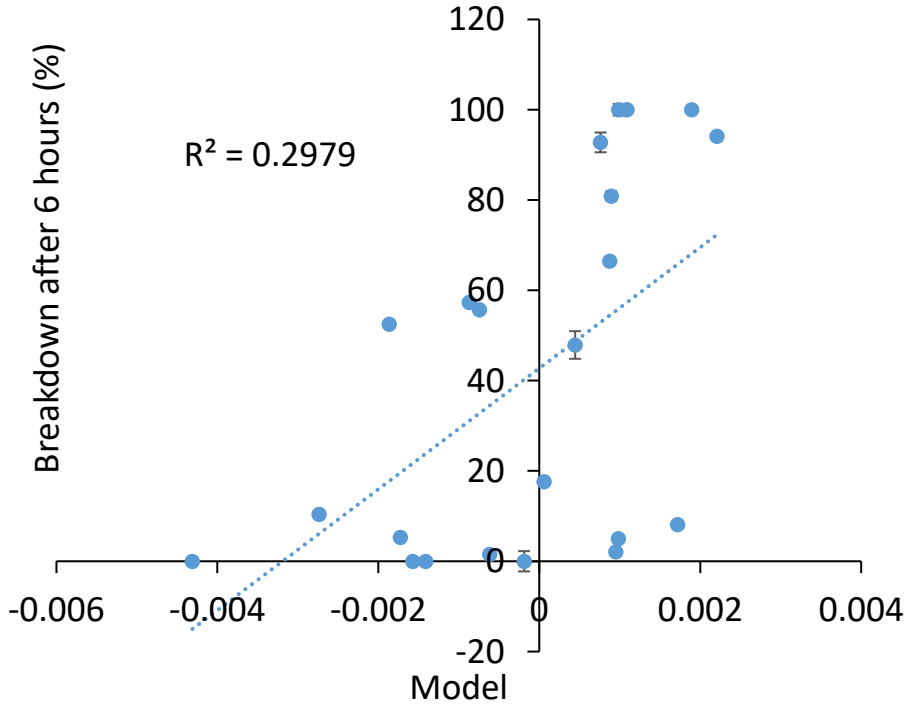

Figure S124: Model 27 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P14)^{-1}$. R^2 = 0.2979.

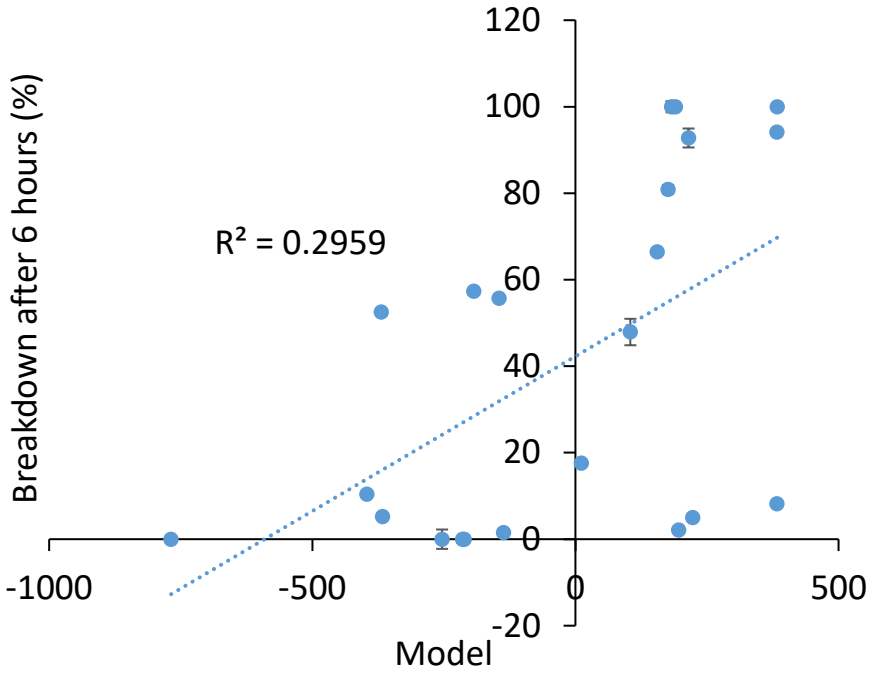

Figure S125: Model 28 vs breakdown after 6 hours (%). Model parameters are P0 = P2 * P13. R^2 = 0.2959.

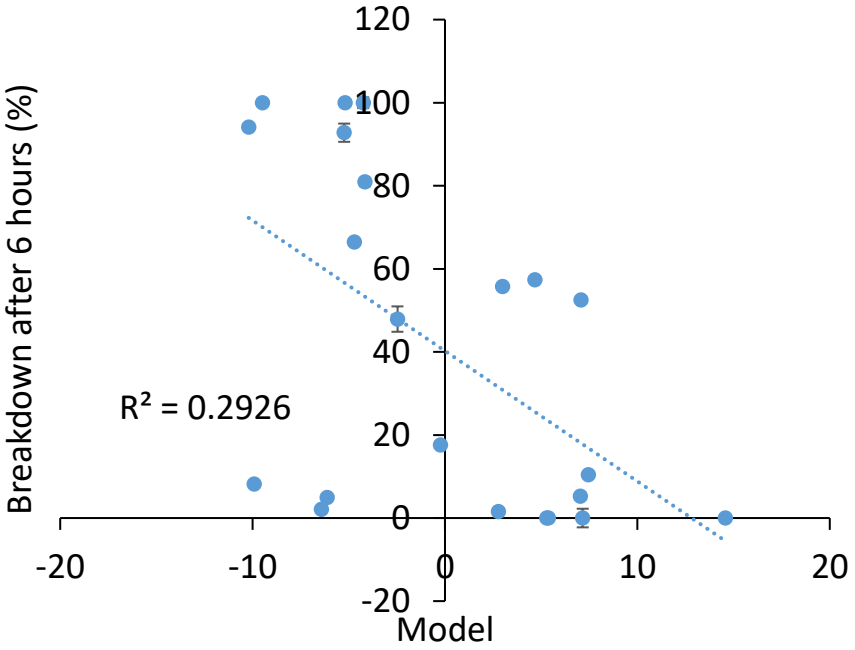

Figure S126: Model 29 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * P19. R^2 = 0.2926.

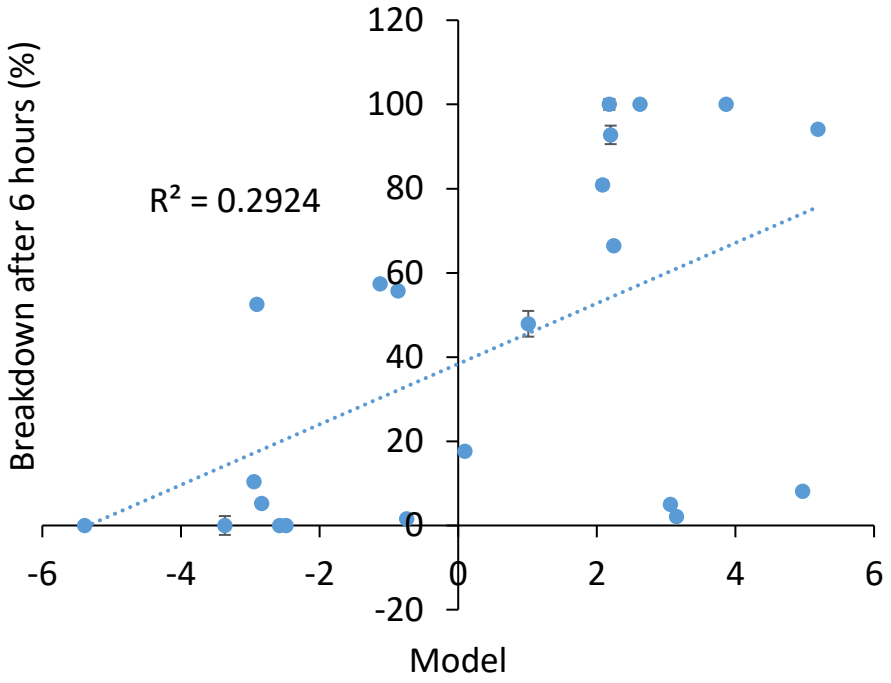

Figure S127: Model 30 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P15)^{-1}$. R^2 = 0.2924.

Table S11: Summary of the parameters used within models 21-30.

Parameter	Model Number										Total
	21	22	23	24	25	26	27	28	29	30	
R^2	0.3307	0.3145	0.3105	0.3092	0.3069	0.3056	0.2979	0.2959	0.2926	0.2924	
Equation	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * P_y$	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * P_y$	$P0 = P_x * P_y$	$P0 = P_x * (P_y)^{-1}$	
P_1											0
P_2								×			1
P_3											0
P_4											0
P_5	×										1
P_6			×								1
P_7											0
P_8											0
P_9											0
P_{10}						×					1
P_{11}											0
P_{12}		×									1
P_{13}	×	×	×	×	×	×	×	×	×	×	10
P_{14}							×				1
P_{15}										×	1
P_{16}				×							1
P_{17}											0
P_{18}											0
P_{19}					×				×		2
P_{20}											0

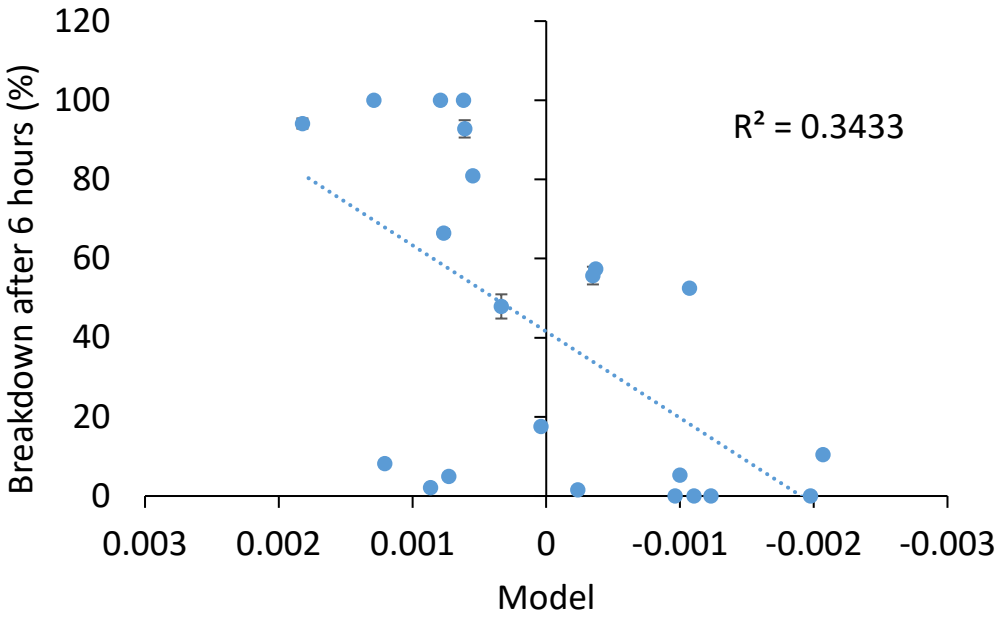

Figure S128: Model 31 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * (P12 * P5)$^{-1}$. R^2 = 0.3433.

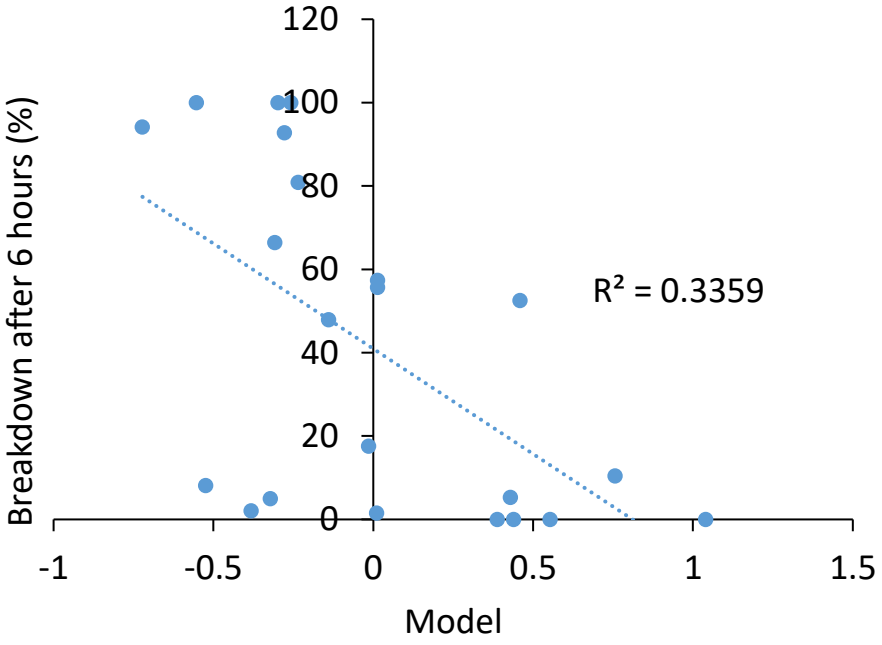

Figure S129: Model 32 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * P10 * (P5)$^{-1}$. R^2 = 0.3359.

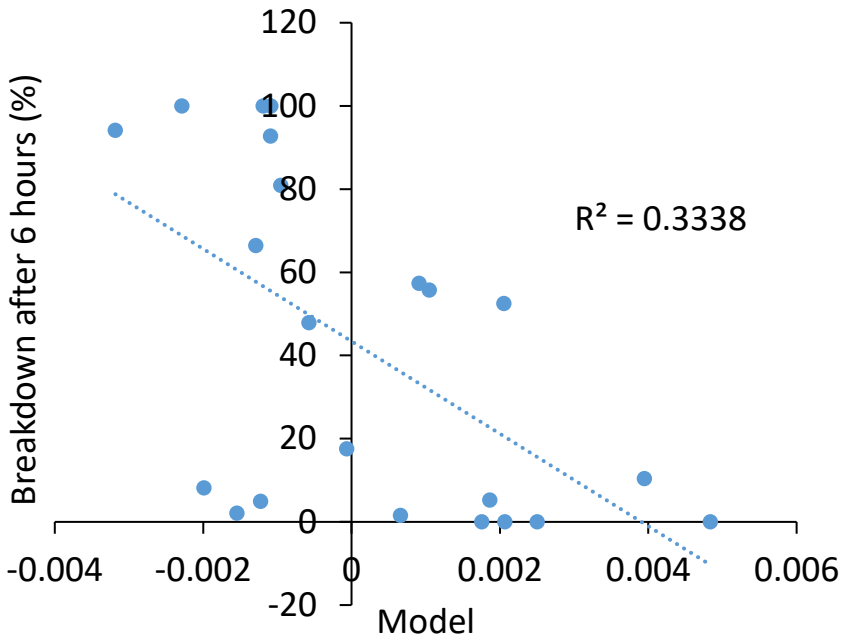

Figure S130: Model 33 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * (P5 * P19)$^{-1}$. R^2 = 0.3338.

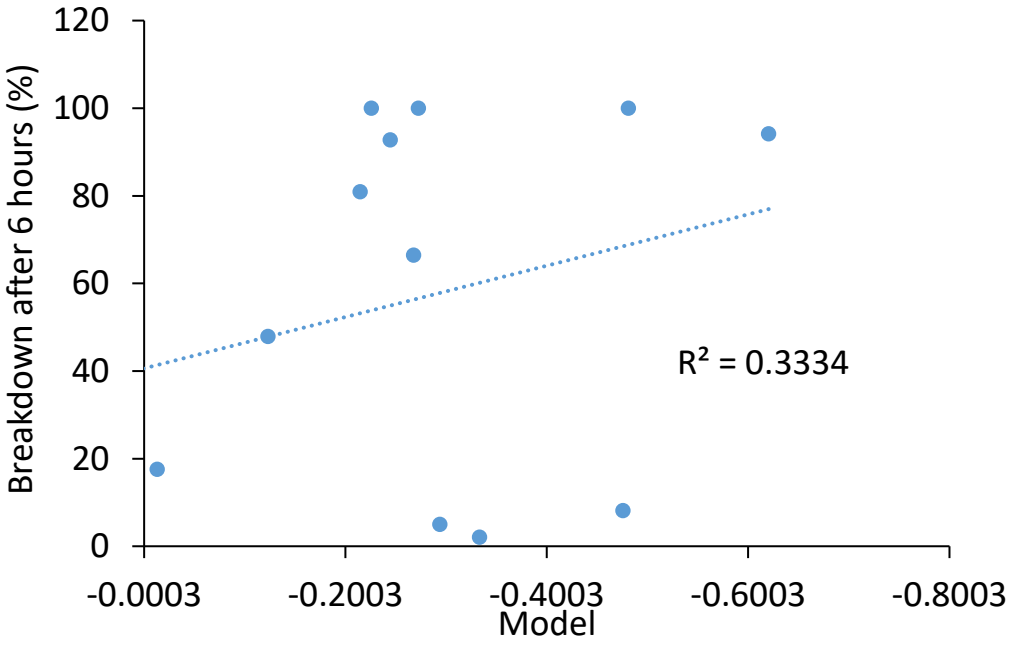

Figure S131: Model 34 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * P10 * (P6)$^{-1}$. R^2 = 0.3334.

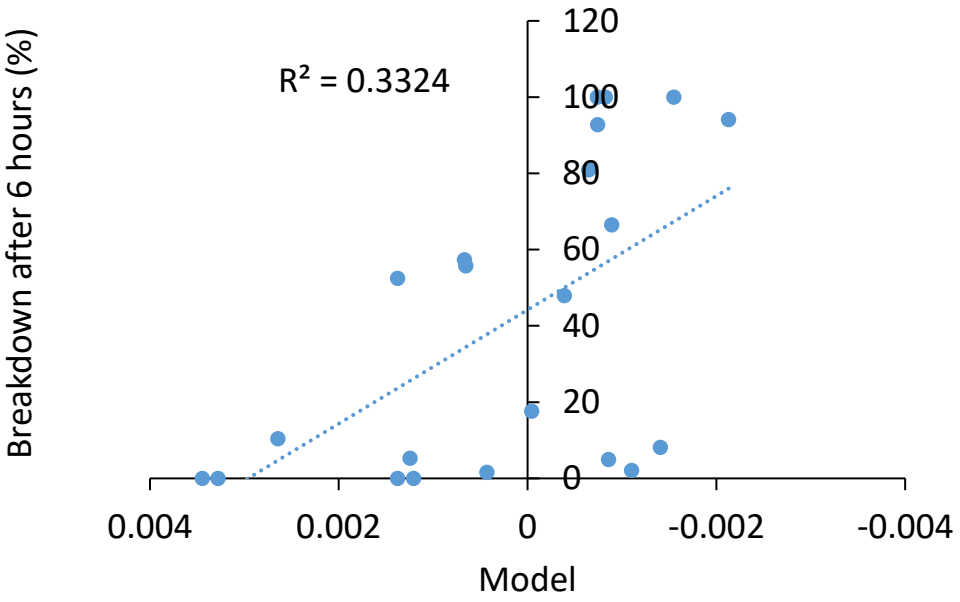

Figure S132: Model 35 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * (P5 * P16)$^{-1}$. R^2 = 0.3324.

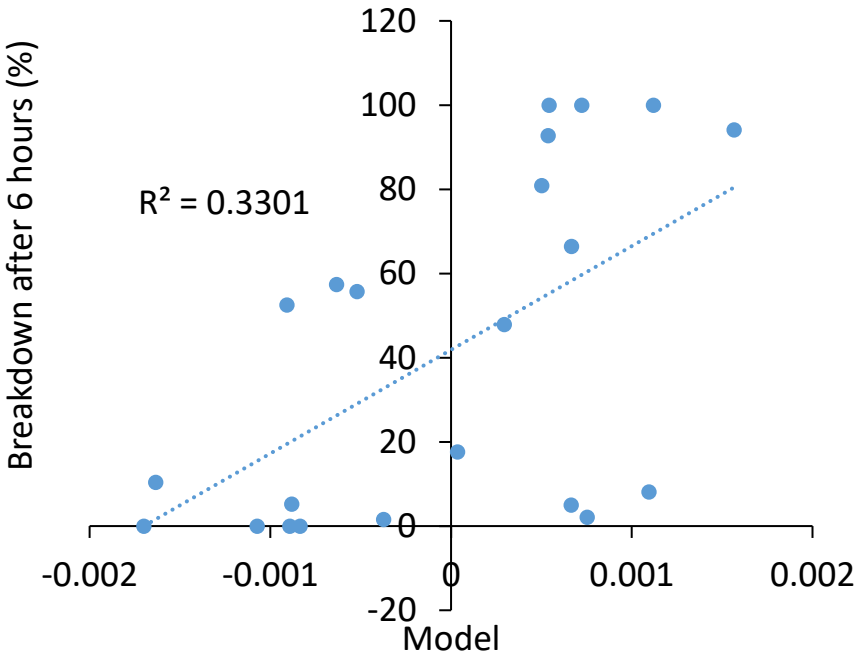

Figure S133: Model 36 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * (P12 * P6)$^{-1}$. R^2 = 0.3301.

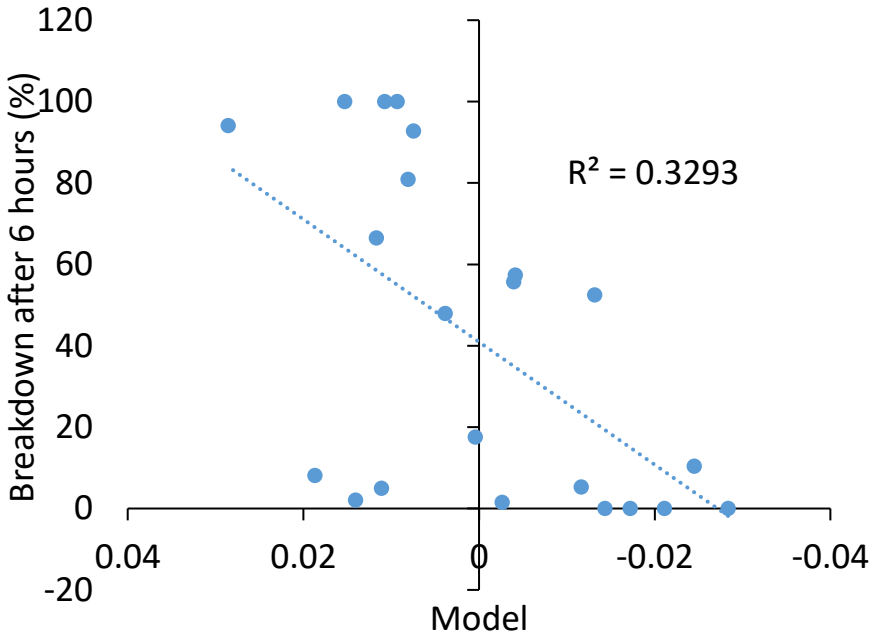

Figure S134: Model 37 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * (P5 * P15. R^2 = 0.3293.

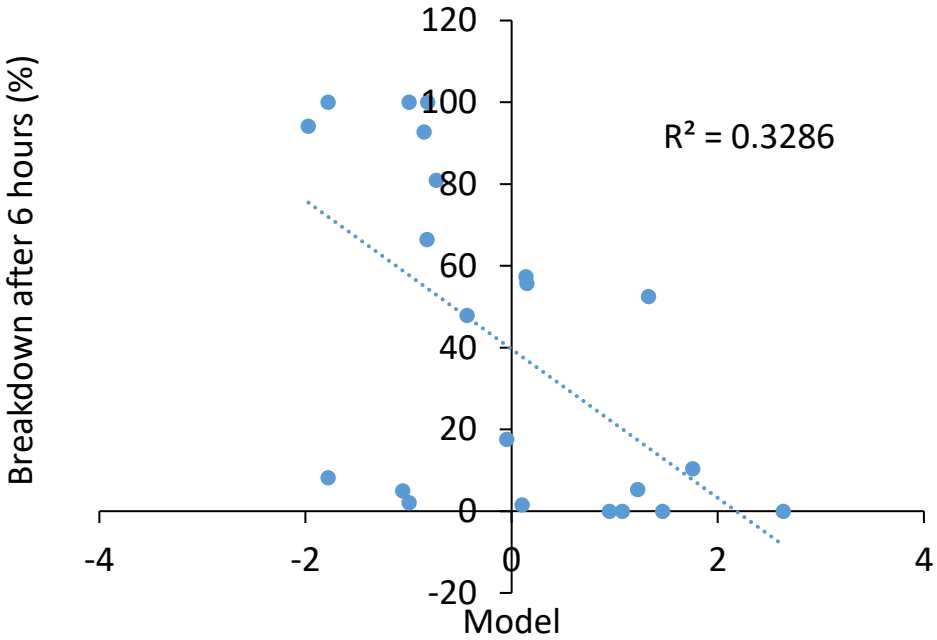

Figure S135: Model 38 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * P7 * $(P5)^{-1}$. R^2 = 0.3286.

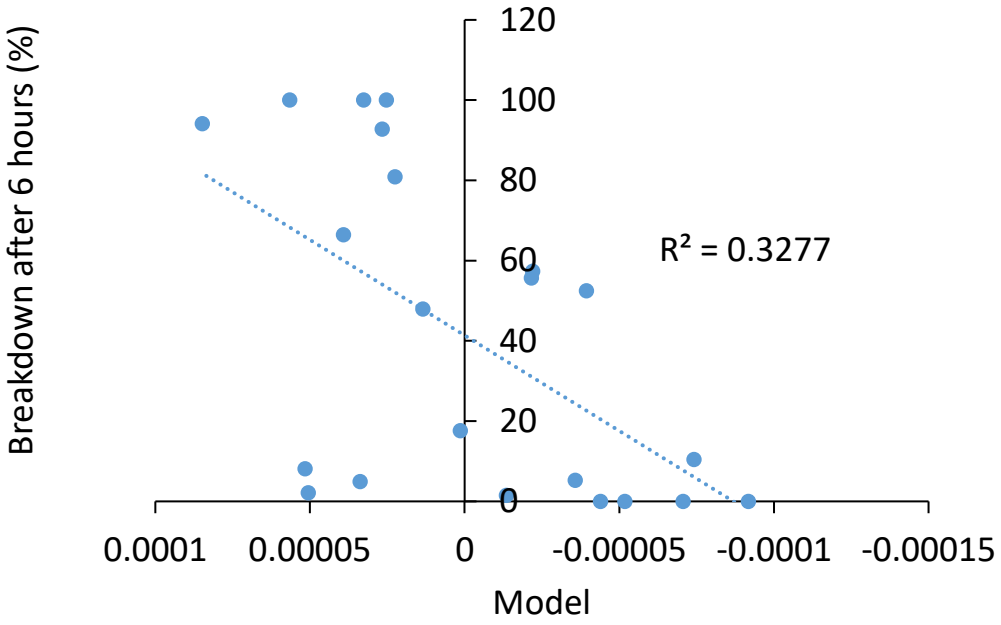

Figure S136: Model 39 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P5 * P2)^{-1}$. R^2 = 0.3277.

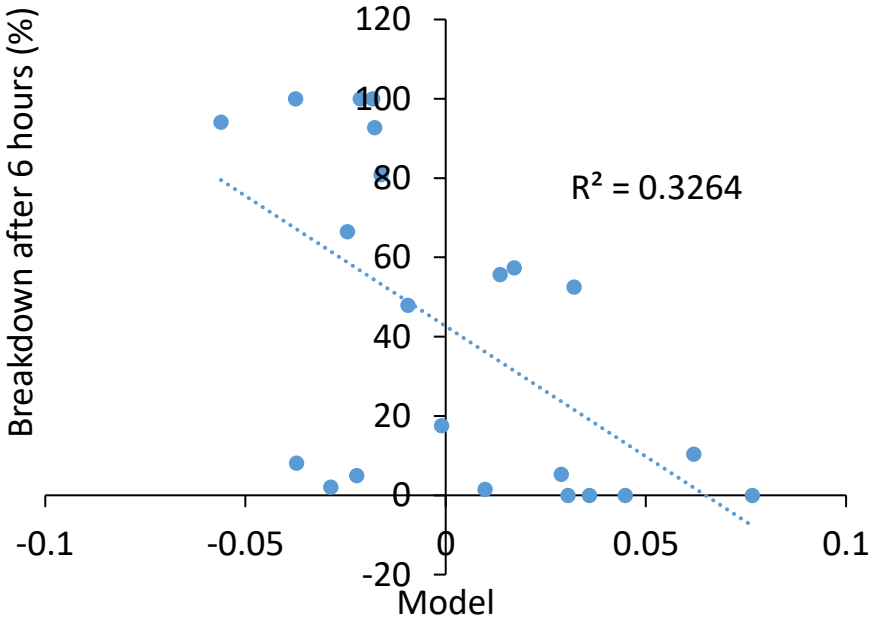

Figure S137: Model 40 vs breakdown after 6 hours (%). Model parameters are P0 = P19 * P13 * $(P5)^{-1}$. R^2 = 0.3264.

Table S12: Summary of the parameters used within models 31-40.

Parameter	Model Number										Total
	31	32	33	34	35	36	37	38	39	40	
R^2	0.3433	0.3359	0.3338	0.3334	0.3324	0.3301	0.3293	0.3286	0.3277	0.3264	
Equation	$P0 = P_x * (P_y * P_z)^{-1}$	$P0 = P_x * P_y * (P_z)^{-1}$	$P0 = P_x * (P_y * P_z)^{-}$	$P0 = P_x * P_y * (P_z)^{-1}$	$P0 = P_x * (P_y * P_z)^{-1}$	$P0 = P_x * (P_y * P_z)^{-1}$	$P0 = P_x * (P_y * P_z)^{-1}$	$P0 = P_x * P_y * (P_z)^{-1}$	$P0 = P_x * (P_y * P_z)^{-1}$	$P0 = P_x * P_y * (P_z)^{-1}$	
P_1											0
P_2									×		1
P_3											0
P_4											0
P_5	×	×	×		×		×	×	×	×	8
P_6				×		×					2
P_7								×			1
P_8											0
P_9											0
P_{10}		×		×							2
P_{11}											0
P_{12}	×					×					2
P_{13}	×	×	×	×	×	×	×	×	×	×	10
P_{14}											0
P_{15}							×				1
P_{16}					×						1
P_{17}											0
P_{18}											0
P_{19}			×							×	2
P_{20}											0

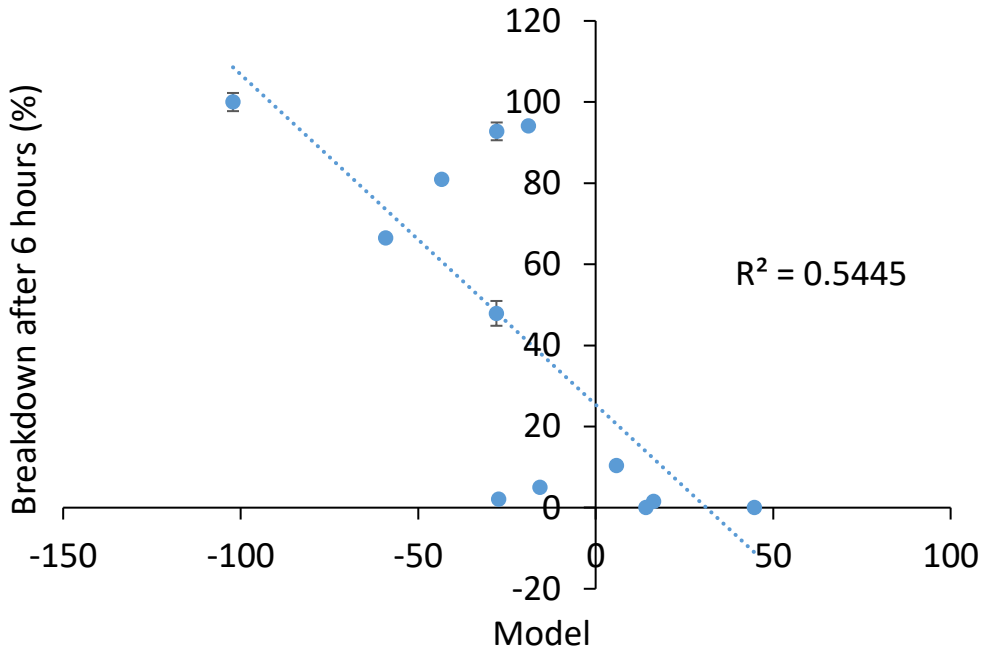

Figure S138: Model 41 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * $(P13)^{-1}$. R^2 = 0.5445.

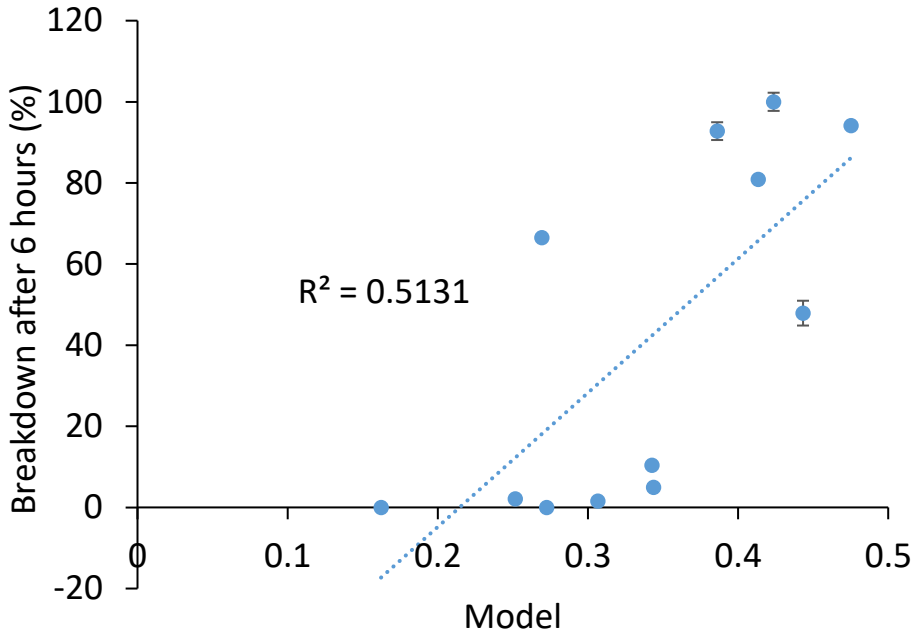

Figure S139: Model 42 vs breakdown after 6 hours (%). Model parameters are P0 = P8 * $(P3)^{-1}$. R^2 = 0.5131.

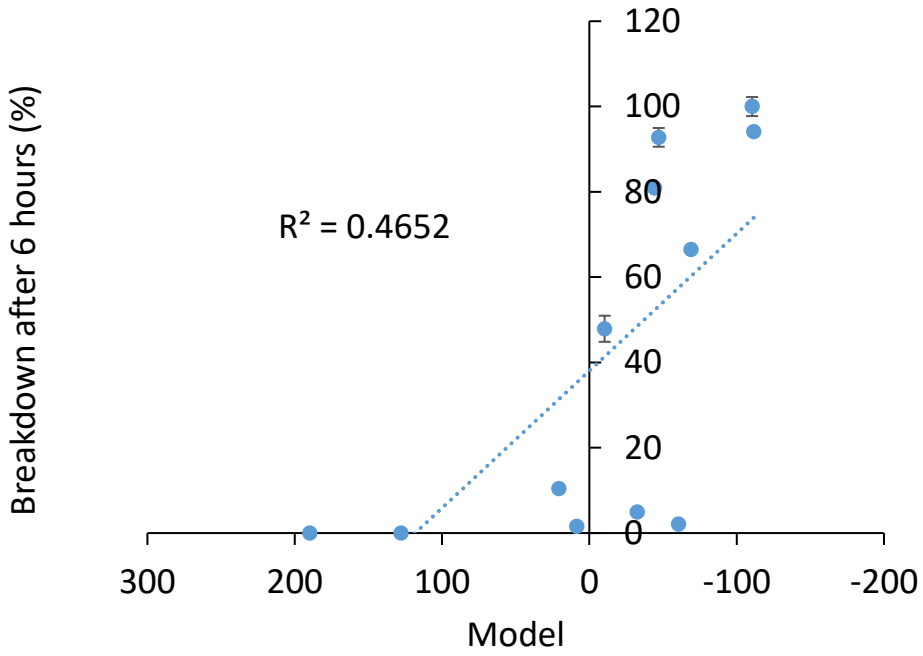

Figure S140: Model 43 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * $(P13)^{-1}$. R^2 = 0.4652.

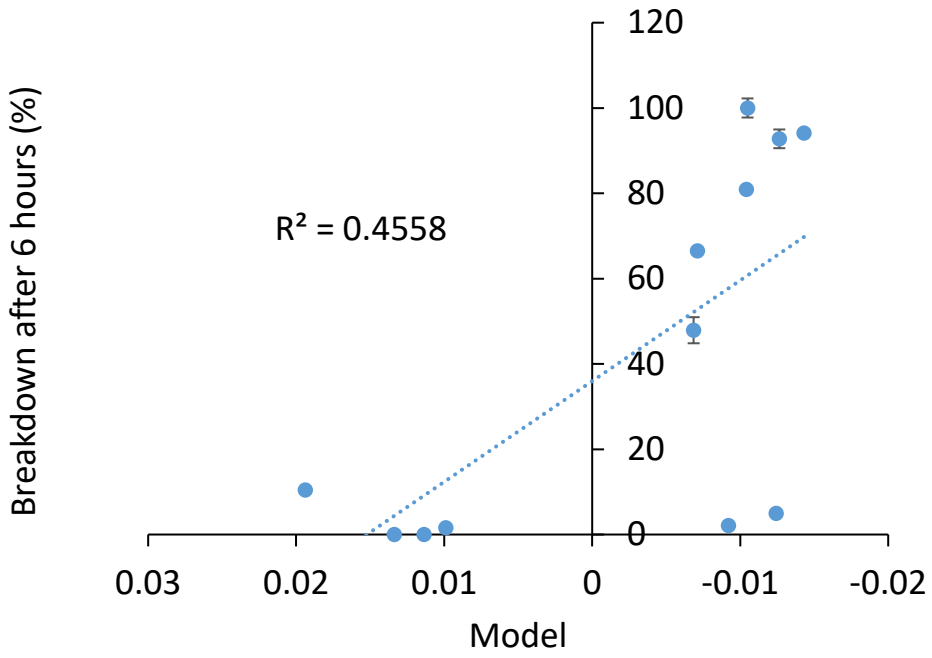

Figure S141: Model 44 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P3)^{-1}$. R^2 = 0.4558.

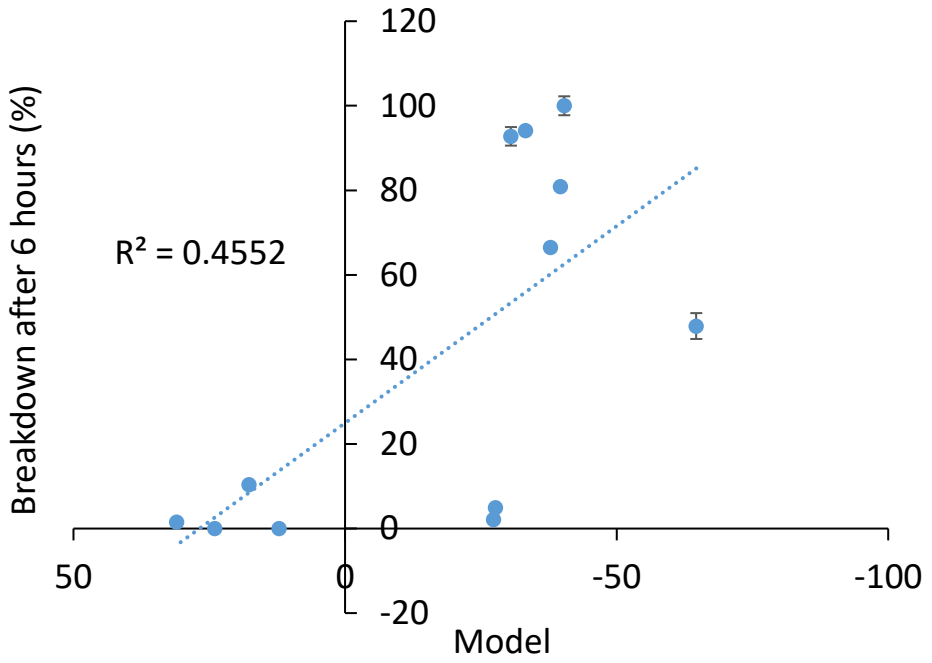

Figure S142: Model 45 vs breakdown after 6 hours (%). Model parameters are P0 = P8 * $(P13)^{-1}$. R^2 = 0.4552.

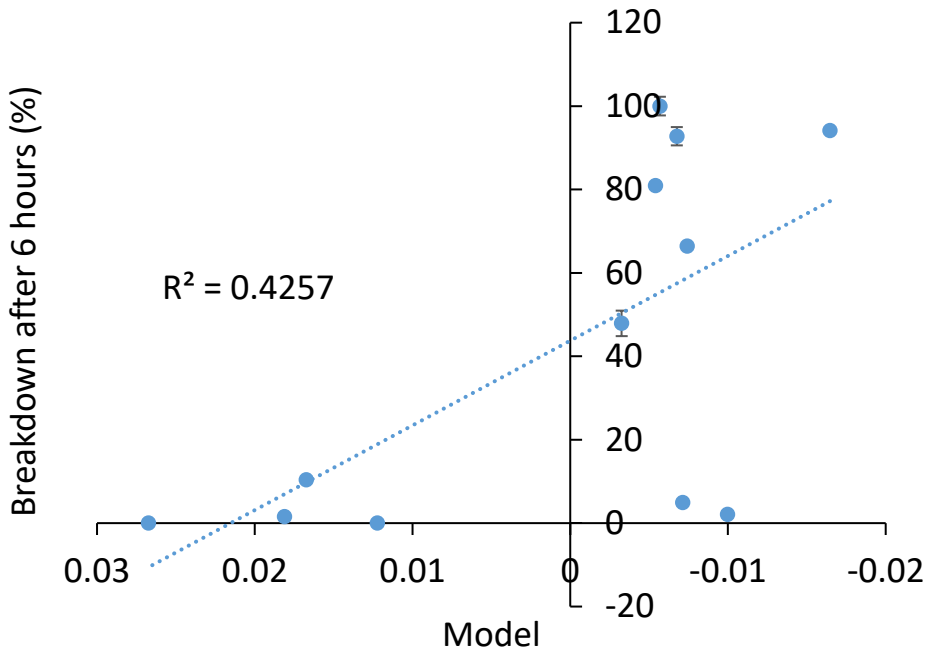

Figure S143: Model 46 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P7)^{-1}$. R^2 = 0.4257.

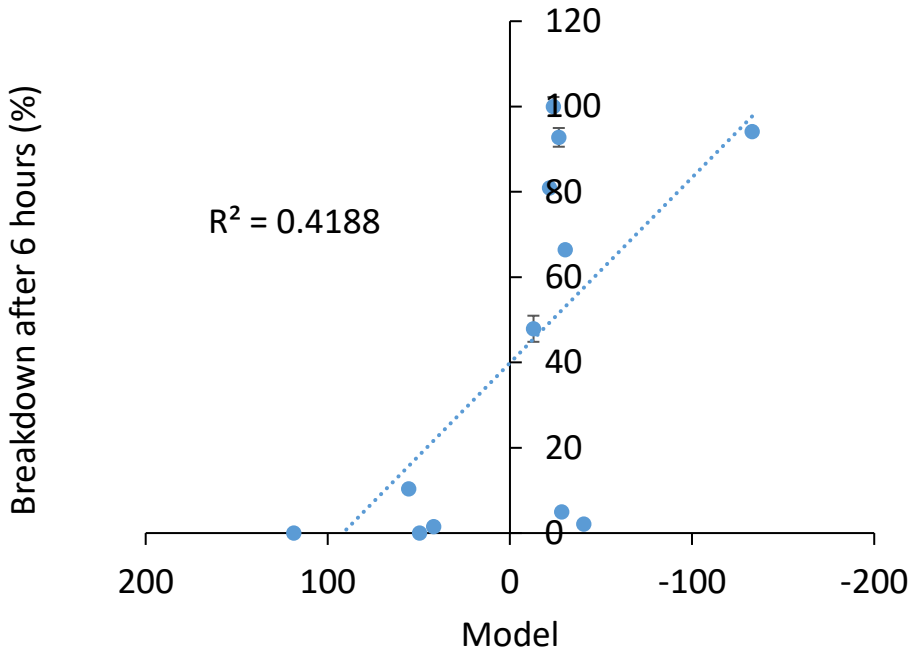

Figure S144: Model 47 vs breakdown after 6 hours (%). Model parameters are P0 = P9 * P13. R^2 = 0.4188.

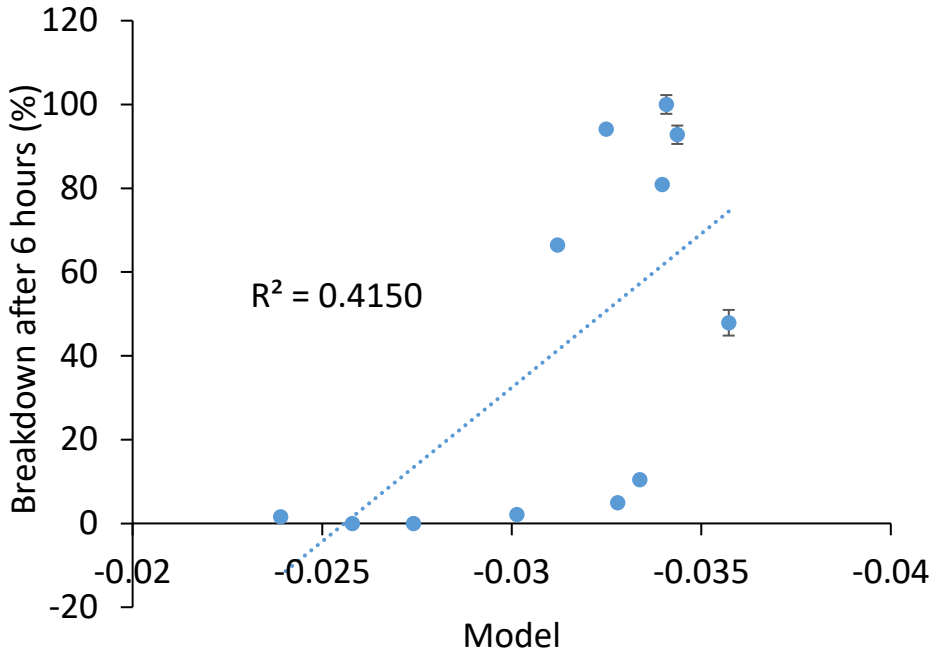

Figure S145: Model 48 vs breakdown after 6 hours (%). Model parameters are P0 = (P19 * P12)$^{-1}$. R^2 = 0.4150.

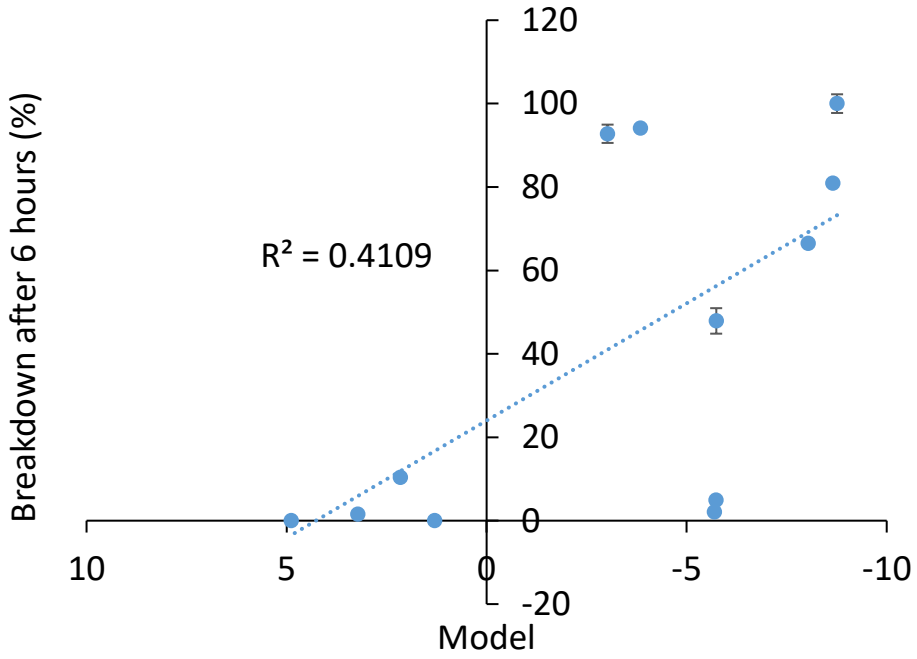

Figure S146: Model 49 vs breakdown after 6 hours (%). Model parameters are P0 = P11 * (P13)$^{-1}$. R^2 = 0.4109.

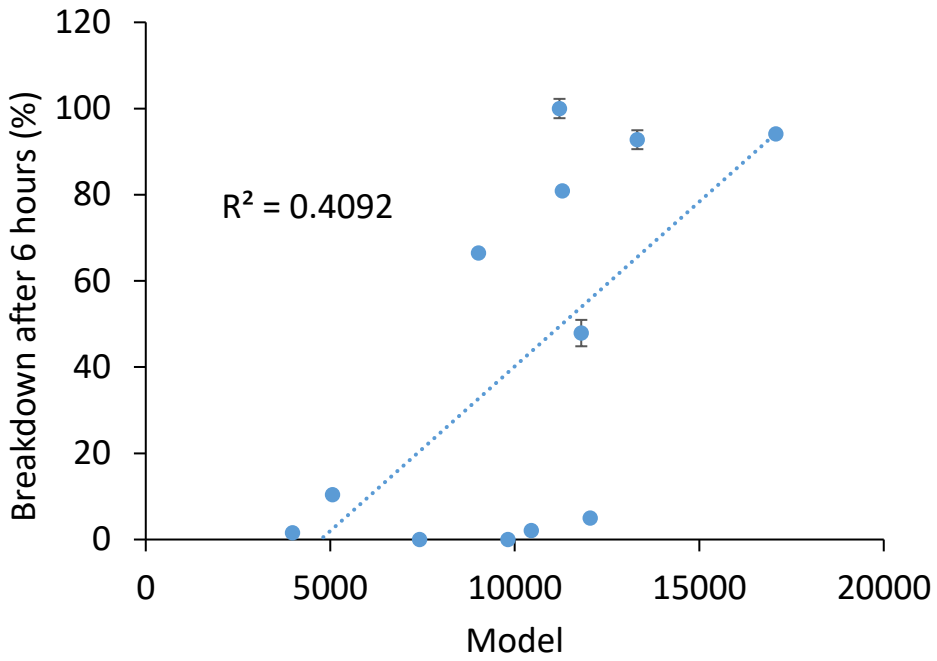

Figure S147: Model 50 vs breakdown after 6 hours (%). Model parameters are P0 = P6 * P8. R^2 = 0.4092.

Table S13: Summary of the parameters used within models 41-50.

Parameter	Model Number										Total
	41	42	43	44	45	46	47	48	49	50	
R^2	0.5445	0.5131	0.4652	0.4558	0.4552	0.4257	0.4189	0.4150	0.4109	0.4092	
Equation	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * P_y$	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * (P_y)^{-1}$	$P0 = P_x * P_y$	$P0 = (P_x * P_y)^{-1}$	$P0 = P_x * (P_y)^{-1}$	$P0 = (P_x * P_y)^{-1}$	
P_1	×		×								2
P_2											0
P_3		×		×							2
P_4											0
P_5											0
P_6										×	1
P_7						×					1
P_8		×			×					×	3
P_9											1
P_{10}							×				0
P_{11}									×		1
P_{12}								×			1
P_{13}	×		×	×	×	×	×		×		7
P_{14}											0
P_{15}											0
P_{16}											0
P_{17}											0
P_{18}											0
P_{19}								×			1
P_{20}											0

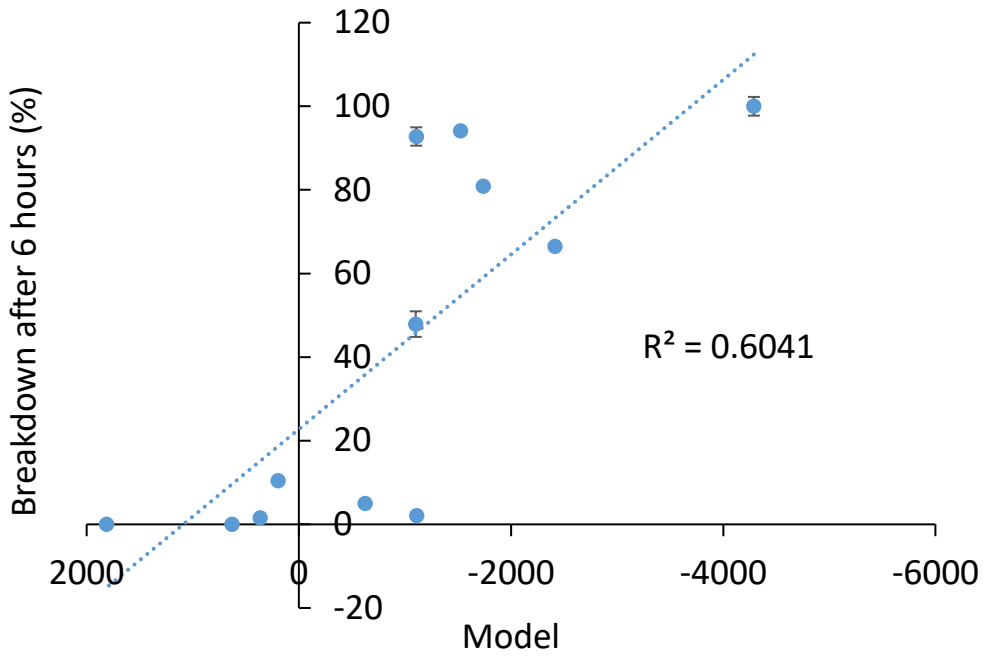

Figure S148: Model 51 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * P8 * $(P13)^{-1}$. R^2 = 0.6041.

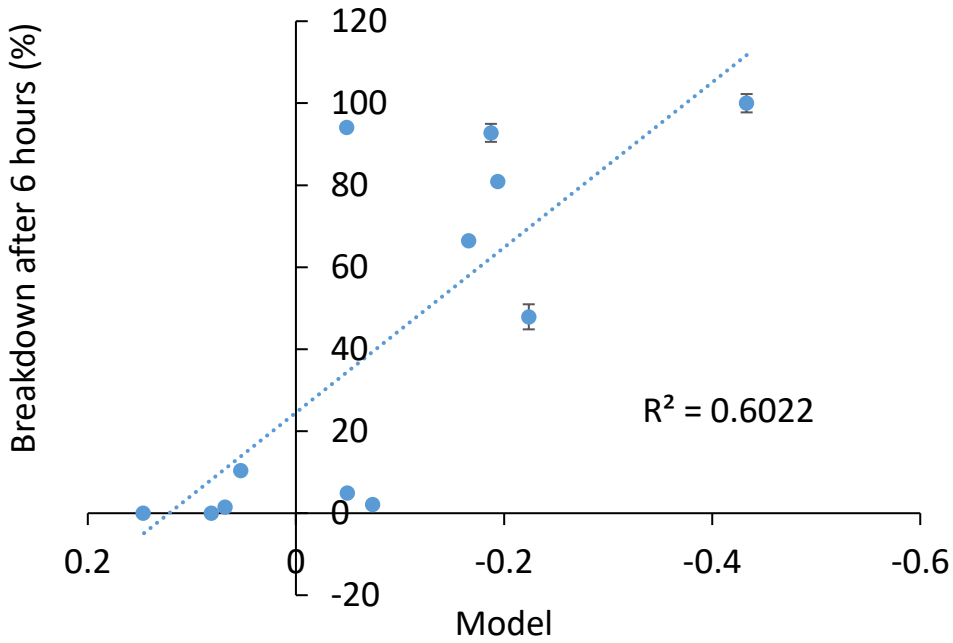

Figure S149: Model 52 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * (P4 * P13)$^{-1}$. R^2 = 0.6022.

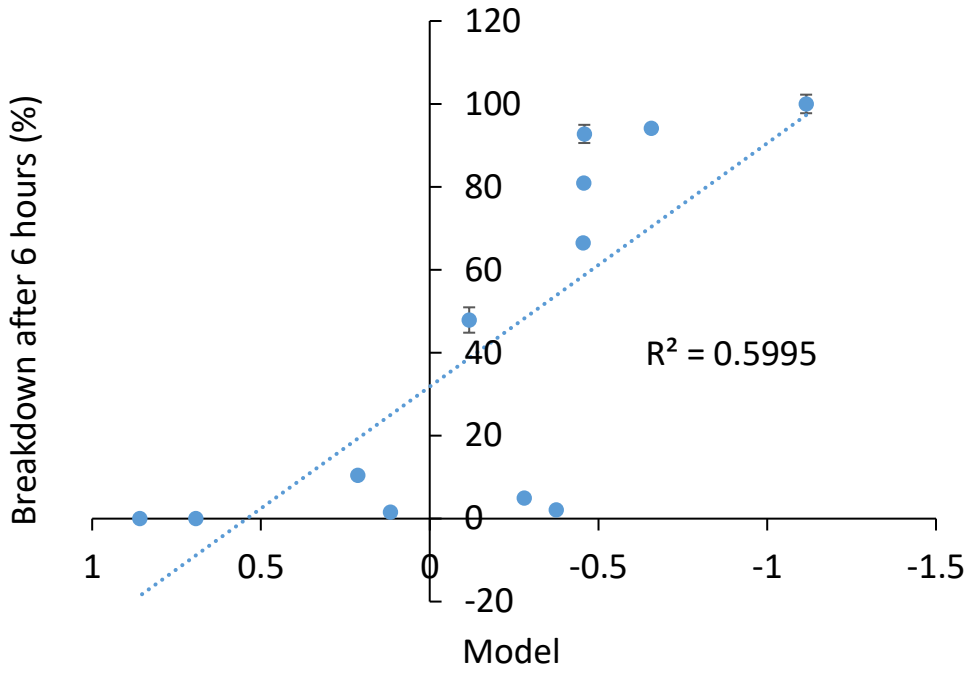

Figure S150: Model 53 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * P13 * $(P3)^{-1}$. R^2 = 0.5995.

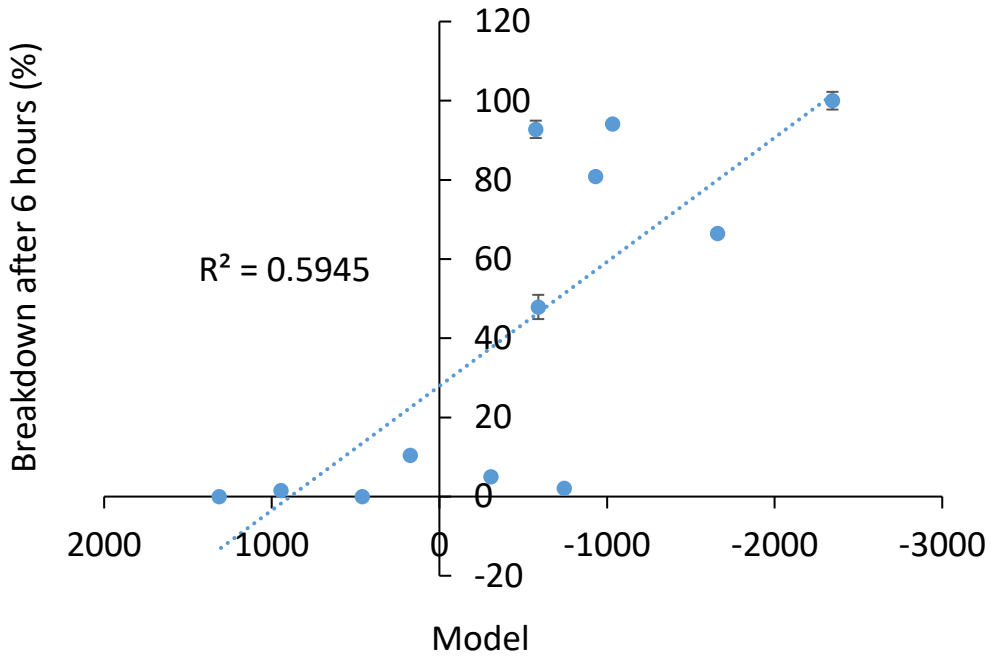

Figure S151: Model 54 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * P9 * $(P13)^{-1}$. R^2 = 0.5945.

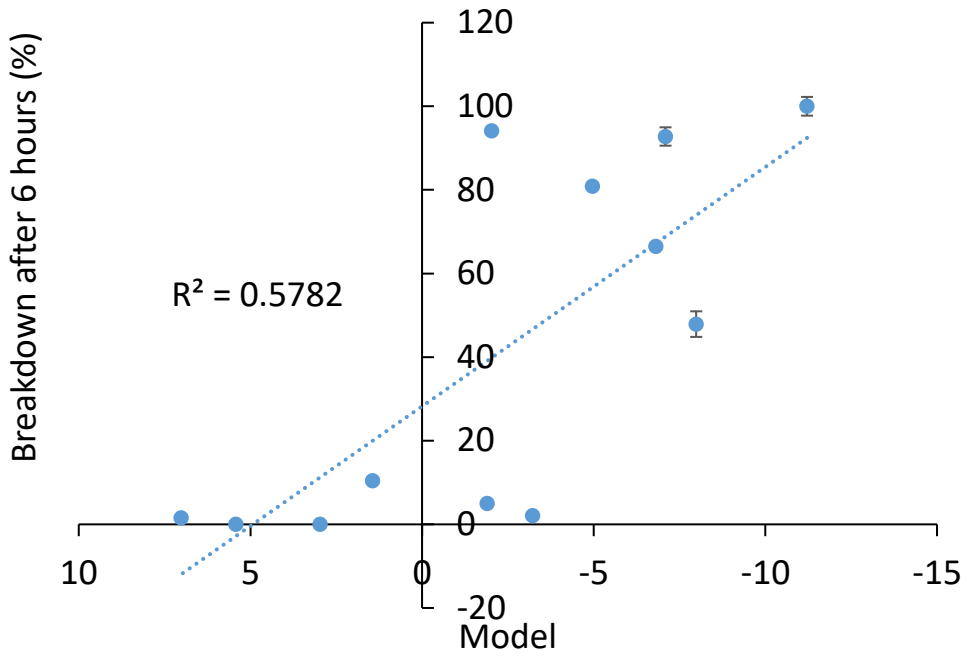

Figure S152: Model 55 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * (P11 * P13)$^{-1}$. R^2 = 0.5782.

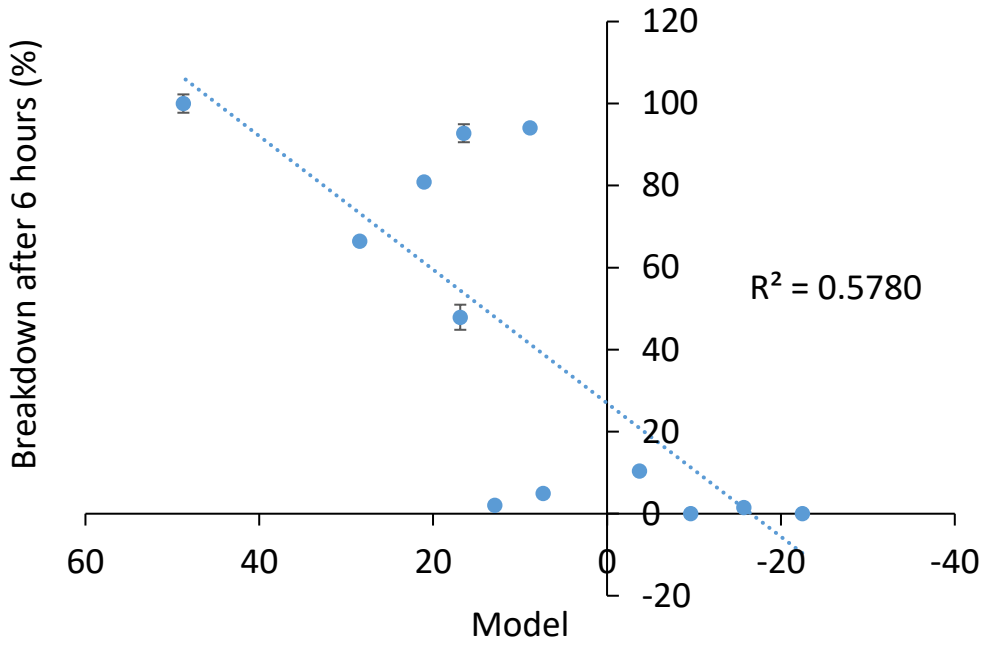

Figure S153: Model 56 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * P15 * (P13)$^{-1}$. R^2 = 0.5780.

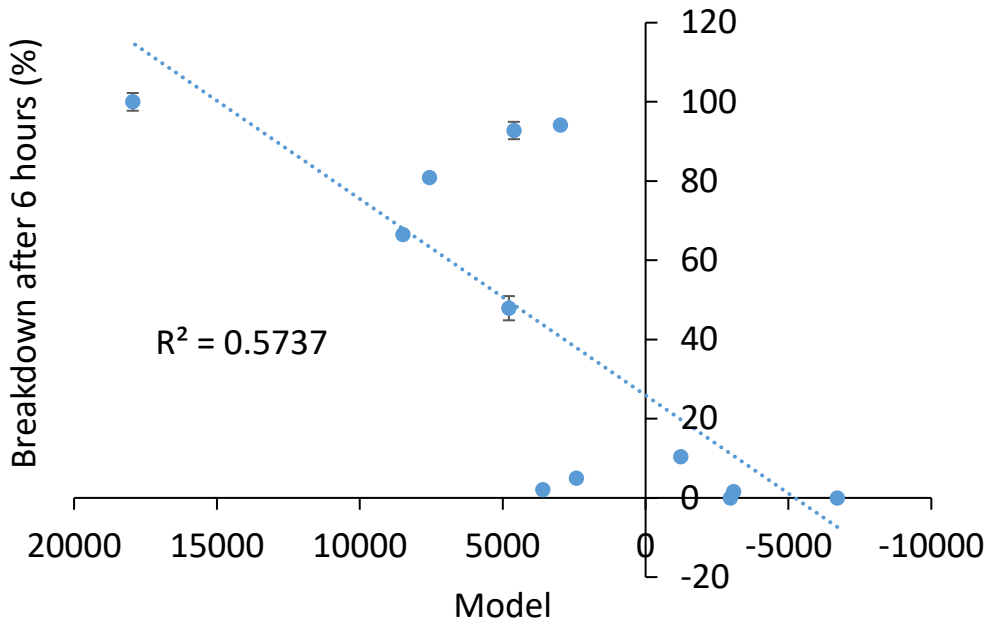

Figure S154: Model 57 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * P2 * $(P13)^{-1}$. R^2 = 0.5737.

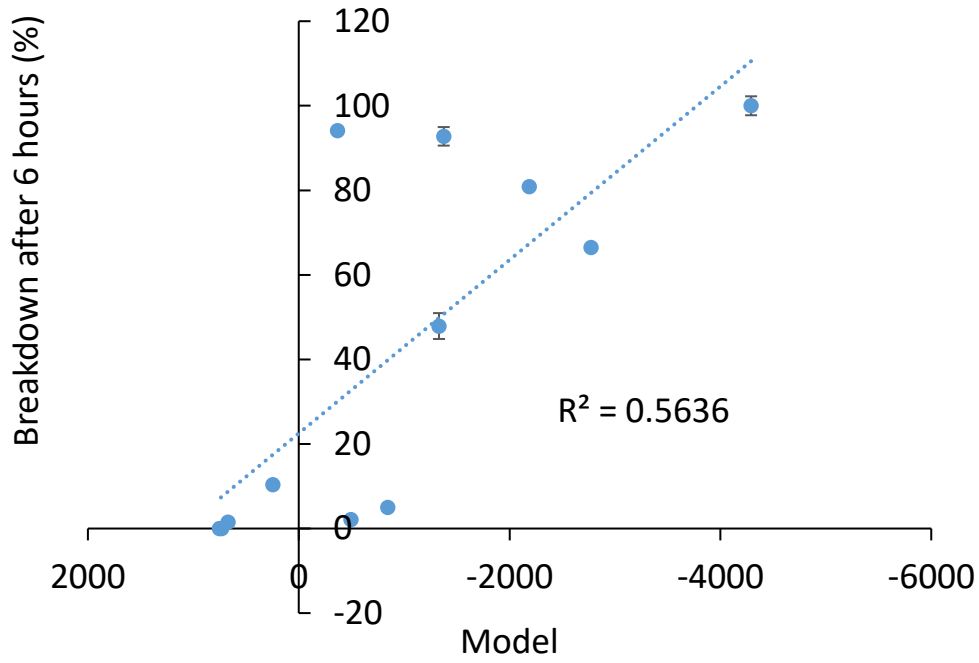

Figure S155: Model 58 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * P20 * $(P13)^{-1}$. R^2 = 0.5636.

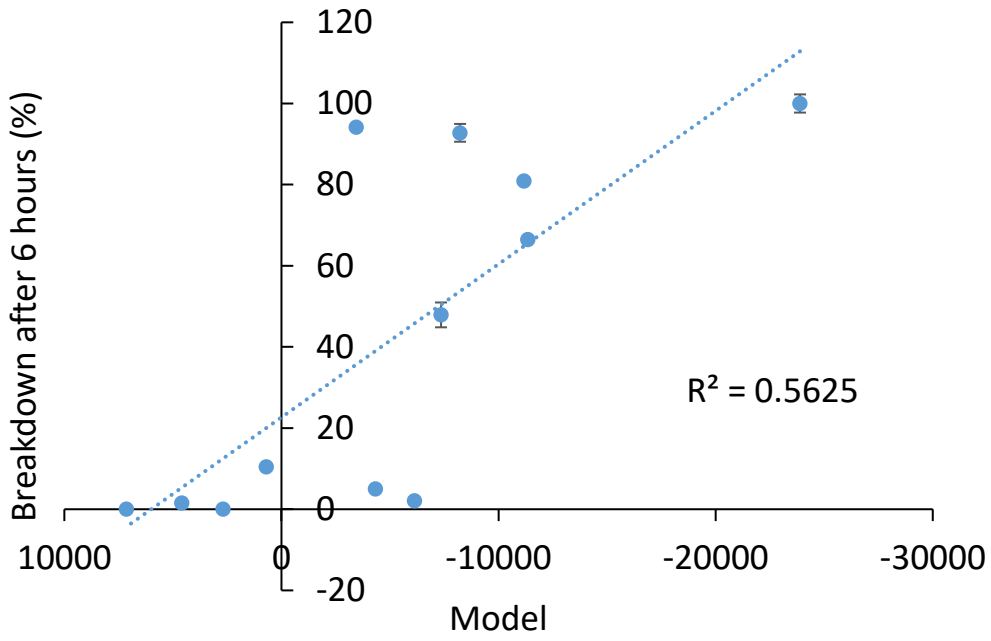

Figure S156: Model 59 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * P5 * $(P13)^{-1}$. R^2 = 0.5625.

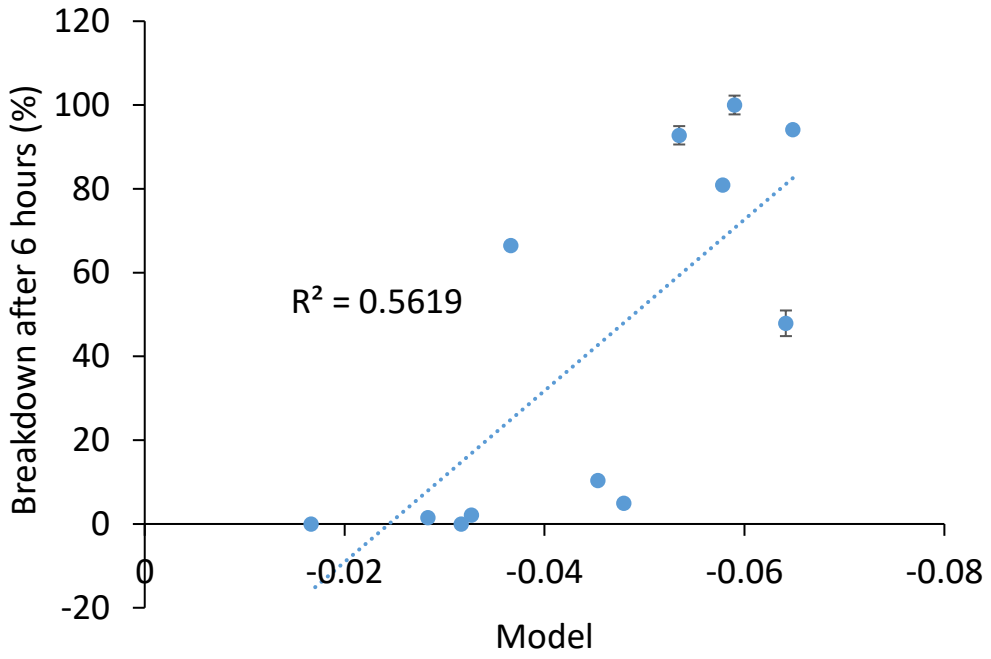

Figure S157: Model 60 vs breakdown after 6 hours (%). Model parameters are P0 = P8 * (P3 * P12)$^{-1}$. R^2 = 0.5619.

Table S14: Summary of the parameters used within models 51-60.

Parameter	Model Number										Total
	51	52	53	54	55	56	57	58	59	60	
R^2	0.6041	0.6022	0.5995	0.5945	0.5782	0.5780	0.5737	0.5636	0.5625	0.5619	
Equation	$P0 = P_X * P_Y * (P_Z)^{-1}$	$P0 = P_X * (P_Y * P_Z)^{-1}$	$P0 = P_X * P_Y * (P_Z)^{-1}$	$P0 = P_X * P_Y * (P_Z)^{-1}$	$P0 = P_X * (P_Y * P_Z)^{-1}$	$P0 = P_X * P_Y * (P_Z)^{-1}$	$P0 = P_X * P_Y * (P_Z)^{-1}$	$P0 = P_X * P_Y * (P_Z)^{-1}$	$P0 = P_X * P_Y * (P_Z)^{-1}$	$P0 = P_X * (P_Y * P_Z)^{-1}$	
P_1	×	×	×	×	×	×	×	×	×		9
P_2							×				1
P_3			×							×	2
P_4		×									1
P_5									×		1
P_6											0
P_7											0
P_8	×									×	2
P_9				×							1
P_{10}											0
P_{11}					×						1
P_{12}										×	1
P_{13}	×	×	×	×	×	×	×	×	×		9
P_{14}											0
P_{15}						×					1
P_{16}											0
P_{17}											0
P_{18}											0
P_{19}											0
P_{20}								×			1

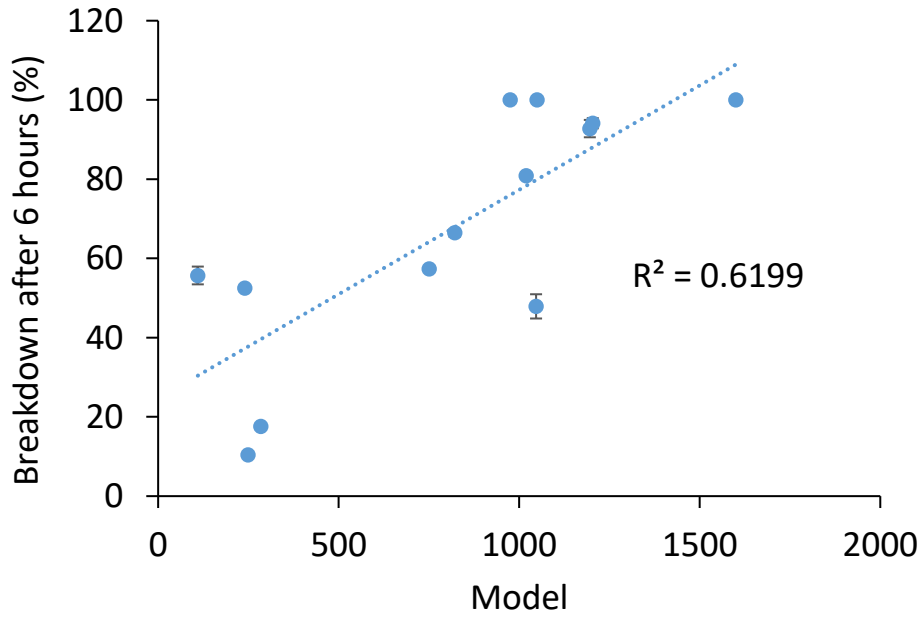

Figure S158: Model 61 vs breakdown after 6 hours (%). Model parameters are P0 = P5 * P18. R^2 = 0.6199.

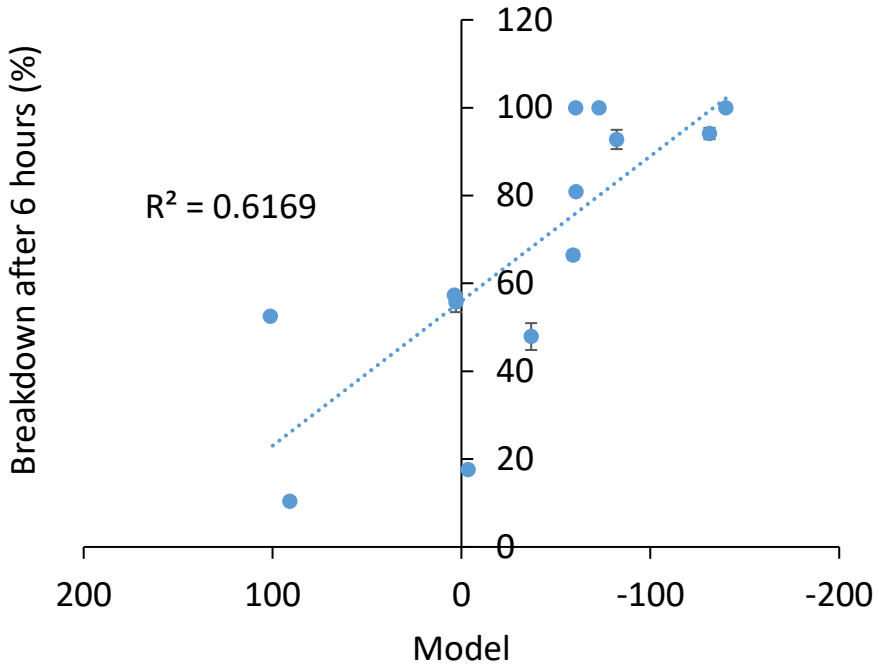

Figure S159: Model 62 vs breakdown after 6 hours (%). Model parameters are P0 = P10 * P13. R^2 = 0.6169.

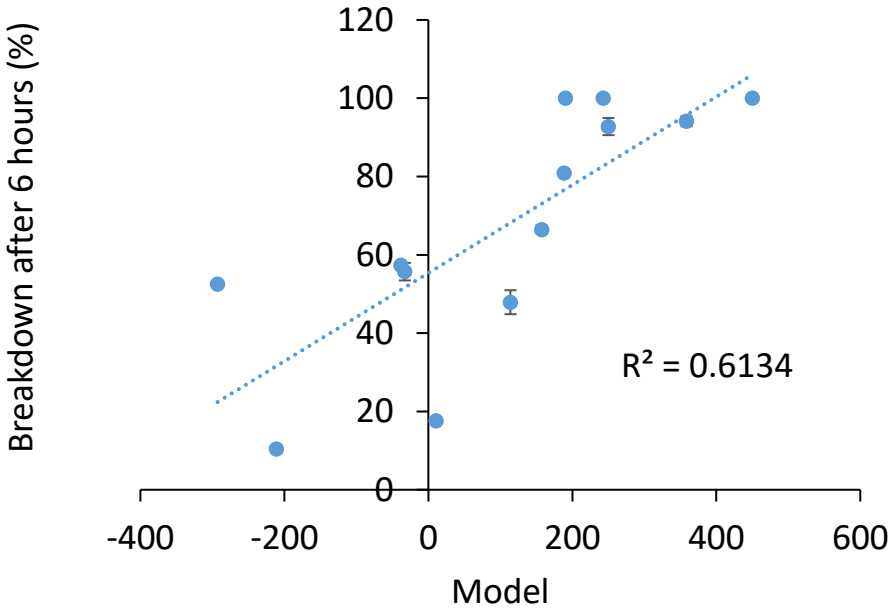

Figure S160: Model 63 vs breakdown after 6 hours (%). Model parameters are P0 = P7 * P13. R^2 = 0.6134.

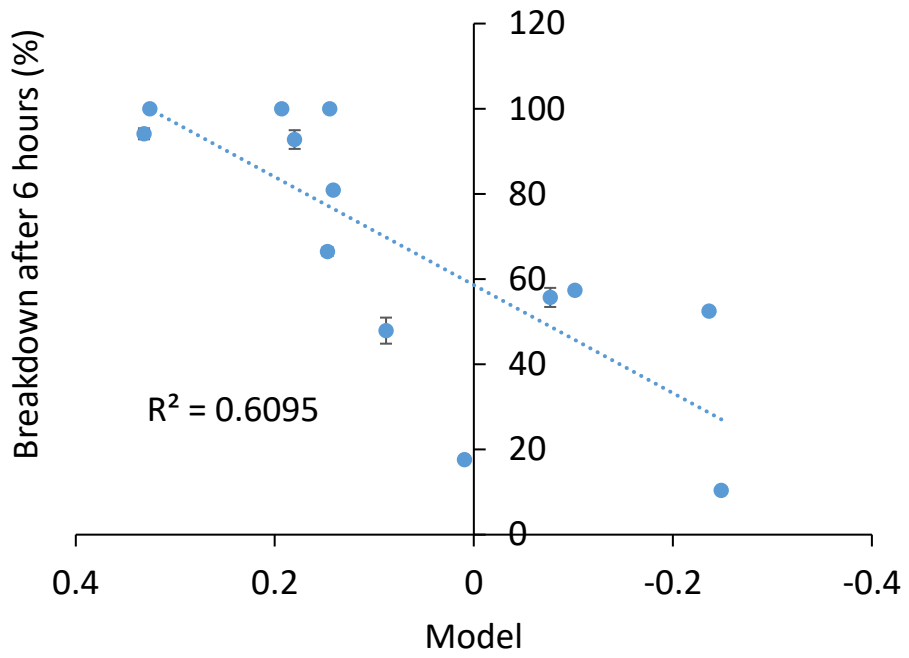

Figure S161: Model 64 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P12)^{-1}$. R^2 = 0.6095.

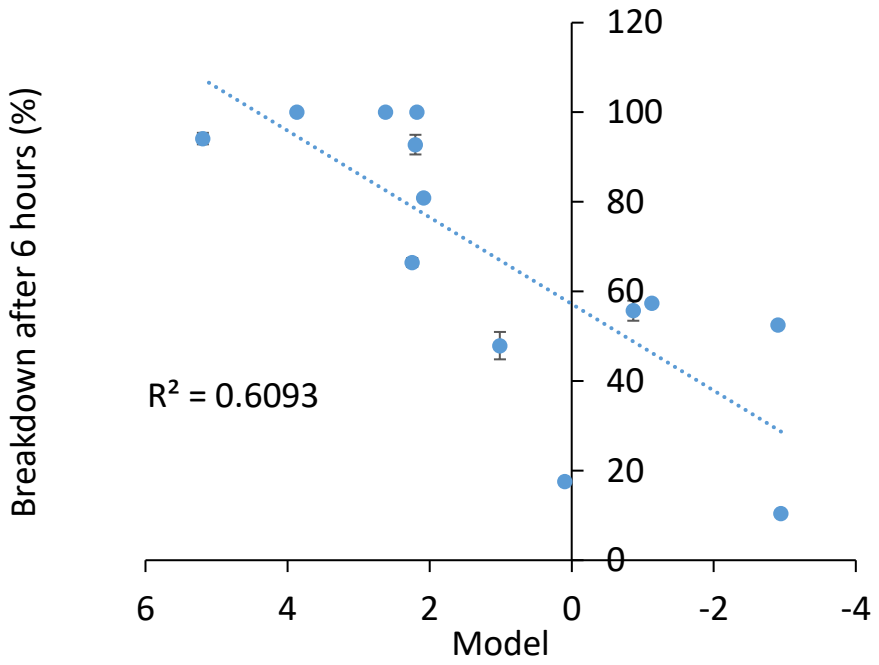

Figure S162: Model 65 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P15)^{-1}$. R^2 = 0.6093.

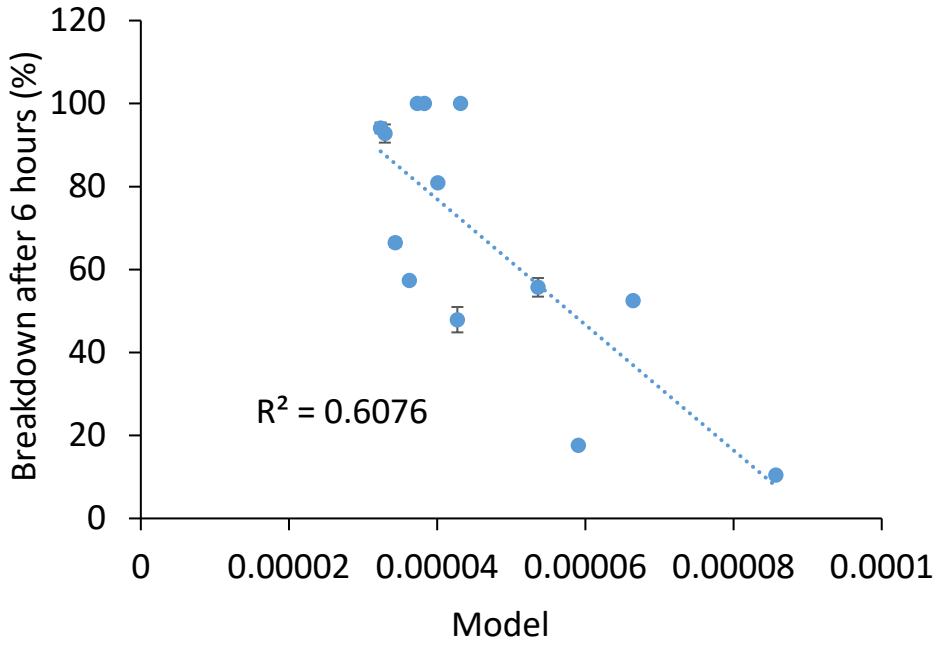

Figure S163: Model 66 vs breakdown after 6 hours (%). Model parameters are P0 = (P5 * P3)$^{-1}$. R^2 = 0.6076.

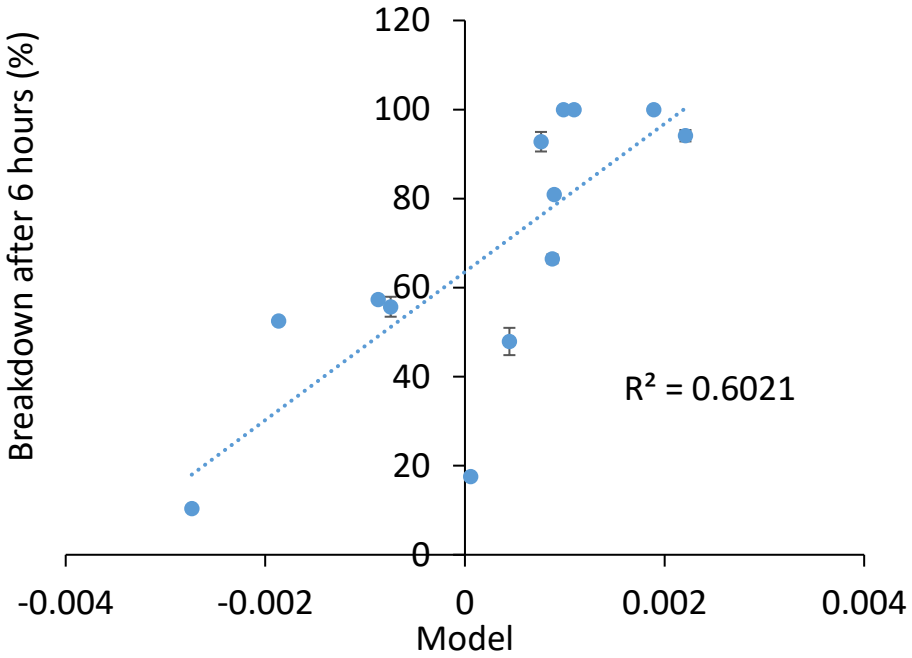

Figure S164: Model 67 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * (P14)$^{-1}$. R^2 = 0.6021.

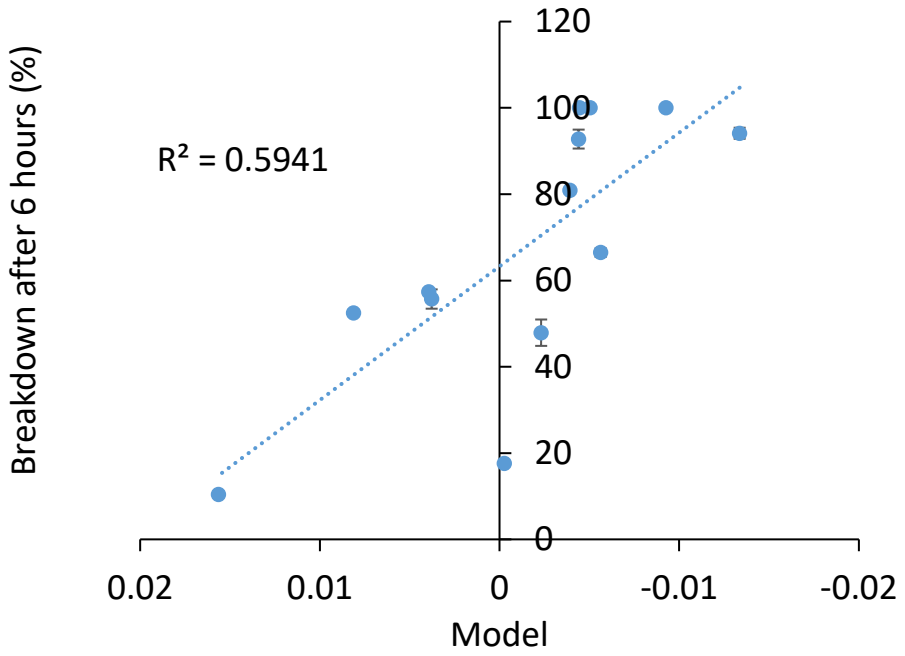

Figure S165: Model 68 vs breakdown after 6 hours (%). Model parameters are P0 = P13 * $(P5)^{-1}$. R^2 = 0.5941.

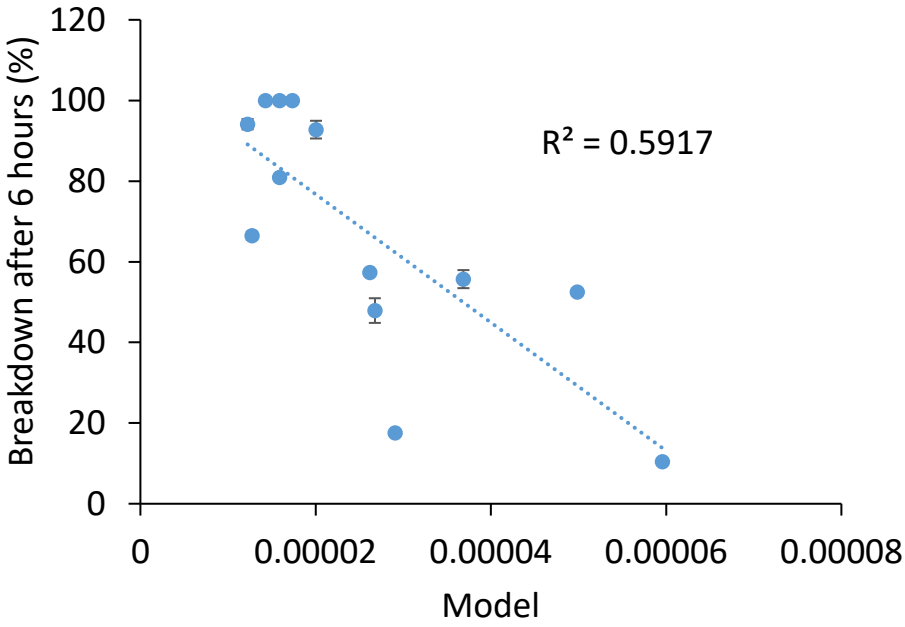

Figure S166: Model 69 vs breakdown after 6 hours (%). Model parameters are P0 = (P6 * $P4)^{-1}$. R^2 = 0.5917.

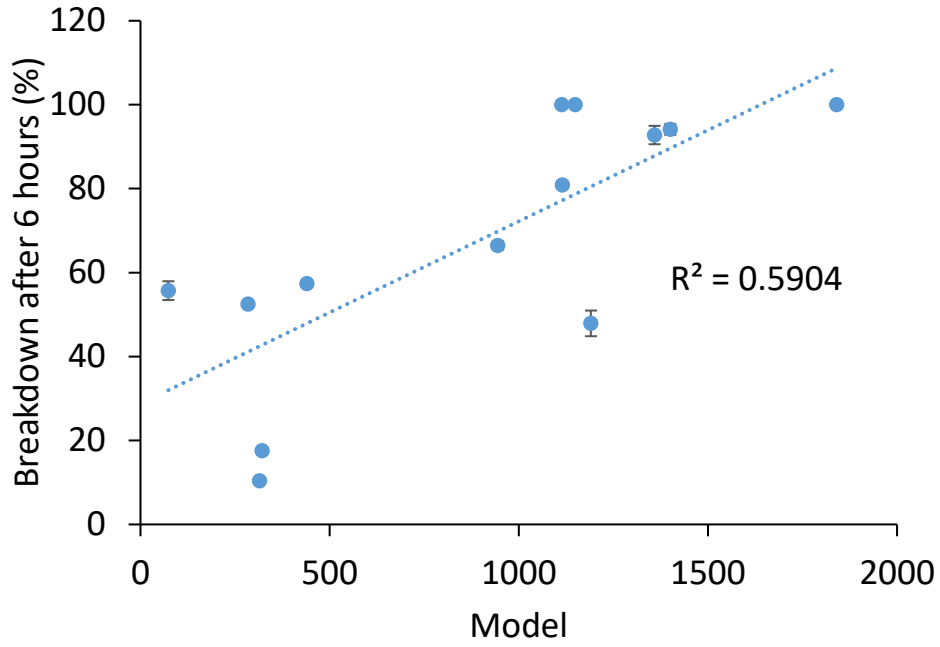

Figure S167: Model 70 vs breakdown after 6 hours (%). Model parameters are P0 = P6 * P18. R^2 = 0.5904.

Table S15: Summary of the parameters used within models 61-70.

Parameter	Model Number										Total
	61	62	63	64	65	66	67	68	69	70	
R^2	0.6199	0.6169	0.6134	0.6095	0.6093	0.6076	0.6021	0.5941	0.5917	0.5904	
Equation	$P0 = P_X * P_Y$	$P0 = P_X * P_Y$	$P0 = P_X * P_Y$	$P0 = P_X * (P_Y)^{-1}$	$P0 = P_X * (P_Y)^{-1}$	$P0 = (P_X * P_Y)^{-1}$	$P0 = P_X * (P_Y)^{-1}$	$P0 = P_X * (P_Y)^{-1}$	$P0 = (P_X * P_Y)^{-1}$	$P0 = P_X * P_Y$	
P_1											0
P_2											0
P_3						×					1
P_4									×		1
P_5	×					×		×			3
P_6									×	×	2
P_7			×								1
P_8											0
P_9											0
P_{10}		×									1
P_{11}											0
P_{12}				×							1
P_{13}		×	×	×	×		×	×			6
P_{14}							×				1
P_{15}					×						1
P_{16}											0
P_{17}											0
P_{18}	×									×	2
P_{19}											0
P_{20}											0

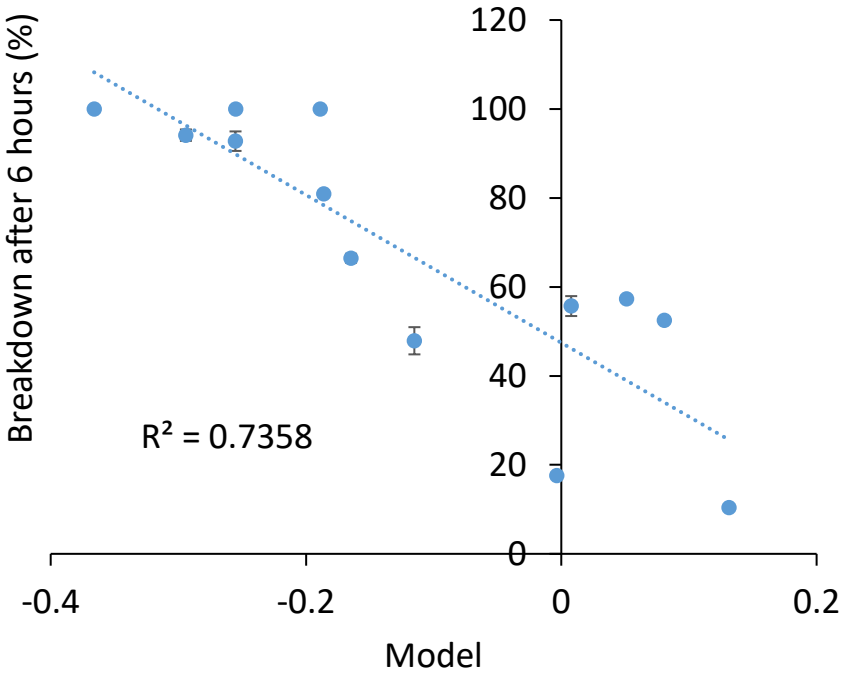

Figure S168: Model 71 vs breakdown after 6 hours (%). Model parameters are P0 = P18 * P13 * $(P9)^{-1}$. R^2 = 0.7358.

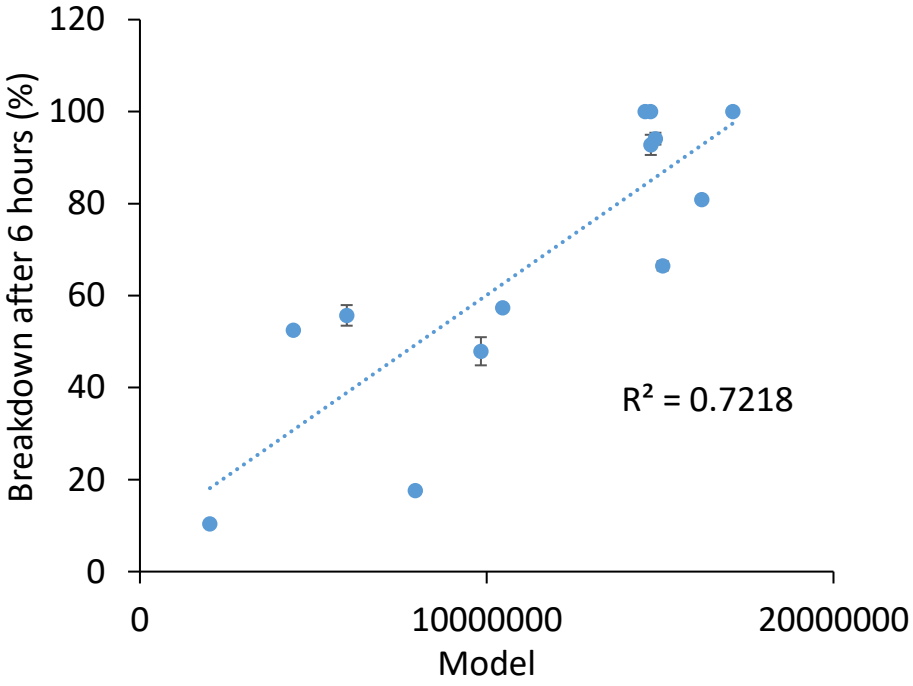

Figure S169: Model 72 vs breakdown after 6 hours (%). Model parameters are P0 = P4 * P5 * P6. R^2 = 0.7218.

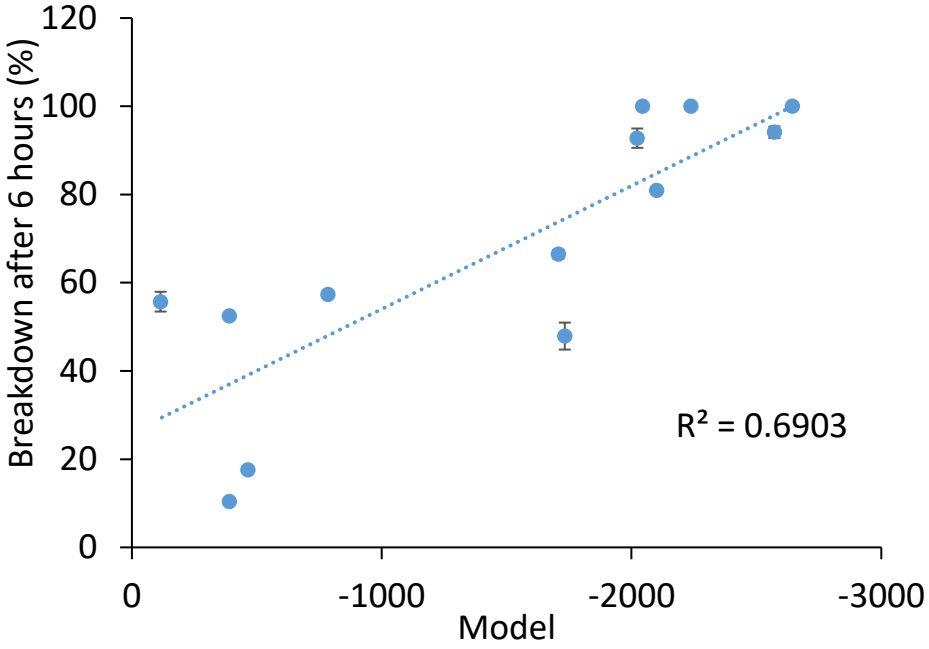

Figure S170: Model 73 vs breakdown after 6 hours (%). Model parameters are P0 = P5 * P18 * $(P15)^{-1}$. R^2 = 0.6903.

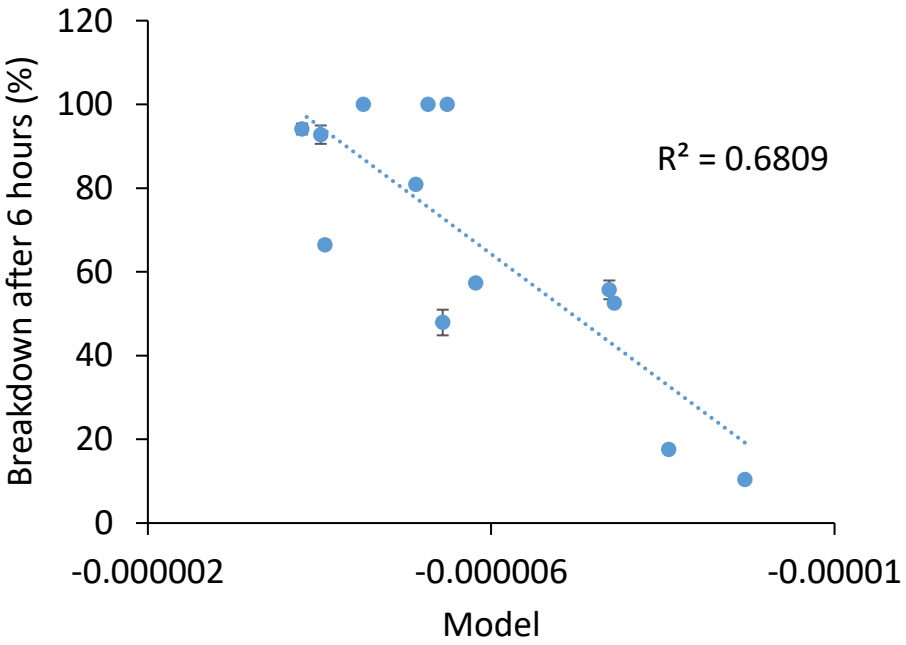

Figure S171: Model 74 vs breakdown after 6 hours (%). Model parameters are P0 = (P3 * P6 * P12)$^{-1}$. R^2 = 0.6809.

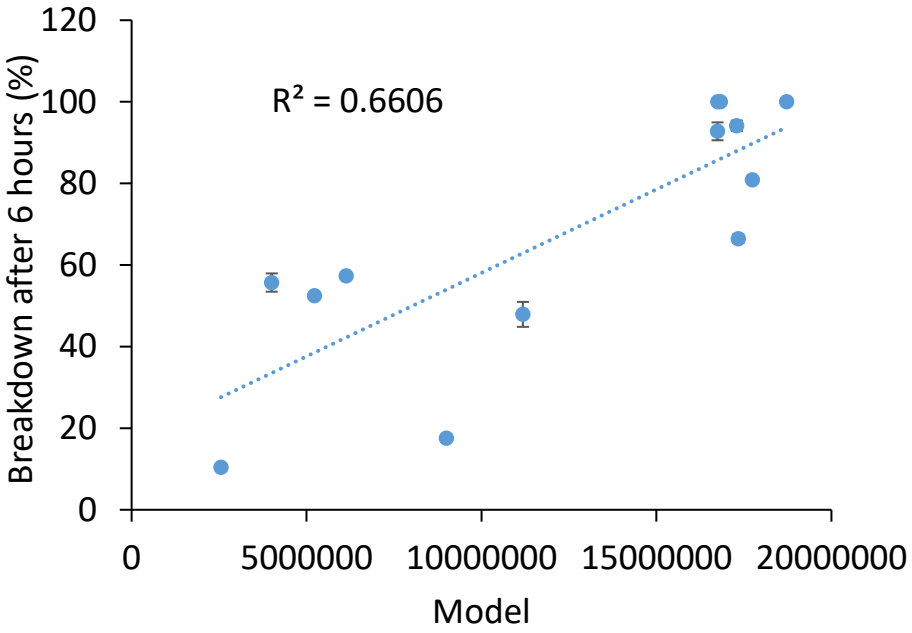

Figure S172: Model 75 vs breakdown after 6 hours (%). Model parameters are P0 = P6 * P6 * P4. R^2 = 0.6606.

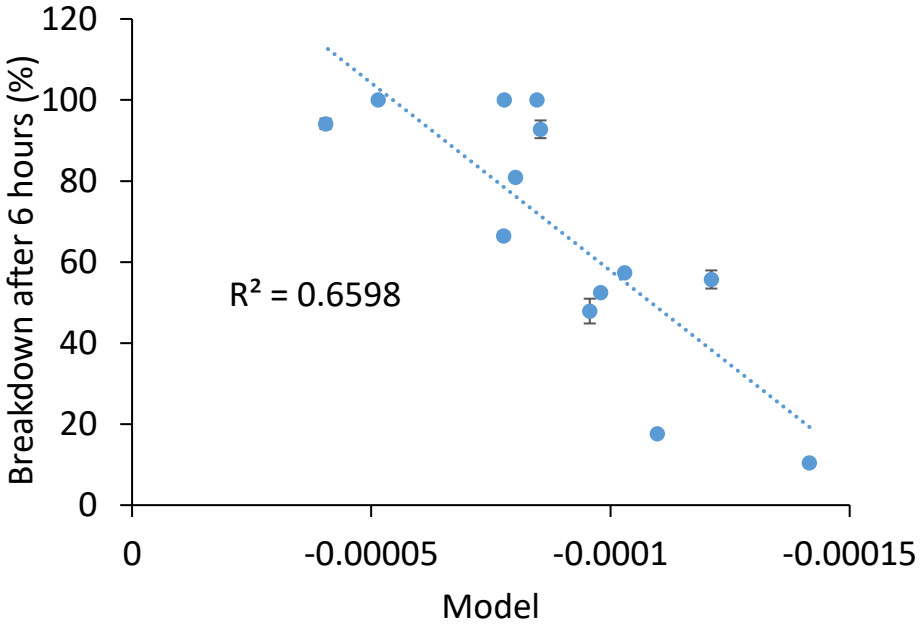

Figure S173: Model 76 vs breakdown after 6 hours (%). Model parameters are P0 = P15 * $(P9 * P6)^{-1}$. R^2 = 0.6598.

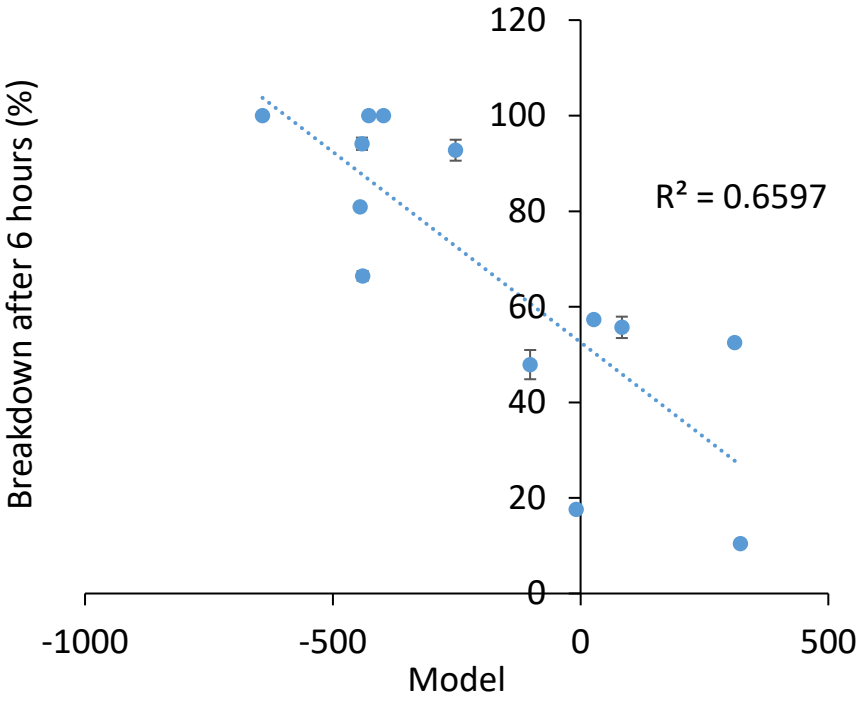

Figure S174: Model 77 vs breakdown after 6 hours (%). Model parameters are P0 = P11 * P13 * $(P20)^{-1}$. R^2 = 0.6597.

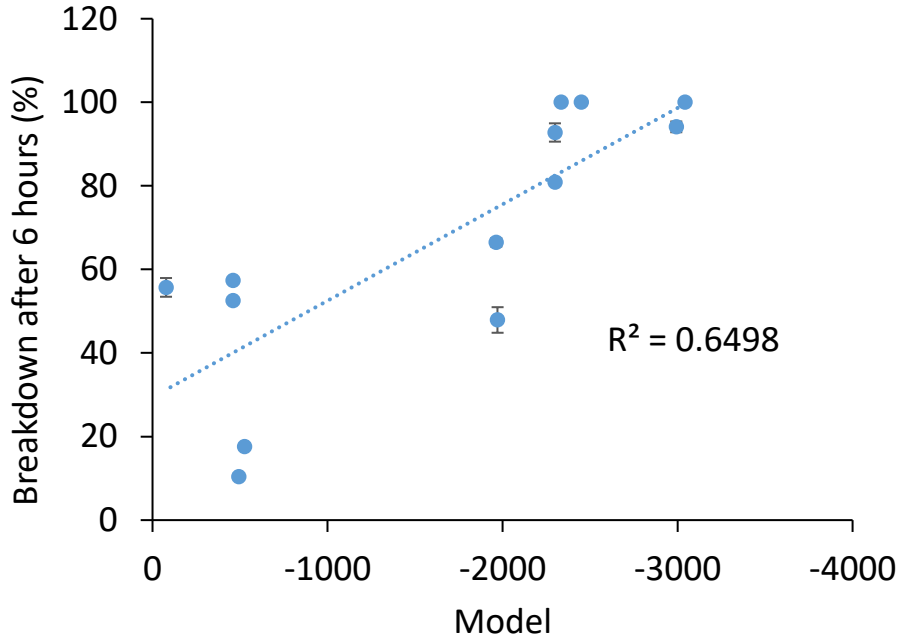

Figure S175: Model 78 vs breakdown after 6 hours (%). Model parameters are P0 = P6 * P18 * $(P15)^{-1}$. R^2 = 0.6498.

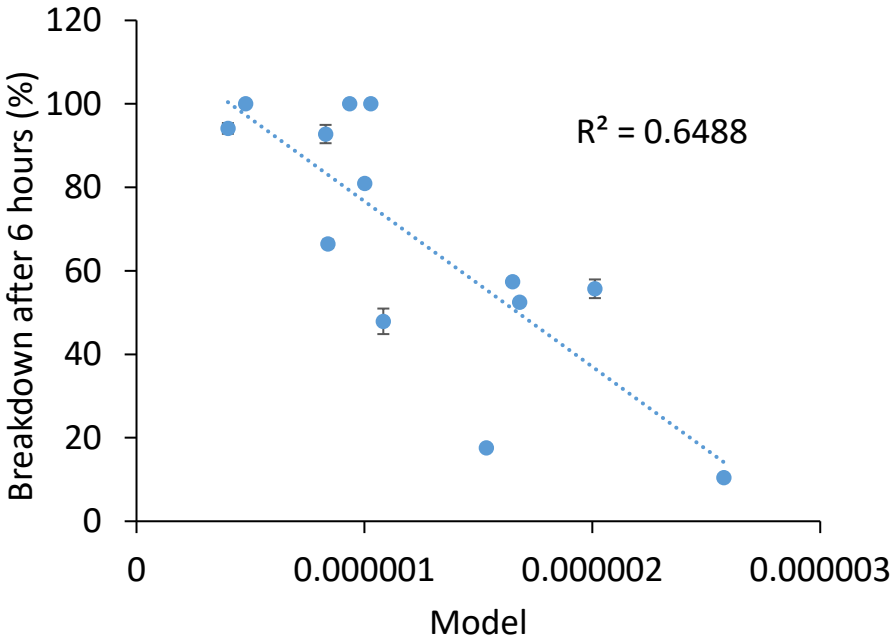

Figure S176: Model 79 vs breakdown after 6 hours (%). Model parameters are P0 = (P3 * P5 * P8)$^{-1}$. R^2 = 0.6488.

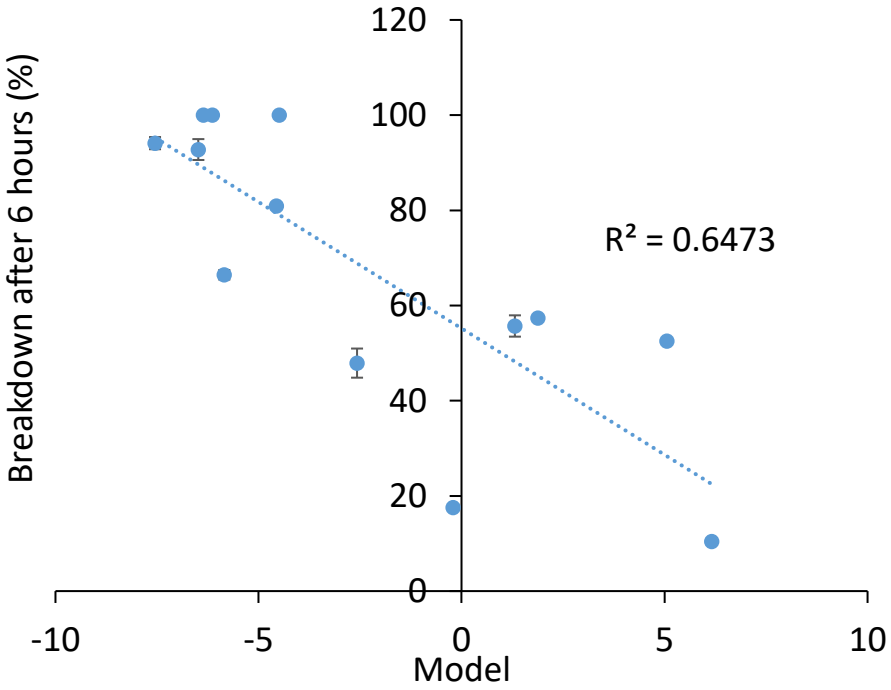

Figure S177: Model 80 vs breakdown after 6 hours (%). Model parameters are P0 = P3 * P13 * (P9)$^{-1}$. R^2 = 0.6473.

Table S16: Summary of the parameters used within models 71-80.

Parameter	Model Number										Total
	71	72	73	74	75	76	77	78	79	80	
R^2	0.7358	0.7218	0.6903	0.6809	0.6606	0.6598	0.6597	0.6498	0.6488	0.6473	
Equation	$P0 = P_x * P_y * (P_z)^{-1}$	$P0 = P_x * P_y * P_z$	$P0 = P_x * P_y * (P_z)^{-1}$	$P0 = (P_x * P_y * P_z)^{-1}$	$P0 = P_x * P_y * P_z$	$P0 = P_x * (P_y * P_z)^{-1}$	$P0 = P_x * P_y * P_z$	$P0 = P_x * P_y * (P_z)^{-1}$	$P0 = (P_x * P_y * P_z)^{-1}$	$P0 = P_x * P_y * (P_z)^{-1}$	
P_1											0
P_2											0
P_3				×					×	×	3
P_4		×			×						2
P_5		×	×						×		3
P_6		×		×	××	×		×			6
P_7											0
P_8									×		1
P_9	×					×				×	3
P_{10}											0
P_{11}							×				1
P_{12}											1
P_{13}	×			×			×			×	3
P_{14}											0
P_{15}			×			×		×			3
P_{16}											0
P_{17}											0
P_{18}	×		×					×			3
P_{19}							×				0
P_{20}											1

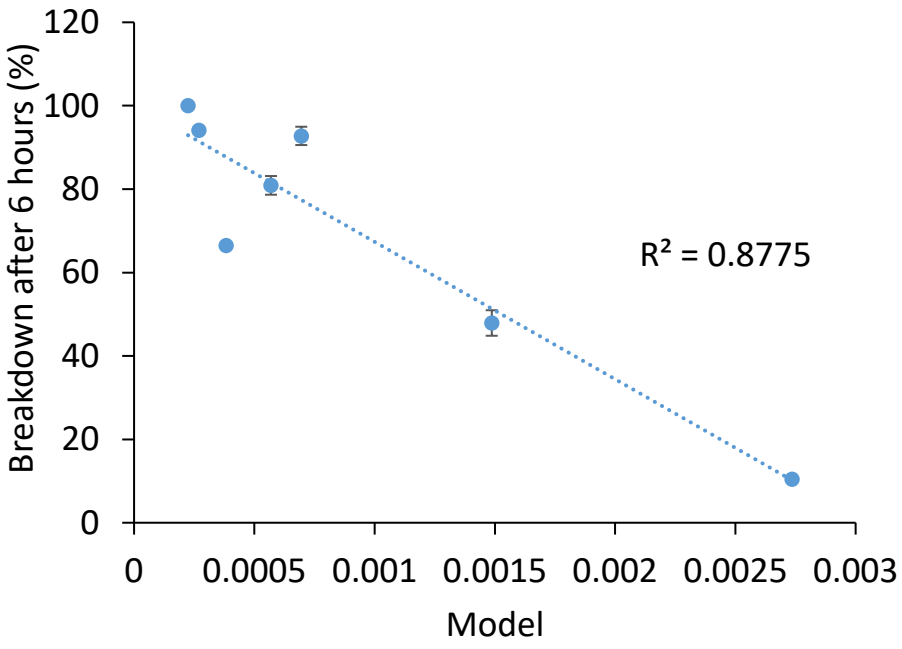

Figure S178: Model 81 vs breakdown after 6 hours (%). Model parameters are P0 = $(P8 * P1)^{-1}$. R^2 = 0.8775.

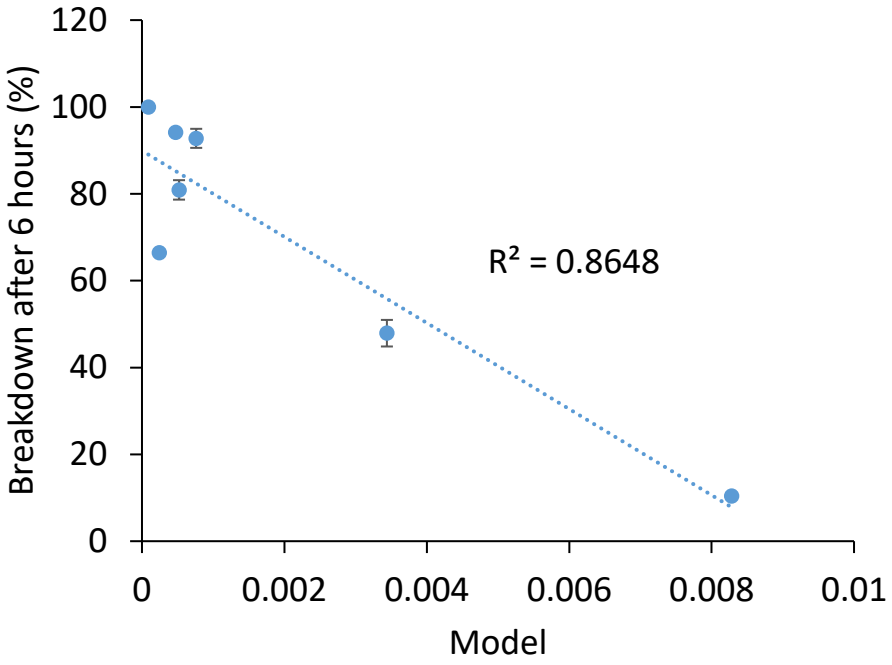

Figure S179: Model 82 vs breakdown after 6 hours (%). Model parameters are P0 = (P1 * P1)$^{-1}$. R^2 = 0.8648.

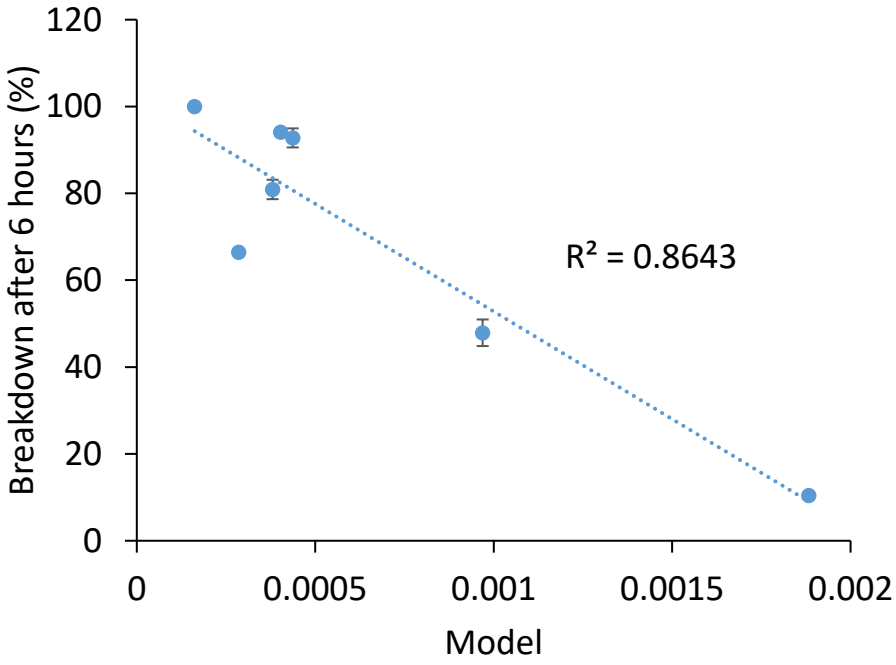

Figure S180: Model 83 vs breakdown after 6 hours (%). Model parameters are P0 = (P10 * P1)$^{-1}$. R^2 = 0.8643.

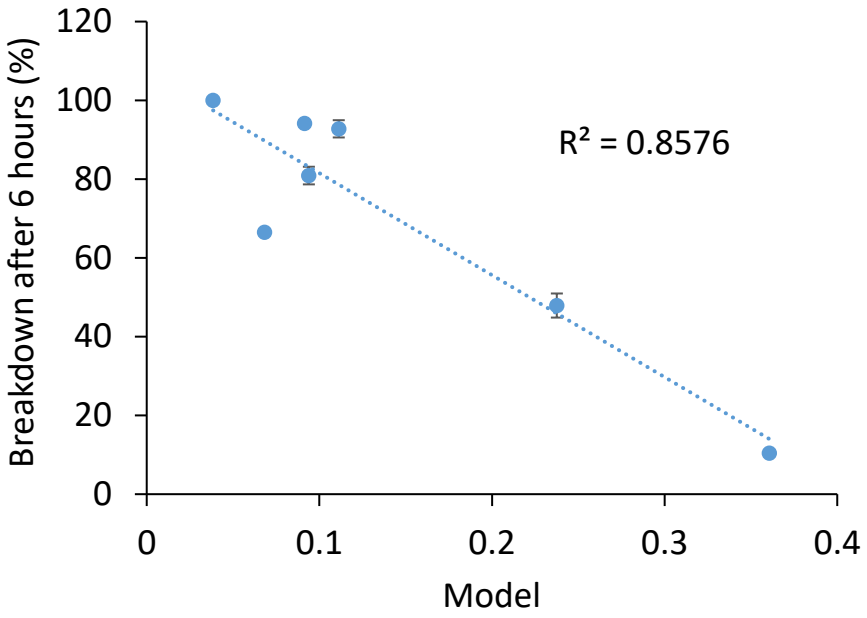

Figure S181: Model 84 vs breakdown after 6 hours (%). Model parameters are P0 = P19 * $(P1)^{-1}$. R^2 = 0.8576.

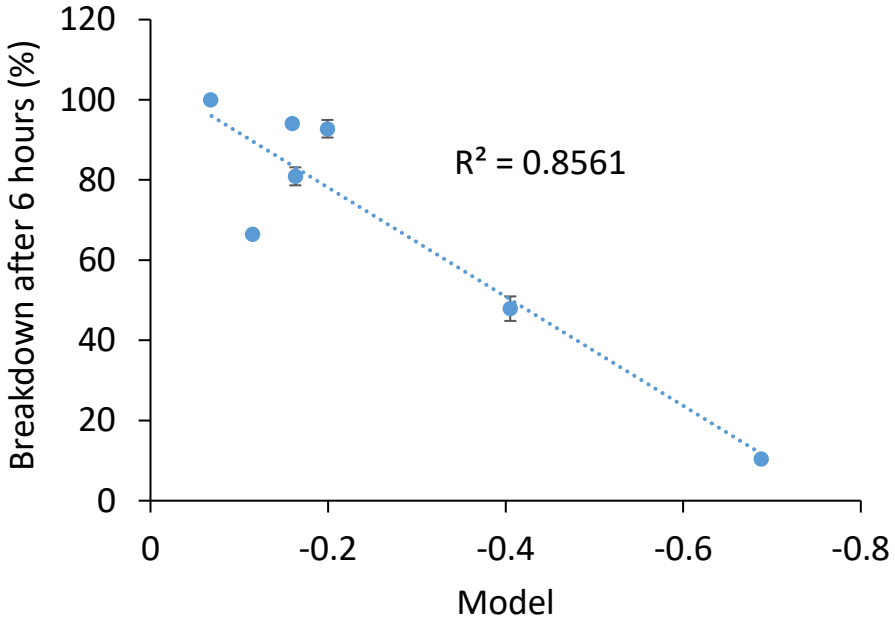

Figure S182: Model 85 vs breakdown after 6 hours (%). Model parameters are P0 = P12 * $(P1)^{-1}$. R^2 = 0.8561.

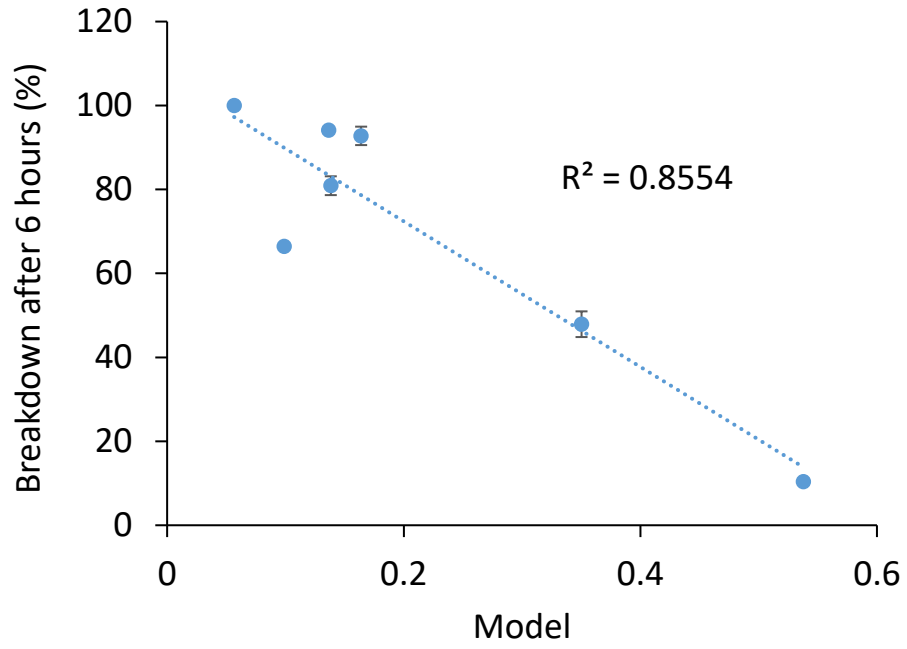

Figure S183: Model 86 vs breakdown after 6 hours (%). Model parameters are P0 = P16 * $(P1)^{-1}$. R^2 = 0.8554.

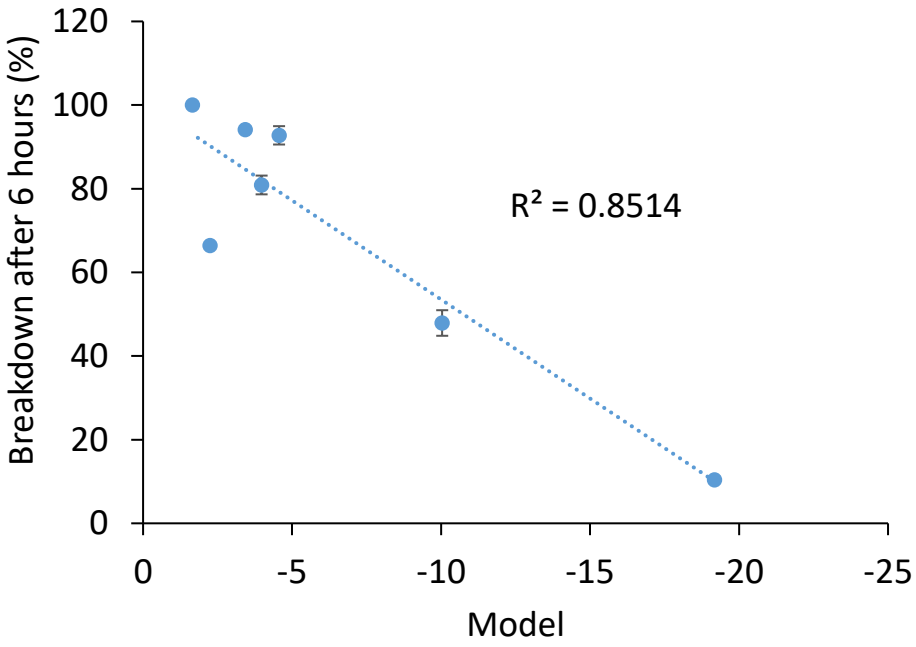

Figure S184: Model 87 vs breakdown after 6 hours (%). Model parameters are P0 = P2 * $(P1)^{-1}$. R^2 = 0.8514.

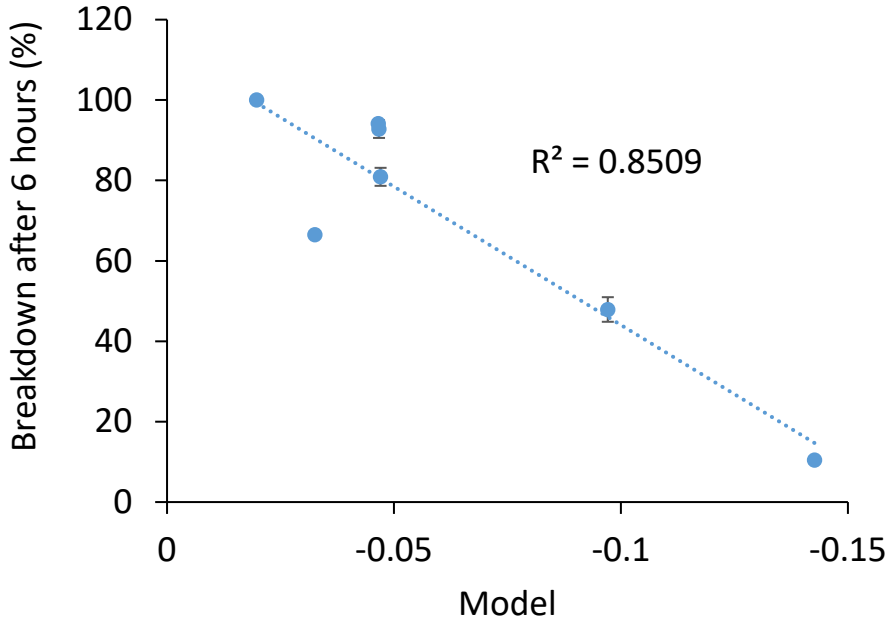

Figure S185: Model 88 vs breakdown after 6 hours (%). Model parameters are P0 = (P15 * P1)$^{-1}$. R^2 = 0.8509.

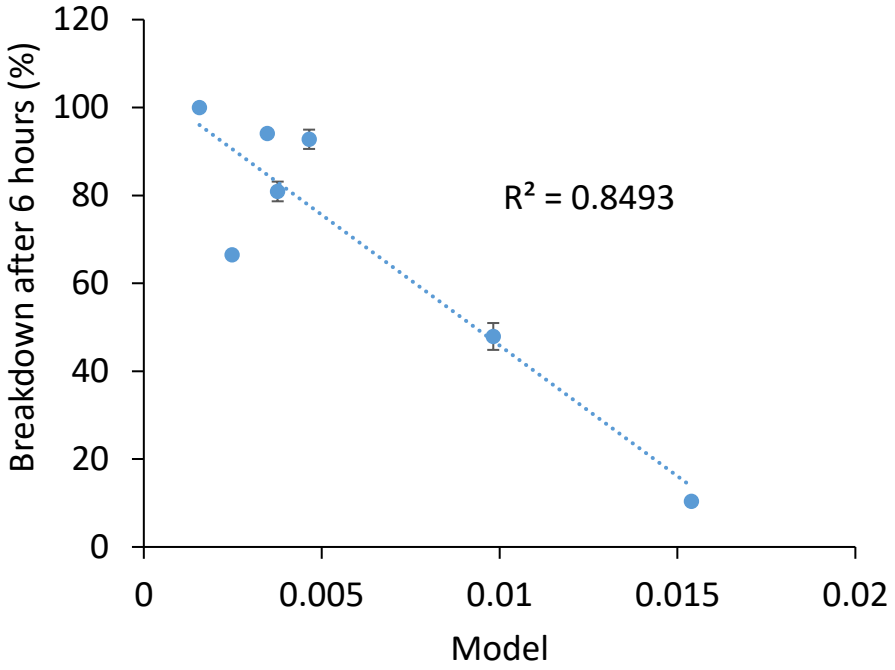

Figure S186: Model 89 vs breakdown after 6 hours (%). Model parameters are P0 = (P16 * P1)$^{-1}$. R^2 = 0.8493.

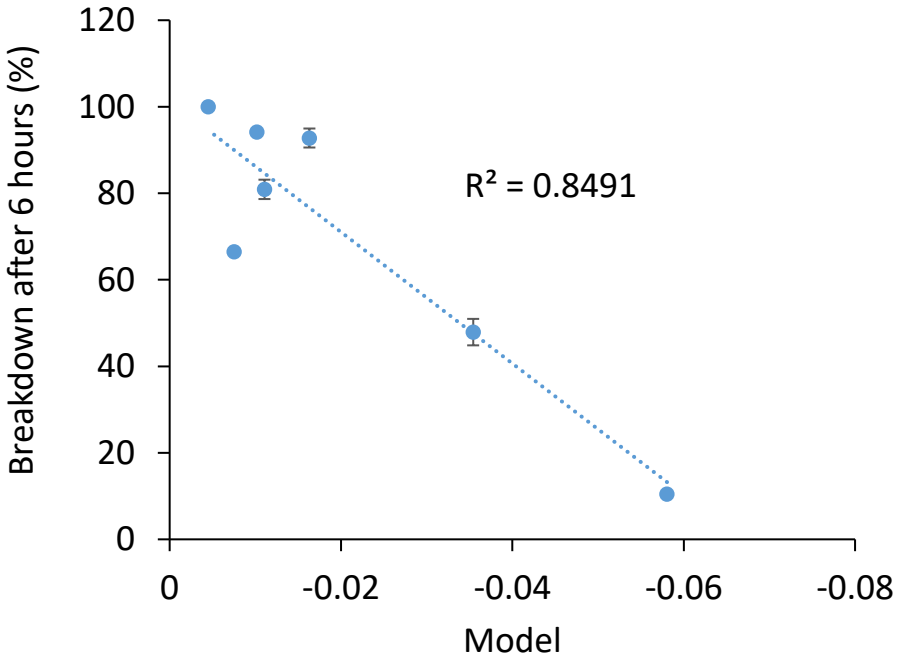

Figure S187: Model 90 vs breakdown after 6 hours (%). Model parameters are P0 = P15 * $(P1)^{-1}$. R^2 = 0.8491.

Table S17: Summary of the parameters used within models 81-90.

Parameter	Model Number										Total
	81	82	83	84	85	86	87	88	89	90	
R^2	0.8775	0.8648	0.8643	0.8576	0.8561	0.8554	0.8514	0.8509	0.8493	0.8491	
Equation	$P0 = (P_X * P_Y)^{-1}$	$P0 = (P_X * P_Y)^{-1}$	$P0 = (P_X * P_Y)^{-1}$	$P0 = P_X * (P_Y)^{-1}$	$P0 = P_X * (P_Y)^{-1}$	$P0 = P_X * (P_Y)^{-1}$	$P0 = P_X * (P_Y)^{-1}$	$P0 = (P_X * P_Y)^{-1}$	$P0 = (P_X * P_Y)^{-1}$	$P0 = P_X * (P_Y)^{-1}$	
P_1	×	××	×	×	×	×	×	×	×	×	11
P_2							×				1
P_3											0
P_4											0
P_5											0
P_6											0
P_7											0
P_8	×										1
P_9											0
P_{10}			×								1
P_{11}											0
P_{12}					×						1
P_{13}											0
P_{14}											0
P_{15}								×		×	2
P_{16}						×			×		2
P_{17}											0
P_{18}											0
P_{19}				×							1
P_{20}											0

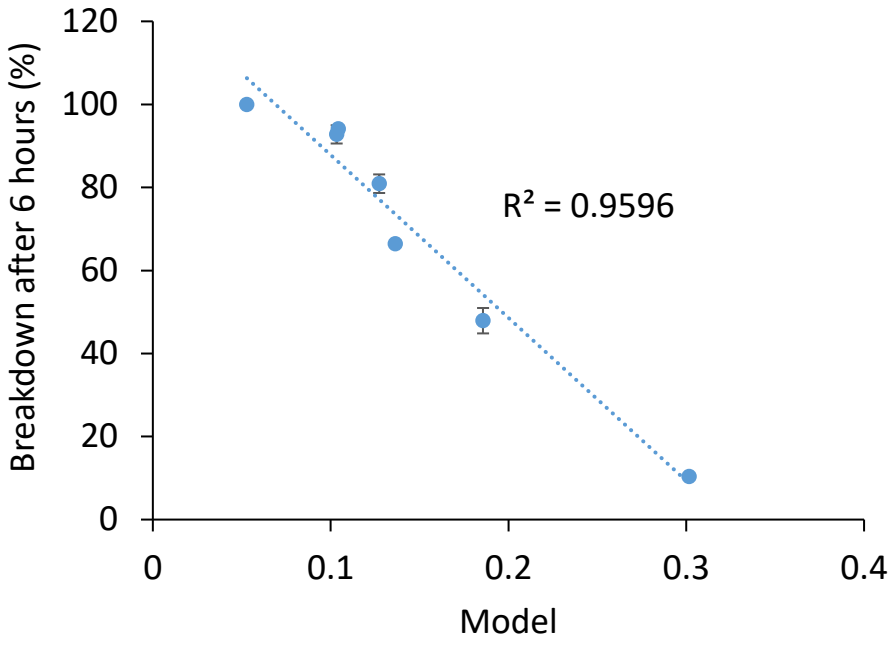

Figure S188: Model 91 vs breakdown after 6 hours (%). Model parameters are P0 = P4 * (P1 * P8)$^{-1}$. R^2 = 0.9596.

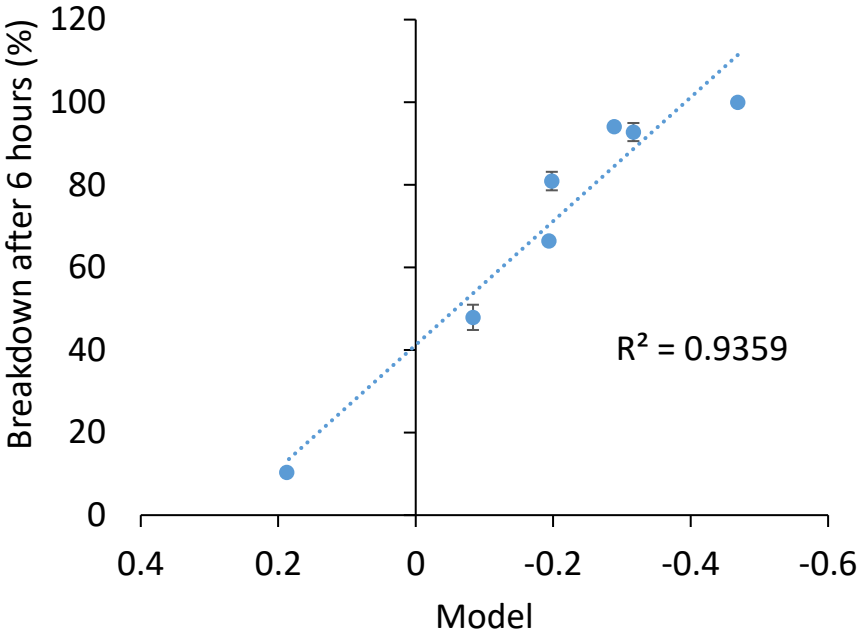

Figure S189: Model 92 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * P13 * (P4)$^{-1}$. R^2 = 0.9359.

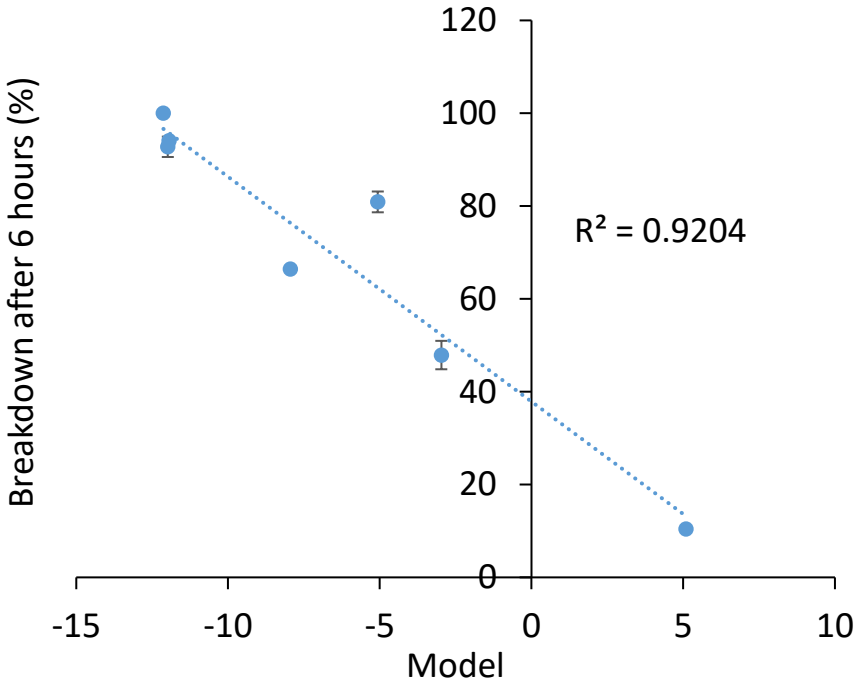

Figure S190: Model 93 vs breakdown after 6 hours (%). Model parameters are P0 = P1 * P13 * $(P11)^{-1}$. R^2 = 0.9204.

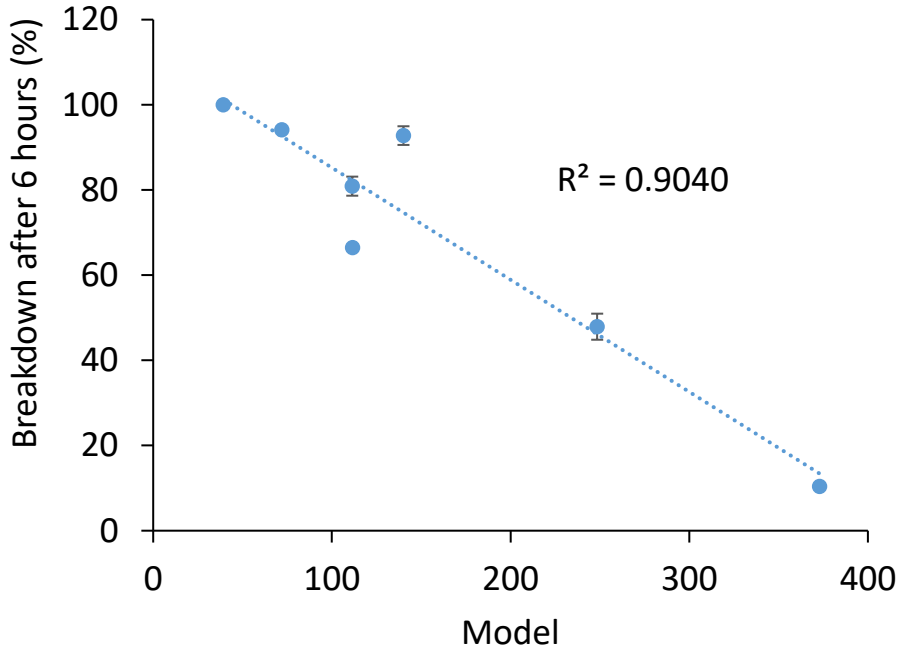

Figure S191: Model 94 vs breakdown after 6 hours (%). Model parameters are P0 = P20 * P3 * $(P1)^{-1}$. R^2 = 0.9040.

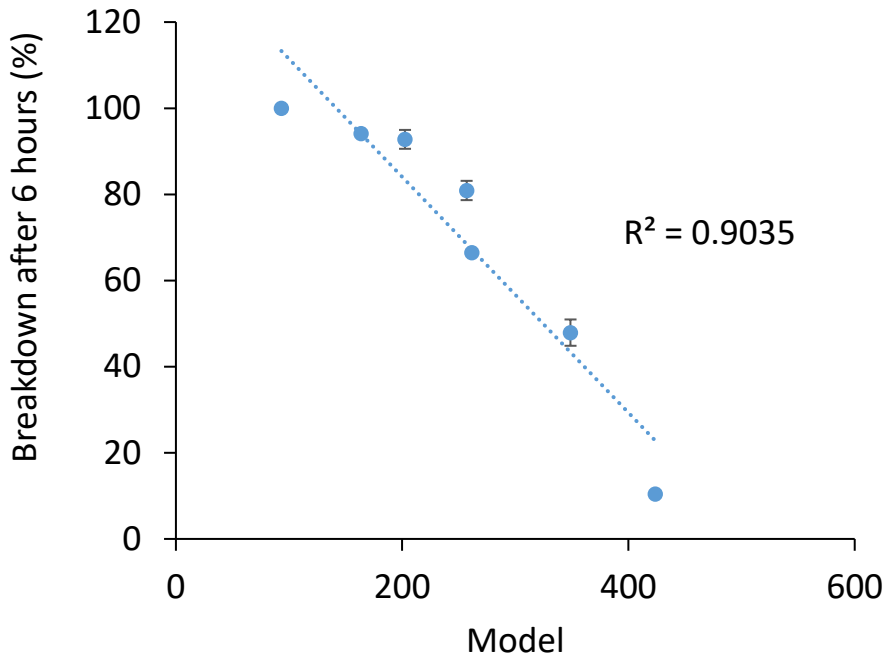

Figure S192: Model 95 vs breakdown after 6 hours (%). Model parameters are P0 = P20 * P4 * $(P1)^{-1}$. R^2 = 0.9035.

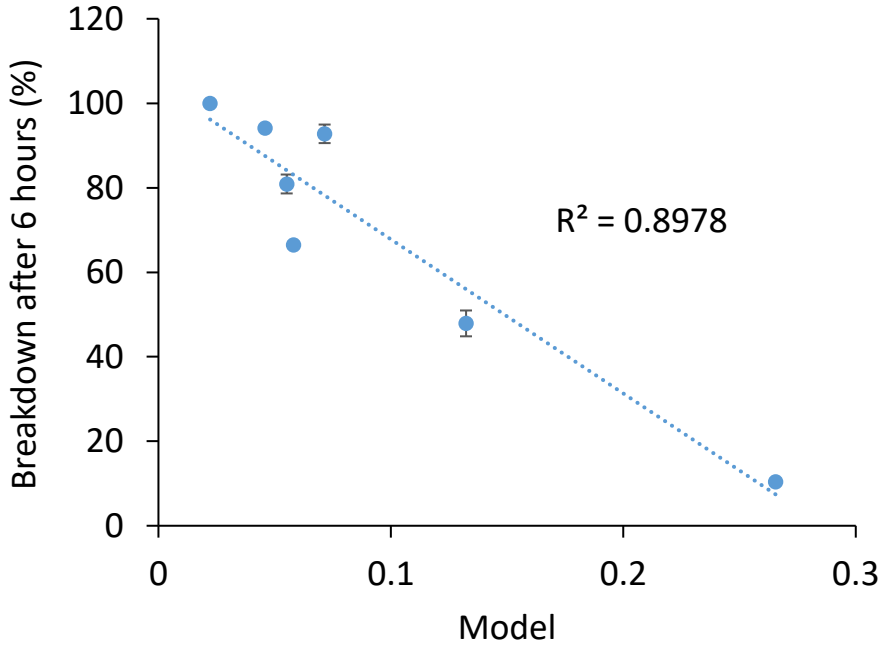

Figure S193: Model 96 vs breakdown after 6 hours (%). Model parameters are P0 = P3 * (P1 * P8)$^{-1}$. R^2 = 0.8978.

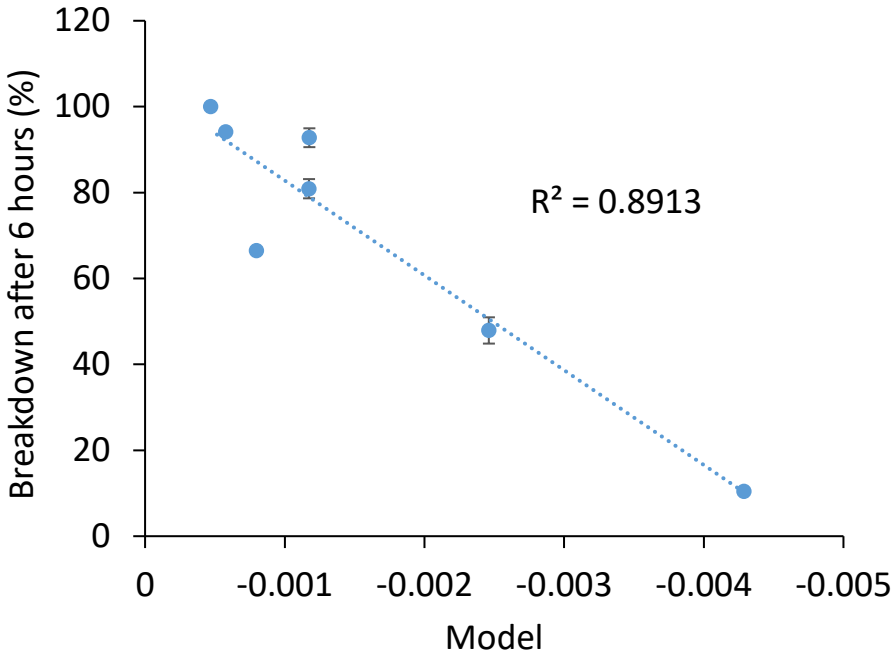

Figure S194: Model 97 vs breakdown after 6 hours (%). Model parameters are P0 = (P1 * P8 * P15)$^{-1}$. R^2 = 0.8913.

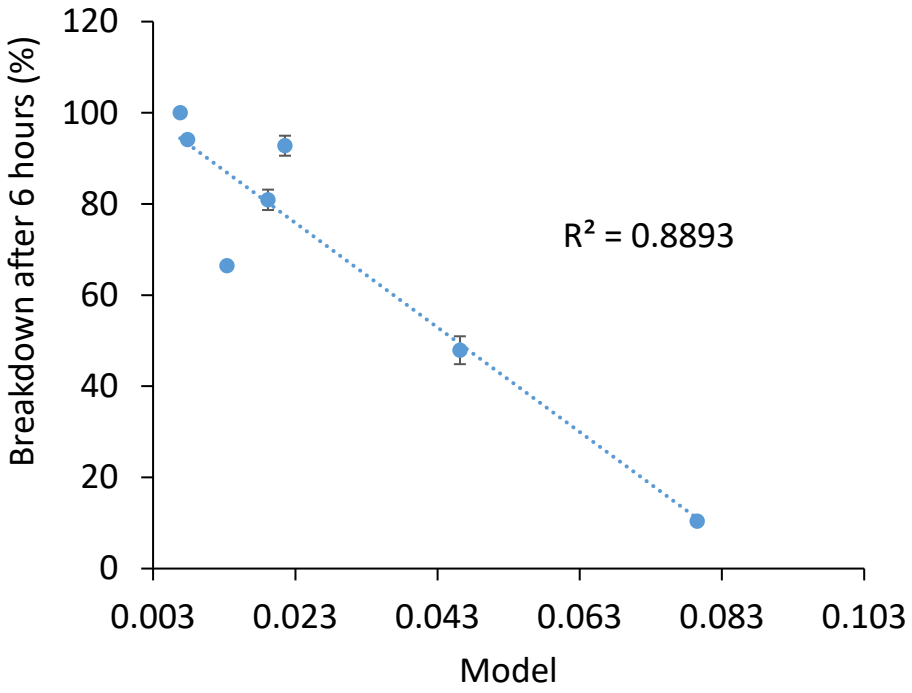

Figure S195: Model 98 vs breakdown after 6 hours (%). Model parameters are P0 = P20 * (P10 * P1)$^{-1}$. R^2 = 0.8893.

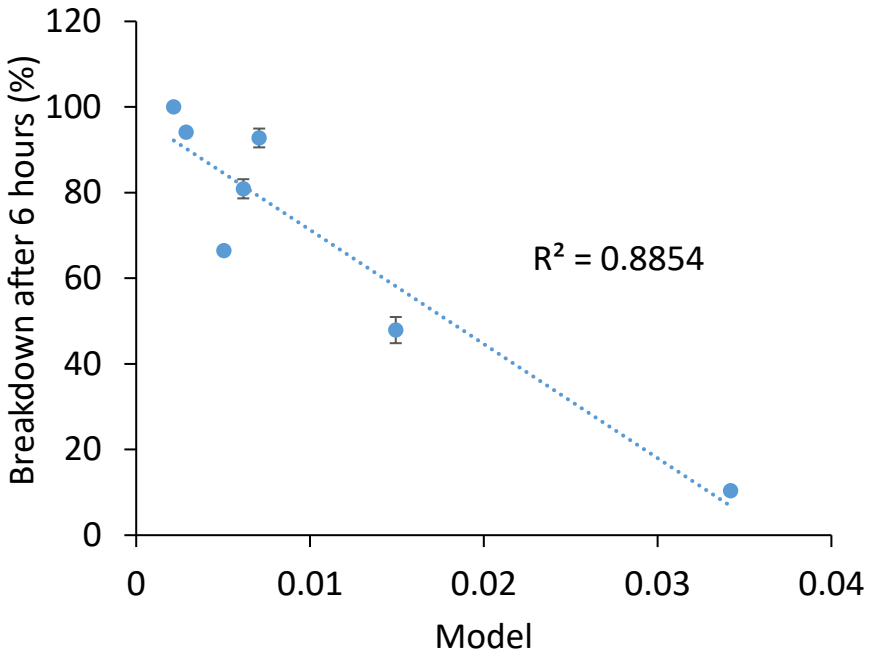

Figure S196: Model 99 vs breakdown after 6 hours (%). Model parameters are P0 = P20 * (P7 * P1)$^{-1}$. R^2 = 0.8854.

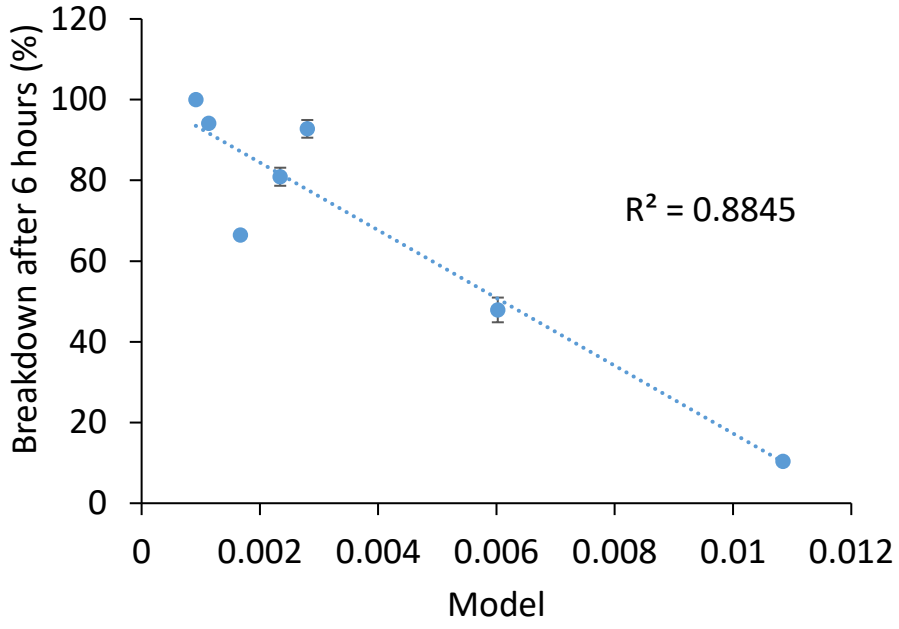

Figure S197: Model 100 vs breakdown after 6 hours (%). Model parameters are P0 = P19 * (P8 * P1)$^{-1}$. R^2 = 0.8845.

Table S18: Summary of the parameters used within models 91-100.

Parameter	Model Number										Total
	91	92	93	94	95	96	97	98	99	100	
R^2	0.9596	0.9359	0.9204	0.9040	0.9035	0.8978	0.8913	0.8893	0.8854	0.8845	
Equation	$P0 = P_X * (P_Y * P_Z)^{-1}$	$P0 = P_X * P_Y * (P_Z)^{-1}$	$P0 = P_X * P_Y * (P_Z)^{-1}$	$P0 = P_X * P_Y * (P_Z)^{-1}$	$P0 = P_X * P_Y * (P_Z)^{-1}$	$P0 = P_x * (P_y * P_z)^{-1}$	$P0 = (P_X * P_Y * P_Z)^{-1}$	$P0 = P_x * (P_y * P_z)^{-1}$	$P0 = P_X * (P_Y * P_Z)^{-1}$	$P0 = P_X * (P_Y * P_Z)^{-1}$	
P_1	×	×	×	×	×	×	×	×	×	×	10
P_2											0
P_3				×		×					2
P_4	×	×			×						3
P_5											0
P_6											0
P_7									×		1
P_8	×					×	×			×	4
P_9											0
P_{10}								×			1
P_{11}			×								1
P_{12}											0
P_{13}		×	×								2
P_{14}											0
P_{15}							×				1
P_{16}											0
P_{17}											0
P_{18}											0
P_{19}										×	1
P_{20}				×	×			×	×		4

PM6 Cartesian coordinates[1]

Table S19: Cartesian coordinates (given in angstroms) generated for compound **1**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	C	C1	-0.8030733	3.8049657	0.6290787
2	C	C2	-0.3999406	3.8400677	-0.8304755
3	O	O1	0.5767425	2.8005450	-1.1482915
4	P	P1	0.0491082	1.2640367	-1.1089634
5	O	O2	1.3271831	0.4417480	-1.6941817
6	C	C14	1.2586515	0.0395943	-3.0962930
7	O	O3	-1.2880013	0.9497258	-1.6360587
8	O	O4	0.2528278	0.9558574	0.5249638
9	C	C5	-0.0022621	-0.3294074	0.9603327
10	C	C6	-1.2115768	-0.9936987	0.7135000
11	C	C7	-1.3987552	-2.2563754	1.2903507
12	C	C8	-0.4127390	-2.8371695	2.0951779
13	C	C9	0.7831560	-2.1409419	2.3354141
14	C	C10	1.0068486	-0.8871801	1.7661768
15	C	C11	1.8443024	-2.7833009	3.1941771
16	F	F1	2.5731146	-3.7054056	2.5429442
17	F	F2	2.7627129	-1.9505041	3.7085898
18	F	F3	1.3789039	-3.4384478	4.2708353
19	C	C12	-2.6960612	-2.9775110	1.0145796
20	F	F4	-3.7938307	-2.2678164	1.3225062
21	F	F5	-2.8686513	-3.3069548	-0.2758594
22	F	F6	-2.8783204	-4.1375869	1.6656873
23	H	H1	-1.0984313	4.8000121	0.9858612
24	H	H2	-1.6478785	3.1318520	0.8297384
25	H	H3	0.0305458	3.4720102	1.2701124
26	H	H4	0.1962563	4.7438438	-1.0792511
27	H	H5	-1.2613654	3.7613546	-1.5215855
28	H	H11	-1.9872202	-0.5359266	0.0798944
29	H	H12	-0.5642908	-3.8273212	2.5352948
30	H	H13	1.9296589	-0.3195055	1.9189679
31	H	H14	2.1256740	-0.6537295	-3.1413225
32	H	H15	0.3221530	-0.5221807	-3.2813212
33	C	C3	1.4309775	1.2283991	-4.0202023
34	H	H6	0.4960707	1.7752612	-4.2018978
35	H	H7	1.8070582	0.9132907	-5.0026875
36	H	H8	2.1604514	1.9483996	-3.6157921

Table S20: Cartesian coordinates (given in angstroms) generated for compound **2**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	C	C1	2.4332411	2.2298561	0.3759211
2	O	O1	1.2278020	1.7442675	-0.2870919
3	P	P1	1.2487569	0.1956023	-0.7925258
4	O	O2	1.5916665	0.3544228	-2.3760324
5	C	C2	1.8154428	-0.8854183	-3.1152603
6	C	C3	0.5048676	-1.5892165	-3.4022936
7	C	C4	3.5812696	2.3901994	-0.6006106
8	O	O3	-0.3936143	-0.0744662	-0.9026563
9	O	O4	2.0193424	-0.7851847	-0.0104856
10	C	C5	-1.1249159	-0.2624726	0.2515616
11	C	C6	-0.6780205	-1.0146175	1.3478563
12	C	C7	-1.5479444	-1.1993468	2.4209243
13	C	C8	-2.8391084	-0.6457365	2.3981464
14	C	C9	-3.2704697	0.0956500	1.2849162
15	C	C10	-2.4151611	0.2949424	0.2059209
16	C	C11	-3.7402499	-0.8732364	3.5728719
17	F	F1	-4.9116515	-0.2149680	3.5651814
18	F	F2	-4.1048095	-2.1567446	3.7466925
19	F	F3	-3.2042087	-0.5347476	4.7598608
20	H	H1	2.6810411	1.5714332	1.2310819
21	H	H2	2.0663880	3.2083107	0.7526541
22	H	H3	2.2840523	-0.4829302	-4.0380850
23	H	H4	2.5437871	-1.5233049	-2.5778639
24	H	H5	0.6017070	-2.2846534	-4.2450168
25	H	H6	0.1279982	-2.1679321	-2.5477777
26	H	H7	-0.2846148	-0.8656810	-3.6637538
27	H	H8	4.3103209	3.1250271	-0.2341922
28	H	H9	3.2284639	2.7506013	-1.5800757
29	H	H10	4.1339544	1.4573165	-0.7745232
30	H	H11	0.3229871	-1.4636038	1.3709078
31	H	H12	-1.2132526	-1.7862765	3.2812282
32	H	H13	-4.2748017	0.5246187	1.2519612
33	H	H14	-2.7202750	0.8682894	-0.6694418

Table S21: Cartesian coordinates (given in angstroms) generated for compound **3**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	C	C1	-0.3616340	3.4647756	-0.6731029
2	O	O1	-0.9858389	2.2541562	-1.2062391
3	P	P1	-0.0167163	0.9680209	-1.4089246
4	O	O2	-0.5937582	0.4117640	-2.8177095
5	C	C2	0.0578692	-0.8059822	-3.3258052
6	C	C3	-0.9429597	-1.3367423	-4.3311205
7	C	C4	-0.0349277	3.3193218	0.7990722
8	O	O3	-0.7571215	-0.1596236	-0.4060088
9	O	O4	1.4356750	1.1163777	-1.2175492
10	C	C5	-0.2273500	-0.6475487	0.7491330
11	C	C6	-1.1802405	-1.3489094	1.5245059
12	C	C7	-0.7735345	-1.9599230	2.6986494
13	C	C8	0.5760243	-1.8670034	3.0989753
14	C	C9	1.5129770	-1.1581470	2.3266069
15	C	C10	1.1161541	-0.5405840	1.1451119
16	N	N1	1.0073866	-2.5267198	4.3382700
17	O	O5	0.1655901	-3.1350746	4.9819259
18	O	O6	2.1834144	-2.4298065	4.6545160
19	H	H1	-1.1820820	4.1931382	-0.8524707
20	H	H2	0.5190801	3.7390329	-1.2848299
21	H	H3	1.0098287	-0.4921140	-3.7988794
22	H	H4	0.2439373	-1.5246389	-2.5059146
23	H	H5	-0.5167931	-2.1430224	-4.9395361
24	H	H6	-1.8481065	-1.7188486	-3.8376208
25	H	H7	-1.2766179	-0.5365126	-5.0104189
26	H	H8	-0.8448207	2.8172971	1.3479035
27	H	H9	0.1037755	4.3035701	1.2687953
28	H	H10	0.8929099	2.7560871	0.9793684
29	H	H11	-2.2132160	-1.3977573	1.1775423
30	H	H12	-1.4839941	-2.5161694	3.3221415
31	H	H13	2.5567933	-1.1014159	2.6610380
32	H	H14	1.8582913	0.0030020	0.5425747

Table S22: Cartesian coordinates (given in angstroms) generated for compound **4**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	C	C1	0.1432895	3.9891492	0.5229926
2	C	C2	-1.0236999	3.1334470	0.9729969
3	O	O1	-1.4374161	2.1971688	-0.0655583
4	P	P1	-0.4402951	0.9374018	-0.3496655
5	O	O2	-1.3669082	0.0717623	-1.3753026
6	C	C3	-0.9819151	0.0640052	-2.7806391
7	C	C4	0.2824490	-0.7384627	-3.0137526
8	O	O3	0.9623575	1.2052511	-0.7145296
9	O	O4	-0.6758432	0.1206327	1.0763156
10	C	C5	-0.0333644	-1.1038023	1.2355909
11	C	C6	-0.8573094	-2.1383769	1.7039361
12	C	C7	-0.2718756	-3.3726841	1.9857666
13	C	C8	1.1021067	-3.5649851	1.7944102
14	C	C9	1.9002314	-2.5174901	1.3232740
15	C	C10	1.3433766	-1.2675609	1.0389829
16	H	H1	0.3317343	4.8061143	1.2293608
17	H	H2	1.0836562	3.4205351	0.4266541
18	H	H3	-0.0430605	4.4386331	-0.4623239
19	H	H4	-1.9551654	3.7271209	1.0879265
20	H	H5	-0.8247634	2.5844054	1.9131736
21	H	H6	-0.9090426	1.1012735	-3.1564392
22	H	H7	-1.8754484	-0.4256226	-3.2238152
23	H	H8	0.2467105	-1.7093787	-2.5001582
24	H	H9	1.1862661	-0.2177320	-2.6502721
25	H	H10	0.4348454	-0.9365403	-4.0812741
26	H	H11	-1.9219656	-1.9605723	1.8398422
27	H	H12	-0.8894416	-4.1910969	2.3548708
28	H	H13	1.5493933	-4.5317875	2.0145196
29	H	H14	2.9695807	-2.6715003	1.1776736
30	H	H15	1.9715184	-0.4493076	0.6754432

Table S23: Cartesian coordinates (given in angstroms) generated for compound **5**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	O	O1	-0.7788801	-0.9882209	-1.5898791
2	P	P1	0.8557843	-0.9149557	-1.3408493
3	O	O2	0.9934885	-1.9627561	-0.0809119
4	C	C1	-1.2400687	-0.5513408	-2.8943978
5	C	C2	1.1781147	-3.3612264	-0.4353257
6	C	C3	-1.2740218	0.9646952	-2.9793326
7	O	O3	1.6898207	-1.1545030	-2.5277476
8	C	C4	-0.1640041	-4.0147972	-0.7096242
9	O	O4	1.0909812	0.5110051	-0.5973944
10	C	C5	0.2100723	0.8547964	0.5291697
11	C	C6	0.1884249	2.3875528	0.4672101
12	C	C7	-0.5069922	2.9625788	1.7056671
13	C	C8	0.1404204	2.4473170	2.9988834
14	C	C9	0.1569343	0.9128085	3.0426959
15	C	C10	0.8568410	0.3238575	1.8130695
16	H	H1	-0.6219207	-1.0069048	-3.6940673
17	H	H2	-2.2587658	-0.9894065	-2.9190051
18	H	H3	1.6505334	-3.7541584	0.4886755
19	H	H4	1.8877846	-3.4619454	-1.2806822
20	H	H5	-0.2766167	1.4050060	-3.1191032
21	H	H6	-1.8886869	1.2988321	-3.8236413
22	H	H7	-1.6985421	1.4051120	-2.0670886
23	H	H8	-0.0908755	-5.1074750	-0.6712574
24	H	H9	-0.5746642	-3.7472362	-1.6923432
25	H	H10	-0.9115429	-3.7023126	0.0349640
26	H	H11	-0.8039093	0.4256215	0.3635173
27	H	H12	1.2306988	2.7611033	0.3932000
28	H	H13	-0.3105498	2.7233686	-0.4598052
29	H	H14	-0.4639949	4.0679015	1.6767510
30	H	H15	-1.5821008	2.6982307	1.6920022
31	H	H16	1.1755348	2.8333162	3.0769252
32	H	H17	-0.4020954	2.8443689	3.8767385
33	H	H18	0.6679015	0.5674174	3.9612605
34	H	H19	-0.8786472	0.5262516	3.1067354
35	H	H20	1.9346554	0.5817209	1.8160626
36	H	H21	0.8188886	-0.7856230	1.8389284

Table S24: Cartesian coordinates (given in angstroms) generated for compound **6**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	C	C1	-1.7079472	3.2133796	1.4643437
2	C	C2	-1.1088344	3.4293691	0.0873007
3	O	O1	-1.0753122	2.1825541	-0.6639671
4	P	P1	0.1432890	1.1564639	-0.2812014
5	O	O2	-0.0343103	-0.0170943	-1.4141946
6	C	C3	0.6845136	0.1896999	-2.6630430
7	C	C4	-0.0019563	1.2339449	-3.5239368
8	O	O3	1.4921260	1.7416579	-0.1542544
9	O	O4	-0.4612722	0.4192526	1.0546766
10	C	C5	0.3986417	-0.5827336	1.6638525
11	C	C6	0.1610529	-1.9362215	0.9950555
12	C	C7	0.9402066	-3.0451741	1.7112471
13	C	C8	0.6966180	-4.4071433	1.0659405
14	H	H1	-1.0250841	2.6947161	2.1512689
15	H	H2	-1.9846410	4.1646820	1.9325239
16	H	H3	-2.6132795	2.5907779	1.4068151
17	H	H4	-0.1007248	3.8872938	0.1225775
18	H	H5	-1.7697133	4.0423005	-0.5599612
19	H	H6	0.6155875	-0.8237122	-3.1087242
20	H	H7	1.7453662	0.4324575	-2.4559354
21	H	H8	-1.0972535	1.1686776	-3.4233070
22	H	H9	0.2369337	1.0976121	-4.5850116
23	H	H10	0.2803315	2.2609887	-3.2581392
24	H	H11	1.4595339	-0.2675812	1.6426561
25	H	H12	0.0378268	-0.5690814	2.7129567
26	H	H13	0.4406782	-1.9013629	-0.0797265
27	H	H14	-0.9254666	-2.1602883	0.9916056
28	H	H15	2.0244606	-2.8145161	1.6977166
29	H	H16	0.6496457	-3.0830795	2.7798308
30	H	H17	1.2760325	-5.1916328	1.5654707
31	H	H18	-0.3596333	-4.6952427	1.1177289
32	H	H19	0.9825689	-4.4109642	0.0078354

Table S25: Cartesian coordinates (given in angstroms) generated for compound **7**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	C	C1	-0.7716292	2.0876130	-0.1676381
2	O	O1	-0.7283514	0.9747739	0.7512739
3	P	P1	0.4714049	-0.1335840	0.4470728
4	O	O2	-0.2884269	-1.2906398	-0.4732545
5	C	C2	-0.0880297	-1.1613841	-1.8972838
6	O	O3	1.6807200	0.4431863	-0.1904413
7	C	C3	0.5693815	-0.9947146	2.0740806
8	H	H1	0.2290578	2.4381933	-0.4605829
9	H	H2	-1.2885362	2.8661959	0.4112000
10	H	H3	-1.3719888	1.8079360	-1.0414889
11	H	H4	-0.2823982	-2.1780024	-2.2679672
12	H	H5	-0.8301070	-0.4636062	-2.3027417
13	H	H6	0.9360911	-0.8535344	-2.1568449
14	H	H7	0.4424505	-0.2882224	2.9076420
15	H	H8	-0.2188240	-1.7578762	2.1661194
16	H	H9	1.5391858	-1.4963343	2.2008544

Table S26: Cartesian coordinates (given in angstroms) generated for compound **8**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	C	C1	-0.6926463	1.2167604	0.0508566
2	C	C2	0.1046331	0.1769149	-0.8028702
3	C	C3	0.2415917	1.9196868	1.0444556
4	C	C4	-1.8041940	0.4773666	0.8168900
5	C	C5	-1.3333529	2.2416990	-0.9023144
6	O	O1	0.7570725	-0.7087015	0.1713540
7	C	C6	1.2542626	0.7516777	-1.6194217
8	P	P1	0.4622476	-2.3162031	0.0146999
9	O	O2	-0.7549398	-2.5744045	1.1312776
10	O	O3	0.0530822	-2.7686755	-1.3361318
11	C	C7	1.9168596	-3.0508219	0.8745238
12	H	H1	-0.5928286	-0.3937801	-1.4614556
13	H	H2	0.8043521	1.1766192	1.6278975
14	H	H3	-0.3145031	2.5457208	1.7481034
15	H	H4	0.9717416	2.5572949	0.5375252
16	H	H5	-1.3819744	-0.2431760	1.5322193
17	H	H6	-2.4774322	-0.0637465	0.1470109
18	H	H7	-2.4158275	1.1763093	1.3971047
19	H	H8	-0.5792918	2.8109806	-1.4562482
20	H	H9	-1.9942851	1.7640249	-1.6325237
21	H	H10	-1.9364753	2.9670195	-0.3445515
22	H	H11	0.9464896	1.6314163	-2.1955319
23	H	H12	1.6481360	0.0111732	-2.3273129
24	H	H13	2.0865164	1.0491652	-0.9668150
25	H	H14	-1.6552686	-2.7334351	0.7578612
26	H	H15	2.3154820	-3.9125316	0.3209694
27	H	H16	2.7267043	-2.3144470	0.9874708
28	H	H17	1.6438486	-3.3939066	1.8849567

Table S27: Cartesian coordinates (given in angstroms) generated for compound **9**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	O	O1	-1.4368442	1.0189884	-0.0394760
2	P	P1	-0.2865275	-0.1509370	-0.0573042
3	O	O2	-1.0229440	-1.2622069	-1.0090478
4	O	O3	1.0891563	0.2487863	-0.4089517
5	C	C1	-1.2743724	2.0734683	0.9474700
6	C	C2	-0.1242525	2.9983540	0.6006456
7	C	C3	-1.1157345	-0.9458968	-2.4262034
8	C	C4	0.2253128	-1.0955332	-3.1198443
9	O	O4	-0.5188978	-0.8279816	1.4186592
10	C	C5	0.4483538	-1.8306381	1.8358660
11	C	C6	1.7515328	-1.1881688	2.2719465
12	H	H1	-2.2567156	2.5844124	0.8659576
13	H	H2	-1.1802586	1.6261655	1.9557535
14	H	H3	-0.1328897	3.8972529	1.2271150
15	H	H4	0.8626213	2.5238961	0.7228672
16	H	H5	-0.1736407	3.3246478	-0.4483020
17	H	H6	-1.5643334	0.0573215	-2.5599638
18	H	H7	-1.8444067	-1.7153103	-2.7588021
19	H	H8	0.1196761	-1.0312672	-4.2086939
20	H	H9	0.6920369	-2.0628078	-2.8849435
21	H	H10	0.9531821	-0.3237874	-2.8151348
22	H	H11	0.5862459	-2.5850301	1.0387189
23	H	H12	-0.0923555	-2.2956718	2.6874130
24	H	H13	2.4092225	-1.9132339	2.7632144
25	H	H14	1.5728286	-0.3661993	2.9773623
26	H	H15	2.3140038	-0.7586230	1.4236781

Table S28: Cartesian coordinates (given in angstroms) generated for compound **10**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	O	O1	-0.8798965	1.1790024	-0.8991552
2	P	P1	-0.0381936	-0.1778632	-0.5216611
3	O	O2	-0.8725237	-1.2894652	-1.3853580
4	O	O3	1.4256193	-0.1115433	-0.7025251
5	C	C1	-0.3756011	2.4125152	-0.3164572
6	C	C2	-0.9765335	2.6000118	1.0780587
7	C	C3	-0.7718608	-1.1865313	-2.8331761
8	C	C4	0.5776761	-1.7084015	-3.3285832
9	O	O4	-0.5582352	-0.5196787	0.9926220
10	C	C5	0.2977720	-1.4219491	1.7597901
11	C	C6	0.5849974	-1.8118031	-4.8490581
12	C	C7	-0.6109517	3.9659086	1.6455803
13	C	C8	0.1896172	-0.8962516	3.1921660
14	C	C9	0.8582976	-1.8462753	4.1770399
15	H	H1	0.7313009	2.4348958	-0.3202841
16	H	H2	-0.7545645	3.1675064	-1.0349826
17	H	H3	-0.6410286	1.7944823	1.7654448
18	H	H4	-2.0788804	2.4816670	1.0209875
19	H	H5	-0.9865720	-0.1524955	-3.1611569
20	H	H6	-1.6096043	-1.8448386	-3.1457098
21	H	H7	1.4125028	-1.0549696	-2.9864318
22	H	H8	0.7851507	-2.6978724	-2.8708881
23	H	H9	1.3434379	-1.4180775	1.3926506
24	H	H10	-0.1467231	-2.4298841	1.6460648
25	H	H11	1.5597354	-2.1646766	-5.2099633
26	H	H12	-0.1714123	-2.5162714	-5.2159794
27	H	H13	0.3970285	-0.8411223	-5.3244224
28	H	H14	0.4749499	4.0976392	1.7263399
29	H	H15	-1.0287142	4.0962388	2.6514736
30	H	H16	-0.9991933	4.7832854	1.0264913
31	H	H17	0.6427077	0.1132192	3.2562501
32	H	H18	-0.8822933	-0.7565561	3.4472599
33	H	H19	0.7818971	-1.4636605	5.2034118
34	H	H20	0.3937953	-2.8409054	4.1669720
35	H	H21	1.9263039	-1.9752800	3.9571893

Table S29: Cartesian coordinates (given in angstroms) generated for compound **11**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	O	O1	0.9331850	0.6988320	1.0196206
2	P	P1	0.2524496	-0.4547442	0.0720660
3	O	O2	-0.5287755	0.5423783	-0.9844745
4	O	O3	1.1020259	-1.5175538	-0.4919519
5	C	C1	2.3408977	1.0388451	0.8570531
6	C	C2	3.2233682	-0.1218089	1.2913402
7	C	C3	-0.8663548	0.0698075	-2.3176546
8	C	C4	-1.7286964	-1.1851377	-2.2639667
9	O	O4	-0.9496254	-0.9962029	1.0263723
10	C	C5	0.3913046	-0.1075650	-3.1579644
11	C	C6	2.6348488	1.5268750	-0.5556219
12	C	C7	-1.8993574	-0.0167650	1.5745916
13	C	C8	-1.3527790	0.4715437	2.9082567
14	C	C9	-3.1742237	-0.8398417	1.7123959
15	H	H1	2.3975727	1.8841344	1.5898232
16	H	H2	3.1787394	-0.9741467	0.5901848
17	H	H3	2.9198739	-0.5108171	2.2716573
18	H	H4	4.2734342	0.1796838	1.3600808
19	H	H5	-1.4630712	0.9495493	-2.6701420
20	H	H6	-1.1469419	-2.0933029	-2.0398961
21	H	H7	-2.2210396	-1.3644042	-3.2266706
22	H	H8	-2.5147618	-1.1067711	-1.5019816
23	H	H9	0.1436314	-0.2859037	-4.2096024
24	H	H10	1.0327735	0.7797976	-3.1093532
25	H	H11	1.0003420	-0.9659754	-2.8238185
26	H	H12	2.7714122	0.7033718	-1.2710093
27	H	H13	1.8235577	2.1653553	-0.9346457
28	H	H14	3.5563220	2.1197531	-0.5814287
29	H	H15	-2.0336057	0.8207653	0.8496994
30	H	H16	-1.0634476	-0.3715264	3.5497225
31	H	H17	-2.0875344	1.0729710	3.4515888
32	H	H18	-0.4483567	1.0869012	2.7741121
33	H	H19	-2.9785290	-1.7660441	2.2723230
34	H	H20	-3.5593396	-1.1451795	0.7327397
35	H	H21	-3.9592987	-0.2868740	2.2365543

Table S30: Cartesian coordinates (given in angstroms) generated for compound **12**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	C	C1	-0.2364318	4.1469637	-1.9402597
2	C	C2	-1.2210373	3.7233411	-1.0277257
3	C	C3	-1.1965228	2.4305860	-0.5200465
4	C	C4	-0.1663522	1.5596212	-0.9296777
5	C	C5	0.8348084	1.9699331	-1.8217465
6	C	C6	0.7895629	3.2697227	-2.3239795
7	C	C7	-0.2797604	5.5461417	-2.4684454
8	F	F1	0.3788682	5.7628820	-3.6201964
9	F	F2	-1.5109741	6.0236517	-2.7274261
10	F	F3	0.2416079	6.4640787	-1.6330731
11	O	O1	-0.2044137	0.3270477	-0.3520165
12	S	S1	0.5350322	-1.0806963	-1.0498229
13	C	C8	0.3417669	-2.1174386	0.2863491
14	C	C9	1.3440649	-2.1978867	1.2650857
15	C	C10	1.1879934	-3.0440744	2.3591455
16	C	C11	0.0214522	-3.8212944	2.4920061
17	C	C12	-0.9807083	-3.7393227	1.5086521
18	C	C13	-0.8204541	-2.8912376	0.4150736
19	C	C14	-0.1364672	-4.7288869	3.6626668
20	O	O2	1.9098982	-0.7249887	-1.2699147
21	O	O3	-0.3202310	-1.4339260	-2.1433416
22	H	H1	-2.0129431	4.4068775	-0.7116794
23	H	H2	-1.9488692	2.0770894	0.1824580
24	H	H3	1.6542858	1.3030156	-2.1085976
25	H	H4	1.5709636	3.5932333	-3.0167227
26	H	H5	2.2569515	-1.5976563	1.1664771
27	H	H6	1.9701273	-3.1045389	3.1152551
28	H	H7	-1.8856732	-4.3390238	1.6006857
29	H	H8	-1.6053170	-2.8350919	-0.3494437
30	H	H9	0.5365203	-5.5981680	3.5821038
31	H	H10	0.1085729	-4.2248835	4.6103807
32	H	H11	-1.1563183	-5.1250706	3.7677761

Table S31: Cartesian coordinates (given in angstroms) generated for compound **13**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	C	C1	0.1873860	0.0000000	4.7857688
2	C	C2	1.3508362	0.0000000	3.9874386
3	C	C3	1.2345670	0.0000000	2.6078773
4	C	C4	-0.0563832	0.0000000	2.0285552
5	C	C5	-1.2220120	0.0000000	2.8160765
6	C	C6	-1.0921309	0.0000000	4.2003988
7	N	N1	0.3165557	0.0000000	6.2463581
8	O	O1	-0.7093142	0.0000000	6.9103625
9	O	O2	1.4441447	0.0000000	6.7187310
10	O	O3	-0.0582042	0.0000000	0.6768679
11	S	S1	-1.5116683	0.0000000	-0.2972170
12	C	C7	-0.7500943	0.0000000	-1.8158245
13	O	O4	-2.1478853	1.2472773	0.0058687
14	O	O5	-2.1478853	-1.2472773	0.0058687
15	C	C8	-0.4323507	1.2136897	-2.4446517
16	C	C9	0.1921803	1.2156240	-3.6887606
17	C	C10	0.5109856	0.0000000	-4.3226601
18	C	C11	0.1921803	-1.2156240	-3.6887606
19	C	C12	-0.4323507	-1.2136897	-2.4446517
20	C	C13	1.1943344	0.0000000	-5.6457704
21	H	H1	2.3348288	0.0000000	4.4714709
22	H	H2	2.1087802	0.0000000	1.9586518
23	H	H3	-2.2177429	0.0000000	2.3698949
24	H	H4	-1.9806248	0.0000000	4.8443706
25	H	H5	-0.6812912	2.1655459	-1.9591043
26	H	H6	0.4361556	2.1616257	-4.1717576
27	H	H7	0.4361556	-2.1616257	-4.1717576
28	H	H8	-0.6812912	-2.1655459	-1.9591043
29	H	H9	0.9460930	0.8829594	-6.2528805
30	H	H10	2.2899524	0.0000000	-5.5187789
31	H	H11	0.9460930	-0.8829594	-6.2528805

Table S32: Cartesian coordinates (given in angstroms) generated for compound **14**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	C	C1	0.5657542	0.0000000	5.2600503
2	C	C2	1.6609919	0.0000000	4.3856455
3	C	C3	1.4649231	0.0000000	3.0066881
4	C	C4	0.1448276	0.0000000	2.5182777
5	C	C5	-0.9653971	0.0000000	3.3707095
6	C	C6	-0.7353143	0.0000000	4.7504324
7	O	O1	0.0603017	0.0000000	1.1489020
8	S	S1	-1.4372982	0.0000000	0.3028019
9	C	C7	-0.7925208	0.0000000	-1.2783219
10	O	O2	-2.0744540	-1.2466879	0.6245265
11	O	O3	-2.0744540	1.2466879	0.6245265
12	C	C8	-0.5255527	-1.2127974	-1.9282771
13	C	C9	0.0006487	-1.2153854	-3.2182407
14	C	C10	0.2686949	0.0000000	-3.8740343
15	C	C11	0.0006487	1.2153854	-3.2182407
16	C	C12	-0.5255527	1.2127974	-1.9282771
17	C	C13	0.8472125	0.0000000	-5.2475861
18	H	H1	0.7297299	0.0000000	6.3344464
19	H	H2	2.6744578	0.0000000	4.7861038
20	H	H3	2.2962916	0.0000000	2.3074218
21	H	H4	-1.9867889	0.0000000	2.9943678
22	H	H5	-1.5867146	0.0000000	5.4316463
23	H	H6	-0.7366270	-2.1638663	-1.4241779
24	H	H7	0.2059836	-2.1610072	-3.7179355
25	H	H8	0.2059836	2.1610072	-3.7179355
26	H	H9	-0.7366270	2.1638663	-1.4241779
27	H	H10	0.5510411	-0.8829382	-5.8320070
28	H	H11	0.5510411	0.8829382	-5.8320070
29	H	H12	1.9487695	0.0000000	-5.2053274

Table S33: Cartesian coordinates (given in angstroms) generated for compound **15**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	O	O1	-0.2817902	0.4312506	-0.1953385
2	S	S1	-1.2471650	-0.9252609	-0.4330855
3	C	C1	-0.4440660	-2.0281895	0.6030350
4	O	O2	-1.0991712	-1.3018158	-1.8191768
5	O	O3	-2.5528268	-0.5715120	0.0728898
6	C	C2	-0.8307287	-2.1368382	1.9454043
7	C	C3	-0.1759669	-3.0280742	2.7926002
8	C	C4	0.8769132	-3.8234495	2.3030477
9	C	C5	1.2594557	-3.7142491	0.9553615
10	C	C6	0.6003770	-2.8201434	0.1118302
11	C	C7	-0.7053086	1.6899142	-0.7852286
12	C	C8	-0.3688413	1.6734765	-2.2809576
13	C	C9	-0.5832882	3.0653490	-2.8846924
14	C	C10	0.2241112	4.1320061	-2.1304607
15	C	C11	-0.1068111	4.1290739	-0.6310228
16	C	C12	0.1039537	2.7417813	-0.0140749
17	C	C13	1.5750390	-4.7715053	3.2182228
18	H	H1	-1.6549157	-1.5243774	2.3298388
19	H	H2	-0.4791865	-3.1093048	3.8350077
20	H	H3	2.0710580	-4.3265991	0.5663363
21	H	H4	0.8983856	-2.7442733	-0.9404599
22	H	H5	-1.7979295	1.8076158	-0.6058847
23	H	H6	0.6796702	1.3460734	-2.4225780
24	H	H7	-0.9800202	0.9156637	-2.8129947
25	H	H8	-0.2926129	3.0564829	-3.9523413
26	H	H9	-1.6600380	3.3226418	-2.8644378
27	H	H10	1.3065443	3.9489783	-2.2740193
28	H	H11	0.0216786	5.1308538	-2.5589922
29	H	H12	0.5228108	4.8703850	-0.1038560
30	H	H13	-1.1542925	4.4539525	-0.4770636
31	H	H14	1.1761361	2.4630618	-0.0319231
32	H	H15	-0.1891358	2.7345894	1.0517918
33	H	H16	2.0635237	-4.2379484	4.0483572
34	H	H17	0.8709261	-5.4876626	3.6688055
35	H	H18	2.3535118	-5.3619463	2.7160590

Table S34: Cartesian coordinates (given in angstroms) generated for compound **16**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	C	C1	-1.8903611	-0.0065515	-1.5559436
2	O	O1	-0.6513013	0.0806548	-0.8158145
3	S	S1	0.6069644	0.9337846	-1.5479480
4	C	C2	1.7817148	0.8162810	-0.3078440
5	O	O2	0.1296241	2.2869507	-1.7050691
6	O	O3	0.9834186	0.1704138	-2.7130206
7	C	C3	1.8434605	1.7919273	0.6945948
8	C	C4	2.7970871	1.6972972	1.7077246
9	C	C5	3.7003128	0.6204345	1.7266502
10	C	C6	3.6362319	-0.3574420	0.7165032
11	C	C7	2.6816907	-0.2576155	-0.2933002
12	C	C8	4.7228433	0.5041958	2.8056372
13	C	C9	-2.8217387	-0.8051954	-0.6447196
14	C	C10	-4.2064498	-0.9729975	-1.2799414
15	C	C11	-5.1419832	-1.7733067	-0.3773679
16	H	H1	-2.2606739	1.0190794	-1.7421535
17	H	H2	-1.6909289	-0.5249597	-2.5123622
18	H	H3	1.1455908	2.6377688	0.6813846
19	H	H4	2.8394068	2.4597204	2.4836089
20	H	H5	4.3335026	-1.1935020	0.7242149
21	H	H6	2.6405497	-1.0183299	-1.0822279
22	H	H7	4.7143317	1.3540355	3.5016376
23	H	H8	4.5651189	-0.4042102	3.4075973
24	H	H9	5.7406832	0.4402050	2.3915432
25	H	H10	-2.8993393	-0.2990028	0.3382581
26	H	H11	-2.3675703	-1.7922414	-0.4261490
27	H	H12	-4.6500484	0.0209536	-1.4890538
28	H	H13	-4.1138871	-1.4776594	-2.2623147
29	H	H14	-5.2850226	-1.2832022	0.5927648
30	H	H15	-6.1309902	-1.8884559	-0.8355176
31	H	H16	-4.7522429	-2.7790305	-0.1813716

Table S35: Cartesian coordinates (given in angstroms) generated for compound **17**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	O	O1	-0.0584815	-1.5969935	1.0000637
2	S	S1	1.2382854	-2.7257442	0.7513987
3	C	C1	0.4855587	-4.0407425	1.5754343
4	O	O2	1.2972337	-2.9308798	-0.6650231
5	O	O3	2.3516706	-2.1962552	1.4695323
6	C	C2	-0.1012207	-0.3874291	0.3656395
7	C	C3	0.2070984	-0.2336023	-0.9940236
8	C	C4	0.0484387	1.0319154	-1.5666821
9	C	C5	-0.4220031	2.1137733	-0.8108849
10	C	C6	-0.7191333	1.9311696	0.5485171
11	C	C7	-0.5630718	0.6836380	1.1530484
12	C	C8	0.3494201	1.2401044	-3.0320596
13	F	F1	-0.7474769	1.2185844	-3.8084336
14	F	F2	1.1655907	0.3391591	-3.5985891
15	F	F3	0.9300762	2.4161764	-3.3248838
16	C	C9	-1.2321921	3.1070767	1.3428686
17	F	F4	-2.5006507	3.4400202	1.0490235
18	F	F5	-0.5455662	4.2469415	1.1589444
19	F	F6	-1.2410065	2.9576231	2.6770293
20	H	H1	-0.5269436	-3.7951432	1.9528502
21	H	H2	1.0411007	-4.3854546	2.4652224
22	H	H3	0.3413900	-4.9359198	0.9448633
23	H	H4	0.5541062	-1.0955485	-1.5842585
24	H	H5	-0.5624357	3.0944378	-1.2759542
25	H	H6	-0.7897858	0.5030929	2.2063566

Table S36: Cartesian coordinates (given in angstroms) generated for compound **18**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	O	O1	0.0797576	-1.5460047	0.8214037
2	S	S1	0.3728114	-2.9292502	-0.1786711
3	C	C1	0.6727504	-4.0196338	1.1266936
4	O	O2	-0.8655285	-3.2000655	-0.8356412
5	O	O3	1.5596118	-2.6451343	-0.9289465
6	C	C2	-0.0396601	-0.2775088	0.3303113
7	C	C3	0.5869683	0.1544835	-0.8461641
8	C	C4	0.4312839	1.4853711	-1.2346885
9	C	C5	-0.3319746	2.3678824	-0.4566550
10	C	C6	-0.9451314	1.9165083	0.7280867
11	C	C7	-0.8057047	0.5936208	1.1295373
12	C	C8	-0.5119353	3.8002237	-0.8535962
13	F	F1	0.0573622	4.1788242	-2.0101022
14	F	F2	-0.0249430	4.6845863	0.0365769
15	F	F3	-1.7950807	4.1777781	-1.0012925
16	H	H1	1.6882281	-4.4525730	1.1169070
17	H	H2	-0.0227424	-4.8761843	1.1571552
18	H	H3	0.5772756	-3.5417253	2.1214079
19	H	H4	1.2075738	-0.5192119	-1.4464655
20	H	H5	0.9186762	1.8242626	-2.1528580
21	H	H6	-1.5372909	2.6038409	1.3381451
22	H	H7	-1.2723060	0.2199101	2.0388562

Table S37: Cartesian coordinates (given in angstroms) generated for compound **19**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	O	O1	0.6129635	0.0000000	-1.4010522
2	S	S1	-0.5474694	0.0000000	-2.7011969
3	C	C1	0.6224346	0.0000000	-3.9680662
4	O	O2	-1.2418140	-1.2432363	-2.5960622
5	O	O3	-1.2418140	1.2432363	-2.5960622
6	C	C2	0.2759606	0.0000000	-0.0881036
7	C	C3	-1.0496862	0.0000000	0.3789683
8	C	C4	-1.2715126	0.0000000	1.7525530
9	C	C5	-0.1798973	0.0000000	2.6393893
10	C	C6	1.1465093	0.0000000	2.1595238
11	C	C7	1.3804787	0.0000000	0.7941288
12	N	N1	-0.4218540	0.0000000	4.0875799
13	O	O4	-1.5816096	0.0000000	4.4708661
14	O	O5	0.5515712	0.0000000	4.8261360
15	H	H1	0.1819063	0.0000000	-4.9798339
16	H	H2	1.2961334	0.8764104	-3.9461589
17	H	H3	1.2961334	-0.8764104	-3.9461589
18	H	H4	-1.9029016	0.0000000	-0.3008718
19	H	H5	-2.2935123	0.0000000	2.1527322
20	H	H6	1.9777597	0.0000000	2.8751648
21	H	H7	2.3902202	0.0000000	0.3865243

Table S38: Cartesian coordinates (given in angstroms) generated for compound **20**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	O	O1	0.6523969	-0.6643286	1.1979397
2	S	S1	1.1259161	-2.1711495	0.5240455
3	C	C1	-0.4312388	-2.8362817	0.1450480
4	O	O2	1.8653257	-1.9175595	-0.6787808
5	O	O3	1.7149262	-2.8381852	1.6421063
6	C	C2	0.2708968	0.4281823	0.4592069
7	C	C3	0.7123208	0.6888375	-0.8422363
8	C	C4	0.2656289	1.8560935	-1.4690630
9	C	C5	-0.5968131	2.7371240	-0.8108493
10	C	C6	-1.0169748	2.4607684	0.4970185
11	C	C7	-0.5923342	1.3029621	1.1453358
12	H	H1	-0.6894685	-2.7699278	-0.9246607
13	H	H2	-1.2607482	-2.3434348	0.6810202
14	H	H3	-0.5233513	-3.9035182	0.4068004
15	H	H4	1.4109541	0.0223121	-1.3578783
16	H	H5	0.6022197	2.0788474	-2.4821450
17	H	H6	-0.9360603	3.6418782	-1.3094967
18	H	H7	-1.6804212	3.1553121	1.0123479
19	H	H8	-0.8931752	1.0720677	2.1642409

Table S39: Cartesian coordinates (given in angstroms) generated for compound **21**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	O	O1	0.3744008	-1.2282015	0.6337470
2	S	S1	-0.3962019	-2.6877744	0.3203073
3	C	C3	0.7706516	-3.7351407	1.0650937
4	O	O2	-0.4238088	-2.8655861	-1.1086203
5	O	O3	-1.6352520	-2.6658998	1.0533127
6	C	C4	-0.2952639	0.0069487	0.2575907
7	C	C5	-0.1364373	0.2139632	-1.2529674
8	C	C6	-0.6309056	1.6100637	-1.6462911
9	C	C7	0.0857422	2.7042536	-0.8418048
10	C	C8	-0.0588499	2.4758330	0.6696540
11	C	C9	0.4332974	1.0816576	1.0753539
12	H	H7	1.2080680	-4.4650597	0.3655601
13	H	H8	0.3574978	-4.3203794	1.9019833
14	H	H9	1.6285790	-3.1829632	1.4886990
15	H	H10	-1.3642347	-0.0746042	0.5579756
16	H	H11	0.9269983	0.0855010	-1.5362798
17	H	H12	-0.6811822	-0.5701802	-1.8186960
18	H	H13	-0.4694405	1.7700859	-2.7292812
19	H	H14	-1.7248230	1.6806374	-1.4889196
20	H	H15	1.1585432	2.7247197	-1.1149130
21	H	H16	-0.3188183	3.6970820	-1.1127997
22	H	H17	0.5090447	3.2466858	1.2239739
23	H	H18	-1.1174654	2.6030416	0.9691979
24	H	H19	1.5251747	0.9893399	0.9128540
25	H	H20	0.2746859	0.9059761	2.1552696

Table S40: Cartesian coordinates (given in angstroms) generated for compound **22**, calculated using semi-empirical PM6 methods, after energy minimisation calculations.

	Atom		X	Y	Z
1	O	O1	0.3117463	0.0000000	-1.2340842
2	S	S1	-0.2686875	0.0000000	-2.8159170
3	C	C3	1.2620884	0.0000000	-3.6320000
4	O	O2	-0.9688215	1.2427959	-3.0027161
5	O	O3	-0.9688215	-1.2427959	-3.0027161
6	C	C4	-0.6761368	0.0000000	-0.1771793
7	C	C5	0.1444019	0.0000000	1.1117600
8	C	C6	-0.7655219	0.0000000	2.3453476
9	C	C7	0.0464845	0.0000000	3.6378231
10	H	H7	1.1703974	0.0000000	-4.7291428
11	H	H8	1.8824241	-0.8774182	-3.3850429
12	H	H9	1.8824241	0.8774182	-3.3850429
13	H	H10	-1.2982847	0.9089958	-0.2803433
14	H	H11	-1.2982847	-0.9089958	-0.2803433
15	H	H12	0.8178412	0.8803105	1.1216247
16	H	H13	0.8178412	-0.8803105	1.1216247
17	H	H14	-1.4326969	0.8848781	2.3242635
18	H	H15	-1.4326969	-0.8848781	2.3242635
19	H	H16	-0.6090355	0.0000000	4.5164809
20	H	H17	0.6916694	-0.8833131	3.7106701
21	H	H18	0.6916694	0.8833131	3.7106701

References

1 R. J. Ellaby, E. R. Clark, N. Allen, F. R. Taylor, K. K. L. Ng, M. Dimitrovski, D. F. Chu, D. P. Mulvihill and J. R. Hiscock, *Org. Biomol. Chem.*, 2021, **19**, 2008–2014.

2 Y. F. Chen, C. L. Kao, W. K. Lee, P. C. Huang, C. Y. Hsu and C. H. Kuei, *J. Chinese Chem. Soc.*, 2016, **63**, 751–757.

3 D. S. Panmand, A. D. Tiwari, S. S. Panda, J. C. M. Monbaliu, L. K. Beagle, A. M. Asiri, C. V. Stevens, P. J. Steel, C. D. Hall and A. R. Katritzky, *Tetrahedron Lett.*, 2014, **55**, 5898–5901.

4 H. Huang and J. Y. Kang, *Org. Lett.*, 2018, **20**, 4938–4941.

5 S. Feng, J. Li and J. Wei, *New J. Chem.*, 2017, **41**, 4743–4746.

6 D. V. Schoonover and H. W. Gibson, *Tetrahedron Lett.*, 2017, **58**, 242–244.

7 J. W. W. Chang, E. Y. Chia, C. L. L. Chai and J. Seayad, *Org. Biomol. Chem.*, 2012, **10**, 2289–2299.

8 T. Noji, H. Fujiwara, K. Okano and H. Tokuyama, *Org. Lett.*, 2013, **15**, 1946–1949.

9 N. Ortega, A. Feher-Voelger, M. Brovetto, J. I. Padrón, V. S. Martín and T. Martín, *Adv. Synth. Catal.*, 2011, **353**, 963–972.

10 J. Wang, Y. Zhao, W. Zhao, P. Wang and J. Li, *J. Carbohydr. Chem.*, 2017, **35**, 445–454.

11 N. Busschaert, I. L. Kirby, S. Young, S. J. Coles, P. N. Horton, M. E. Light and P. A. Gale, *Angew. Chemie - Int. Ed.*, 2012, **51**, 4426–4430.

12 C. A. Hunter, *Angew. Chem. Int. Ed*, 2004, **43**, 5310–5324.

13 J. J. P. Stewart, *J Mol Model*, 2007, **13**, 1173–1213.

14 Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215–241.

15 A. D. McLean and G. S. Chandler, *J. Chem. Phys.*, 1980, **72**, 5639–5648.

16 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian 16; Revision A.03; Gaussian Inc.; Wallingford CT; 2016.