Supporting information:

Controlling Antimicrobial Activity of Quinolones Using Visible/NIR Light-Activated BODIPY Photocages

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1. General information

All chemicals were obtained from commercial sources and used as received unless stated otherwise. Room temperature reactions were carried out between 22-25 °C. Thin-layer chromatography (TLC) was performed using silica gel 60 pre-coated aluminum plates (Macherey-Nagel 0.20 mm thickness) with a fluorescence indicator UV254. Solvents were ACS grade and used without further purification. For the detection of components, UV light at 254 nm was used. All chromatographic solvents were ACS grade and used without further purification. Column chromatography was performed on silica gel 60 (0.040-0.063 mm) and the indicated eluent in each case.

^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVANCE III HD (300 MHz), or Bruker AVANCE NEO (400 MHz) spectrometers at 25 °C. Chemical shifts (δ) are reported in parts per million (ppm) with the solvent resonance as the internal standard (δ_H 7.26 for $CHCl_3$, and 2.50 for DMSO-d_6; δ_C 77.16 for $CHCl_3$). Coupling constants (J) are reported in Hertz (Hz). The following abbreviations are used to indicate signal multiplicity: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublets), and quint (quintet).

Molecular absorption spectra were obtained by using a spectrometer provided with an Ocean Optics USB4000-UV-Vis detector and coupled to a deuterium/tungsten halogen lamp. Quartz cuvettes with 1 cm optical path length were used. Solutions were prepared in a concentration range of 5×10^{-5} M approximately.

High-resolution electrospray mass spectra (HR ESI-MS) were recorded on a Bruker MicrOTOF-Q spectrometer. Accurate mass measurements were achieved by using sodium formate as an external reference. HR ESI-MS performed at Iowa State University were recorded on an Agilent QTOF 6540 spectrometer.

2. Synthesis

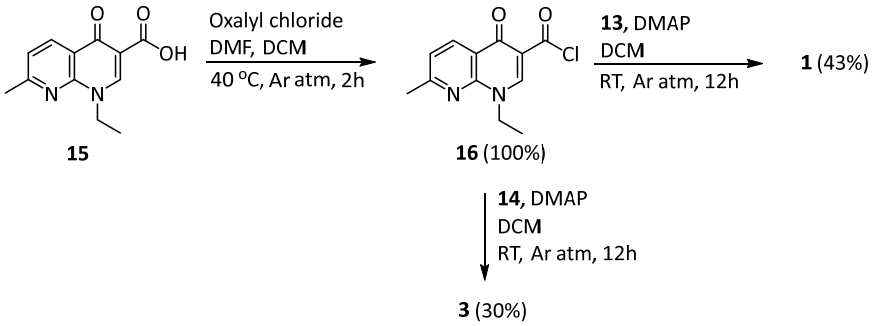


Figure S1. Synthetic route of compounds **1** and **3**, photoreleasable derivatives of nalidixic acid.

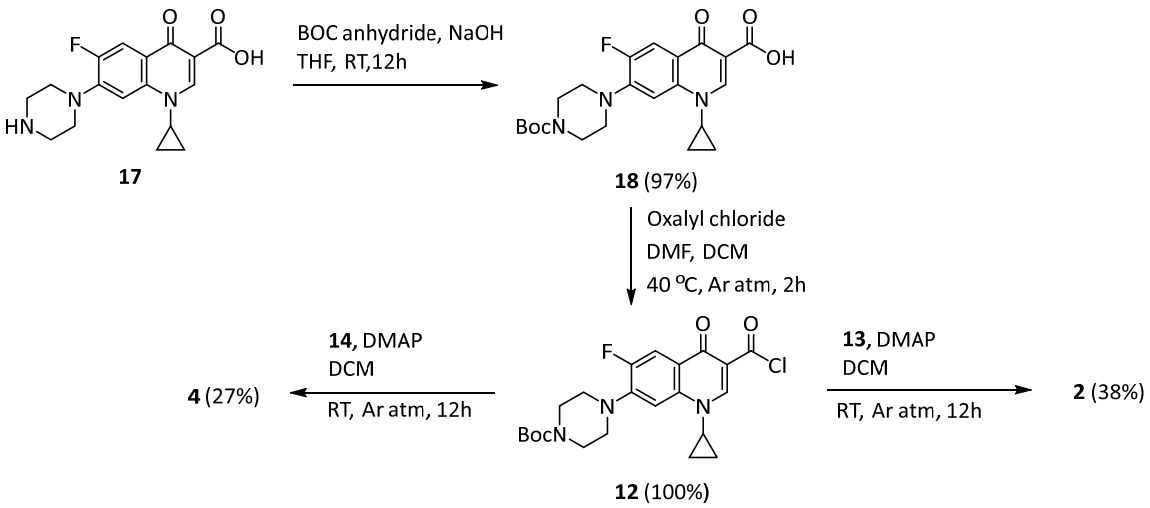
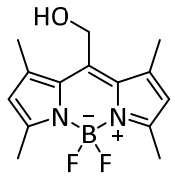


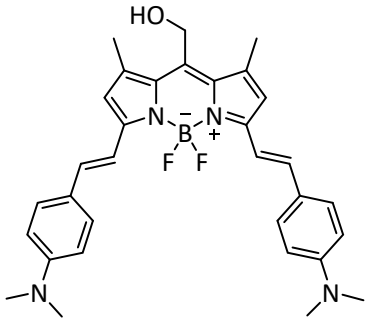
Figure S2. Synthetic route of compounds **2** and **4**, photoreleasable derivatives of Boc-ciprofloxacin.

(5,5-difluoro-1,3,7,9-tetramethyl-5*H*-4l4,5l4-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinin-10-yl) methanol (13):



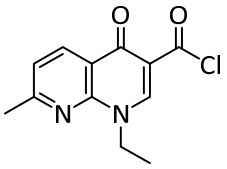
Compound prepared according to a previously described procedure (75% yield).[1]
^{1}H-NMR (300 MHz, $CDCl_3$): δ 6.09 (s, 2H), 4.91 (s, 2H), 2.53 (s, 6H), 2.51 (s, 6H).
^{1}H-NMR spectrum in agreement with published data.[1]

(3,7-bis(4-(dimethylamino)styryl)-5,5-difluoro-1,9-dimethyl-5*H*-4l4,5l4- dipyrrolo[1,2-*c*:2', 1'-*f*][1,3,2]diazaborinin-10-yl)methanol (14):



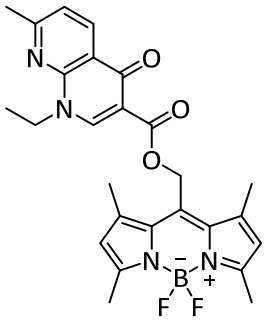
Compound prepared according to a previously described procedure (92% yield).[2]
^{1}H-NMR (300 MHz, DMSO-d_6): δ 7.48-7.43 (m, 6H), 7.27 (d, *J* = 16 Hz, 2H), 6.94 (s, 2H), 6.79 (d, *J* = 8.9 Hz, 4H), 5.45 (t, *J* = 4.9 Hz, 1H), 4.74 (d, *J* = 4.8 Hz, 2H), 3.00 (s, 12H), 2.54 (s, 6H).
^{1}H-NMR spectrum in agreement with published data.[2]

1-ethyl-7-methyl-4-oxo-1,4-dihydro-1,8-naphthyridine-3-carbonyl chloride (16):



To a solution of nalidixic acid (0.43 mmol, 0.1 g) in dry DCM (4 ml) under argon atmosphere was added oxalyl chloride (1.29 mmol, 0.11 ml) and one drop of DMF. The resulting mixture was stirred for 2 hours at 40 °C. After that time, the solvent was evaporated *in vacuo* to give 0.11 g of a dark blue solid that was immediately used in the next step.

(5,5-difluoro-1,3,7,9-tetramethyl-5*H*-4l4,5l4-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinin-10-yl) methyl 1-ethyl-7-methyl-4-oxo-1,4-dihydro-1,8-naphthyridine-3-carboxylate (1):



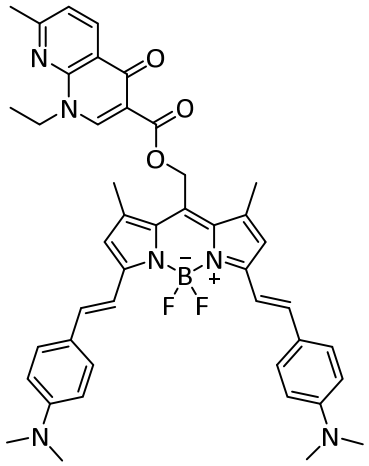
Compound **13** (80 mg, 0.29 mmol) was dissolved in dry DCM (4 ml) under argon atmosphere and 4-(dimethylamino)pyridine (70 mg, 0.58 mmol) was added. This mixture was added over a solution containing compound **16** (111 mg, 0.43 mmol) in dry DCM (3 ml) under argon atmosphere. The reaction mixture was stirred in the dark for 12 hours at room temperature. After that time, the solvent was evaporated *in vacuo*, and the resulting residue was purified by column chromatography (DCM:EtOAc 5:2) to obtain 61 mg (43%) of a red solid.

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.63 (d, *J* = 8.1 Hz, 1H), 8.55 (s, 1H), 7.24 (d, *J* = 8.1 Hz, 1H), 6.08 (s, 2H), 5.51 (s, 2H), 4.46 (q, *J* = 7.1 Hz, 2H), 2.65 (s, 3H), 2.54 (s, 6H), 2.44 (s, 6H), 1.47 (t, *J* = 7.1 Hz, 3H).

^{13}C-NMR (100 MHz, $CDCl_3$): δ 174.8, 164.2, 163.0, 156.6, 148.7, 142.1, 137.0, 134.0, 133.1, 122.4, 121.6, 121.5, 110.6, 58.1, 47.0, 25.2, 15.9, 15.4, 14.8.

HR-MS (ESI, [M+H]+): Calcd. for $C_{26}H_{27}BF_2N_4O_3$ + H: 493.2217; Found: 493.2226

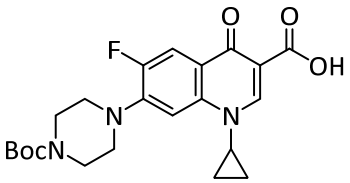
(3,7-bis(4-(dimethylamino)styryl)-5,5-difluoro-1,9-dimethyl-5*H*-4l4,5l4- dipyrrolo[1,2-*c*:2',1'-*f*] [1,3,2]diazaborinin-10-yl)methyl 1-ethyl-7-methyl-4-oxo- 1,4-dihydro-1,8-naphthyridine-3-carboxylate (3):



Compound **14** (83 mg, 0.15 mmol) was dissolved in dry DCM (4 ml) under argon atmosphere and 4-(dimethylamino)pyridine (37 mg, 0.30 mmol) was added. This mixture was added over a solution containing compound **16** (56 mg, 0.23 mmol) in dry DCM (3 ml) under argon atmosphere. The reaction mixture was stirred in the dark for 12 hours at room temperature. After that time, the solvent was evaporated *in vacuo*, and the resulting residue was purified by column chromatography (DCM:EtOAc:Toluene 2:3:1) to obtain 34 mg (30%) of a dark green solid.

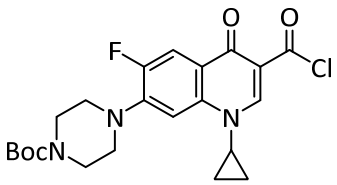
^{1}H-NMR (300 MHz, $CDCl_3$): δ 8.64 (d, *J* = 8.1 Hz, 1H), 8.57 (s, 1H), 7.53 (d, *J* = 8.9 Hz, 6H), 7.25-7.15 (m, 3H), 6.71 (d, *J* = 8.9 Hz, 6H), 5.53 (s, 2H), 4.45 (q, *J* = 7.1 Hz, 2H), 3.04 (s, 12H), 2.64 (s, 3H), 2.46 (s, 6H), 1.45 (t, *J* = 7.1 Hz, 3H).
^{13}C-NMR (75 MHz, CDCl3): δ 175.0, 163.7, 162.9, 153.4, 151.1, 148.7, 148.6, 139.5, 137.2, 137.0, 129.4, 129.3, 125.2, 121.5, 121.4, 118.4, 115.0, 112.2, 110.6, 58.4, 46.9, 40.4, 25.2, 16.1, 15.4.
HR-MS (ESI, [M+Na]+): Calcd. for $C_{44}H_{45}BF_2N_6O_3$ +Na: 777.3514; Found: 777.3497

7-(4-(*tert*-butoxycarbonyl)piperazin-1-yl)-1-cyclopropyl-6-fluoro-4-oxo-1,4- dihydroquinoline-3-carboxylic acid (18):



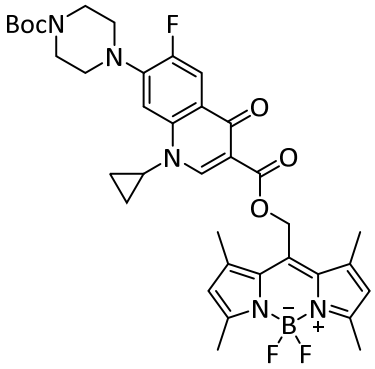
Ciprofloxacin (2 g, 6.0 mmol) and di-*tert*-butyl decarbonate (1.4 g, 6.6 mmol) were dissolved in THF (60 ml). Next, a solution of sodium hydroxide (0.48 g, 12.0 mmol) in water (12 ml) was added, and the mixture was stirred overnight at room temperature. After that time, the solvent was removed *in vacuo*, and the residue was taken into aqueous saturated ammonium chloride (200 ml). The aqueous phase was extracted with DCM (200 ml) three times. The organic layer was washed with brine (400 ml) and dried over anhydrous $MgSO_4$. The solvent was evaporated *in vacuo* to obtain 2.51 g (97%) of white solid.
^{1}H-NMR (300 MHz, $CDCl_3$): δ 14.94 (s, 1H), 8.71 (s, 1H), 7.96 (d, *J* = 12.9 Hz, 1H), 7.35 (d, *J* = 7.1 Hz, 1H), 3.72 – 3.61 (m, 4H), 3.59-3.50 (m, 1H), 3.34 – 3.21 (m, 4H), 1.49 (s, 9H), 1.41- 1.35 (m, 2H), 1.26 – 1.15 (m, 2H).

***Tert*-butyl 4-(3-(chlorocarbonyl)-1-cyclopropyl-6-fluoro-4-oxo-1,4- dihydroquinolin-7-yl) piperazine-1-carboxylate (12):**



To a solution of compound **18** (0.15 g, 0.35 mmol) in dry DCM (5 ml) under argon atmosphere, oxalyl chloride (88 µl, 1.05 mmol) and one drop of DMF were added. The reaction was stirred for 2 hours at 40 °C. After that time, the solvent was removed *in vacuo* to give 0.16 g (100%) of an orange solid that was immediately used in the next step.

(5,5-difluoro-1,3,7,9-tetramethyl-5*H*-4l4,5l4-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2] diazaborinin-10-yl) methyl 7-(4-(*tert*-butoxycarbonyl)piperazin-1-yl)-1 cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylate (2):



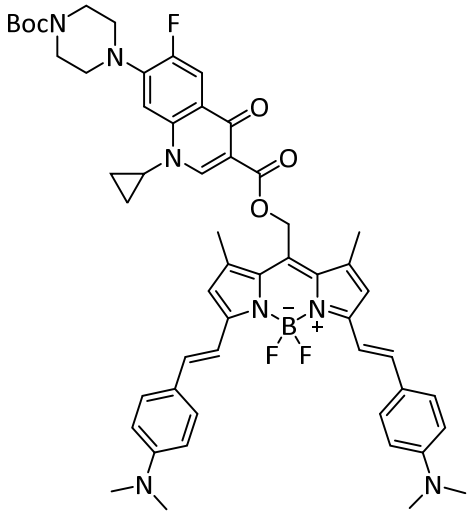
Compound **13** (67 mg, 0.24 mmol) was dissolved in dry DCM (4 ml) under argon atmosphere and 4-(dimethylamino)pyridine (57 mg, 0.47 mmol) was added. This mixture was added over a solution containing compound **12** (160 mg, 0.36 mmol) in dry DCM (3 ml) under argon atmosphere. The reaction mixture was stirred in the dark for 12 hours at room temperature. After that time, the solvent was evaporated *in vacuo*, and the resulting residue was purified by column chromatography (DCM:EtOAc 5:2) to obtain 63 mg (38%) of a red solid.

^{1}H-NMR (300 MHz, $CDCl_3$): δ 8.45 (s, 1H), 8.05 (d, *J* = 13.1 Hz, 1H), 7.24 (d, 1H), 6.08 (s, 2H), 5.51 (s, 2H), 3.68 – 3.60 (m, 4H), 3.45 – 3.33 (m, 1H), 3.24 – 3.16 (m, 4H), 2.53 (s, 6H), 2.45 (s, 6H), 1.49 (s, 9H), 1.34 – 1.26 (m, 2H), 1.12 – 1.02 (m, 2H).

^{13}C-NMR (75 MHz, $CDCl_3$): δ 173.1, 164.6, 156.5, 155.2, 154.7, 151.9, 148.2, 144.8, 142.1, 138.1, 134.1, 133.1, 122.4, 113.8, 109.3, 105.1, 80.4, 58.1, 50.1, 43.6, 34.7, 28.6, 15.9, 14.8, 8.5.

HR-MS (ESI, [M+H]+): Calcd. for $C_{36}H_{41}BF_3N_5O_5$ +H: 692.3225; Found: 692.3235

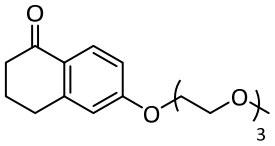
(3,7-bis(4-(dimethylamino)styryl)-5,5-difluoro-1,9-dimethyl-5*H*-4l4,5l4- dipyrrolo[1,2-*c*:2',1'-*f*] [1,3,2]diazaborinin-10-yl)methyl 7-(4-(*tert*-butoxycarbonyl)piperazin-1-yl)-1-cyclopropyl-6-fluoro -4-oxo-1,4- dihydroquinoline-3-carboxylate (4):



Compound **14** (83 mg, 0.15 mmol) was dissolved in dry DCM (4 ml) under argon atmosphere and 4-(dimethylamino)pyridine (37 mg, 0.30 mmol) was added. This mixture was added over a solution

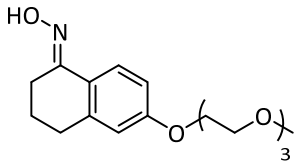
containing compound **12** (103 mg, 0.23 mmol) in dry DCM (3 ml) under argon atmosphere. The reaction mixture was stirred in the dark for 12 hours at room temperature. After that time, the solvent was evaporated *in vacuo*, and the resulting residue was purified by column chromatography (DCM:EtOAc:Toluene 2:3:1) to obtain 34 mg (30%) of a dark green solid.
^{1}H-NMR (300 MHz, $CDCl_3$): δ 8.45 (s, 1H), 8.07 (d, *J* = 13.1 Hz, 1H), 7.53 (d, *J* = 8.9 Hz, 6H), 7.25 – 7.17 (m, 3H), 6.71 (d, *J* = 8.7 Hz, 6H), 5.54 (s, 2H), 3.66 – 3.59 (m, 4H), 3.42 – 3.32 (m, 1H), 3.22 – 3.16 (m, 4H), 3.03 (s, 12H), 2.48 (s, 6H), 1.49 (s, 9H), 1.26 – 1.21 (m, 2H), 1.09 – 1.02 (m, 2H).
^{13}C-NMR (75 MHz, $CDCl_3$): δ 173.3, 164.1, 154.8, 153.4, 151.1, 148.0, 144.7, 144.6, 139.6, 138.1, 137.1, 134.8, 129.4, 129.3, 127.9, 125.2, 123.3, 118.4, 115.0, 113.9, 113.6, 112.2, 109.4, 105.2, 80.3, 58.4, 50.1, 43.6, 40.4, 34.7, 28.6, 16.1, 8.6.
HR-MS (ESI, [M+H]+): Calcd. for $C_{54}H_{59}BF_3N_7O_5$ +H: 954.4704; Found: 954.4659

6-(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)-3,4-dihydronaphthalen-1(2*H*)-one (7):



To a solution of 6-hydroxy-1-tetralone **6** (1 g, 6.2 mmol) in anhydrous DMF (15 ml) under argon atmosphere was added sodium carbonate (1.3 g, 12.3 mmol), 1-chloro-2-[2-(2-methoxyethoxy)ethoxy]ethane (1.2 g, 6.7 mmol), and sodium iodide as a catalyst. The resulting mixture was stirred for 16 hours at 100 °C. After that time, the solvent was removed *in vacuo*, and the resulting product was neutralized with 1M HCl. Then, it was extracted with DCM (60 ml) twice, and the organic layers were washed with brine (60 ml). Next, the organic layer was dried over anhydrous $MgSO_4$, and the solvent was evaporated *in vacuo* to give 1.8 g (95%) of a clear oil.
^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.99 (d, *J* = 8.7 Hz, 1H), 6.83 (dd, *J* = 8.8, 2.5 Hz, 1H), 6.71 (d, *J* = 2.5 Hz, 1H), 4.20 – 4.15 (m, 2H), 3.88-3.84 (m, 2H), 3.75-3.72 (m, 2H), 3.70 – 3.61 (m, 4H), 3.56-3.53 (m, 2H), 3.37 (s, 3H), 2.92-2.89 (m, 2H), 2.62-2.58 (m, 2H), 2.10 (quint, *J* = 6.4 Hz, 2H).
^{13}C-NMR (100 MHz, $CDCl_3$): δ 197.3, 162.9, 147.0, 129.7, 126.6, 113.6, 113.4, 72.1, 71.0, 70.8, 70.7, 69.7, 67.7, 59.2, 39.0, 30.3, 23.5.
HR-MS (ESI, [M+H]+): Calcd. for $C_{17}H_{24}O_5$ +H: 309.1697; Found: 309.1701

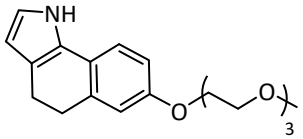
6-(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)-3,4-dihydronaphthalen-1(2*H*)-one oxime (8):



Sodium acetate (0,29 g, 3.6 mmol) was dissolved in water (3 ml) and added over a solution of hydroxylamine hydrochloride (0.25 g, 3.6 mmol) in water (3 ml). The resulting mixture was added over a solution of compound **7** (1 g, 3.2 mmol) in methanol (10 ml) and heated at 35 °C. Next, the sample was stirred for 2 hours at 80 °C. After that time, the reaction was cooled at room temperature, and the solvent was removed *in vacuo*. Next, water (30 ml) was added to the residue, and the aqueous phase was extracted with DCM (50 ml) twice. The combined organic layers were washed with brine (50 ml) and dried over anhydrous $MgSO_4$. Then, the solvent was evaporated *in vacuo* to result in 0.99 g (94%) of a clear oil.

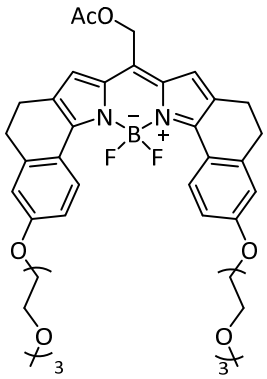
^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.77 (d, *J* = 8.7 Hz, 1H), 6.76 (dd, *J* = 8.8, 2.7 Hz, 1H), 6.66 (d, *J* = 2.6 Hz, 1H), 4.16 – 4.09 (m, 2H), 3.87 – 3.82 (m, 2H), 3.75 – 3.71 (m, 2H), 3.70 – 3.62 (m, 4H), 3.58 – 3.52 (m, 2H), 3.37 (s, 3H), 2.79 (t, *J* = 6.6 Hz, 2H), 2.70 (t, *J* = 6.1 Hz, 2H), 1.85 (quint, *J* = 6.5 Hz, 2H).
^{13}C-NMR (100 MHz, $CDCl_3$): δ 159.6, 155.2, 141.6, 125.7, 123.5, 113.8, 113.6, 72.0, 70.9, 70.8, 70.7, 69.8, 67.4, 59.1, 30.2, 23.9, 21.5.
HR-MS (ESI, [M+H]+): Calcd. for $C_{17}H_{25}NO_5$ +H: 324.1805; Found: 324.1811

7-(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)-4,5-dihydro-1*H*-benzo[g]indole (9):



In a three-neck flask, under argon atmosphere, compound **8** (1 g, 3.1 mmol) was dissolved in DMSO (25 ml). Next, lithium hydroxide monohydrate (0.7 g, 16.7 mmol) was added, and a light flow of acetylene was passed through the reaction mixture. The mixture was heated at 135 °C while keeping the acetylene flow for 6 hours. After that time, the reaction mixture was allowed to reach room temperature, and distilled water (60 ml) was added. Then, the aqueous phase was extracted with diethyl ether (100 ml) five times. The combined organic layers were extracted with water (100 ml) once. Finally, the organic layer was dried over anhydrous $MgSO_4$ and the solvent was removed *in vacuo*. The obtained residue was purified by column chromatography (DCM:EtOAc 5:1)to give 0.31 g (30%) of a clear oil.
^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.34 (s, 1H), 7.06 (d, *J* = 8.3 Hz, 1H), 6.80 (d, *J* = 2.5 Hz, 1H), 6.72 (d, *J* = 2.7 Hz, 1H), 6.71 (t, *J* = 2.7 Hz, 1H), 6.10 (t, *J* = 2.5 Hz, 1H), 4.14 – 4.07 (m, 2H), 3.86 – 3.82 (m, 2H), 3.76 – 3.72 (m, 2H), 3.71-3.64 (m, 4H), 3.59 – 3.52 (m, 2H), 3.38 (s, 3H), 2.89 (t, *J* = 7.5 Hz, 2H), 2.72 (t, *J* = 7.3 Hz, 2H).
^{13}C-NMR (100 MHz, $CDCl_3$): δ 156.6, 136.8, 127.8, 123.1, 119.3, 118.5, 117.4, 115.6, 112.1, 108.0, 72.1, 70.9, 70.8, 70.7, 69.9, 67.6, 59.2, 30.6, 21.9.
HR-MS (ESI, [M+H]+): Calcd. for $C_{19}H_{25}NO_4$ +H: 332.1856; Found: 332.1855

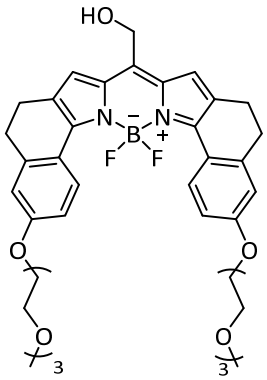
8-((acetyloxy)methyl)-17,17-difluoro-3,13-bis(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)-5,10,11,17-tetrahydro-6H benzo[g]benzo[6',7']indolo[1',2':3,4] [1,3,2] diazaborinino[1,6-a]indol-16-ium (10):



To a solution of compound **9** (0.94 mmol, 0.31 g) in dry DCM (10 ml) under argon atmosphere, was added acetoxyacetyl chloride (0.56 mmol, 60 µl) and the mixture was stirred in the dark at 40 °C for 2 hours. Then, TEA (1.7 mmol, 0.23 ml) was added. The resulting mixture was allowed to stir for 15

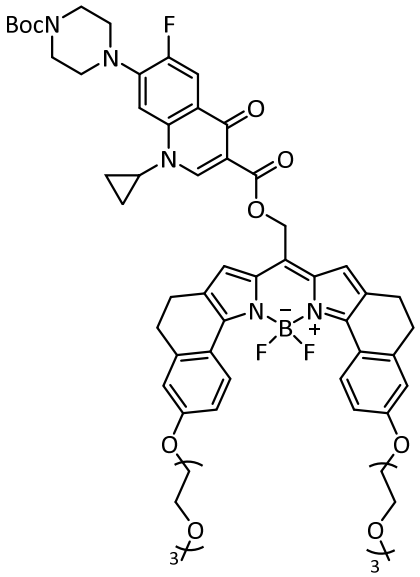
minutes. Next, boron trifluoride diethyl etherate (1.7 mmol, 0.21 ml) was added. After 1 hour of stirring, another portion of TEA (1.7 mmol, 0.23 ml) and boron trifluoride diethyl etherate (1.7 mmol, 0.21 ml) were added, and the stirring continued for one more hour. After that time, the solvent was evaporated *in vacuo*, and the obtained residue was purified by column chromatography (DCM:MeOH 32:1) to give 85 mg (23%) of a deep blue-green solid.
^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.68 (d, *J* = 9.0 Hz, 2H), 6.98 (s, 2H), 6.95 (dd, *J* = 8.9, 2.7 Hz, 2H), 6.82 (d, *J* = 2.7 Hz, 2H), 5.25 (s, 2H), 4.24 – 4.19 (m, 4H), 3.91 – 3.86 (m, 4H), 3.78 – 3.73 (m, 4H), 3.72 – 3.65 (m, 8H), 3.58 – 3.53 (m, 4H), 3.38 (s, 6H), 2.88 (t, *J* = 7.0 Hz, 4H), 2.73 (t, *J* = 6.4 Hz, 4H), 2.10 (s, 3H).
^{13}C-NMR (100 MHz, $CDCl_3$): δ 170.7, 160.2, 152.6, 143.1, 136.2, 132.6, 130.4, 128.3, 122.1, 121.6, 115.1, 113.1, 72.1, 71.0, 70.8, 70.7, 69.7, 67.5, 59.9, 59.2, 31.0, 22.5, 21.1.
HR-MS (ESI, [M+H]+): Calcd. for $C_{42}H_{51}BF_2N_2O_{10}$ +H: 790.3568; Found: 790.3562

17,17-difluoro-8-(hydroxymethyl)-3,13-bis(2-(2-(2-methoxyethoxy)ethoxy) ethoxy)-5,10,11,17-tetrahydro-6H-benzo[g]benzo[6',7']indolo[1',2':3,4] [1,3,2]diazaborinino [1,6-a]indol-16-ium (11):



To a solution of compound **10** (0.11 mmol, 85 mg) in a mixture of DCM (25 ml) and MeOH (10 ml) was added a solution of potassium carbonate (0.39 mmol, 53 mg) in water (1 ml). The reaction mixture was stirred in the dark at room temperature for 3 hours. After that time, the organic solvent was removed *in vacuo*, and the residue was extracted with DCM (40 ml) twice. Next, the combined organic layers were washed with 1M HCl (10 ml) and brine (20 ml). The organic layer was dried over anhydrous $MgSO_4$, and the solvent was removed *in vacuo*. The resulting residue was purified by column chromatography (DCM:MeOH 40:1) to obtain 48 mg (58%) of a dark green solid.
^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.68 (d, *J* = 9.0 Hz, 2H), 7.04 (s, 2H), 6.96 (dd, *J* = 8.9, 2.7 Hz, 2H), 6.82 (d, *J* = 2.7 Hz, 2H), 4.81 (s, 2H), 4.28 – 4.14 (m, 4H), 3.93 – 3.84 (m, 4H), 3.80 – 3.72 (m, 4H), 3.72 – 3.64 (m, 8H), 3.59 – 3.52 (m, 4H), 3.38 (s, 6H), 2.88 (t, *J* = 7.0 Hz, 4H), 2.73 (t, *J* = 7.0 Hz, 4H).
^{13}C-NMR (100 MHz, $CDCl_3$): δ 160.1, 152.4, 143.0, 135.5, 133.5, 132.4, 121.8, 121.8, 121.7, 115.1, 113.1, 72.1, 71.0, 70.8, 70.7, 69.8, 67.6, 59.9, 59.2, 31.0, 22.6.
HR-MS (ESI, [M+H]+): Calcd. for $C_{40}H_{49}BF_2N_2O_9$ +H: 790.3568; Found: 790.3562

8-((((7-(4-(*tert*-butoxycarbonyl)piperazin-1-yl)-1-cyclopropyl-6-fluoro-4-oxo- 1,4-dihydroquinolin-3-yl)carbonyl)oxy)methyl)-17,17-difluoro-3,13-bis(2-(2-(2- methoxyethoxy)ethoxy)ethoxy)-5,10, 11,17-tetrahydro-6H benzo[g]benzo [6',7'] indolo [1',2':3,4][1,3,2]diazaborinino[1,6-a]indol-16-ium (5):



Compound **11** (48 mg, 0.06 mmol) was dissolved in dry DCM (3 ml) under argon atmosphere and 4-(dimethylamino)pyridine (16 mg, 0.13 mmol) was added. This mixture was added over a solution containing compound **12** (39 mg, 0.09 mmol) in dry DCM (2 ml) under argon atmosphere. The reaction mixture was stirred in the dark for 12 hours at room temperature. After that time, the solvent was evaporated *in vacuo*, and the resulting residue was purified by column chromatography (DCM:MeOH 40:1) to obtain 21 mg (28%) of a dark green solid.

^{1}H-NMR (400 MHz, $CDCl_3$): δ 8.68 (d, *J* = 9.0 Hz, 2H), 8.46 (s, 1H), 8.07 (d, *J* = 13.1 Hz, 1H), 7.24 (d, *J* = 7.0 Hz, 1H), 7.18 (s, 2H), 6.95 (dd, *J* = 8.9, 2.7 Hz, 2H), 6.82 (d, *J* = 2.7 Hz, 2H), 5.49 (s, 2H), 4.25 – 4.16 (m, 4H), 3.91 – 3.81 (m, 4H), 3.79 – 3.73 (m, 4H), 3.72 – 3.61 (m, 12H), 3.59 – 3.52 (m, 4H), 3.38 (s, 6H), 3.45-3.33 (m, 1H), 3.20 (m, 4H), 2.88 (t, *J* = 6.2 Hz, 4H), 2.74 (t, *J* = 7.1 Hz, 4H), 1.49 (s, 9H), 1.31 – 1.26 (m, 2H), 1.10-1.05 (m, 2H).

^{13}C-NMR (100 MHz, $CDCl_3$): δ 173.2, 164.3, 160.1, 154.8, 154.7, 152.4, 152.3, 148.5, 144.6, 143.1, 138.1, 136.2, 132.6, 130.3, 129.3, 122.6, 121.7, 115.1, 113.8, 113.6, 113.1, 109.5, 105.3, 80.4, 72.1, 71.0, 70.8, 70.7, 69.8, 67.5, 60.1, 59.2, 53.6, 50.1, 34.8, 31.0, 29.8, 28.5, 22.6, 8.4.

HR-MS (ESI, [M+H]+): Calcd. for $C_{62}H_{73}BF_3N_5O_{13}$ +H: 1163.5359; Found: 1163.5340

3. HPLC Conditions

A Phenomenex C18 column (250 mm x 4.6 mm x 5 µm) was employed as the stationary phase. The mobile phase consisted of different mixtures of acetonitrile and water containing 0.1% of trifluoroacetic acid. The flow in all cases was 1 ml/minute, and the injection volume was 20 µl, previously filtered through a 0.45 µm PTFE membrane filter. The gradient methods used for each compound are described next.

Table S1. HPLC method A, used for the analysis of compounds **1** and **2**.

Time (min)	Mobile phase composition (%)	
	Acetonitrile	Water (0.1% TFA)
0	80	20
5	40	60
7	40	60
14	10	90
15	10	90

For compounds **1** and **2**, the detection was carried out in dual-mode at 254 or 282, and 520 nm to monitor the release of the antibiotic as well as the remaining protected compound. Retention times are indicated next: t_{R1} = 12.8 min, t_{R2} = 14.7 min, $t_{R\text{Nalidixic acid}}$ = 8.0 min, $t_{R\text{Boc-ciprofloxacin}}$ = 11.3 min.

Table S2. HPLC method B, used for the analysis of compounds **3**, **4**, and **5**.

Time (min)	Mobile phase composition (%)	
	Acetonitrile	Water (0.1% TFA)
0	80	20
5	40	60
7	40	60
14	10	90
20	10	90

For compounds **3** and **4**, the detection was carried out in dual-mode at 254 or 282, and 730 nm in order to monitor the release of the antibiotic and the remaining protected compound. For compound **5**, the selected wavelengths in dual-mode were 282 and 675 nm. Retention times are indicated next: t_{R3} = 15.8 min, t_{R4}= 16.8 min, t_{R5} = 15.9 min, $t_{R\textbf{Nalidixic acid}}$ = 8.0 min, $t_{R\textbf{Boc-ciprofloxacin}}$ = 11.3 min.

The following data correspond to the minimum purity of the samples as measured by HPLC:

- Compound 1: purity > 92%
- Compound 2: purity > 92%
- Compound 3: purity > 95%
- Compound 4: purity > 95%
- Compound 5: purity > 95%

4. Photorelease studies

All compounds (**1**-**5**) were irradiated at a concentration of 256 mg/L in mixtures of DMSO/H_2O with the LED lamp indicated in table 3. The release process was followed by HPLC (**1**-**4**) employing method A or B as indicated in HPLC conditions section, or ^{1}H-NMR (**5**).

Table S3. Irradiation conditions of photoreleasable quinolones

Compound	**DMSO/H_2O**	**Volume (ml)**	**LED lamp**
1	60:40	1	Green (λ = 520 nm)
2	60:40	1	Green (λ = 520 nm)
3	80:20	1	NIR (λ = 730 nm)
4	80:20	1	NIR (λ = 730 nm)
5	60:40	1	Red (λ = 625 nm)

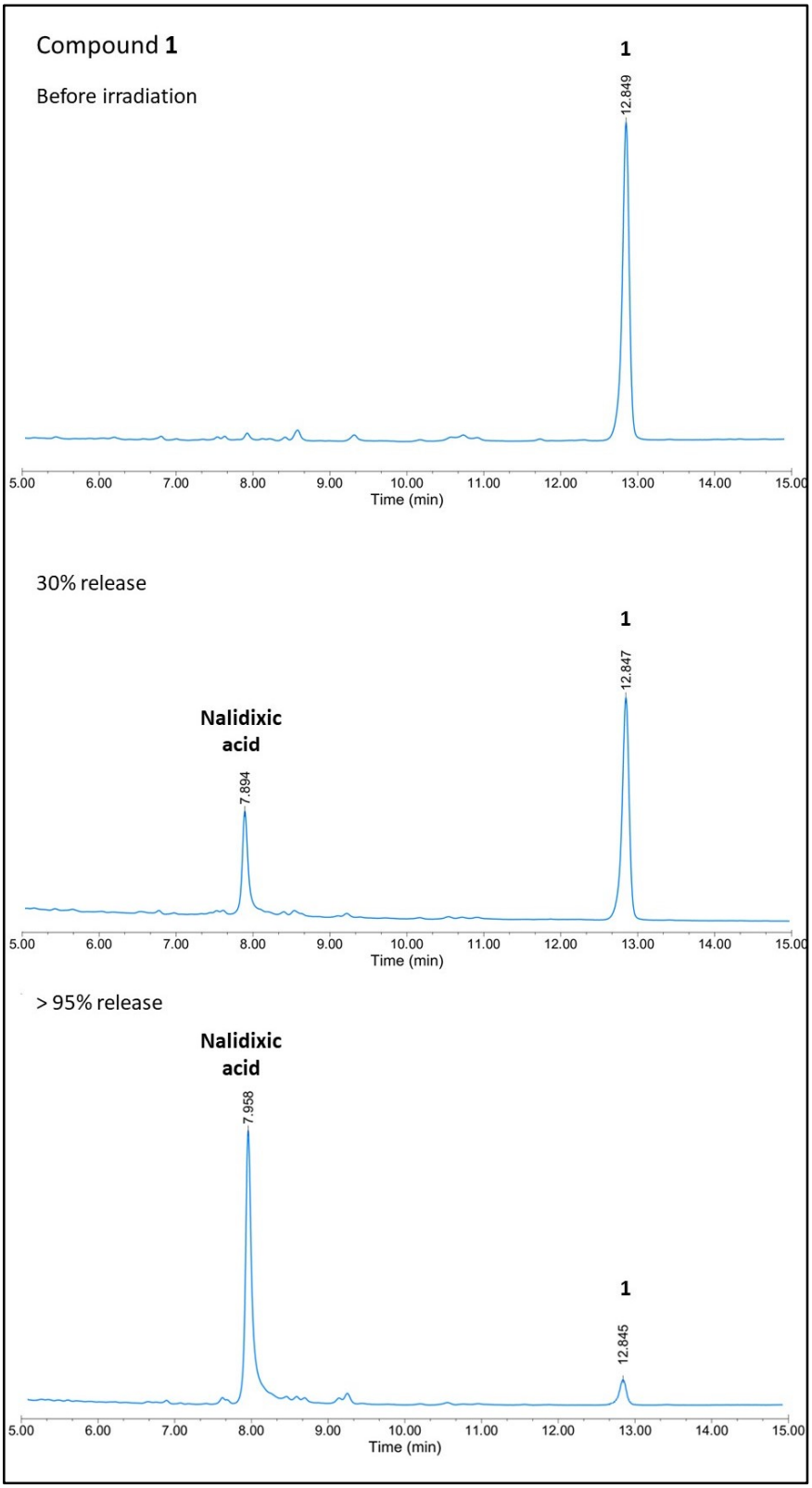


Figure S3. Release process of compound **1** upon irradiation with green light. The peak corresponding to compound **1** decreases while the peak of nalidixic acid grows. Release yield > 95%.

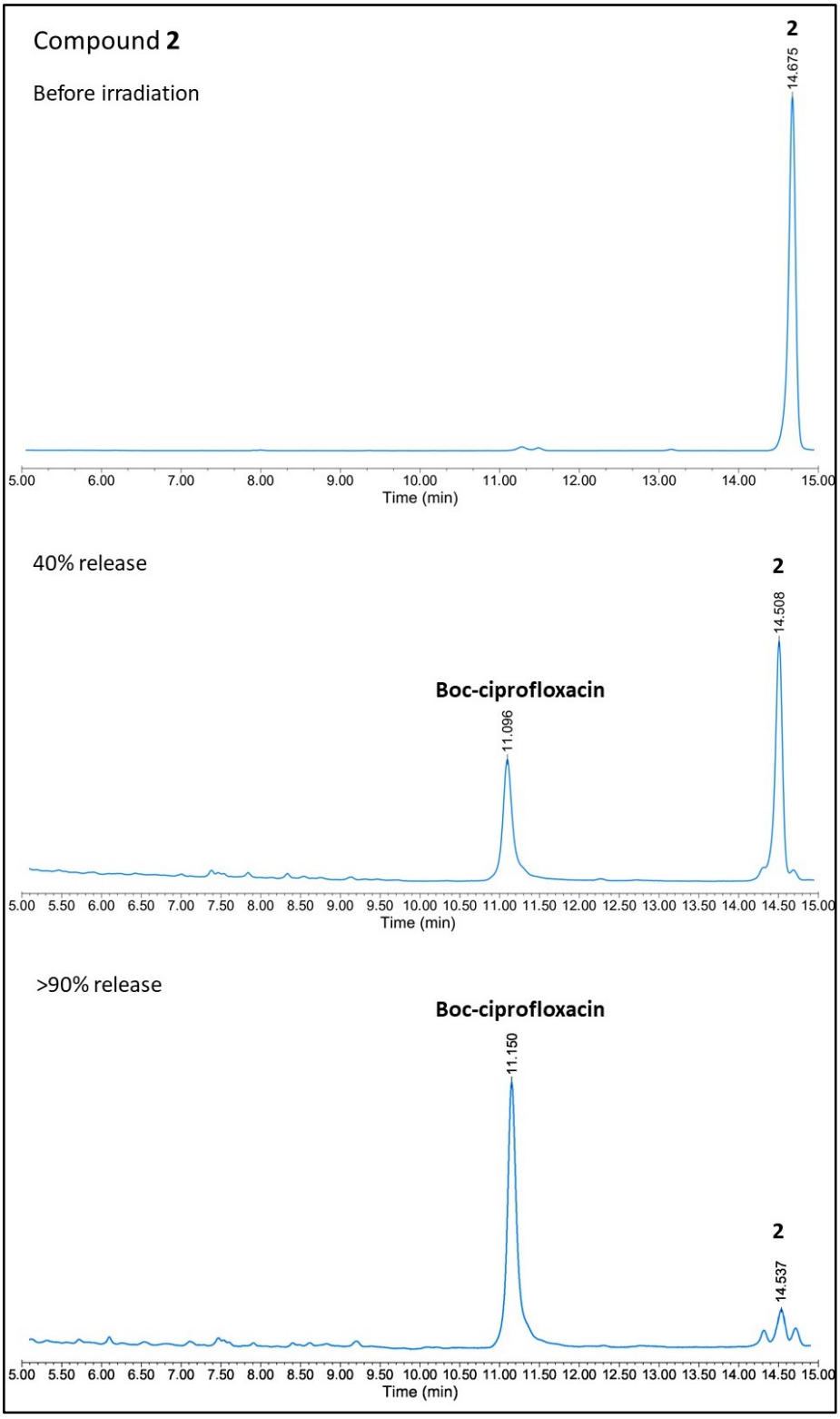


Figure S4. Release process of compound **2** upon irradiation with green light. The peak corresponding to compound **2** decreases while the peak of Boc-ciprofloxacin grows. Release yield > 90%.

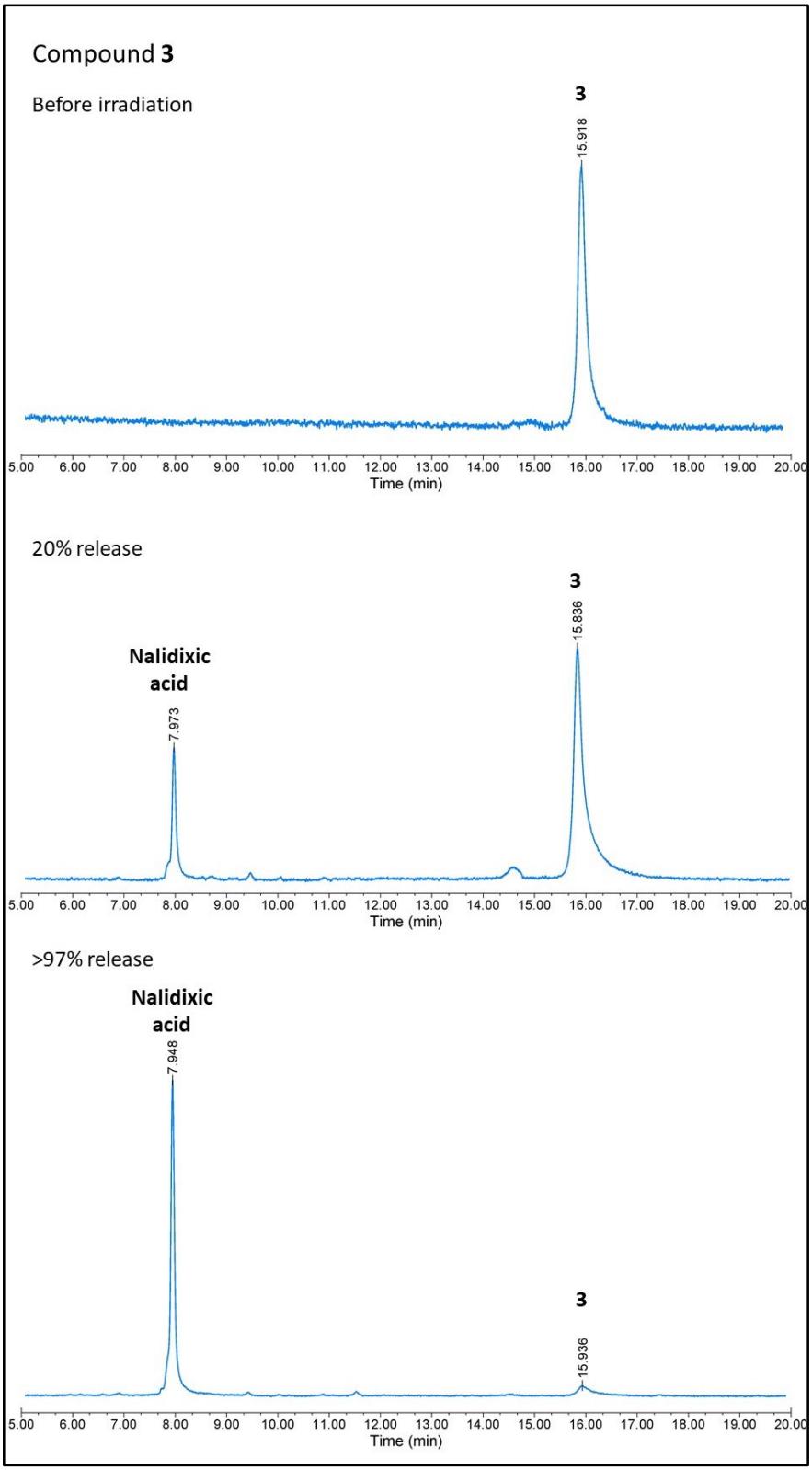


Figure S5. Release process of compound **3** upon irradiation with NIR light. The peak corresponding to compound **3** decreases while the peak of nalidixic acid grows. Release yield > 97%.

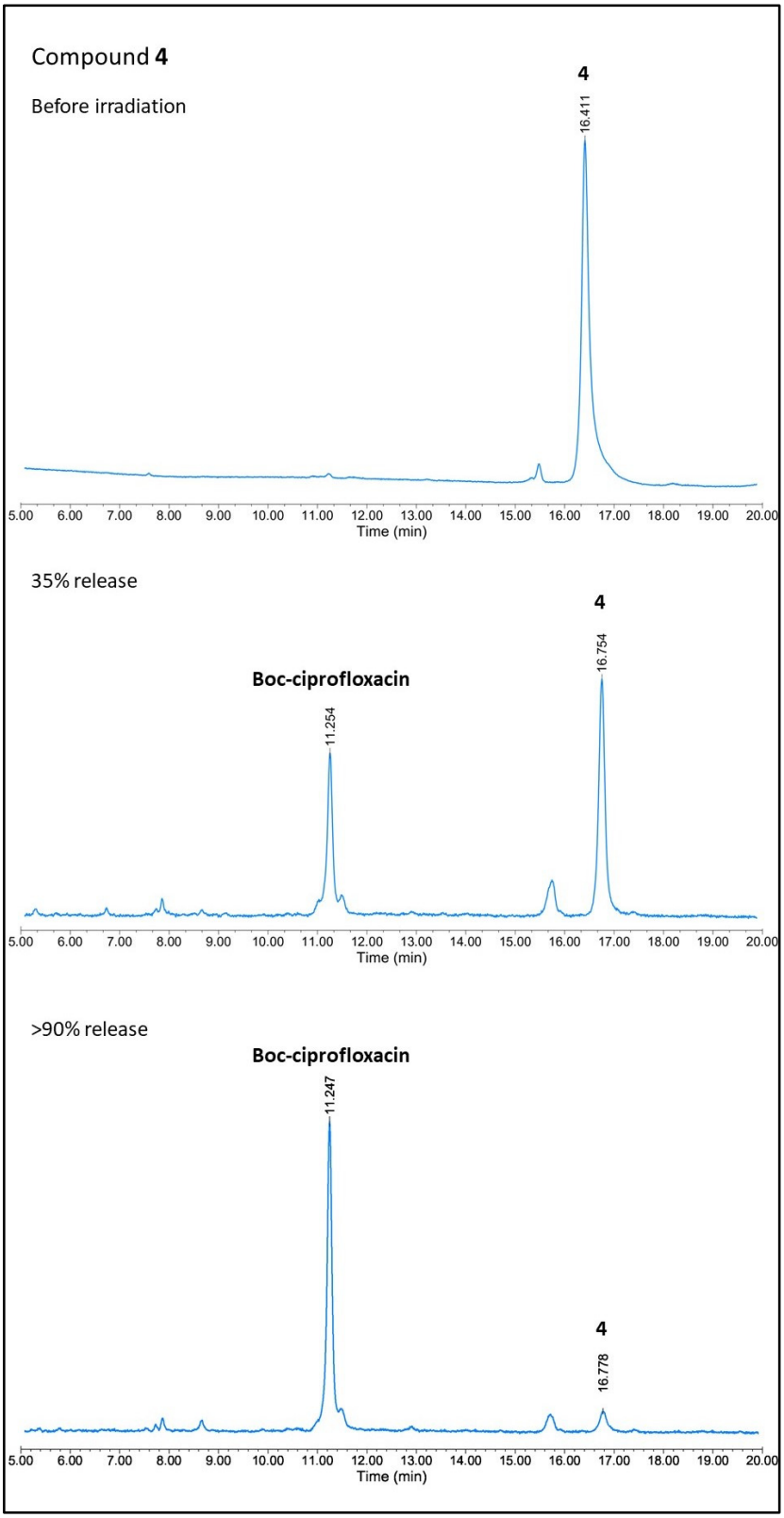


Figure S6. Release process of compound **4** upon irradiation with NIR light. The peak corresponding to compound **4** decreases while the peak of Boc-ciprofloxacin grows. Release yield > 90%.

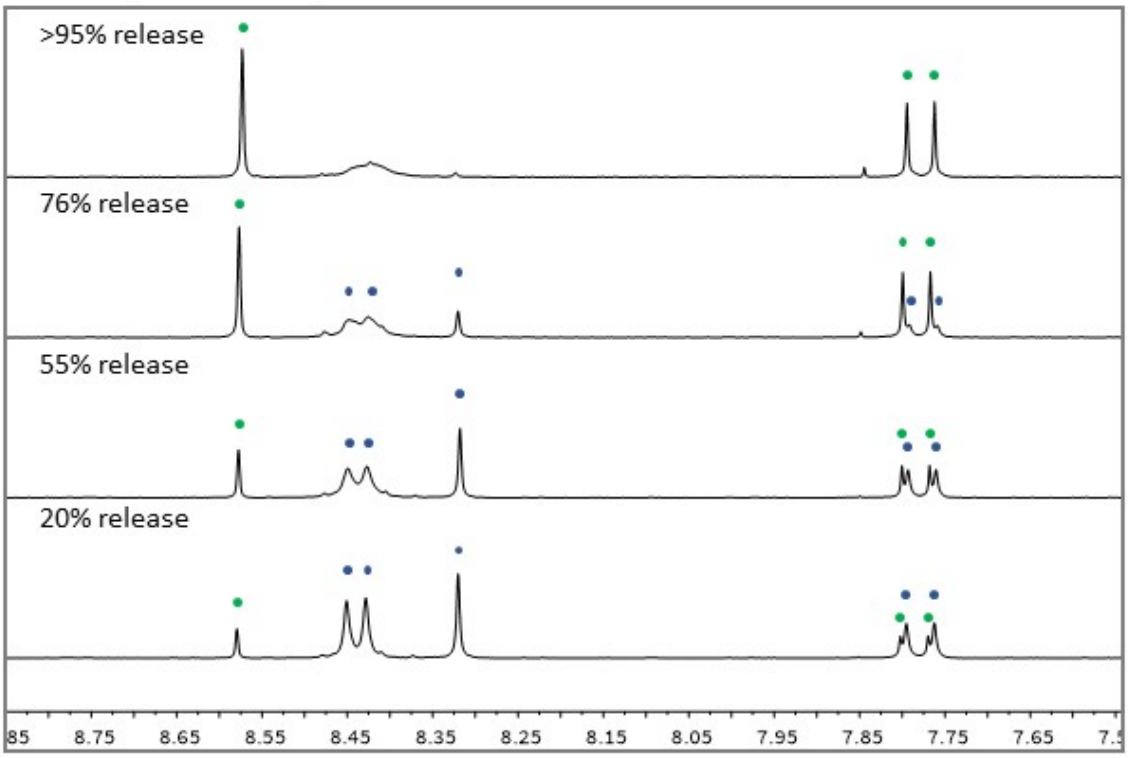


Figure S7. Release process of compound **5** upon irradiation with red light. The peaks corresponding to compound **5** (in blue) gradually disappear while the peaks of Boc-ciprofloxacin (in green) grow. Release yield > 95%.

5. Quantum yield measurements

The adequate light source was selected according to the sample under study. Compounds **1** and **2** were irradiated with green light using a 30W RGB LED. Compounds **3** and **4** were irradiated using a 515mW far-red LED. Compound **15** was irradiated with a 30W RGB LED in red light mode. The LED of choice was incorporated in the setup represented in Figure S8. Samples were prepared in a concentration close to 5 x 10^{-5} M and dissolved in different mixtures of DMSO and water according to their solubility (see Table S3). All samples were equipped with a magnetic stirrer to ensure homogeneous irradiation of the total volume. Prior to the irradiation process, the sample was analyzed by HPLC to check that the protected form of the antibiotic was being irradiated. The HPLC conditions for each compound can be found in the previous section.

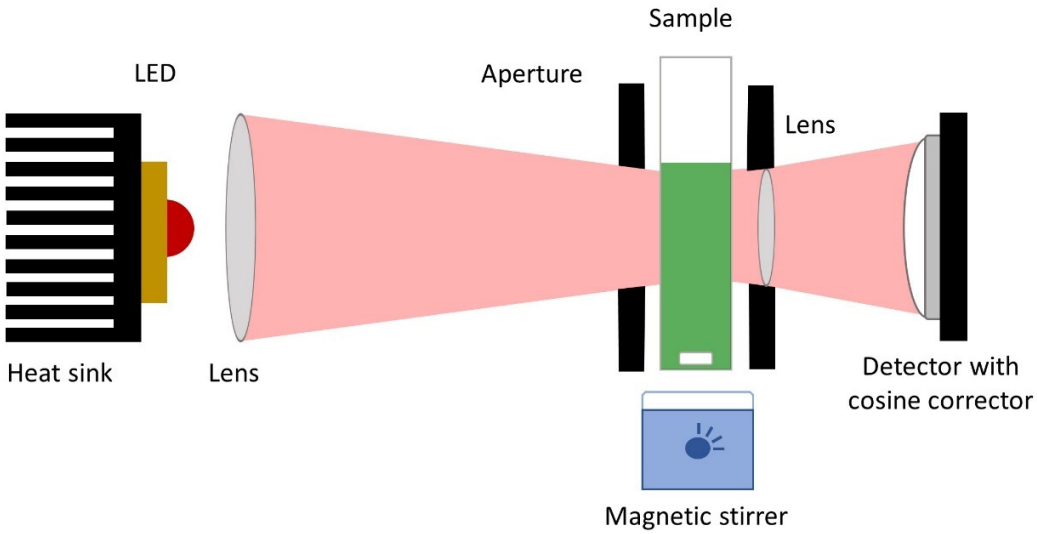


Figure S8. Schematic representation of the instrumental setup used to measure the quantum yield.[3] The light emitted by the LED is focused through a lens and imaged into the sample equipped with a magnetic stirrer. The radiation not absorbed by the sample is collected by a cosine corrector.

Once the LED was placed in the setup, the light was blocked with a laser dimming paper in front of the lens. This allowed the determination of the ambient light, which was later substrated from subsequent measurements. Next, the paper was removed, and a reference cuvette containing the solvent used to dissolve the samples was inserted. The light not absorbed by the sample was collected by a cosine corrector coupled to an Ocean Optics USB4000-UV-Vis detector. The transmitted radiant flux (P_{ref}), was obtained in moles of photons·s^{-1}·m^{-2}.

Then, the reference was exchanged by a cuvette containing the sample that was irradiated for a determined time. During that time, the light not absorbed by the sample (P_{sample}) was monitored by continuous acquisition of the transmitted radiant flux in moles of photons·s^{-1}·m^{-2}. Note that upon irradiation, the conversion from the protected antibiotic to the released form should be below 10% to avoid competitive absorption between the initial product and the byproduct of the photocage. After irradiation, the sample's conversion was quantified by HPLC, which allowed the calculation of the number of antibiotic molecules released.

The light absorbed by the sample can be calculated as the difference between the light not absorbed by the reference and the light not absorbed by the sample, as expressed in equation 1:

$$P_{abs} = P_{ref} - P_{sample}$$

Equation 1. Equation expressing the moles of photons·s^{-1}·m^{-2} absorbed by the sample. P_{ref} corresponds with the transmitted radiant flux measured for the reference with solvent, P_{sample} refers to the transmitted radiant flux recorded when the sample was inserted in the setup.

To conclude the experiment, the number of photons absorbed by the sample, as well as the number of molecules of antibiotic released, were introduced in equation 1 to obtain the quantum yield.

6. Determination of minimal inhibitory concentration (MIC)

The minimal inhibitory concentration (MIC) was determined by the microdilution method in cation adjusted Mueller-Hinton broth (Becton Dickinson).[4] *Escherichia coli* ATCC 25922 strain was cultured in Brain-Heart Infusion (BHI) agar (Becton Dickinson) for 24h at 37 °C. Overnight colonies of a pure culture on agar were used to prepare an inoculum adjusted to the turbidity of a 0.5 McFarland in sterile saline solution (1 x 10^8 CFU/ml). This suspension was diluted in cation adjusted Mueller-Hinton broth until a density of 5 x 10^5 CFU/mL and exposed to a serial twofold dilution of each compound tested (0.03-32 mg/L) with a final volume of 0.1 mL in a 96 well microdilution tray. The MIC value was determined as the lowest concentration of compound where no visible growth was apparent. Positive (with bacteria and cation adjusted Mueller-Hinton broth) and negative (only with cation adjusted Mueller-Hinton broth) control wells were included in all assays. Moreover, control tests of solvents (mixtures of water and DMSO 40:60 or 20:80) were included to check the survival of the bacterium in these concentrations.

In the experiments in which the compounds were activated in presence of the bacteria, for the irradiation of the plates, we used a 100W RGB LED in green mode and a 50W RGB LED in red mode. The plates were placed on top of each LED and inside an incubator at a controlled temperature of 37 °C (Figure S9). The irradiation of the plates took place for an hour. After that time, the LEDS were switched off and the plates were kept in the incubator for a total time of 24 hours.

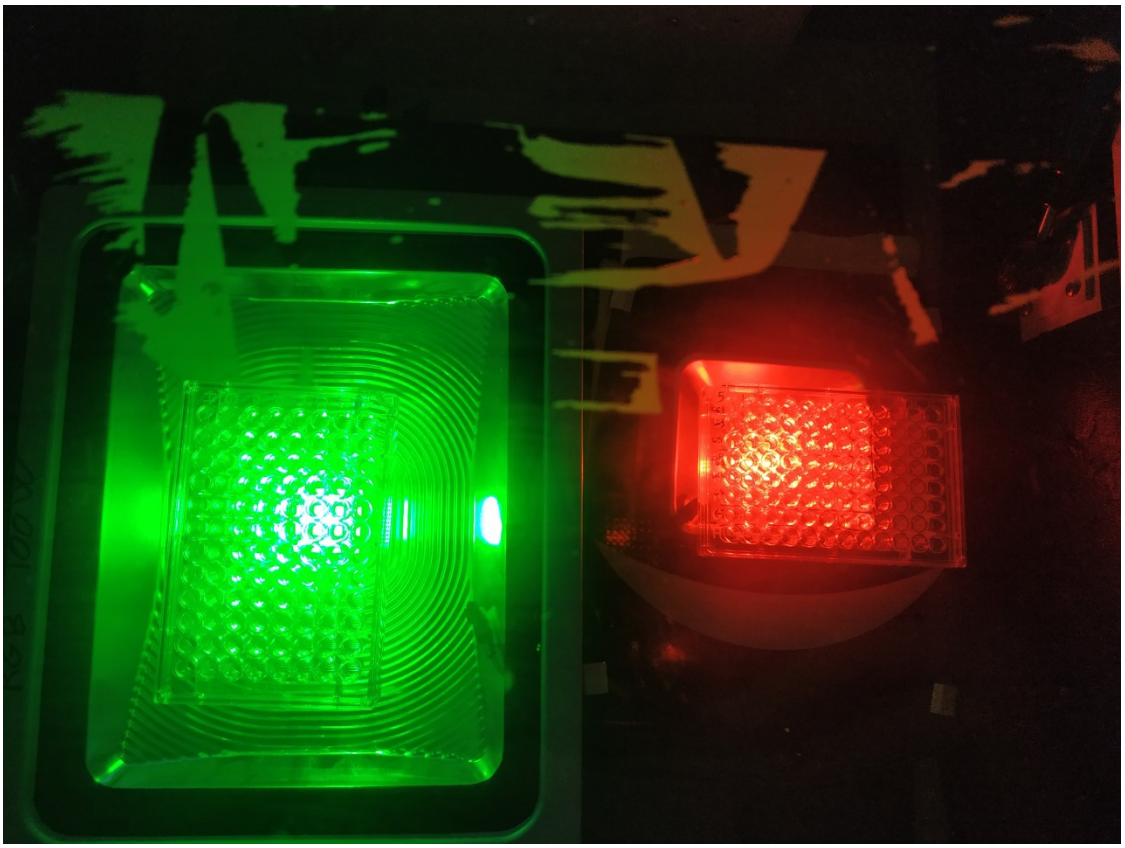
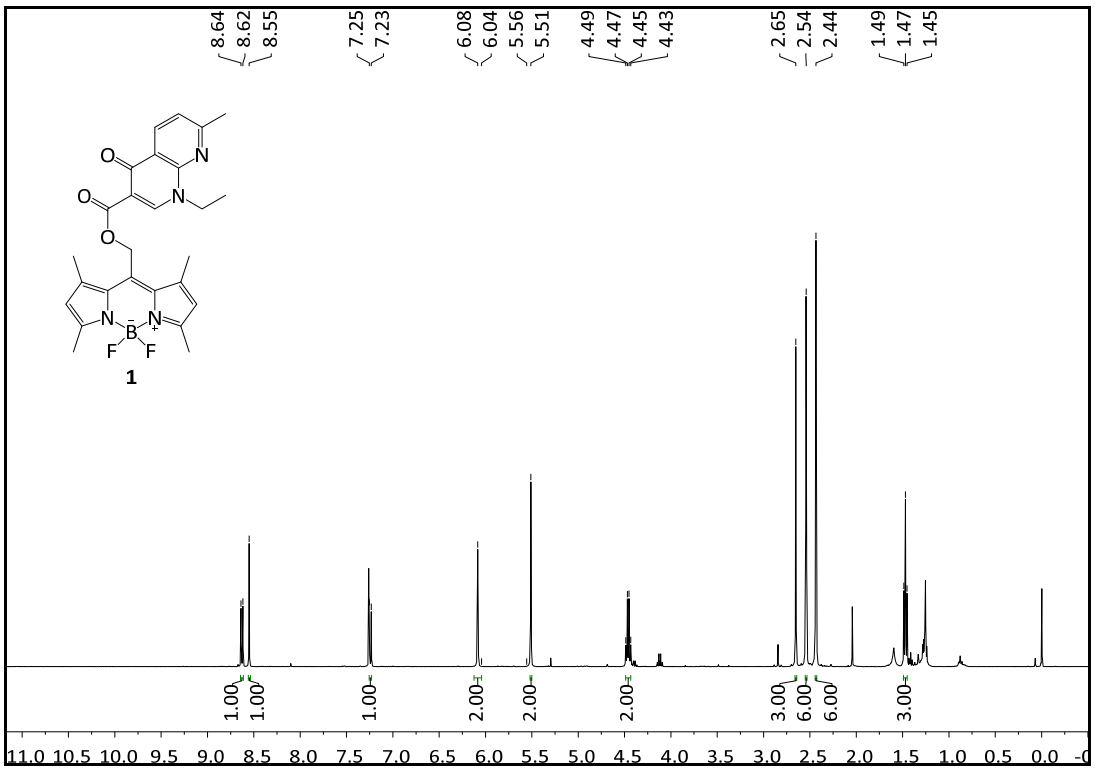
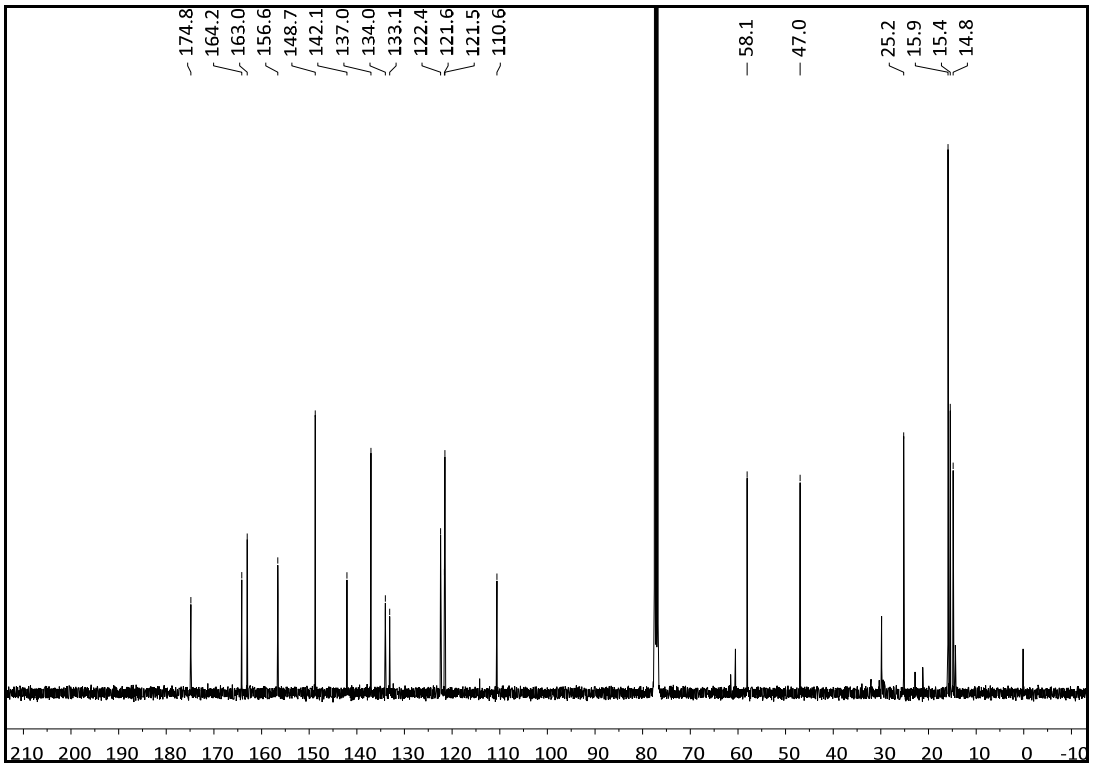
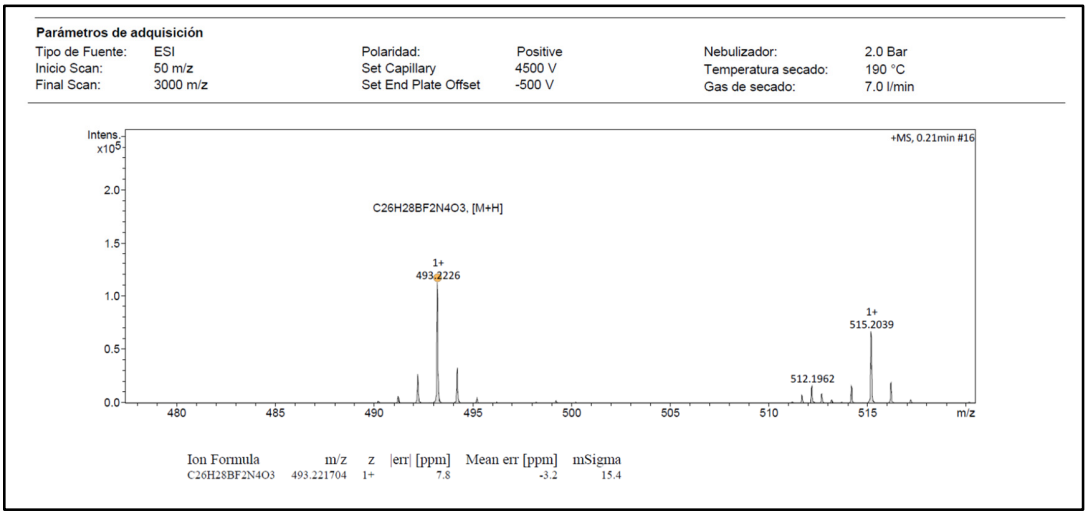


Figure S9 . Irradiation of the photoreleasable quinolones in a biological environment. On the left, compound **2** irradiated with green light. On the right, compound **5** irradiated with red light.

7. Characterization data



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1+
515.2039
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m/z
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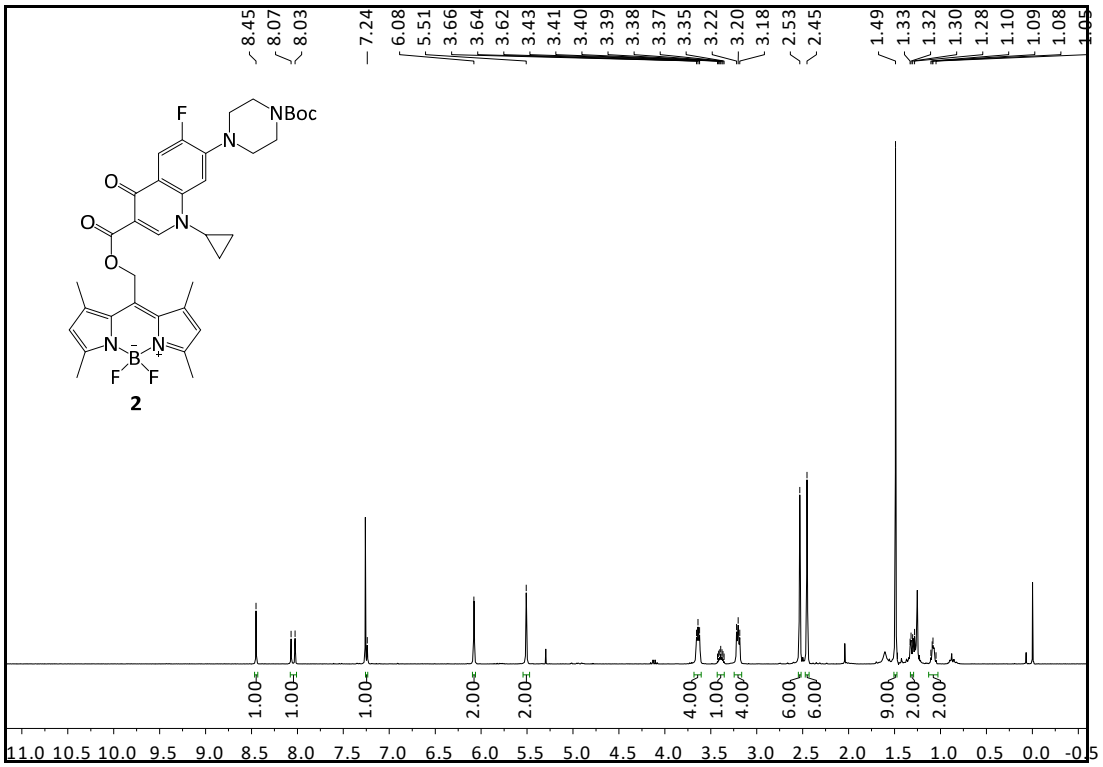
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O
O
N
O
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B
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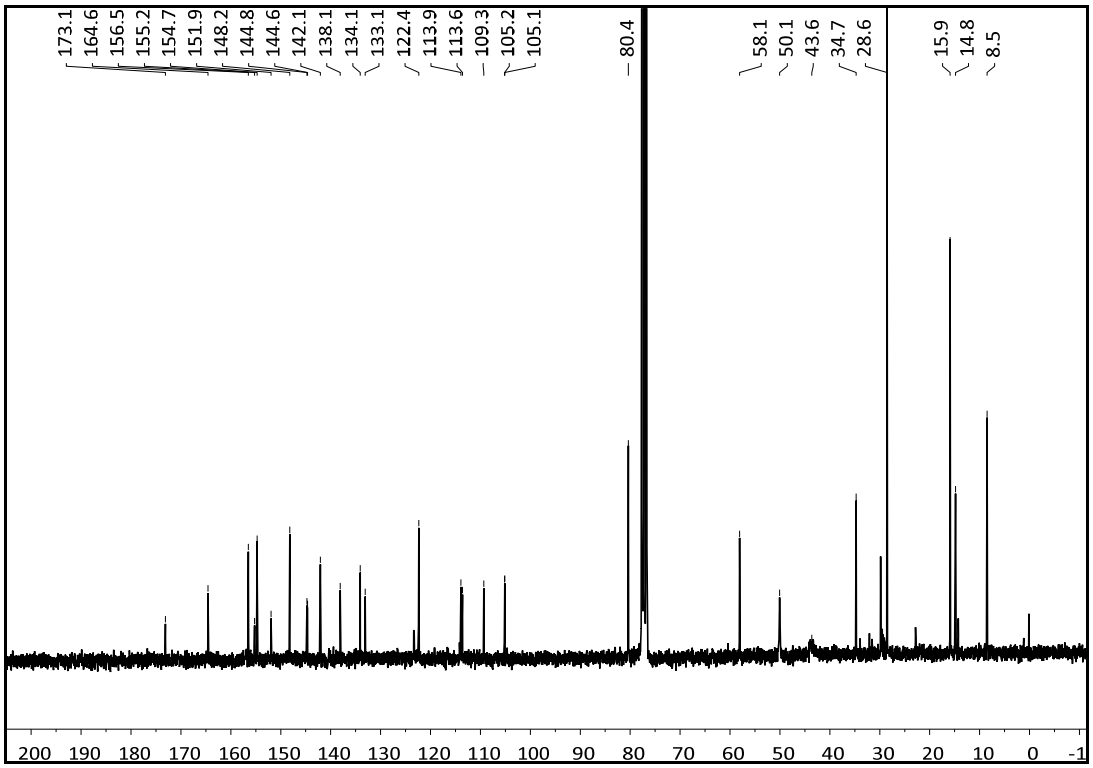

Parámetros de adquisición

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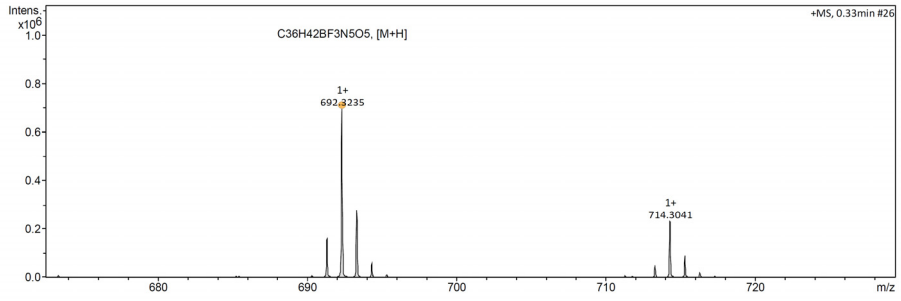

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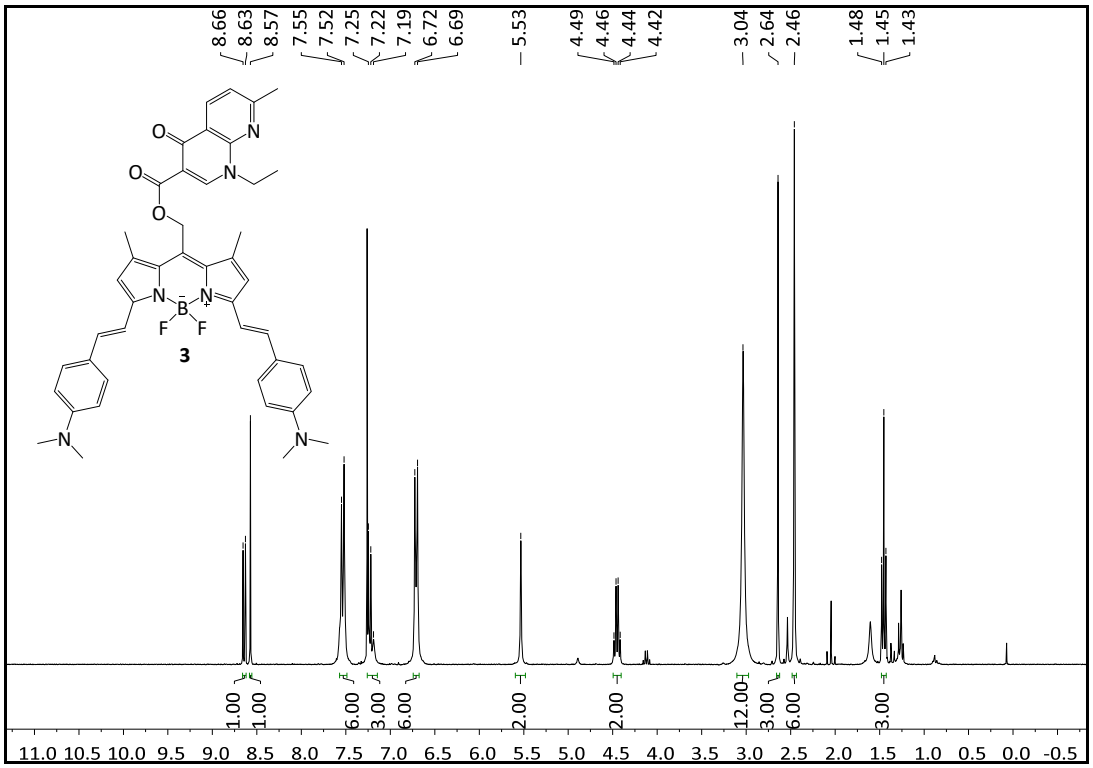
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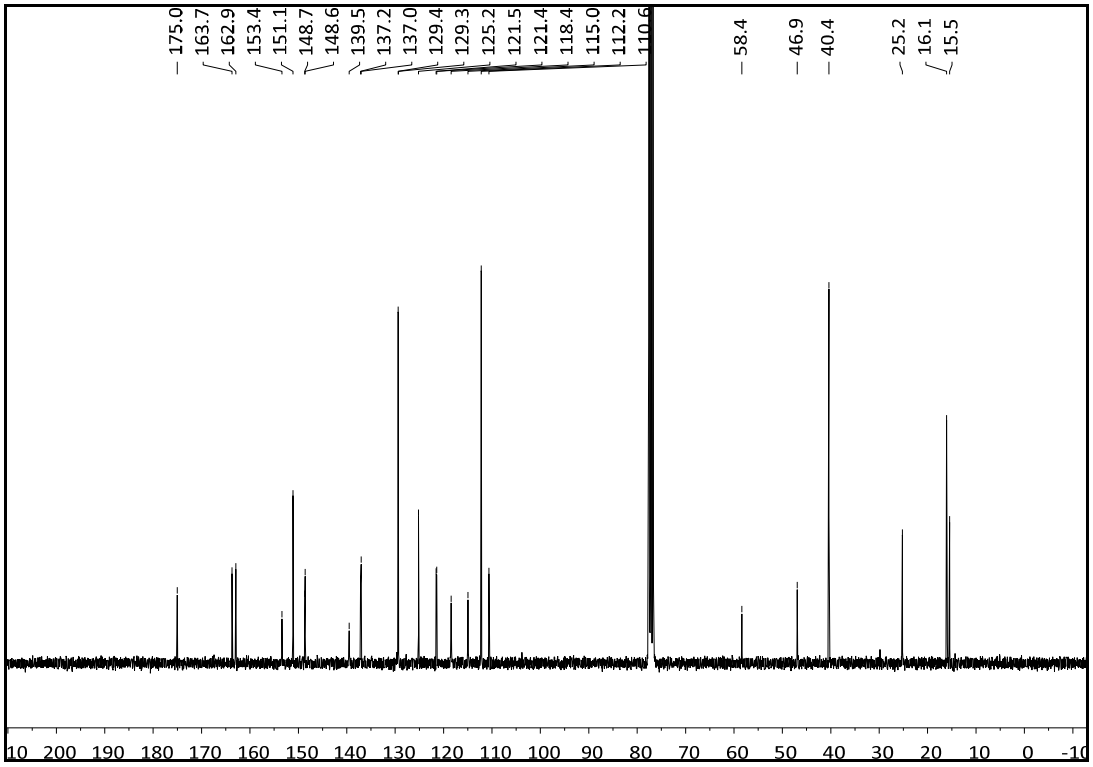
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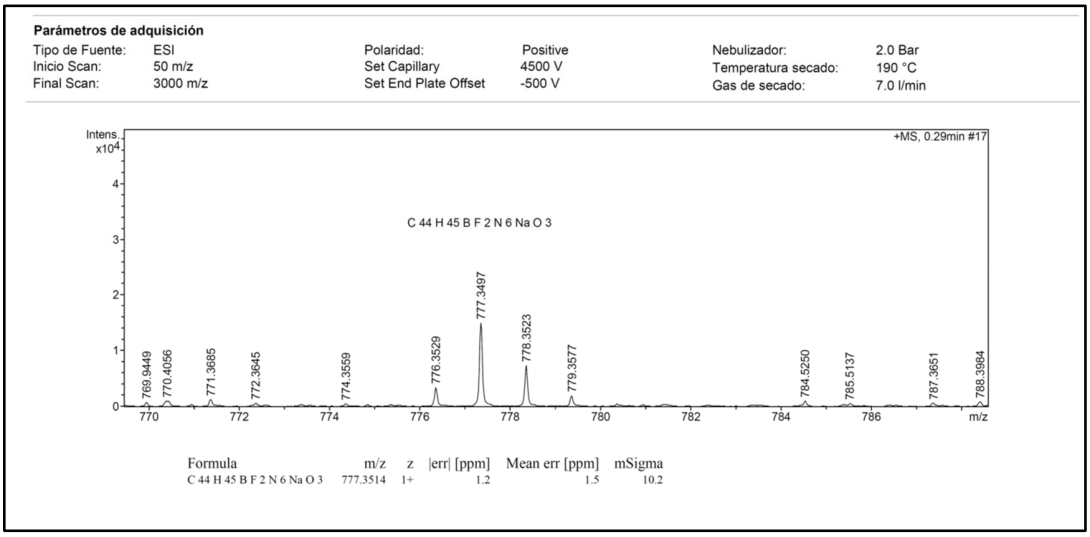
Parámetros de adquisición
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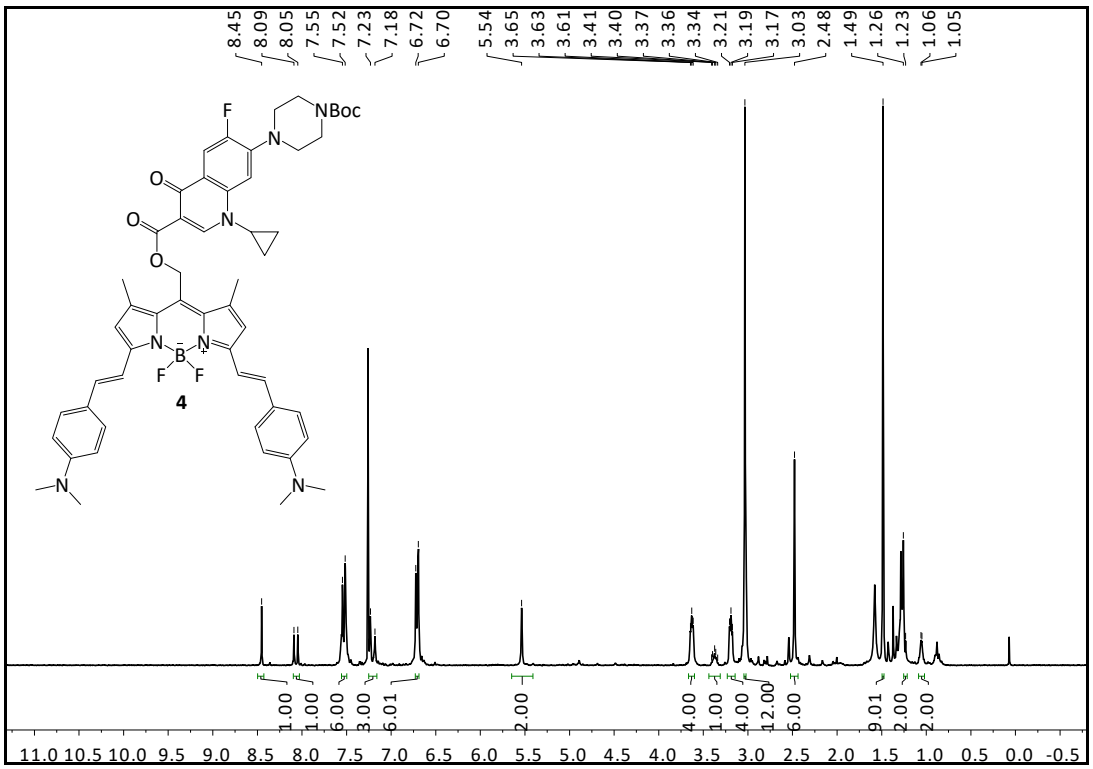
Inicio Scan: 50 m/z
Final Scan: 3000 m/z
Polaridad: Positive
Set Capillary 4500 V
Set End Plate Offset -500 V
Nebulizador: 2.0 Bar
Temperatura secado: 190 °C
Gas de secado: 7.0 l/min
Intens. x10^4
+MS, 0.29min #17
C 44 H 45 B F 2 N 6 Na O 3
769.9449
770.4056
771.3685
772.3645
774.3559
776.3529
777.3497
778.3523
779.3577
784.5250
785.5137
787.3651
788.3984
m/z
Formula m/z z |err| [ppm] Mean err [ppm] mSigma
C 44 H 45 B F 2 N 6 Na O 3 777.3514 1+ 1.2 1.5 10.2


8.45
8.09
8.05
7.55
7.52
7.23
7.18
6.72
6.70
5.54
3.65
3.63
3.61
3.41
3.40
3.37
3.36
3.34
3.21
3.19
3.17
3.03
2.48
1.49
1.26
1.23
1.06
1.05
F
NBoc
N
O
O
N
O
N
B
F
F
N
N
4
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1.00
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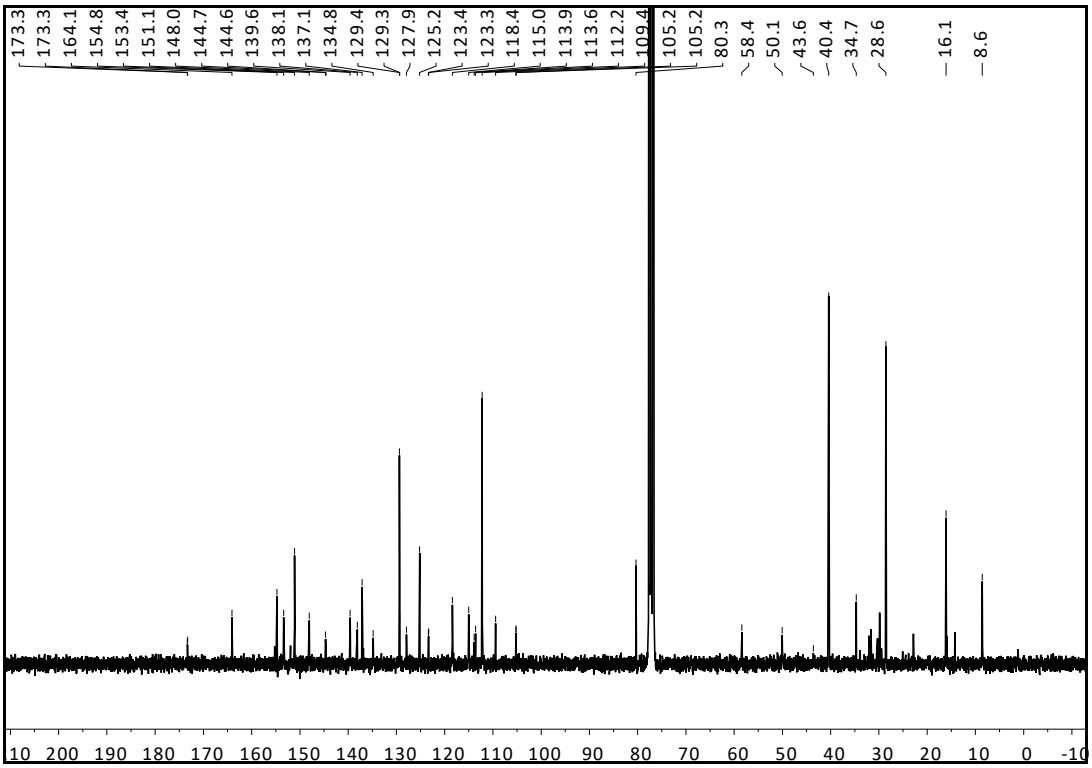
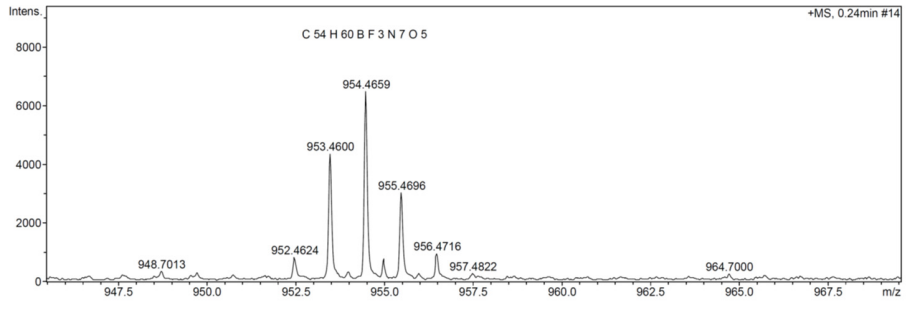
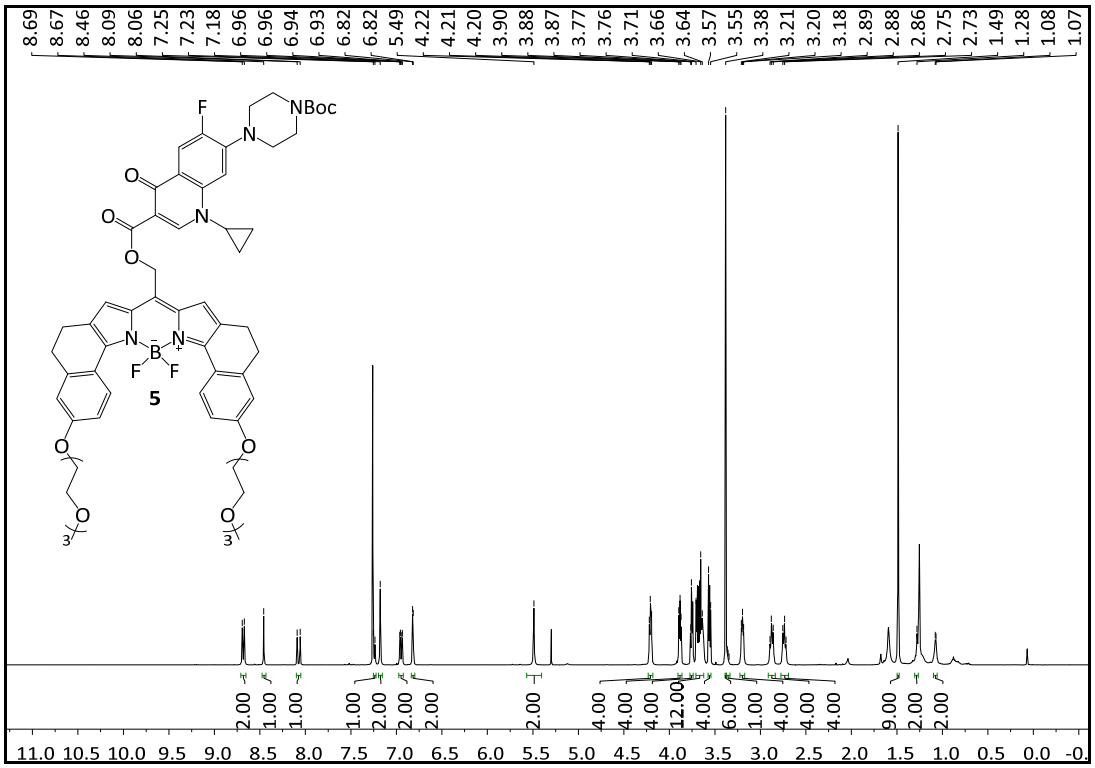


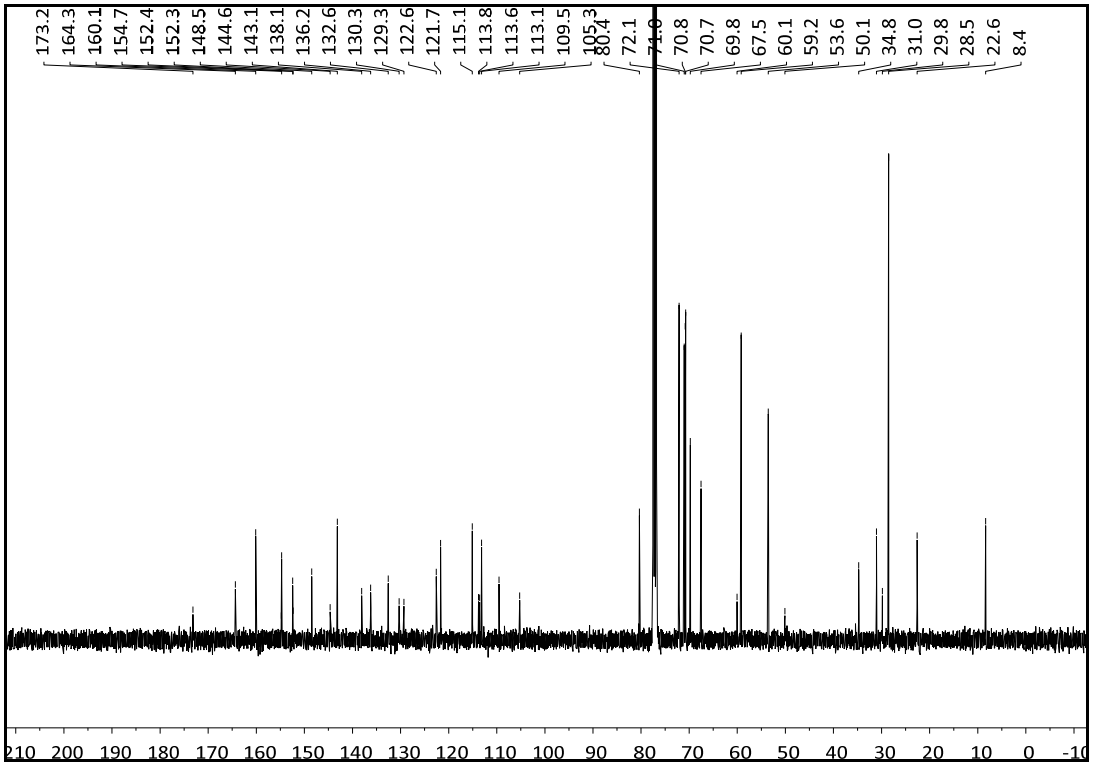
Parámetros de adquisición

Tipo de Fuente:	ESI	Polaridad:	Positive	Nebulizador:	2.0 Bar
Inicio Scan:	50 m/z	Set Capillary	4500 V	Temperatura secado:	190 °C
Final Scan:	3000 m/z	Set End Plate Offset	-500 V	Gas de secado:	7.0 l/min

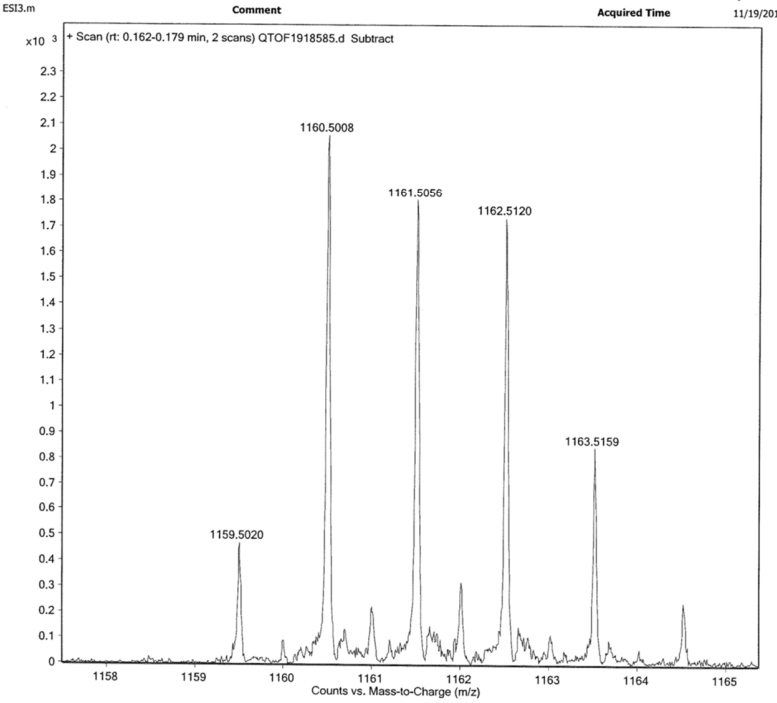


Formula	m/z	z	|err| [ppm]	Mean err [ppm]	mSigma
C 54 H 60 B F 3 N 7 O 5	954.4704	1+	3.8	7.0	193.0


F
NBoc
N
O
O
N
O
N
B
N
F
F
5
O
O
O
O
3
3



Sample Name	18	**Position**	Vial 1	**Instrument Name**	QTOF
User Name	CIF-PC\admin	**Inj Vol**	1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	QTOF1918585.d
ACQ Method	ESI3.m	**Comment**		**Acquired Time**	11/19/2019 2:49:37 PM



Formula (M)	m/z	m/z (Calc)	Diff (ppm)
C62 H69 B F3 N5 O13	1159.502	1159.5046	2.25

8. Computational Results

Computational Methods

The geometries have been optimized in the ground state (S_0) at the B3LYP[5,6]/6-31+g(d) level of theory. A single point calculation in the S_0 minimum has been performed at the CAM-B3LYP[7]/6-31+g(d) level of theory to compute the excitation energies and evaluate the electronic nature of the $S_0 \rightarrow S_1$ transition. To analyze the photorelease path, both optimizations and relaxed scans along the photorelease coordinate (C-O distance) have been performed in S_1 and T_1. Calculations in the ground state (S_0) and first triplet state (T_1) have been performed with the B3LYP functional whereas the ones performed in the first singlet excited state (S_1) were performed with the CAM-B3LYP functional. In all cases, the 6-31+g(d) has been selected as the basis set. Moreover, we have also evaluated the solvent effect considering it in two different ways: on one hand implicitly (dichloromethane, DMSO and water) by applying the polarizable continuum model through the integral equation formalism variant (IEF-PCM[8]); on the other hand, two water molecules were explicitly included while keeping the IEF-PCM implicit water description for the surroundings. Frequency calculations have been performed to verify the minimum or transition state character of the optimized stationary points and to get the free energies. The density functional theory (DFT) and its time-dependent version (TD-DFT) were applied for ground and excited states, respectively, as implemented in Gaussian 16 software.[9] It should be remarked that for **5**, the tetraoxaundecane chain present in the synthetic analogue has been simplified with a methoxy group, to decrease the computational time. This simplification should not influence the absorption energy neither the mechanism, as the chain does not contribute to the electronic conjugation extent of the chromophore. The spin-orbit coupling values were computed at the CAM-B3LYP/def2-SVPD level of theory, including water as implicit solvent by the conductor-like polarizable continuum model, CPCM, as implemented in Orca 4.2.1.[12]

The electronic nature of the vertical transition has been analyzed for the three compounds studied from a computational point of view, compounds **2**, **4** and **5**. In all cases the first singlet excited state is optically bright (large oscillation strength value, f, in Table S4) and corresponds to a π,π* electronic transition (Figure S10). As experimentally observed, the computed absorption energy of **4** is smaller (that is the wavelength is longer) compared to **5**, whereas the one computed for compound **2** is the largest (shorter wavelength).

Table S4. Experimental and computed absorption ($S_0 \rightarrow S_1$) energies in eV (nm) and the corresponding oscillator strength (f), considering dichloromethane as the solvent.

Compound	**2**	**4**	**5**
Experimental λ_{max} eV (nm)	2.38 (520)	1.67 (744)	1.85 (671)
Computed Excitation energy eV (nm)	2.74 (452)	1.87 (663)	2.09 (592)
f	0.628	1.197	0.904

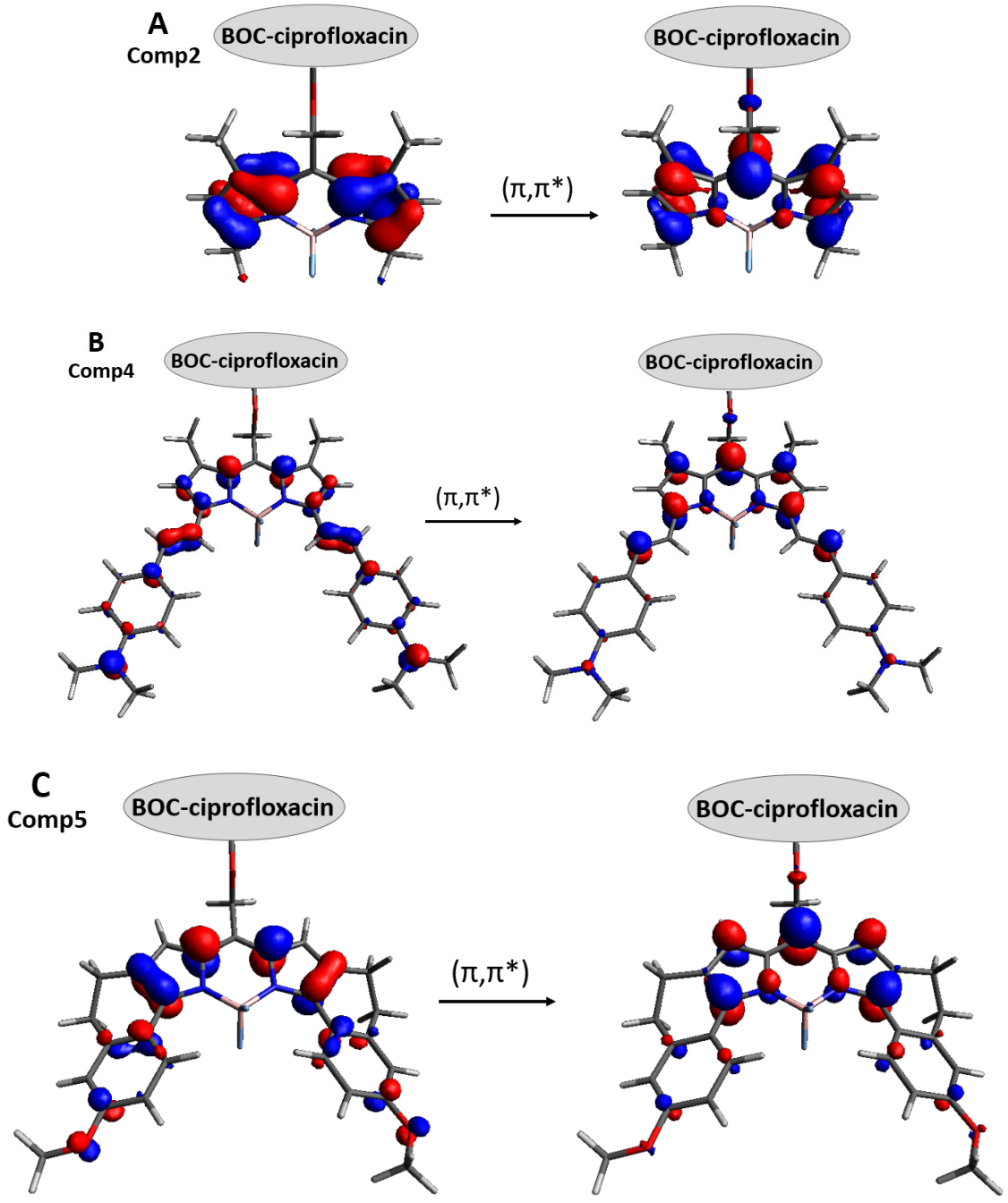


Figure S10. Molecular orbitals involved in the $S_0 \rightarrow S_1$ vertical transition of compound A) **2**, B) **4** and C) **5**.

In addition, relaxed scans have been performed from the S_1 and T_1 minima (Figures S11 and S12, respectively), considering diverse solvents. In particular, the solvents tested are implicit dichloromethane, DMSO and water and explicit water.

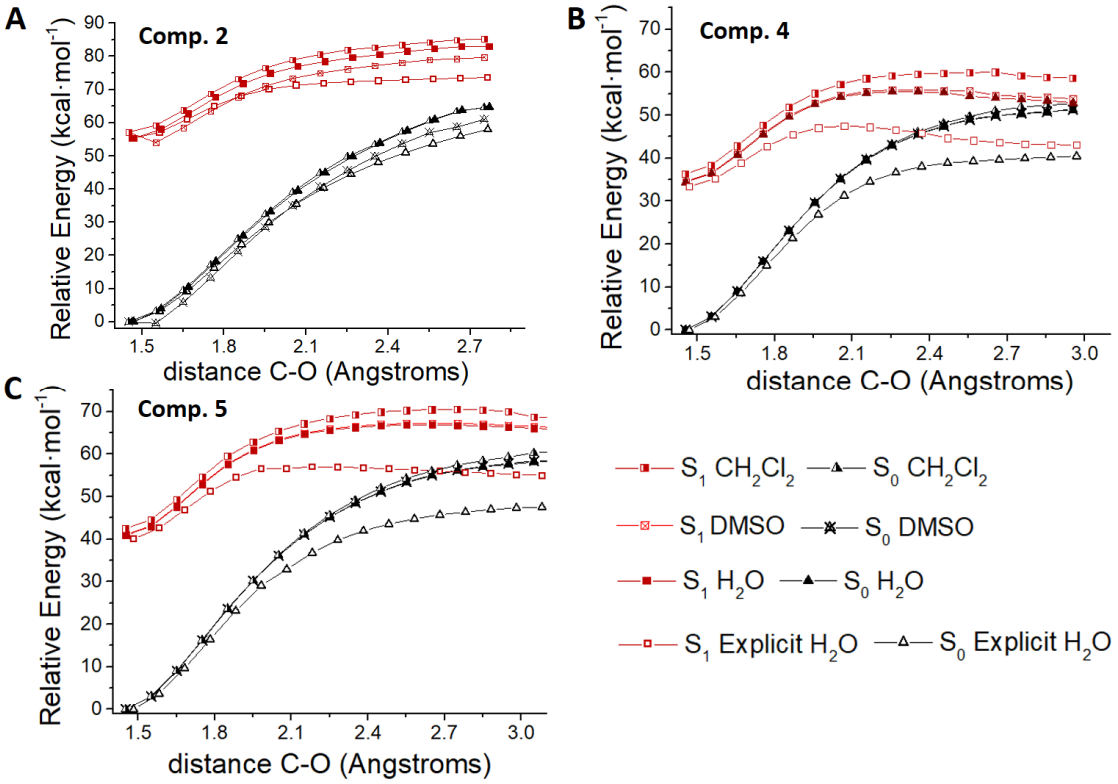


Figure S11. Relaxed scan along the photorelease coordinate (distance C-O) in S_1 considering diverse solvents for A) compound **2**, B) **4** and C) **5**.

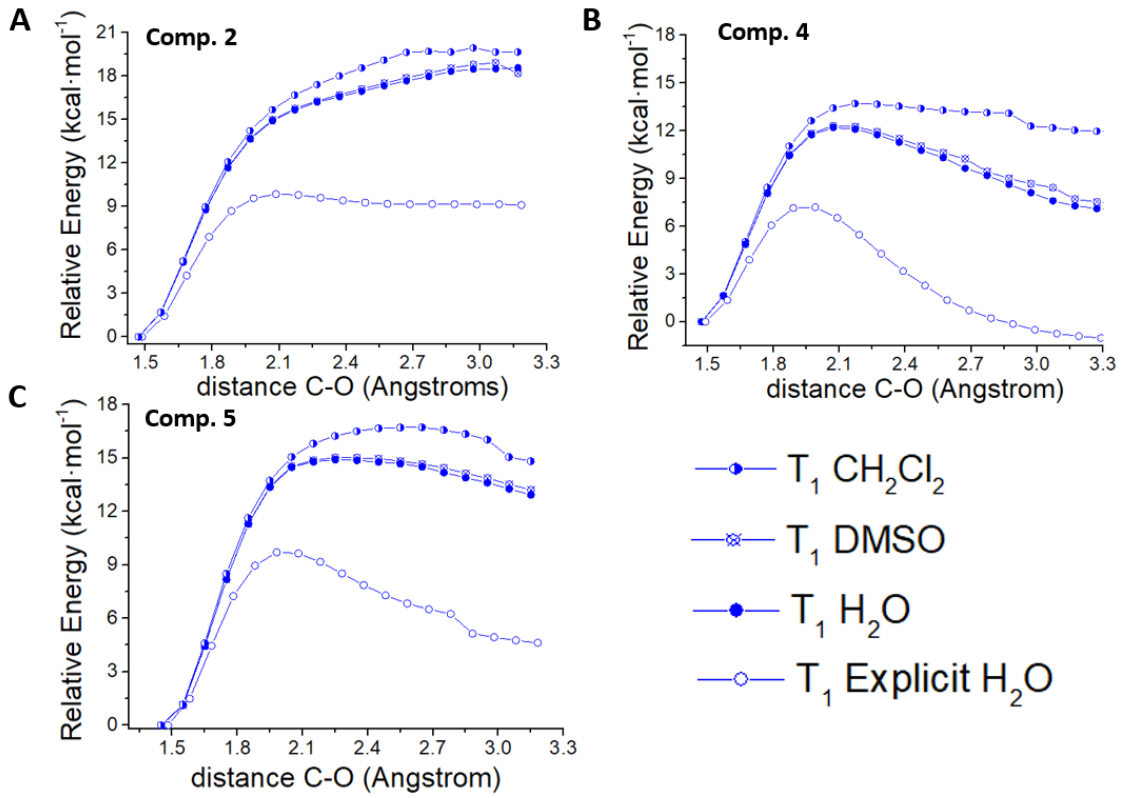


Figure S12. Relaxed scan along the photorelease coordinate (distance C-O) in T_1 considering diverse solvents for A) compound **2**, B) **4** and C) **5**.

Table S5. Energy of the first triplet (T_1) and singlet excited state (S_1) relative to the ground state (S_0) computed at the S_1 minimum. The results shown have been computed considering explicit water as the solvent.

Comp.	Solvent	Relative S_0 energy (kcal/mol)	Relative S_1 energy (kcal/mol)	Relative T_1 energy (kcal/mol)	ΔE_{S1-T1} (kcal/mol)
2	Explicit water	0	55.3	29.7	25.6
	Implicit water	0	55.5	30.5	25.0
4	Explicit water	0	33.4	16.7	16.7
	Implicit water	0	34.4	17.7	16.7
5	Explicit water	0	45.9	21.7	24.2
	Implicit water	0	46.5	22.6	23.9

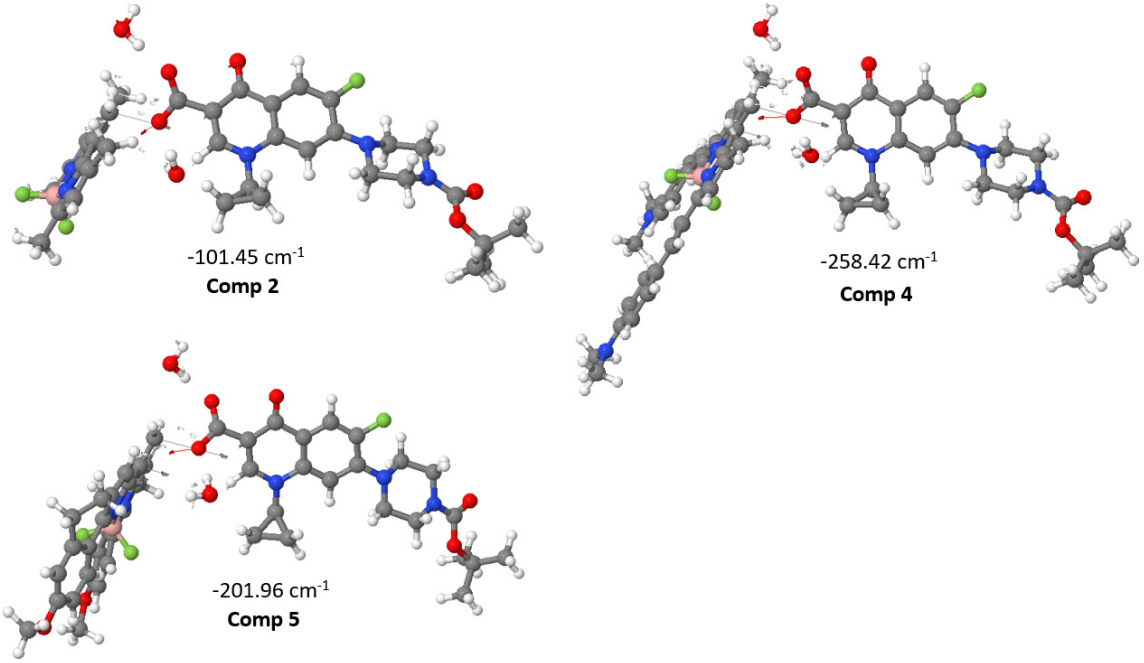


Figure S13. Transition state structures optimized in T_1 considering explicit water molecules as the solvent. The vector of the negative frequency corresponds to the photorelease process.

Table S6. Charge analysis for the ciprofloxacin, PPG and, when applying, the water molecules computed for the minimum, transition state and products in T_1. The charge of each moiety is computed as the sum of the Mulliken charges of each atom included in the moiety.

		Min T_1		**TS T_1**		**Products T_1**	
		Implicit water	Explicit water	Implicit water	Explicit water	Implicit water	Explicit water
2	*Ciprofloxacin*	-0.59	-0.45	-	-0.87	-0.97	-0.97
	PPG	0.59	0.25	-	0.76	0.97	1.00
	WAT1		0.16		0.09		-0.006
	WAT2		0.04		0.02		-0.03
4	*Ciprofloxacin*	-0.71	-0.47	-0.85	-0.81	-1.0	-0.98
	PPG	0.71	0.26	0.85	0.64	1.0	1.00
	WAT1	-	0.17	-	0.14		0.00
	WAT2	-	0.04	-	0.03		-0.02
5	*Ciprofloxacin*	-0.49	-0.43	-0.87	-0.81	-0.95	-0.94
	PPG	0.49	0.24	0.87	0.68	0.95	0.99
	WAT1	-	0.16	-	0.11	-	-0.01
	WAT2	-	0.03	-	0.02	-	-0.04

Table S7. S_1- T_1 spin-orbit coupling values (in cm^{-1}) calculated at the CAM-B3LYP/def2-SVPD level of theory, including water as implicit solvent, without (implicit) or with (micro-solvation) two explicit water molecules.

Solvation method	**Compound 2**	**Compound 4**	**Compound 5**
Micro-solvation	0.118	0.024	0.037
Implicit	0.118	0.022	0.051

9. Cartesian Coordinates

Compound 2							
Min S_0 (implicit water)				Min S_1 (implicit water)			
6	-1.948701	0.940695	-0.221898	6	-2.192738	0.949198	-0.294893
6	-2.556749	2.120571	0.248514	6	-2.696932	2.179861	0.177083
6	-2.500179	3.083773	-0.755056	6	-2.501460	3.146427	-0.793010
7	-1.511791	1.147623	-1.486180	7	-1.685472	1.135118	-1.537707
6	-1.833667	2.461177	-1.866237	6	-1.862971	2.472378	-1.900543
1	-2.988178	2.247429	1.233678	1	-3.150449	2.327058	1.149402
6	-3.039562	4.477490	-0.601256	6	-2.874019	4.588524	-0.657052
1	-3.357468	4.632197	0.434215	1	-3.119680	4.804772	0.386081
1	-3.914867	4.656546	-1.238505	1	-3.754217	4.851362	-1.256555
1	-2.293508	5.243376	-0.837279	1	-2.059744	5.255993	-0.955006
5	-0.798782	0.109968	-2.380905	5	-1.062326	0.046956	-2.419141
7	-0.425213	0.811826	-3.704715	7	-0.501427	0.739374	-3.666234
6	-1.477890	2.935858	-3.140604	6	-1.438218	2.944427	-3.167046
6	-0.766136	2.130829	-4.046897	6	-0.687539	2.082040	-4.003710
6	-1.868398	4.337648	-3.545115	6	-1.764866	4.331723	-3.607130
6	0.258970	0.258287	-4.733387	6	0.226128	0.141492	-4.640792
6	-0.245847	2.386841	-5.362101	6	-0.005737	2.318391	-5.255808
6	0.383966	1.211446	-5.762278	6	0.540095	1.102271	-5.625457
6	-0.298164	3.630815	-6.202459	6	0.136575	3.593552	-6.024261
1	0.894320	1.047342	-6.703179	1	1.125724	0.903963	-6.514535
1	-1.313510	3.849396	-6.557041	1	-0.788876	3.875933	-6.541029
1	0.331178	3.498553	-7.087706	1	0.908027	3.473416	-6.789599
1	0.064084	4.513294	-5.665388	1	0.426837	4.432267	-5.384233
8	-0.777804	5.215829	-3.173539	8	-0.707969	5.227135	-3.175656
1	-2.778472	4.661810	-3.045843	1	-2.704854	4.676939	-3.181358
1	-2.040386	4.412427	-4.616611	1	-1.853492	4.399320	-4.689441
6	-0.951197	6.540392	-3.462479	6	-0.865823	6.532236	-3.498112
6	0.186824	7.361544	-3.002821	6	0.240524	7.369898	-2.999135
8	-1.952385	6.942615	-4.031755	8	-1.831464	6.918593	-4.128001
6	0.362453	8.743632	-3.442136	6	0.333806	8.786986	-3.313231
6	1.100170	6.798022	-2.130427	6	1.205432	6.783827	-2.212325
7	2.158941	7.441447	-1.601568	7	2.252611	7.424716	-1.673181
1	0.987048	5.770140	-1.814947	1	1.147753	5.728901	-1.983290
6	1.557127	9.407863	-2.882861	6	1.519633	9.454842	-2.747073
8	-0.387498	9.341365	-4.235658	8	-0.475537	9.419882	-4.003367
6	2.435518	8.765000	-1.984847	6	2.456677	8.781608	-1.952439
6	3.070644	6.722767	-0.718664	6	3.225955	6.681420	-0.893031
6	2.525213	5.781336	0.321483	6	2.754756	5.657890	0.095057

6	3.148916	7.088897	0.742785	6	3.353169	6.947578	0.578958
1	3.994524	6.439093	-1.217218	1	4.133958	6.465633	-1.449193
1	2.475967	7.864150	1.098119	1	2.673527	7.675694	1.010368
1	4.131652	7.086267	1.205520	1	4.352235	6.944546	1.002587
1	3.073984	4.857669	0.478700	1	3.336102	4.745127	0.168425
1	1.448432	5.690226	0.427918	1	1.686796	5.525307	0.233505
6	1.844288	10.735682	-3.253251	6	1.726893	10.817445	-3.010027
6	2.952292	11.369952	-2.755309	6	2.823099	11.453735	-2.506484
6	3.874842	10.745128	-1.875437	6	3.806717	10.798496	-1.730830
6	3.580420	9.426105	-1.505800	6	3.591290	9.448521	-1.467168
1	1.167566	11.258963	-3.919934	1	0.997694	11.361984	-3.598642
1	4.257210	8.900428	-0.848735	1	4.318941	8.900266	-0.888438
9	3.154348	12.676790	-3.093686	9	2.958297	12.786110	-2.731615
7	4.972488	11.452257	-1.373241	7	4.895142	11.512216	-1.225612
6	5.919393	12.020832	-2.354845	6	5.761845	12.178611	-2.208122
6	5.679101	10.887980	-0.219409	6	5.681865	10.883107	-0.170184
6	6.786528	13.097616	-1.708333	6	6.626841	13.229319	-1.531753
1	5.370447	12.459885	-3.186881	1	5.153741	12.658020	-2.973018
1	6.562195	11.217052	-2.751517	1	6.405812	11.430618	-2.697812
6	6.544021	11.957139	0.451713	6	6.547820	11.920374	0.533633
1	6.314438	10.035773	-0.516113	1	6.324124	10.082731	-0.573115
1	4.946396	10.533918	0.510647	1	5.006323	10.443699	0.567093
7	7.452233	12.569931	-0.518398	7	7.372280	12.636545	-0.430981
1	7.122431	11.501648	1.253255	1	7.187479	11.426196	1.261080
1	5.894861	12.731811	0.886752	1	5.902588	12.633944	1.064528
1	6.160515	13.959150	-1.430621	1	5.991687	14.042160	-1.152479
1	7.545747	13.434839	-2.414022	1	7.333312	13.647148	-2.247305
6	8.738329	12.947801	-0.240673	6	8.655505	13.028643	-0.200834
8	9.438824	13.596789	-1.018977	8	9.287596	13.757254	-0.959622
8	9.135396	12.505189	0.972133	8	9.139073	12.509510	0.938534
6	10.507289	12.724058	1.487511	6	10.522102	12.736216	1.378545
6	10.456407	12.034386	2.853839	6	10.586365	11.948260	2.681868
6	10.776297	14.223186	1.650790	6	10.754529	14.220659	1.639703
6	11.529212	12.037933	0.575935	6	11.498737	12.161821	0.357823
1	11.271746	10.981502	0.438388	1	11.263769	11.112144	0.154107
1	12.519249	12.087260	1.043466	1	12.513630	12.209340	0.764861
1	11.582592	12.520689	-0.401836	1	11.472810	12.719862	-0.578814
1	9.991323	14.689056	2.257454	1	9.998692	14.608911	2.329972
1	10.825595	14.729438	0.684858	1	10.721969	14.798848	0.715797
1	11.732403	14.363468	2.167936	1	11.737404	14.354812	2.102321
1	9.696035	12.494742	3.494032	1	9.856233	12.330705	3.401441
1	11.427891	12.125151	3.351139	1	11.584237	12.037318	3.120822
1	10.222594	10.969875	2.743855	1	10.379594	10.888630	2.504179
9	0.364519	-0.372352	-1.737569	9	-0.033218	-0.617684	-1.723086
9	-1.655887	-0.989256	-2.634426	9	-2.032288	-0.915231	-2.779738
6	-1.781977	-0.347633	0.516405	6	-2.184241	-0.359118	0.404704
1	-2.190151	-1.190068	-0.052263	1	-2.640475	-1.142475	-0.211200
1	-0.723165	-0.563922	0.700317	1	-1.159325	-0.685277	0.619309
1	-2.296204	-0.292559	1.479269	1	-2.731791	-0.284189	1.346032
6	0.781690	-1.141507	-4.728052	6	0.604993	-1.292715	-4.615515
1	1.531022	-1.281654	-3.940617	1	1.279108	-1.508071	-3.777655
1	-0.019413	-1.865964	-4.544596	1	-0.273947	-1.934102	-4.484084
1	1.244314	-1.368379	-5.691947	1	1.105901	-1.564314	-5.546531
Min T_1 (implicit water)				Products T_1 (implicit water)			
6	-1.970151	0.875856	-0.219058	6	-1.730941	0.065024	-0.725867
6	-2.494678	2.078312	0.286860	6	-2.081808	1.306839	-0.128203
6	-2.408651	3.057337	-0.692045	6	-2.375708	2.211016	-1.121626
7	-1.547988	1.096818	-1.522510	7	-1.792077	0.198972	-2.086243

6	-1.802696	2.409070	-1.859537	6	-2.191631	1.481234	-2.380546
1	-2.890152	2.207092	1.286798	1	-2.102377	1.490538	0.937874
6	-2.845515	4.480112	-0.519683	6	-2.755765	3.639283	-0.909110
1	-3.081740	4.664619	0.532821	1	-2.679218	3.878624	0.155197
1	-3.748325	4.712768	-1.100042	1	-3.792536	3.831877	-1.214244
1	-2.068936	5.192554	-0.819353	1	-2.101930	4.325896	-1.466304
5	-0.918151	0.040161	-2.445161	5	-1.506357	-0.931868	-3.113413
7	-0.525135	0.752166	-3.750105	7	-1.498798	-0.258486	-4.516008
6	-1.480009	2.918943	-3.148238	6	-2.351225	1.914212	-3.752136
6	-0.790363	2.069161	-4.058116	6	-1.895450	1.027737	-4.800805
6	-1.842464	4.315414	-3.532241	6	-2.943075	3.125194	-4.052085
6	0.143091	0.165547	-4.815936	6	-1.130462	-0.867644	-5.682193
6	-0.241743	2.332173	-5.392443	6	-1.745262	1.250443	-6.241425
6	0.316439	1.135975	-5.818484	6	-1.274197	0.064587	-6.749916
6	-0.231799	3.608446	-6.177102	6	-2.001535	2.489339	-7.038366
1	0.817248	0.965223	-6.763339	1	-1.037043	-0.146908	-7.784098
1	-1.228256	3.873579	-6.554956	1	-3.071081	2.728765	-7.086797
1	0.424152	3.497451	-7.046066	1	-1.650422	2.342813	-8.062954
1	0.132201	4.456037	-5.586127	1	-1.480838	3.358959	-6.621791
8	-0.738625	5.219629	-3.179008	8	-0.537142	5.717409	-2.449048
1	-2.737600	4.663120	-3.020761	1	-3.303457	3.788295	-3.281318
1	-2.024112	4.413063	-4.600633	1	-3.095623	3.446746	-5.070724
6	-0.926077	6.538362	-3.450743	6	-0.690769	6.973452	-2.529310
6	0.213926	7.369474	-3.000291	6	0.539409	7.830164	-2.236077
8	-1.939103	6.948804	-3.997751	8	-1.767798	7.579717	-2.784464
6	0.397815	8.743463	-3.459581	6	0.966652	8.929447	-3.082423
6	1.119661	6.817852	-2.113773	6	1.262587	7.527076	-1.111031
7	2.175907	7.467024	-1.583773	7	2.336790	8.231424	-0.650542
1	1.001827	5.794227	-1.786159	1	0.986366	6.673985	-0.503462
6	1.587281	9.415107	-2.897352	6	2.158376	9.652814	-2.598810
8	-0.339746	9.330680	-4.273250	8	0.422884	9.244784	-4.166774
6	2.456649	8.784500	-1.981882	6	2.826667	9.299903	-1.402896
6	3.079854	6.758896	-0.685163	6	3.032174	7.783638	0.545379
6	2.525766	5.830554	0.362143	6	2.242268	7.327885	1.743837
6	3.147098	7.142788	0.772370	6	3.003113	8.629416	1.795849
1	4.007745	6.468315	-1.172347	1	3.955562	7.250717	0.326182
1	2.471943	7.922851	1.112721	1	2.419280	9.544970	1.762145
1	4.126098	7.145105	1.243000	1	3.916171	8.688865	2.381612
1	3.072612	4.908548	0.535182	1	2.625868	6.469301	2.287013
1	1.448106	5.741456	0.460929	1	1.158857	7.388422	1.701910
6	1.878539	10.737872	-3.282900	6	2.664155	10.738606	-3.343464
6	2.981364	11.379001	-2.782461	6	3.773955	11.417744	-2.916707
6	3.895049	10.766164	-1.885130	6	4.491505	11.070162	-1.741736
6	3.597141	9.452406	-1.500706	6	3.986343	9.996683	-1.002037
1	1.208552	11.251846	-3.963490	1	2.150665	11.044893	-4.248469
1	4.267294	8.935771	-0.829781	1	4.503492	9.683703	-0.106853
9	3.186974	12.681489	-3.136234	9	4.188641	12.503547	-3.638546
7	4.987841	11.480709	-1.381756	7	5.606975	11.822786	-1.342423
6	5.945120	12.033036	-2.362528	6	6.736915	11.893761	-2.290932
6	5.682581	10.932081	-0.213322	6	6.084190	11.649057	0.031991
6	6.808069	13.117731	-1.723645	6	7.674006	13.042675	-1.928749
1	5.404814	12.460877	-3.206019	1	6.360766	12.049152	-3.301645
1	6.590230	11.222494	-2.741419	1	7.294838	10.941845	-2.273305
6	6.542987	12.009438	0.450445	6	7.013266	12.799853	0.424081
1	6.319380	10.074702	-0.491575	1	6.618530	10.690759	0.154616
1	4.942414	10.589558	0.514744	1	5.227399	11.653677	0.711188
7	7.461486	12.606443	-0.519825	7	8.109586	12.927790	-0.537555
1	7.112937	11.564775	1.264031	1	7.420752	12.613333	1.415966
1	5.891162	12.791539	0.867844	1	6.439879	13.738588	0.453277

1	6.180948	13.984182	-1.464375	1	7.155629	14.002410	-2.075544
1	7.574553	13.443489	-2.426862	1	8.552750	13.021958	-2.573194
6	8.746288	12.984200	-0.236364	6	9.394889	13.259139	-0.203990
8	9.455947	13.619098	-1.018015	8	10.270421	13.507688	-1.034586
8	9.131106	12.558599	0.986478	8	9.576876	13.259670	1.134702
6	10.499374	12.779918	1.510288	6	10.896969	13.515074	1.756790
6	10.433965	12.111151	2.886354	6	10.583540	13.388409	3.250440
6	10.773049	14.280277	1.653341	6	11.372177	14.933143	1.425275
6	11.526159	12.076103	0.617849	6	11.900299	12.441447	1.324494
1	11.265421	11.018793	0.493875	1	11.501710	11.440735	1.526904
1	12.512440	12.128330	1.092934	1	12.825577	12.560314	1.899788
1	11.589792	12.543978	-0.366526	1	12.139591	12.520123	0.262157
1	9.984778	14.758272	2.246136	1	10.603446	15.666924	1.693351
1	10.832640	14.771741	0.680379	1	11.609498	15.039348	0.365067
1	11.725229	14.424641	2.176593	1	12.272491	15.156901	2.008939
1	9.669791	12.583961	3.512806	1	9.833444	14.126619	3.554368
1	11.401392	12.205799	3.390787	1	11.493143	13.558913	3.835966
1	10.197007	11.045984	2.790373	1	10.203985	12.387921	3.484838
9	0.224435	-0.532205	-1.832477	9	-0.259045	-1.507107	-2.855908
9	-1.841207	-1.006170	-2.706639	9	-2.509860	-1.908610	-3.051727
6	-1.852031	-0.438922	0.467385	6	-1.346020	-1.191874	-0.039470
1	-2.354167	-1.232340	-0.099526	1	-1.869401	-2.054970	-0.463554
1	-0.802269	-0.740099	0.572558	1	-0.270688	-1.376820	-0.163342
1	-2.300042	-0.380620	1.462514	1	-1.565290	-1.120444	1.027604
6	0.577357	-1.257481	-4.825776	6	-0.652838	-2.268596	-5.766236
1	1.303654	-1.457523	-4.028214	1	0.357813	-2.348690	-5.343993
1	-0.269515	-1.934741	-4.660412	1	-1.293899	-2.944473	-5.191145
1	1.037831	-1.499399	-5.786971	1	-0.620299	-2.593061	-6.808100
Min S_0 (explicit water)				Min S_1 (explicit water)			
6	-1.577312	0.872572	-0.174316	6	-1.494839	0.777540	-0.253079
6	-2.125918	2.044323	0.383440	6	-1.941193	1.957863	0.378883
6	-2.198233	3.019518	-0.605948	6	-2.009920	2.970965	-0.559520
7	-1.306156	1.095435	-1.481066	7	-1.284484	1.040634	-1.565704
6	-1.673510	2.413005	-1.800569	6	-1.592556	2.379886	-1.811300
1	-2.434266	2.156078	1.415423	1	-2.180788	2.040282	1.431670
6	-2.735793	4.402212	-0.369741	6	-2.434925	4.375406	-0.270432
1	-2.947606	4.531870	0.695744	1	-2.504094	4.518750	0.811008
1	-3.674455	4.579539	-0.909796	1	-3.421142	4.607585	-0.690281
1	-2.028744	5.184982	-0.662744	1	-1.727842	5.114865	-0.658363
5	-0.691657	0.075350	-2.465327	5	-0.813540	0.022498	-2.610359
7	-0.549407	0.774577	-3.835733	7	-0.639056	0.775947	-3.934049
6	-1.490185	2.899380	-3.105647	6	-1.465568	2.927347	-3.112962
6	-0.932348	2.096287	-4.116926	6	-0.940442	2.121590	-4.154752
6	-1.887884	4.317885	-3.430667	6	-1.859089	4.338699	-3.380564
6	-0.041785	0.219229	-4.960790	6	-0.169687	0.238501	-5.086003
6	-0.633961	2.349922	-5.501474	6	-0.615413	2.423452	-5.531818
6	-0.082017	1.172264	-5.996915	6	-0.148340	1.242229	-6.077746
6	-0.835088	3.584554	-6.334373	6	-0.719680	3.720862	-6.269396
1	0.264453	1.004879	-7.009054	1	0.190135	1.094991	-7.095704
1	-1.897728	3.805739	-6.495328	1	-1.759200	4.005906	-6.471785
1	-0.383938	3.434015	-7.319636	1	-0.217540	3.628819	-7.235994
1	-0.372466	4.474043	-5.894012	1	-0.247869	4.548905	-5.730371
8	-0.730838	5.167370	-3.170095	8	-0.715629	5.208348	-3.098859
1	-2.717036	4.658902	-2.816071	1	-2.685011	4.661600	-2.750611
1	-2.177810	4.426139	-4.471842	1	-2.150874	4.486121	-4.415573
6	-0.902074	6.502039	-3.415625	6	-0.872373	6.521316	-3.388427
6	0.243825	7.312798	-2.975300	6	0.257983	7.347817	-2.944428
8	-1.920515	6.929373	-3.938190	8	-1.869979	6.935581	-3.951642

6	0.521110	8.617509	-3.572195	6	0.551744	8.625784	-3.573820
6	1.047305	6.833455	-1.957254	6	1.028406	6.906537	-1.894303
7	2.086639	7.502205	-1.423625	7	2.050042	7.588468	-1.358658
1	0.852792	5.867370	-1.511874	1	0.824050	5.955312	-1.422836
6	1.694955	9.303122	-3.000496	6	1.711800	9.326329	-2.999312
8	-0.130606	9.121042	-4.504671	8	-0.071663	9.099943	-4.531706
6	2.462038	8.750074	-1.952582	6	2.443709	8.809344	-1.921511
6	2.878598	6.879097	-0.368580	6	2.803991	7.006936	-0.262111
6	2.196122	6.114768	0.733870	6	2.075735	6.319815	0.853067
6	2.846625	7.443492	1.029933	6	2.743004	7.643150	1.096105
1	3.826301	6.492132	-0.735488	1	3.751658	6.583359	-0.582434
1	2.185483	8.286177	1.211212	1	2.096928	8.508083	1.208481
1	3.783465	7.468229	1.579100	1	3.661497	7.678164	1.672913
1	2.680925	5.201626	1.065614	1	2.529236	5.417858	1.249631
1	1.110878	6.080934	0.751194	1	0.990750	6.309001	0.834716
6	2.078760	10.557612	-3.512050	6	2.110646	10.555261	-3.546840
6	3.173627	11.206765	-3.004743	6	3.192311	11.212573	-3.038835
6	3.989889	10.665870	-1.976185	6	3.975037	10.704428	-1.976669
6	3.597101	9.421100	-1.465516	6	3.567815	9.489518	-1.431740
1	1.486770	11.015424	-4.297034	1	1.540655	10.984973	-4.362470
1	4.189766	8.959462	-0.689859	1	4.137546	9.053966	-0.625203
9	3.467757	12.448658	-3.487559	9	3.512684	12.426669	-3.554872
7	5.080446	11.384746	-1.478559	7	5.060557	11.434247	-1.489769
6	6.125449	11.790206	-2.441762	6	6.125745	11.752981	-2.451951
6	5.668564	10.945309	-0.209499	6	5.616269	11.032602	-0.201575
6	6.989712	12.906838	-1.862837	6	7.015510	12.862818	-1.916681
1	5.663485	12.140855	-3.363590	1	5.688226	12.072659	-3.395927
1	6.758329	10.919657	-2.682411	1	6.732435	10.852755	-2.639813
6	6.530965	12.056681	0.393027	6	6.501951	12.136963	0.361262
1	6.281438	10.037789	-0.345462	1	6.203249	10.103862	-0.292011
1	4.865816	10.716771	0.496467	1	4.799519	10.856470	0.501926
7	7.538153	12.507533	-0.567890	7	7.529823	12.507096	-0.602514
1	7.024315	11.683804	1.288611	1	6.972168	11.792217	1.279161
1	5.888757	12.904235	0.675724	1	5.885457	13.016101	0.594235
1	6.384862	13.818445	-1.743013	1	6.439988	13.796574	-1.847329
1	7.814895	13.125496	-2.540547	1	7.856300	13.023474	-2.589693
6	8.817379	12.864986	-0.236757	6	8.814363	12.816404	-0.275184
8	9.605399	13.381541	-1.030355	8	9.630172	13.259832	-1.077718
8	9.100473	12.563702	1.049139	8	9.074590	12.562456	1.016915
6	10.439794	12.789810	1.641331	6	10.407890	12.757568	1.601528
6	10.252783	12.281800	3.073854	6	10.199078	12.326982	3.048800
6	10.771391	14.285307	1.639985	6	10.801389	14.229430	1.533773
6	11.489964	11.951872	0.905604	6	11.420655	11.848124	0.913877
1	11.188743	10.898416	0.878051	1	11.074714	10.809610	0.932990
1	12.443659	12.017400	1.441719	1	12.372821	11.898123	1.451382
1	11.641180	12.304538	-0.116549	1	11.588636	12.147487	-0.121264
1	9.969338	14.855380	2.122642	1	10.022274	14.852875	1.984088
1	10.914962	14.663820	0.626206	1	10.964382	14.552822	0.505303
1	11.693811	14.450467	2.208419	1	11.726155	14.381074	2.099323
1	9.470587	12.850048	3.588850	1	9.440132	12.949724	3.531853
1	11.187613	12.396064	3.632759	1	11.135315	12.428449	3.605150
1	9.974951	11.222203	3.077967	1	9.877709	11.282329	3.099343
8	2.156616	4.029446	-3.444461	8	1.984632	3.974771	-2.740420
1	2.179994	3.105246	-3.740033	1	2.039942	3.015088	-2.860340
1	1.211317	4.261439	-3.431966	1	1.067053	4.209261	-2.961665
8	-4.499641	6.544676	-5.147497	8	-4.253792	6.136222	-5.248272
1	-4.739799	7.420078	-5.488940	1	-4.519784	6.860254	-5.833162
1	-3.619641	6.663363	-4.739141	1	-3.437042	6.440692	-4.807152
9	0.574778	-0.349292	-2.000120	9	0.407686	-0.558137	-2.212813

9	-1.529260	-1.058874	-2.580512	9	-1.760764	-1.013987	-2.752747
6	-1.315558	-0.423382	0.521047	6	-1.269140	-0.553910	0.360023
1	-1.844888	-1.249840	0.034172	1	-1.838717	-1.332220	-0.160742
1	-0.248058	-0.671142	0.508747	1	-0.213003	-0.842746	0.297325
1	-1.646413	-0.360262	1.560697	1	-1.566965	-0.539126	1.409954
6	0.469324	-1.182255	-5.040242	6	0.244993	-1.179451	-5.217102
1	1.309295	-1.337936	-4.353865	1	1.098514	-1.402511	-4.565613
1	-0.308322	-1.904825	-4.768943	1	-0.562764	-1.857927	-4.919347
1	0.806172	-1.396819	-6.057492	1	0.526034	-1.394413	-6.249623
Min T_1 (explicit water)				TS T_1 (explicit water)			
6	-1.584850	0.679536	-0.276388	6	-1.537996	0.597141	-0.244902
6	-2.062422	1.845161	0.348858	6	-1.921365	1.796887	0.401517
6	-2.109180	2.871525	-0.581993	6	-2.077204	2.784768	-0.549340
7	-1.325954	0.972675	-1.608070	7	-1.448500	0.838178	-1.594916
6	-1.632628	2.294413	-1.843462	6	-1.776505	2.152747	-1.832239
1	-2.341233	1.916231	1.392788	1	-2.058294	1.904965	1.469678
6	-2.566599	4.267723	-0.289759	6	-2.464519	4.200739	-0.260661
1	-2.701709	4.388935	0.789295	1	-2.475429	4.363985	0.820530
1	-3.529746	4.497031	-0.764829	1	-3.468287	4.434822	-0.638454
1	-1.846621	5.022712	-0.623334	1	-1.765974	4.915798	-0.707759
5	-0.804281	-0.029431	-2.652107	5	-1.079739	-0.216263	-2.666808
7	-0.620710	0.741347	-3.970575	7	-0.954886	0.538417	-4.012588
6	-1.467643	2.874618	-3.134467	6	-1.783451	2.690049	-3.170272
6	-0.928242	2.068459	-4.178264	6	-1.283829	1.855018	-4.234640
6	-1.853431	4.290660	-3.389508	6	-2.229798	3.989618	-3.426282
6	-0.123468	0.203512	-5.148994	6	-0.520414	-0.013715	-5.193813
6	-0.593208	2.389061	-5.570095	6	-1.024020	2.158023	-5.640871
6	-0.106736	1.215377	-6.125270	6	-0.558127	0.984184	-6.197289
6	-0.709725	3.691933	-6.301153	6	-1.188564	3.451730	-6.374259
1	0.240888	1.086155	-7.142636	1	-0.258613	0.834176	-7.226426
1	-1.754373	3.977278	-6.482479	1	-2.245664	3.722044	-6.493332
1	-0.224677	3.604946	-7.278160	1	-0.758081	3.361670	-7.375490
1	-0.229936	4.518224	-5.764371	1	-0.691136	4.280500	-5.858944
8	-0.704578	5.182154	-3.086376	8	-0.540547	5.243218	-3.243617
1	-2.682894	4.616542	-2.766089	1	-2.751899	4.549705	-2.668861
1	-2.130205	4.460972	-4.425593	1	-2.404566	4.320105	-4.435794
6	-0.875611	6.502436	-3.362061	6	-0.757958	6.517721	-3.299239
6	0.258259	7.337517	-2.920974	6	0.399088	7.385405	-2.878634
8	-1.883023	6.924069	-3.915800	8	-1.839575	7.043454	-3.635506
6	0.569226	8.603510	-3.580283	6	0.736478	8.623817	-3.563909
6	1.015245	6.916437	-1.845087	6	1.149421	6.973845	-1.802622
7	2.040204	7.609390	-1.310286	7	2.178092	7.672231	-1.259314
1	0.795066	5.980692	-1.349718	1	0.926931	6.035901	-1.310031
6	1.734751	9.307472	-3.013190	6	1.891986	9.340203	-2.991027
8	-0.046036	9.061347	-4.560635	8	0.151205	9.055630	-4.579178
6	2.456316	8.812326	-1.905655	6	2.597291	8.864102	-1.862808
6	2.773685	7.050836	-0.180324	6	2.908583	7.116062	-0.129302
6	2.026235	6.389202	0.946544	6	2.157761	6.457946	0.997755
6	2.698303	7.721426	1.168796	6	2.833399	7.788346	1.219841
1	3.725440	6.615432	-0.475441	1	3.861215	6.677201	-0.418190
1	2.052748	8.590721	1.256151	1	2.190886	8.660204	1.304678
1	3.611595	7.766815	1.755042	1	3.745204	7.830985	1.808805
1	2.472512	5.493547	1.367978	1	2.600267	5.562079	1.422930
1	0.940611	6.382122	0.917953	1	1.072308	6.453611	0.964976
6	2.159119	10.518713	-3.592862	6	2.324322	10.543210	-3.584283
6	3.250885	11.179696	-3.094492	6	3.404537	11.216594	-3.078896
6	4.024139	10.692946	-2.007350	6	4.159900	10.750794	-1.970326
6	3.589112	9.494116	-1.426797	6	3.722160	9.560476	-1.378446

1	1.601697	10.933556	-4.425588	1	1.779756	10.941032	-4.433779
1	4.147549	9.074146	-0.603467	1	4.269451	9.156567	-0.539492
9	3.586760	12.380483	-3.649512	9	3.748133	12.410210	-3.648668
7	5.117868	11.421296	-1.528555	7	5.242846	11.496275	-1.485574
6	6.199134	11.727123	-2.488798	6	6.345266	11.767933	-2.431028
6	5.660401	11.055842	-0.216405	6	5.758730	11.160902	-0.155373
6	7.082797	12.856257	-1.966005	6	7.223926	12.907479	-1.922735
1	5.771479	12.024865	-3.445211	1	5.938699	12.040934	-3.404133
1	6.810899	10.823805	-2.650494	1	6.955793	10.857503	-2.555366
6	6.541318	12.181684	0.330238	6	6.632169	12.297453	0.380618
1	6.249246	10.124193	-0.272145	1	6.346482	10.226844	-0.176478
1	4.833577	10.900053	0.481613	1	4.918056	11.023110	0.529935
7	7.585826	12.533106	-0.632179	7	7.697404	12.621547	-0.569302
1	6.999932	11.859467	1.263158	1	7.071409	11.997715	1.330266
1	5.919015	13.065740	0.534607	1	6.008793	13.188160	0.550322
1	6.503705	13.791249	-1.926115	1	6.648934	13.845926	-1.922630
1	7.931061	13.002639	-2.634579	1	8.086936	13.030572	-2.577021
6	8.872758	12.855996	-0.296791	6	8.972016	12.969691	-0.212399
8	9.699278	13.281737	-1.105195	8	9.813705	13.380801	-1.012759
8	9.115809	12.632713	1.013165	8	9.185398	12.787862	1.109162
6	10.453295	12.834336	1.618002	6	10.504032	13.027381	1.740819
6	10.215093	12.435470	3.077176	6	10.235199	12.667093	3.204724
6	10.858714	14.308447	1.522871	6	10.889626	14.504311	1.612610
6	11.473876	11.898046	0.963798	6	11.555114	12.088846	1.140288
1	11.121790	10.860825	1.002539	1	11.216764	11.047950	1.198113
1	12.420144	11.955220	1.513824	1	12.485048	12.175001	1.713874
1	11.659769	12.170969	-0.076846	1	11.765725	12.336096	0.097998
1	10.077749	14.948307	1.949398	1	10.089147	15.143913	2.001716
1	11.038230	14.609407	0.489082	1	11.089524	14.778195	0.575000
1	11.778285	14.467100	2.097763	1	11.792623	14.693742	2.204215
1	9.452051	13.074112	3.535265	1	9.451483	13.306610	3.625106
1	11.143862	12.543752	3.647235	1	11.147666	12.806261	3.794087
1	9.886118	11.392959	3.147007	1	9.920185	11.622001	3.296830
8	2.052837	3.891893	-2.871694	8	1.927464	3.893637	-3.397791
1	2.018319	2.923500	-2.822652	1	1.953129	3.473924	-4.271322
1	1.125037	4.169534	-2.981333	1	1.072396	4.380854	-3.370918
8	-4.485253	6.429596	-4.995890	8	-3.965957	6.346578	-5.259670
1	-4.771301	7.292402	-5.333933	1	-4.030564	7.071989	-5.899636
1	-3.591924	6.583244	-4.627867	1	-3.198769	6.577213	-4.682710
9	0.428099	-0.585562	-2.229491	9	0.141980	-0.828422	-2.341776
9	-1.727560	-1.091925	-2.823392	9	-2.084676	-1.199925	-2.749809
6	-1.367806	-0.664754	0.322277	6	-1.257249	-0.723214	0.375766
1	-1.938632	-1.435188	-0.210253	1	-1.815898	-1.523635	-0.121906
1	-0.312044	-0.958366	0.268487	1	-0.192573	-0.974374	0.288233
1	-1.676798	-0.659852	1.370466	1	-1.525258	-0.703868	1.434325
6	0.306189	-1.214315	-5.283772	6	-0.086972	-1.428177	-5.330653
1	1.139811	-1.443168	-4.608257	1	0.849908	-1.601076	-4.785918
1	-0.507692	-1.903735	-5.028144	1	-0.831021	-2.114675	-4.911855
1	0.623993	-1.410974	-6.310676	1	0.072302	-1.670674	-6.383590

Products T_1 (explicit water)			
6	-4.741481	-2.002753	-1.713004
6	-4.591688	-1.320346	-0.471207
6	-3.871577	-0.169555	-0.682975
7	-4.102384	-1.287198	-2.686271
6	-3.570241	-0.153904	-2.115669
1	-4.982535	-1.674295	0.473619
6	-3.472931	0.810471	0.373472

1	-3.713829	0.403590	1.358852
1	-4.010025	1.761555	0.269084
1	-2.399232	1.027140	0.347004
5	-4.049504	-1.662182	-4.196637
7	-3.020205	-0.696128	-4.849367
6	-2.845947	0.808963	-2.916416
6	-2.479887	0.422828	-4.262095
6	-2.555363	2.068386	-2.431371
6	-2.514989	-0.805403	-6.116620
6	-1.542583	1.038470	-5.204462
6	-1.596385	0.259257	-6.336010
6	-0.654781	2.220559	-4.996922
1	-1.030987	0.403205	-7.247214
1	-1.218252	3.158572	-4.913431
1	0.035548	2.310988	-5.839879
1	-0.063231	2.117767	-4.079037
8	1.152807	5.350546	-2.296964
1	-2.848772	2.363819	-1.434776
1	-2.092624	2.837165	-3.035702
6	0.903443	6.534809	-2.680928
6	1.951911	7.595001	-2.400993
8	-0.168842	6.905681	-3.239323
6	2.376139	8.574383	-3.385960
6	2.514999	7.604829	-1.149581
7	3.416113	8.522370	-0.702628
1	2.238634	6.850238	-0.423475
6	3.389852	9.530627	-2.901965
8	1.973038	8.610745	-4.570418
6	3.897825	9.494914	-1.582775
6	3.959304	8.401416	0.641447
6	3.045440	8.066826	1.790554
6	3.640990	9.448533	1.681225
1	4.958072	7.969679	0.657472
1	2.972603	10.252971	1.387323
1	4.438823	9.739234	2.358856
1	3.431117	7.382474	2.540342
1	1.982037	7.968510	1.593766
6	3.883341	10.521273	-3.775348
6	4.832556	11.411989	-3.350044
6	5.391888	11.384766	-2.045084
6	4.896621	10.404696	-1.178848
1	3.486775	10.583066	-4.783044
1	5.298632	10.333409	-0.178941
9	5.233692	12.394182	-4.212950
7	6.344085	12.340198	-1.660062
6	7.591274	12.394454	-2.450134
6	6.620315	12.482172	-0.227788
6	8.331884	13.705331	-2.200108
1	7.359052	12.315864	-3.511681
1	8.239688	11.545161	-2.175012
6	7.350318	13.798452	0.047965
1	7.228267	11.641624	0.149842
1	5.673673	12.494488	0.319231
7	8.560684	13.897233	-0.768887
1	7.618364	13.848837	1.101630
1	6.682665	14.642013	-0.183094
1	7.740192	14.545088	-2.595033
1	9.295168	13.690707	-2.709897
6	9.741533	14.439535	-0.339894

8	10.704253	14.645019	-1.080926				
8	9.717277	14.698142	0.985914				
6	10.893994	15.228308	1.713325				
6	10.372803	15.325095	3.150070				
6	11.262476	16.616360	1.180369				
6	12.057849	14.236062	1.628514				
1	11.739725	13.242823	1.965477				
1	12.867760	14.573318	2.285431				
1	12.445706	14.158265	0.610918				
1	10.389641	17.278869	1.202672				
1	11.643293	16.565924	0.158567				
1	12.036813	17.054273	1.820631				
1	9.511544	15.999648	3.206555				
1	11.159882	15.714213	3.804612				
1	10.069919	14.340021	3.521330				
8	3.570527	4.197608	-1.751056				
1	3.599291	3.436320	-2.350577				
1	2.712292	4.656457	-1.953415				
8	-2.103140	5.063219	-3.768697				
1	-2.768985	5.571239	-4.257687				
1	-1.372418	5.712690	-3.564207				
9	-3.618652	-2.983396	-4.341755				
9	-5.312619	-1.498790	-4.781072				
6	-5.451946	-3.280596	-1.959366				
1	-6.093739	-3.217038	-2.844074				
1	-4.728781	-4.085741	-2.145509				
1	-6.054285	-3.549401	-1.089454				
6	-2.888305	-1.885723	-7.061150				
1	-2.448004	-2.838989	-6.740083				
1	-3.973307	-2.030105	-7.093258				
1	-2.521584	-1.652997	-8.062703				

Compound 4							
Min S_0 (implicit water)				Min S_1 (implicit water)			
6	-1.795776	-4.258962	3.928837	6	-1.684993	-4.295499	3.827375
6	-2.453537	-3.092802	4.406820	6	-2.295195	-3.128451	4.355116
6	-2.540460	-1.952551	3.621726	6	-2.377956	-1.974991	3.606157
6	-1.238820	-4.195100	2.618511	6	-1.170794	-4.216218	2.504412
6	-1.336651	-3.046936	1.850750	6	-1.262728	-3.055173	1.771601
6	-1.989880	-1.882814	2.321485	6	-1.869014	-1.886306	2.290337
1	-2.897105	-3.079652	5.395247	1	-2.704044	-3.131069	5.357412
1	-3.052041	-1.080738	4.024805	1	-2.852085	-1.100291	4.044318
1	-0.893035	-3.057388	0.858995	1	-0.853285	-3.052208	0.766498
6	-2.119006	-0.657237	1.559580	6	-1.988773	-0.654427	1.569816
7	-1.700213	-5.394528	4.691573	7	-1.594853	-5.442614	4.554837
1	-0.726535	-5.054232	2.201873	1	-0.696349	-5.078482	2.053490
6	-2.286943	-5.433511	6.026181	6	-2.136977	-5.499108	5.902139
6	-1.019026	-6.575920	4.173779	6	-0.962488	-6.623290	3.990016
1	0.032901	-6.365011	3.939458	1	0.083795	-6.430478	3.725354
1	-1.505035	-6.957760	3.265852	1	-1.488453	-6.971358	3.093028
1	-1.046431	-7.361644	4.928867	1	-0.982870	-7.424149	4.727372
1	-3.371544	-5.263012	5.995201	1	-3.215179	-5.299792	5.909564
1	-1.838221	-4.679189	6.686490	1	-1.646333	-4.774855	6.563279
1	-2.110516	-6.415922	6.464423	1	-1.973699	-6.495399	6.309847
6	-1.651991	-0.411043	0.300745	6	-1.546602	-0.401327	0.293668
1	-2.653121	0.140640	2.074703	1	-2.484592	0.149939	2.110122
6	-1.822959	0.839971	-0.384428	6	-1.692296	0.838486	-0.366242

1	-1.116904	-1.186120	-0.236268	1	-1.050821	-1.188482	-0.262471
6	-2.467332	2.023014	0.064957	6	-2.281874	2.043862	0.099940
6	-2.399093	2.979884	-0.933242	6	-2.209604	2.994889	-0.889412
7	-1.354264	1.070636	-1.649868	7	-1.250785	1.068595	-1.653667
6	-1.689969	2.373307	-2.031837	6	-1.553263	2.366406	-2.014215
1	-2.930726	2.158809	1.033434	1	-2.711048	2.192129	1.082339
6	-2.967107	4.364867	-0.794325	6	-2.711421	4.400064	-0.746892
1	-3.311868	4.515258	0.233436	1	-2.982250	4.584869	0.296245
1	-3.830157	4.528896	-1.451858	1	-3.606718	4.588222	-1.350583
1	-2.229101	5.143425	-1.013787	1	-1.957997	5.141115	-1.030491
5	-0.582519	0.064653	-2.525402	5	-0.539569	0.049922	-2.541074
7	-0.214871	0.763803	-3.848302	7	-0.172848	0.741193	-3.851994
6	-1.315806	2.865537	-3.296353	6	-1.211904	2.865562	-3.290106
6	-0.567844	2.073589	-4.187768	6	-0.485185	2.045136	-4.180317
6	-1.725630	4.257411	-3.703248	6	-1.614405	4.244624	-3.693552
6	0.504727	0.213435	-4.874782	6	0.528909	0.164944	-4.891740
6	-0.023510	2.346405	-5.494223	6	0.062789	2.313096	-5.491357
6	0.630089	1.193525	-5.894834	6	0.673748	1.152763	-5.902263
6	-0.079995	3.598753	-6.323985	6	0.036622	3.581131	-6.290201
6	1.006849	-1.132224	-4.847697	6	0.980143	-1.172877	-4.874393
1	1.157370	1.064807	-6.831098	1	1.192675	1.016296	-6.842163
1	-1.090305	3.803518	-6.700235	1	-0.959979	3.805138	-6.687679
1	0.571994	3.487046	-7.195906	1	0.710118	3.484787	-7.146262
1	0.254205	4.482368	-5.770451	1	0.363347	4.446775	-5.706138
6	1.712681	-1.701042	-5.868226	6	1.663651	-1.772246	-5.904749
1	0.796429	-1.707385	-3.953070	1	0.758634	-1.744959	-3.980866
6	2.248786	-3.046009	-5.922804	6	2.142279	-3.121438	-5.944880
1	1.909226	-1.099687	-6.755317	1	1.873297	-1.181048	-6.794295
6	2.109102	-3.999879	-4.886456	6	1.976564	-4.054916	-4.894173
6	2.959884	-3.463904	-7.070950	6	2.826678	-3.583489	-7.092182
6	2.638927	-5.275226	-4.986249	6	2.453495	-5.342748	-4.980368
6	3.356031	-5.690098	-6.145943	6	3.140626	-5.798337	-6.138510
6	3.498400	-4.736653	-7.190849	6	3.311142	-4.869045	-7.196971
1	1.571774	-3.740374	-3.978464	1	1.459533	-3.761465	-3.986153
1	2.497783	-5.960612	-4.158953	1	2.296112	-6.011684	-4.143887
7	3.883641	-6.951855	-6.246365	7	3.613942	-7.071705	-6.226010
1	3.090903	-2.763627	-7.893515	1	2.975951	-2.899345	-7.923694
1	4.031511	-4.993144	-8.098634	1	3.826011	-5.161129	-8.103341
6	3.708938	-7.912812	-5.162912	6	3.421926	-8.004225	-5.127663
6	4.604264	-7.352251	-7.449386	6	4.309612	-7.513036	-7.423307
1	5.482516	-6.716221	-7.622792	1	5.211474	-6.916833	-7.605894
1	3.962739	-7.304412	-8.339822	1	3.666082	-7.447676	-8.308728
1	4.948114	-8.380186	-7.333336	1	4.609749	-8.552116	-7.297889
1	2.647343	-8.124879	-4.977177	1	2.357698	-8.172028	-4.923839
1	4.157604	-7.552223	-4.227785	1	3.898640	-7.645106	-4.207999
1	4.198911	-8.847844	-5.434703	1	3.871372	-8.960298	-5.390942
8	-0.675485	5.172938	-3.289331	8	-0.567534	5.177876	-3.307522
1	-2.660043	4.557158	-3.234670	1	-2.539403	4.556413	-3.214938
1	-1.861458	4.340595	-4.779024	1	-1.763634	4.328439	-4.766798
6	-0.883548	6.492300	-3.568173	6	-0.784707	6.477083	-3.601099
6	0.222358	7.344477	-3.081815	6	0.302912	7.349710	-3.115957
8	-1.886537	6.871187	-4.152364	8	-1.782134	6.842611	-4.194394
6	0.290927	8.771144	-3.390075	6	0.409016	8.743256	-3.516745
6	1.214762	6.764097	-2.312123	6	1.233026	6.817322	-2.254115
7	2.265227	7.420536	-1.782442	7	2.253558	7.495714	-1.708034
1	1.179061	5.707037	-2.088773	1	1.165829	5.778212	-1.963215
6	1.478970	9.453543	-2.837181	6	1.567227	9.450549	-2.941271
8	-0.542253	9.398362	-4.069607	8	-0.365501	9.324788	-4.288098
6	2.446237	8.786856	-2.056074	6	2.467380	8.832763	-2.062844

6	3.264981	6.682139	-1.019282	6	3.189635	6.808233	-0.836917
6	2.832238	5.623267	-0.041075	6	2.674177	5.847678	0.191604
6	3.408362	6.923328	0.463091	6	3.246990	7.168441	0.619384
1	4.172082	6.497917	-1.590229	1	4.123432	6.561272	-1.334216
1	2.716490	7.624068	0.921786	1	2.546664	7.919510	0.971015
1	4.414902	6.937933	0.871211	1	4.225059	7.197262	1.088627
1	3.437814	4.723089	0.002933	1	3.252949	4.944176	0.350364
1	1.769876	5.460141	0.113553	1	1.601129	5.719100	0.287652
6	1.667186	10.825042	-3.094358	6	1.786493	10.794126	-3.281851
6	2.767750	11.477560	-2.603730	6	2.858173	11.465128	-2.770547
6	3.779557	10.831811	-1.845335	6	3.804145	10.864873	-1.908497
6	3.582322	9.469113	-1.585447	6	3.577285	9.534204	-1.568769
1	0.920859	11.364954	-3.666793	1	1.085607	11.297277	-3.937835
1	4.328136	8.926960	-1.023264	1	4.276932	9.027022	-0.922100
9	2.873236	12.820551	-2.825033	9	3.004632	12.780263	-3.076269
7	4.867981	11.555345	-1.346979	7	4.867940	11.613361	-1.399652
6	5.711392	12.272735	-2.325358	6	5.782199	12.210959	-2.383568
6	5.682422	10.932722	-0.299132	6	5.602493	11.053810	-0.269890
6	6.554340	13.339160	-1.631614	6	6.623412	13.300608	-1.739236
1	5.082925	12.749858	-3.076114	1	5.211615	12.641766	-3.204333
1	6.372924	11.552960	-2.836101	1	6.442269	11.430162	-2.794364
6	6.527438	11.988565	0.417686	6	6.441780	12.132923	0.402257
1	6.344205	10.153796	-0.715385	1	6.258250	10.227069	-0.589247
1	5.022385	10.466608	0.437182	1	4.891709	10.665479	0.462991
7	7.329565	12.747036	-0.542783	7	7.314458	12.778882	-0.569334
1	7.184895	11.499181	1.133762	1	7.043865	11.686632	1.190165
1	5.864976	12.675637	0.965168	1	5.777872	12.883369	0.853244
1	5.898248	14.127332	-1.232258	1	5.977426	14.138978	-1.442990
1	7.242486	13.790539	-2.346193	1	7.364005	13.667874	-2.448039
6	8.611555	13.170253	-0.317807	6	8.592651	13.170038	-0.312197
8	9.219943	13.927315	-1.075823	8	9.266136	13.838764	-1.090340
8	9.117699	12.641798	0.817662	8	9.021007	12.722536	0.878579
6	10.512874	12.885500	1.253090	6	10.387662	12.960891	1.361237
6	10.596617	12.074202	2.549212	6	10.385905	12.259543	2.714674
6	10.725035	14.375769	1.536805	6	10.631034	14.456422	1.534347
6	11.493447	12.338607	0.211162	6	11.397415	12.308816	0.422782
1	11.274044	11.287122	-0.006807	1	11.156074	11.250745	0.278741
1	12.512491	12.396411	0.610371	1	12.395212	12.371497	0.868236
1	11.451906	12.909870	-0.718351	1	11.418110	12.804034	-0.548595
1	9.970366	14.742450	2.241981	1	9.851342	14.899023	2.162592
1	10.674044	14.969442	0.622156	1	10.648360	14.972267	0.573806
1	11.711935	14.518709	1.991671	1	11.594336	14.609007	2.031174
1	9.865211	12.434023	3.281013	1	9.633148	12.697871	3.376760
1	11.597048	12.172152	2.983810	1	11.366287	12.363926	3.188278
1	10.405485	11.012810	2.357194	1	10.169771	11.193370	2.597570
9	0.593943	-0.365949	-1.855750	9	0.627451	-0.439041	-1.896314
9	-1.380050	-1.083477	-2.778121	9	-1.373594	-1.073875	-2.782113
	Min T_1 (implicit water)				TS T_1 (implicit water)		
6	-1.796701	-4.347280	3.837959	6	-1.234142	-4.286660	3.926734
6	-2.440841	-3.187587	4.355528	6	-1.751383	-3.075979	4.475127
6	-2.525553	-2.027377	3.606304	6	-1.889135	-1.946791	3.692203
6	-1.250709	-4.251849	2.523571	6	-0.871877	-4.273342	2.544430
6	-1.344800	-3.084632	1.789131	6	-1.015815	-3.135761	1.778008
6	-1.985335	-1.923047	2.297826	6	-1.529059	-1.924371	2.317959
1	-2.874388	-3.199565	5.348351	1	-2.043392	-3.028151	5.517037
1	-3.025370	-1.162658	4.037782	1	-2.287235	-1.041295	4.144572
1	-0.910151	-3.072504	0.793852	1	-0.724279	-3.183794	0.733184
6	-2.110640	-0.685229	1.578080	6	-1.696244	-0.714221	1.569126

7	-1.704619	-5.502339	4.567268	7	-1.090614	-5.409761	4.686863
1	-0.749972	-5.103834	2.079333	1	-0.475401	-5.166687	2.077566
6	-2.279535	-5.575198	5.906925	6	-1.466499	-5.399564	6.099423
6	-1.035700	-6.675528	4.012931	6	-0.559781	-6.640017	4.101919
1	0.014715	-6.463592	3.775042	1	0.457089	-6.492413	3.717717
1	-1.533671	-7.028902	3.100546	1	-1.195120	-6.998614	3.282657
1	-1.061792	-7.479720	4.747987	1	-0.525670	-7.411701	4.870168
1	-3.361857	-5.392344	5.889429	1	-2.532580	-5.173767	6.226504
1	-1.815532	-4.845556	6.583444	1	-0.882689	-4.659930	6.661188
1	-2.109625	-6.572066	6.313260	1	-1.272417	-6.383190	6.525661
6	-1.644184	-0.417034	0.303261	6	-1.391349	-0.515813	0.236129
1	-2.630247	0.109079	2.111952	1	-2.105687	0.123794	2.130706
6	-1.792006	0.820558	-0.359277	6	-1.580272	0.708548	-0.444874
1	-1.126183	-1.198271	-0.242201	1	-0.979462	-1.335784	-0.341061
6	-2.407936	2.021414	0.092914	6	-2.095954	1.943392	0.037737
6	-2.325197	2.978326	-0.895493	6	-2.107545	2.861561	-0.993336
7	-1.320205	1.063016	-1.652770	7	-1.269089	0.889969	-1.789349
6	-1.629817	2.355740	-2.014839	6	-1.581741	2.174762	-2.153114
1	-2.862279	2.162631	1.065465	1	-2.421293	2.133853	1.052202
6	-2.855219	4.377750	-0.759200	6	-2.575741	4.281388	-0.854100
1	-3.171588	4.547472	0.275081	1	-2.787194	4.494382	0.198401
1	-3.729224	4.560085	-1.397775	1	-3.499320	4.470850	-1.416335
1	-2.102959	5.135328	-1.004911	1	-1.824671	5.000099	-1.199341
5	-0.576321	0.049856	-2.531253	5	-0.671163	-0.186858	-2.714434
7	-0.196110	0.751017	-3.840945	7	-0.403604	0.459922	-4.086365
6	-1.268061	2.869323	-3.288618	6	-1.371604	2.634969	-3.506239
6	-0.515984	2.049515	-4.171553	6	-0.711505	1.749274	-4.437231
6	-1.665997	4.251531	-3.690604	6	-1.771897	3.913343	-3.898499
6	0.534621	0.175752	-4.884879	6	0.204295	-0.173172	-5.166690
6	0.048982	2.327663	-5.485861	6	-0.269798	1.969809	-5.797173
6	0.679016	1.171138	-5.892067	6	0.285625	0.778821	-6.220729
6	0.016355	3.596455	-6.290211	6	-0.344609	3.213004	-6.636077
6	1.001103	-1.156248	-4.864676	6	0.625332	-1.522325	-5.136998
1	1.209603	1.041969	-6.826966	1	0.720048	0.600222	-7.195747
1	-0.983906	3.818726	-6.683920	1	-1.375640	3.458852	-6.922192
1	0.686269	3.498633	-7.150636	1	0.221477	3.063707	-7.560848
1	0.343997	4.466439	-5.710626	1	0.072539	4.084230	-6.119589
6	1.711220	-1.755444	-5.890045	6	1.220763	-2.170355	-6.202239
1	0.774333	-1.733887	-3.975223	1	0.460529	-2.063814	-4.212412
6	2.204708	-3.105048	-5.920062	6	1.668135	-3.531141	-6.238438
1	1.929334	-1.163541	-6.777737	1	1.376918	-1.607520	-7.120996
6	2.032120	-4.044609	-4.868514	6	1.557040	-4.439363	-5.149778
6	2.914261	-3.563960	-7.060556	6	2.265613	-4.035570	-7.424722
6	2.525472	-5.333362	-4.947745	6	2.004248	-5.741139	-5.236709
6	3.237659	-5.785591	-6.098060	6	2.604953	-6.240290	-6.433437
6	3.414727	-4.850360	-7.157229	6	2.719631	-5.335521	-7.529897
1	1.497825	-3.757817	-3.967414	1	1.109345	-4.114328	-4.215462
1	2.360463	-6.002975	-4.112052	1	1.892681	-6.386868	-4.374288
7	3.728169	-7.061319	-6.178080	7	3.048726	-7.526822	-6.520882
1	3.070331	-2.879276	-7.891495	1	2.369354	-3.373913	-8.281665
1	3.946277	-5.136431	-8.056982	1	3.165214	-5.659445	-8.462502
6	3.525128	-8.001802	-5.080207	6	2.910676	-8.439016	-5.386776
6	4.445734	-7.500901	-7.370710	6	3.664688	-8.014454	-7.753559
1	5.343755	-6.894027	-7.544459	1	4.558594	-7.432110	-8.008617
1	3.811093	-7.445010	-8.264883	1	2.963483	-7.966145	-8.596077
1	4.756134	-8.537082	-7.237585	1	3.962198	-9.053330	-7.615117
1	2.457770	-8.182028	-4.896876	1	1.858039	-8.572213	-5.108222
1	3.980224	-7.637111	-4.150340	1	3.461232	-8.073221	-4.511202
1	3.991647	-8.952809	-5.336356	1	3.315998	-9.411733	-5.663093

8	-0.614671	5.198865	-3.285295	8	-0.157574	5.209592	-3.548779
1	-2.594876	4.567168	-3.221416	1	-2.411177	4.508842	-3.269885
1	-1.799369	4.346850	-4.765716	1	-1.783234	4.189887	-4.938465
6	-0.838731	6.509571	-3.560585	6	-0.425563	6.464924	-3.679628
6	0.260045	7.379217	-3.077237	6	0.679516	7.393576	-3.214083
8	-1.847899	6.886107	-4.139866	8	-1.496441	6.939616	-4.109444
6	0.327060	8.801531	-3.403894	6	1.034328	8.617022	-3.914350
6	1.247306	6.814268	-2.290800	6	1.362112	7.042340	-2.074737
7	2.290965	7.481522	-1.758695	7	2.324744	7.792856	-1.475537
1	1.212685	5.759927	-2.054549	1	1.136432	6.107701	-1.577304
6	1.507344	9.496103	-2.848379	6	2.113241	9.396150	-3.275290
8	-0.499940	9.418182	-4.101314	8	0.524955	8.995247	-4.992123
6	2.469643	8.844023	-2.048962	6	2.743826	8.982214	-2.079746
6	3.285984	6.756446	-0.977410	6	2.992675	7.290546	-0.284361
6	2.847471	5.710684	0.012312	6	2.189299	6.624111	0.800752
6	3.417290	7.018801	0.502561	6	2.793861	7.985220	1.041082
1	4.198252	6.565786	-1.538039	1	3.980959	6.885756	-0.492813
1	2.720749	7.724786	0.945893	1	2.113203	8.831744	1.060355
1	4.420555	7.040871	0.918391	1	3.658094	8.076114	1.693049
1	3.454225	4.812333	0.074161	1	2.635048	5.755969	1.277119
1	1.784120	5.547858	0.160316	1	1.110326	6.573569	0.689526
6	1.693063	10.864865	-3.122063	6	2.544772	10.599603	-3.869100
6	2.786264	11.528393	-2.629783	6	3.551631	11.333023	-3.299842
6	3.793330	10.896984	-1.853257	6	4.232282	10.931265	-2.120311
6	3.598829	9.537309	-1.577008	6	3.797965	9.739683	-1.529831
1	0.950335	11.394043	-3.709026	1	2.055632	10.949853	-4.771626
1	4.341125	9.005551	-1.000427	1	4.291465	9.383258	-0.637633
9	2.888697	12.868914	-2.868525	9	3.891470	12.525234	-3.876749
7	4.874706	11.631541	-1.354444	7	5.239634	11.738027	-1.571517
6	5.724353	12.337741	-2.335609	6	6.405731	12.027628	-2.431098
6	5.682583	11.023973	-0.292756	6	5.655623	11.460652	-0.193918
6	6.560427	13.414452	-1.649397	6	7.195458	13.215204	-1.887588
1	5.100658	12.804245	-3.096951	1	6.070887	12.257653	-3.441982
1	6.390903	11.612738	-2.832311	1	7.059002	11.139700	-2.477796
6	6.520693	12.090214	0.416649	6	6.437286	12.645923	0.376861
1	6.348794	10.240946	-0.694115	1	6.278682	10.551137	-0.137588
1	5.018009	10.566022	0.444618	1	4.766698	11.307021	0.423933
7	7.328685	12.837568	-0.547575	7	7.565092	12.985950	-0.491739
1	7.173585	11.611147	1.143788	1	6.806827	12.391208	1.368407
1	5.853235	12.783284	0.950314	1	5.768740	13.515291	0.466302
1	5.900132	14.206452	-1.264804	1	6.587072	14.129198	-1.963007
1	7.252984	13.858007	-2.364615	1	8.104588	13.355533	-2.472323
6	8.609404	13.263164	-0.320361	6	8.794618	13.385400	-0.043264
8	9.222481	14.010779	-1.083990	8	9.686359	13.801987	-0.784520
8	9.108790	12.748517	0.824458	8	8.904202	13.247405	1.296229
6	10.501538	12.996871	1.264901	6	10.158268	13.548289	2.025477
6	10.577723	12.200443	2.570677	6	9.779130	13.225407	3.473641
6	10.712535	14.490255	1.532606	6	10.511133	15.031795	1.879783
6	11.488005	12.437898	0.235022	6	11.282180	12.625204	1.544902
1	11.269435	11.384110	0.027589	1	10.972163	11.576179	1.613451
1	12.504647	12.499806	0.639707	1	12.159992	12.761696	2.186819
1	11.452289	12.998737	-0.701059	1	11.568362	12.844092	0.514298
1	9.953725	14.865377	2.228838	1	9.661933	15.658113	2.176207
1	10.667403	15.073242	0.610799	1	10.792746	15.278287	0.854328
1	11.696705	14.638179	1.991774	1	11.353401	15.268309	2.540017
1	9.842532	12.568941	3.294322	1	8.946226	13.853954	3.807015
1	11.575833	12.302830	3.009563	1	10.635566	13.409412	4.130886
1	10.387044	11.137029	2.389715	1	9.485900	12.174760	3.574144
9	0.591402	-0.423453	-1.864168	9	-1.567827	-1.277247	-2.847822

9	-1.396164	-1.087613	-2.789835	9	0.538467 -0.682688 -2.165984
Products T_1 (implicit water)					
6	-3.939495	-9.053435	5.596117		
6	-4.503076	-7.834796	6.086632		
6	-4.555674	-6.713242	5.289790		
6	-3.439383	-9.052632	4.253910		
6	-3.499767	-7.922523	3.472448		
6	-4.059588	-6.703359	3.954723		
1	-4.896650	-7.780737	7.093826		
1	-4.990406	-5.801947	5.693004		
1	-3.106058	-7.976393	2.462447		
6	-4.146305	-5.502987	3.191324		
7	-3.879666	-10.167420	6.369497		
1	-3.002769	-9.951310	3.836499		
6	-4.388795	-10.148403	7.742541		
6	-3.304038	-11.409321	5.848246		
1	-2.250777	-11.273207	5.576575		
1	-3.854570	-11.760073	4.967853		
1	-3.363821	-12.176752	6.618519		
1	-5.460791	-9.920014	7.762796		
1	-3.857117	-9.406751	8.349787		
1	-4.237836	-11.129885	8.189357		
6	-3.710451	-5.314564	1.890646		
1	-4.604605	-4.659016	3.703217		
6	-3.825441	-4.090903	1.196004		
1	-3.249778	-6.139225	1.359283		
6	-4.377946	-2.852731	1.629624		
6	-4.250531	-1.924737	0.614066		
7	-3.369955	-3.907738	-0.102661		
6	-3.601575	-2.609889	-0.474452		
1	-4.830654	-2.669761	2.595163		
6	-4.742767	-0.509035	0.697052		
1	-5.304078	-0.371043	1.626007		
1	-5.407753	-0.252940	-0.135994		
1	-3.920536	0.217312	0.700938		
5	-2.717428	-4.999716	-0.976982		
7	-2.476141	-4.403486	-2.380259		
6	-3.201384	-2.129551	-1.791493		
6	-2.706965	-3.106193	-2.754542		
6	-3.255615	-0.796451	-2.102986		
6	-1.993992	-5.107840	-3.475341		
6	-2.381730	-2.961800	-4.150511		
6	-1.946274	-4.202999	-4.573162		
6	-2.490386	-1.757752	-5.040385		
6	-1.628332	-6.470239	-3.418159		
1	-1.626405	-4.448247	-5.577279		
1	-3.491438	-1.311676	-5.013073		
1	-2.283105	-2.048312	-6.074636		
1	-1.770475	-0.975096	-4.770277		
6	-1.134941	-7.180157	-4.499747		
1	-1.746356	-6.969942	-2.463772		
6	-0.740730	-8.549793	-4.512716		
1	-1.028462	-6.657199	-5.448168		
6	-0.795697	-9.411613	-3.378336		
6	-0.254866	-9.120012	-5.724200		
6	-0.399714	-10.726898	-3.446209		
6	0.088494	-11.291983	-4.668481		
6	0.145285	-10.434551	-5.810808		

1	-1.157520	-9.034347	-2.427083
1	-0.463340	-11.336556	-2.553598
7	0.481112	-12.589549	-4.737134
1	-0.198004	-8.493729	-6.611096
1	0.506124	-10.811243	-6.759656
6	0.420540	-13.452338	-3.555082
6	0.970771	-13.153266	-5.996964
1	1.866808	-12.625364	-6.343371
1	0.203502	-13.098585	-6.777889
1	1.227316	-14.199824	-5.839991
1	-0.608562	-13.551735	-3.190843
1	1.046090	-13.057553	-2.746319
1	0.788148	-14.442227	-3.821147
8	-2.203003	3.845090	-2.126872
1	-3.591469	-0.056913	-1.392632
1	-2.936740	-0.420800	-3.062939
6	-2.464786	5.005343	-1.691004
6	-1.280267	5.829310	-1.187969
8	-3.609921	5.528429	-1.593094
6	-1.025980	7.194178	-1.609994
6	-0.426930	5.230365	-0.297674
7	0.631366	5.840560	0.312167
1	-0.573011	4.193854	-0.018827
6	0.149543	7.825623	-0.981790
8	-1.701332	7.808956	-2.468932
6	0.959609	7.150430	-0.038641
6	1.477692	5.079075	1.216512
6	0.852092	4.147503	2.220824
6	1.511758	5.421627	2.686699
1	2.412115	4.760775	0.758011
1	0.858887	6.221321	3.025081
1	2.472766	5.369534	3.190809
1	1.354290	3.199644	2.390435
1	-0.231327	4.100852	2.277048
6	0.493384	9.150330	-1.322584
6	1.585670	9.752232	-0.757420
6	2.441806	9.095090	0.165404
6	2.097049	7.783867	0.505989
1	-0.131256	9.694811	-2.022604
1	2.724296	7.236015	1.193805
9	1.843135	11.058820	-1.071484
7	3.532355	9.775752	0.729930
6	4.553959	10.285058	-0.207367
6	4.155760	9.186543	1.917909
6	5.438735	11.326448	0.472334
1	4.068360	10.741591	-1.069395
1	5.176983	9.447781	-0.565959
6	5.035670	10.218474	2.626570
1	4.766425	8.304583	1.656796
1	3.372907	8.868617	2.611921
7	6.018497	10.781385	1.699184
1	5.552415	9.742688	3.458012
1	4.403253	11.026039	3.025019
1	4.841407	12.219533	0.710970
1	6.247820	11.620209	-0.196373
6	7.303650	11.106221	2.039404
8	8.070947	11.716493	1.293051
8	7.619241	10.659189	3.274646
6	8.970098	10.827895	3.859233

6	8.820617	10.153180	5.225816				
6	9.290223	12.316534	4.026346				
6	10.010054	10.093645	3.007407				
1	9.717053	9.047535	2.862282				
1	10.975052	10.106160	3.526900				
1	10.135093	10.566039	2.031132				
1	8.495679	12.817914	4.590758				
1	9.406697	12.812593	3.060926				
1	10.224768	12.423274	4.588956				
1	8.044971	10.647508	5.820757				
1	9.766805	10.212387	5.774002				
1	8.553033	9.097134	5.111262				
9	-3.577483	-6.117802	-1.071243				
9	-1.496352	-5.424600	-0.404947				
Min S_0 (explicit water)				Min S_1 (explicit water)			
6	-1.044450	-4.176343	4.109990	6	-1.040071	-4.213389	3.978642
6	-1.584302	-2.987314	4.672672	6	-1.564876	-3.039388	4.578888
6	-1.756353	-1.848910	3.899598	6	-1.733227	-1.886463	3.844370
6	-0.695760	-4.137093	2.728396	6	-0.701205	-4.140940	2.599491
6	-0.874650	-2.990036	1.974255	6	-0.875664	-2.980024	1.882404
6	-1.410187	-1.802884	2.529363	6	-1.397975	-1.804401	2.473174
1	-1.869876	-2.955696	5.717350	1	-1.840722	-3.037211	5.625621
1	-2.173063	-0.959408	4.367997	1	-2.138704	-1.006736	4.337900
1	-0.590906	-3.019610	0.925903	1	-0.599987	-2.982018	0.832692
6	-1.615279	-0.577477	1.785798	6	-1.597244	-0.572471	1.772401
7	-0.866650	-5.309994	4.859816	7	-0.868133	-5.360072	4.690476
1	-0.281759	-5.014522	2.245892	1	-0.297171	-5.008292	2.093147
6	-1.234296	-5.321234	6.271241	6	-1.214895	-5.404606	6.101405
6	-0.318651	-6.518133	4.252768	6	-0.332418	-6.550146	4.049887
1	0.691351	-6.348211	3.856726	1	0.678181	-6.377161	3.661463
1	-0.953739	-6.882851	3.434404	1	-0.970241	-6.881740	3.222253
1	-0.258534	-7.300425	5.009491	1	-0.281530	-7.354816	4.781517
1	-2.305822	-5.124395	6.411043	1	-2.280504	-5.200454	6.259519
1	-0.668724	-4.571422	6.840309	1	-0.632942	-4.677647	6.680077
1	-1.012027	-6.302924	6.689654	1	-0.998487	-6.398443	6.489717
6	-1.330716	-0.348659	0.469879	6	-1.319184	-0.323822	0.449534
1	-2.044481	0.237580	2.367650	1	-2.011597	0.237098	2.370373
6	-1.566537	0.903878	-0.190659	6	-1.537291	0.916947	-0.187236
1	-0.899922	-1.139622	-0.133594	1	-0.904119	-1.115123	-0.163783
6	-2.117707	2.101815	0.337785	6	-2.061146	2.124308	0.345999
6	-2.162668	3.056801	-0.662565	6	-2.100114	3.076772	-0.643994
7	-1.270668	1.123062	-1.509352	7	-1.251367	1.146568	-1.518389
6	-1.619661	2.434514	-1.844862	6	-1.580602	2.447548	-1.837356
1	-2.448409	2.246524	1.357931	1	-2.376470	2.271996	1.370654
6	-2.697319	4.446515	-0.455407	6	-2.596842	4.476681	-0.443812
1	-2.925055	4.593536	0.604810	1	-2.779411	4.647734	0.620507
1	-3.626600	4.620897	-1.012335	1	-3.541889	4.662854	-0.966872
1	-1.982508	5.221910	-0.749082	1	-1.877386	5.229487	-0.779389
5	-0.656170	0.095538	-2.479283	5	-0.666095	0.120723	-2.486078
7	-0.486868	0.774273	-3.852580	7	-0.480410	0.801358	-3.840548
6	-1.408591	2.916014	-3.150537	6	-1.383243	2.946973	-3.144634
6	-0.839390	2.095575	-4.144281	6	-0.808997	2.110226	-4.128703
6	-1.789416	4.331059	-3.491309	6	-1.761263	4.347772	-3.480411
6	0.034718	0.190677	-4.976033	6	0.055198	0.206917	-4.965914
6	-0.507564	2.339233	-5.527129	6	-0.450497	2.361571	-5.507299
6	0.026172	1.159303	-6.014839	6	0.071837	1.186988	-5.993273
6	-0.659408	3.581912	-6.360286	6	-0.572357	3.620880	-6.311787
6	0.488484	-1.170747	-5.015543	6	0.483541	-1.137555	-5.002212

1	0.383987	1.004096	-7.024222	1	0.444211	1.035863	-6.998092
1	-1.711148	3.834131	-6.544735	1	-1.614535	3.879806	-6.530855
1	-0.190757	3.422733	-7.336308	1	-0.066008	3.486669	-7.271488
1	-0.181191	4.456178	-5.905699	1	-0.112321	4.481848	-5.816405
6	0.995507	-1.768638	-6.133708	6	1.009139	-1.751350	-6.114098
1	0.409641	-1.733545	-4.092287	1	0.379919	-1.702259	-4.082979
6	1.471316	-3.129976	-6.263759	6	1.460154	-3.106126	-6.211806
1	1.060058	-1.178345	-7.047111	1	1.101025	-1.166771	-7.027522
6	1.477885	-4.074212	-5.209041	6	1.429661	-4.032911	-5.142264
6	1.965205	-3.575994	-7.511387	6	1.974618	-3.581639	-7.440065
6	1.943456	-5.366161	-5.383842	6	1.875128	-5.326428	-5.285426
6	2.442925	-5.808922	-6.643352	6	2.390998	-5.795619	-6.524733
6	2.435447	-4.865846	-7.707448	6	2.424805	-4.873190	-7.602745
1	1.108347	-3.793484	-4.226660	1	1.045667	-3.729128	-4.173733
1	1.920414	-6.043583	-4.538519	1	1.825973	-5.990085	-4.431655
7	2.909304	-7.086211	-6.817798	7	2.832441	-7.074519	-6.668347
1	1.977482	-2.884095	-8.351210	1	2.016579	-2.902785	-8.288095
1	2.799245	-5.143895	-8.689435	1	2.807202	-5.175431	-8.569341
6	2.881641	-8.039238	-5.713531	6	2.785434	-7.999023	-5.547295
6	3.378864	-7.523369	-8.127738	6	3.344207	-7.533024	-7.949297
1	4.228949	-6.919603	-8.471497	1	4.221972	-6.954604	-8.260612
1	2.584125	-7.462599	-8.883822	1	2.583208	-7.458621	-8.735101
1	3.705867	-8.561084	-8.060857	1	3.639744	-8.577202	-7.861158
1	1.856483	-8.232747	-5.368949	1	1.757530	-8.159626	-5.200931
1	3.471123	-7.680981	-4.859752	1	3.383362	-7.636186	-4.703225
1	3.312048	-8.983205	-6.048070	1	3.191623	-8.958960	-5.861670
8	-0.644664	5.196028	-3.191892	8	-0.627376	5.229835	-3.177968
1	-2.639282	4.678653	-2.909231	1	-2.611417	4.700518	-2.902649
1	-2.037963	4.441934	-4.542262	1	-2.002085	4.466163	-4.531571
6	-0.793199	6.516224	-3.500774	6	-0.772591	6.533742	-3.492887
6	0.335528	7.342663	-3.039262	6	0.349163	7.366671	-3.033785
8	-1.780324	6.930982	-4.091637	8	-1.754604	6.945364	-4.087224
6	0.662561	8.609584	-3.689527	6	0.660975	8.635749	-3.671491
6	1.070516	6.916188	-1.949237	6	1.092511	6.937904	-1.959624
7	2.084134	7.606082	-1.391733	7	2.100449	7.626194	-1.405004
1	0.838548	5.979079	-1.461829	1	0.874406	5.991975	-1.483475
6	1.813939	9.312387	-3.093166	6	1.804378	9.344413	-3.073717
8	0.069647	9.069372	-4.682273	8	0.065047	9.098253	-4.652628
6	2.510147	8.814096	-1.970928	6	2.506827	8.841619	-1.969836
6	2.795686	7.042121	-0.250130	6	2.827333	7.056448	-0.284418
6	2.028040	6.366585	0.854642	6	2.072917	6.377117	0.818145
6	2.687107	7.700841	1.102509	6	2.730501	7.704383	1.066185
1	3.756067	6.614818	-0.528475	1	3.783951	6.632580	-0.576507
1	2.034397	8.565449	1.183101	1	2.079560	8.568480	1.154283
1	3.587253	7.746730	1.708696	1	3.633945	7.747025	1.665810
1	2.470726	5.469964	1.277759	1	2.518680	5.479986	1.233973
1	0.943326	6.353232	0.803259	1	0.988780	6.363027	0.772852
6	2.248235	10.527534	-3.656810	6	2.215903	10.567835	-3.624277
6	3.324136	11.190673	-3.127692	6	3.280564	11.234370	-3.093131
6	4.070269	10.703050	-2.022144	6	4.032843	10.741682	-2.002093
6	3.626926	9.498358	-1.459806	6	3.614449	9.531311	-1.455747
1	1.710030	10.944325	-4.501132	1	1.668249	10.986166	-4.460866
1	4.166001	9.077250	-0.624220	1	4.162066	9.107297	-0.627964
9	3.668782	12.395309	-3.668444	9	3.612700	12.443275	-3.614269
7	5.143903	11.436345	-1.508142	7	5.099338	11.482776	-1.490601
6	6.250427	11.760166	-2.432560	6	6.193129	11.795558	-2.421721
6	5.650256	11.071602	-0.181615	6	5.616174	11.101790	-0.180360
6	7.100908	12.899813	-1.878861	6	7.055952	12.920503	-1.874330
1	5.849548	12.055025	-3.401339	1	5.784874	12.097632	-3.384415

1	6.879414	10.865843	-2.577058	1	6.812498	10.897528	-2.575782
6	6.496425	12.207617	0.397583	6	6.473508	12.221115	0.396490
1	6.253951	10.148798	-0.223520	1	6.213517	10.177148	-0.240062
1	4.804572	10.900436	0.489660	1	4.778709	10.927313	0.498798
7	7.565284	12.580535	-0.529818	7	7.528978	12.589285	-0.538162
1	6.930990	11.887059	1.342575	1	6.917164	11.891982	1.333208
1	5.854128	13.080621	0.587495	1	5.841699	13.097036	0.598875
1	6.508129	13.826859	-1.856566	1	6.471434	13.850641	-1.839344
1	7.968336	13.059160	-2.519388	1	7.917594	13.077396	-2.521425
6	8.827535	12.946556	-0.146705	6	8.793199	12.934007	-0.168751
8	9.668693	13.400035	-0.924204	8	9.627656	13.384347	-0.947850
8	9.029137	12.730283	1.171283	8	9.011317	12.705487	1.135777
6	10.334242	12.981373	1.826576	6	10.317273	12.941350	1.765538
6	10.055428	12.574479	3.276333	6	10.066075	12.526793	3.210755
6	10.688215	14.469432	1.744402	6	10.677674	14.421264	1.689619
6	11.413332	12.083535	1.213719	6	11.376051	12.046949	1.129408
1	11.098818	11.033944	1.240229	1	11.054483	11.000704	1.151996
1	12.334798	12.175914	1.799881	1	12.306292	12.128028	1.700436
1	11.629399	12.363264	0.180785	1	11.574939	12.335069	0.096606
1	9.868188	15.080175	2.139104	1	9.867992	15.031833	2.102069
1	10.896674	14.776415	0.717801	1	10.870205	14.733926	0.662919
1	11.578248	14.662045	2.354317	1	11.577337	14.603459	2.285806
1	9.252646	13.184773	3.704126	1	9.275503	13.137753	3.656680
1	10.957234	12.717036	3.881081	1	10.978778	12.659143	3.798808
1	9.762593	11.520588	3.335454	1	9.768148	11.475438	3.265724
8	2.172479	3.933944	-3.071771	8	2.021104	3.928807	-2.791183
1	2.160388	2.968418	-3.168831	1	2.014031	2.960727	-2.827672
1	1.242755	4.203413	-3.178860	1	1.108930	4.196297	-2.999728
8	-4.348256	6.458166	-5.278016	8	-4.194734	6.143744	-5.260746
1	-4.557959	7.286528	-5.736700	1	-4.512609	6.900997	-5.773129
1	-3.468252	6.604448	-4.877595	1	-3.351244	6.432737	-4.860194
9	0.602664	-0.347291	-1.993030	9	0.576731	-0.365470	-2.001732
9	-1.500301	-1.040639	-2.592309	9	-1.526397	-1.001948	-2.604702
Min T_1 (explicit water)				TS T_1 (explicit water)			
6	-1.042338	-4.281280	4.000360	6	-0.893194	-4.236799	4.031874
6	-1.563355	-3.101584	4.604896	6	-1.395202	-3.045025	4.632358
6	-1.733549	-1.942293	3.869671	6	-1.594835	-1.903317	3.880745
6	-0.709596	-4.206270	2.614906	6	-0.610840	-4.191289	2.632158
6	-0.885311	-3.039217	1.896054	6	-0.816476	-3.041787	1.897300
6	-1.403570	-1.857706	2.491436	6	-1.316354	-1.849336	2.488829
1	-1.834591	-3.098068	5.653798	1	-1.626881	-3.020965	5.690195
1	-2.134732	-1.062215	4.367878	1	-1.979157	-1.013038	4.373536
1	-0.614321	-3.042782	0.844300	1	-0.584622	-3.065761	0.836727
6	-1.603960	-0.618635	1.792537	6	-1.546955	-0.628418	1.773468
7	-0.868485	-5.435602	4.714496	7	-0.690797	-5.372570	4.760700
1	-0.310005	-5.073951	2.103619	1	-0.228042	-5.069018	2.125732
6	-1.209457	-5.482503	6.133214	6	-0.989348	-5.395743	6.191075
6	-0.334028	-6.631481	4.069459	6	-0.173362	-6.581746	4.123123
1	0.676008	-6.458314	3.675966	1	0.817873	-6.409292	3.685744
1	-0.976589	-6.962651	3.243590	1	-0.847256	-6.936661	3.333423
1	-0.280503	-7.436388	4.802167	1	-0.083281	-7.366943	4.873009
1	-2.274807	-5.274392	6.296804	1	-2.049318	-5.185001	6.380619
1	-0.621389	-4.757525	6.710737	1	-0.383926	-4.661197	6.736703
1	-0.994258	-6.479059	6.518098	1	-0.762274	-6.385757	6.585166
6	-1.325363	-0.363405	0.461399	6	-1.328508	-0.403517	0.427559
1	-2.016503	0.189762	2.394311	1	-1.933399	0.193469	2.373978
6	-1.540615	0.877093	-0.176560	6	-1.575154	0.827676	-0.221080
1	-0.910411	-1.156634	-0.150746	1	-0.943476	-1.208979	-0.187479

6	-2.066756	2.088267	0.353221	6	-2.072431	2.048891	0.311561
6	-2.100431	3.044879	-0.638722	6	-2.159205	2.982602	-0.701540
7	-1.245720	1.112040	-1.522742	7	-1.352837	1.033007	-1.581291
6	-1.570266	2.411970	-1.838760	6	-1.699257	2.320090	-1.904833
1	-2.388755	2.235270	1.376340	1	-2.336993	2.219854	1.347018
6	-2.606444	4.445326	-0.437628	6	-2.643646	4.390973	-0.508517
1	-2.807390	4.609465	0.625874	1	-2.812053	4.575139	0.557102
1	-3.544983	4.632101	-0.975463	1	-3.594345	4.578494	-1.024227
1	-1.885146	5.204822	-0.757976	1	-1.920546	5.132939	-0.864659
5	-0.661636	0.080095	-2.495779	5	-0.806953	-0.023574	-2.558264
7	-0.478685	0.764589	-3.856376	7	-0.662160	0.636861	-3.941050
6	-1.367601	2.921341	-3.151204	6	-1.581225	2.799792	-3.258417
6	-0.798733	2.073614	-4.141464	6	-1.009626	1.926830	-4.252305
6	-1.739017	4.324777	-3.482934	6	-1.974857	4.109478	-3.596707
6	0.051157	0.159485	-4.999661	6	-0.148399	0.014717	-5.076869
6	-0.446975	2.326215	-5.532873	6	-0.697248	2.157150	-5.648227
6	0.065020	1.144944	-6.025619	6	-0.172238	0.973053	-6.127173
6	-0.569782	3.587777	-6.340460	6	-0.875614	3.395361	-6.480116
6	0.470334	-1.187862	-5.042081	6	0.288107	-1.329471	-5.093714
1	0.427463	0.992522	-7.034330	1	0.169277	0.802991	-7.139995
1	-1.614140	3.856760	-6.544603	1	-1.933764	3.637623	-6.642576
1	-0.079343	3.446658	-7.308971	1	-0.424332	3.239429	-7.464959
1	-0.094990	4.447502	-5.854121	1	-0.400010	4.273664	-6.030077
6	0.987558	-1.812935	-6.162709	6	0.790872	-1.967276	-6.211807
1	0.369418	-1.754663	-4.123019	1	0.213431	-1.876955	-4.160969
6	1.427307	-3.177385	-6.260764	6	1.247519	-3.323598	-6.294342
1	1.079541	-1.230733	-7.078308	1	0.855958	-1.400126	-7.138831
6	1.394991	-4.108412	-5.188056	6	1.248052	-4.235610	-5.203468
6	1.932412	-3.660891	-7.496204	6	1.736946	-3.819112	-7.532534
6	1.829965	-5.411831	-5.334998	6	1.698969	-5.532624	-5.336075
6	2.336245	-5.889018	-6.580623	6	2.189651	-6.023002	-6.585071
6	2.371603	-4.962336	-7.661593	6	2.191989	-5.114510	-7.684118
1	1.019279	-3.802861	-4.215920	1	0.885542	-3.917855	-4.230491
1	1.778608	-6.074235	-4.479190	1	1.674009	-6.181679	-4.469266
7	2.767841	-7.179443	-6.727647	7	2.635925	-7.305519	-6.717827
1	1.976232	-2.983133	-8.346102	1	1.754569	-3.154364	-8.393243
1	2.745562	-5.266655	-8.631888	1	2.553024	-5.430778	-8.655202
6	2.719973	-8.108314	-5.602189	6	2.626617	-8.217095	-5.575206
6	3.267469	-7.646943	-8.017160	6	3.123989	-7.788760	-8.007832
1	4.149875	-7.077034	-8.335716	1	3.993909	-7.212254	-8.346451
1	2.500458	-7.564673	-8.798191	1	2.343819	-7.728765	-8.776888
1	3.552686	-8.695108	-7.929456	1	3.423575	-8.831326	-7.906151
1	1.691367	-8.261848	-5.250419	1	1.608060	-8.377842	-5.200134
1	3.324973	-7.748683	-4.760104	1	3.245266	-7.833761	-4.754423
1	3.118814	-9.071512	-5.919612	1	3.031886	-9.179305	-5.886415
8	-0.592930	5.225818	-3.177532	8	-0.438379	5.273678	-3.350534
1	-2.584770	4.685868	-2.903283	1	-2.602765	4.667817	-2.921985
1	-1.975466	4.454818	-4.534198	1	-2.109595	4.370321	-4.633063
6	-0.750138	6.536314	-3.490466	6	-0.649298	6.554415	-3.463147
6	0.371609	7.379711	-3.030871	6	0.490448	7.421765	-3.011711
8	-1.738122	6.950534	-4.085264	8	-1.708528	7.062953	-3.873216
6	0.704339	8.634625	-3.699822	6	0.846927	8.657016	-3.694184
6	1.093718	6.976003	-1.924828	6	1.202763	7.020292	-1.905499
7	2.100149	7.678196	-1.366800	7	2.207214	7.726731	-1.331221
1	0.857508	6.047147	-1.423838	1	0.964794	6.085264	-1.414657
6	1.848350	9.350225	-3.103700	6	1.974313	9.384836	-3.081383
8	0.123000	9.076287	-4.708162	8	0.298471	9.076949	-4.734114
6	2.532131	8.874338	-1.964117	6	2.639089	8.920170	-1.924239
6	2.798569	7.136483	-0.206939	6	2.899894	7.181777	-0.171931

6	2.018344	6.481563	0.901440	6	2.114364	6.517912	0.927683
6	2.674052	7.820599	1.131774	6	2.765473	7.856805	1.171175
1	3.762395	6.704255	-0.465317	1	3.867693	6.753339	-0.423356
1	2.020347	8.686392	1.188302	1	2.109964	8.721212	1.228706
1	3.566928	7.878179	1.747670	1	3.653634	7.911759	1.794244
1	2.456320	5.593437	1.346853	1	2.551083	5.628410	1.371759
1	0.934376	6.466362	0.837040	1	1.031057	6.500300	0.854233
6	2.288543	10.554597	-3.685894	6	2.418069	10.589433	-3.662499
6	3.358332	11.228451	-3.158030	6	3.469842	11.276358	-3.116836
6	4.092513	10.762616	-2.035285	6	4.184171	10.823501	-1.976125
6	3.643341	9.569313	-1.454273	6	3.736195	9.629810	-1.398265
1	1.759688	10.954351	-4.544255	1	1.903655	10.978420	-4.534583
1	4.173340	9.164783	-0.604764	1	4.253363	9.235219	-0.536107
9	3.709151	12.422493	-3.718617	9	3.822679	12.471624	-3.677005
7	5.161469	11.506317	-1.525028	7	5.235252	11.584025	-1.447984
6	6.278348	11.806558	-2.444922	6	6.372537	11.874650	-2.345032
6	5.653519	11.167624	-0.186292	6	5.698605	11.260710	-0.095701
6	7.127660	12.954561	-1.906794	6	7.205855	13.032176	-1.802240
1	5.888043	12.082591	-3.423565	1	6.004161	12.137352	-3.335948
1	6.905477	10.907202	-2.564673	1	7.005203	10.975843	-2.439295
6	6.498071	12.312587	0.377407	6	6.525362	12.415036	0.475032
1	6.254548	10.242247	-0.202903	1	6.304395	10.338081	-0.088890
1	4.800661	11.013045	0.479945	1	4.831649	11.108071	0.552693
7	7.577558	12.661844	-0.546891	7	7.624578	12.758956	-0.428178
1	6.921909	12.010757	1.333370	1	6.928731	12.125529	1.443609
1	5.857263	13.191799	0.542002	1	5.877474	13.293304	0.615387
1	6.538040	13.883866	-1.909501	1	6.613578	13.959380	-1.830940
1	8.001871	13.097625	-2.541911	1	8.094402	13.170180	-2.418330
6	8.838444	13.027874	-0.159643	6	8.872625	13.140211	-0.015262
8	9.689227	13.461306	-0.938156	8	9.739160	13.569859	-0.778444
8	9.027120	12.835989	1.164063	8	9.030370	12.967827	1.315246
6	10.327710	13.092518	1.826092	6	10.312147	13.244406	2.005128
6	10.033919	12.714504	3.280708	6	9.984879	12.886621	3.457719
6	10.690399	14.576886	1.718997	6	10.667138	14.729573	1.883960
6	11.407499	12.177687	1.240108	6	11.412756	12.328858	1.460425
1	11.086705	11.130521	1.282543	1	11.099093	11.279961	1.512262
1	12.323725	12.275540	1.833555	1	12.313552	12.443763	2.074129
1	11.635319	12.437357	0.204464	1	11.663670	12.573574	0.426450
1	9.870339	15.199288	2.094981	1	9.833164	15.351778	2.228364
1	10.909257	14.863214	0.688595	1	10.911068	15.001166	0.855206
1	11.576236	14.776389	2.332788	1	11.535093	14.945235	2.517497
1	9.230488	13.336759	3.689628	1	9.167461	13.509460	3.836953
1	10.931022	12.863940	3.890768	1	10.865572	13.051420	4.087419
1	9.735121	11.663395	3.357035	1	9.691068	11.834775	3.542799
8	2.129652	3.906368	-2.903001	8	2.086907	3.979038	-3.561143
1	2.085302	2.937097	-2.901496	1	1.920688	3.177416	-4.081591
1	1.208307	4.195475	-3.038318	1	1.212284	4.422675	-3.495092
8	-4.316826	6.383846	-5.171859	8	-3.909782	6.412161	-5.441908
1	-4.617466	7.236636	-5.522317	1	-4.069229	7.219887	-5.953997
1	-3.428360	6.559239	-4.800555	1	-3.121646	6.611570	-4.885177
9	0.587151	-0.408181	-2.013145	9	0.451686	-0.500797	-2.109945
9	-1.530627	-1.042914	-2.613735	9	-1.689181	-1.132656	-2.630845
Products T_1 (explicit water)							
6	-0.568322	-4.350627	6.192108				
6	-1.647034	-3.482659	6.547560				
6	-2.468747	-2.949158	5.580103				
6	-0.384779	-4.634985	4.800319				
6	-1.216055	-4.093763	3.847722				

6	-2.294277	-3.227988	4.194347
1	-1.829799	-3.234168	7.585453
1	-3.280195	-2.292246	5.883626
1	-1.033338	-4.342221	2.807022
6	-3.186457	-2.641479	3.250204
7	0.250191	-4.884961	7.134017
1	0.418368	-5.287061	4.480513
6	0.042947	-4.590383	8.553498
6	1.352915	-5.769561	6.751024
1	2.060311	-5.254835	6.090762
1	0.981326	-6.666483	6.242067
1	1.885148	-6.079766	7.648958
1	-0.946614	-4.925728	8.885104
1	0.137553	-3.516394	8.751337
1	0.797346	-5.115283	9.137533
6	-3.165148	-2.809823	1.876063
1	-3.956344	-1.999880	3.674398
6	-4.083625	-2.196077	0.996995
1	-2.408609	-3.445411	1.430716
6	-5.169899	-1.323403	1.287630
6	-5.782836	-0.960588	0.103951
7	-4.048621	-2.367196	-0.380137
6	-5.053843	-1.627666	-0.945099
1	-5.470781	-1.000248	2.275479
6	-6.983519	-0.063517	0.018999
1	-7.335287	0.170847	1.028153
1	-7.813463	-0.532996	-0.522156
1	-6.757835	0.888014	-0.478111
5	-3.043566	-3.261839	-1.135968
7	-3.417992	-3.237857	-2.632837
6	-5.242484	-1.607809	-2.390781
6	-4.421882	-2.499510	-3.201584
6	-6.144587	-0.755811	-2.972193
6	-2.790083	-3.981306	-3.622860
6	-4.461626	-2.783515	-4.613900
6	-3.450574	-3.694725	-4.850638
6	-5.390872	-2.263367	-5.671971
6	-1.697805	-4.839011	-3.369578
1	-3.205333	-4.125597	-5.812335
1	-6.444019	-2.425434	-5.413638
1	-5.196672	-2.782507	-6.615269
1	-5.254262	-1.190325	-5.854706
6	-1.056160	-5.577528	-4.349351
1	-1.357331	-4.909603	-2.343129
6	0.044895	-6.463397	-4.163801
1	-1.413821	-5.487809	-5.373289
6	0.658898	-6.726221	-2.904293
6	0.585035	-7.145254	-5.291574
6	1.718071	-7.594636	-2.780265
6	2.254577	-8.276928	-3.919649
6	1.645251	-8.017401	-5.186385
1	0.290960	-6.235552	-2.008765
1	2.145784	-7.757249	-1.798877
7	3.299175	-9.135438	-3.799172
1	0.143419	-6.970656	-6.269569
1	2.011840	-8.506984	-6.079860
6	3.904658	-9.397136	-2.491426
6	3.834691	-9.825559	-4.974616
1	4.195177	-9.109197	-5.721638

1	3.074609	-10.466676	-5.436444
1	4.671531	-10.450642	-4.666986
1	3.172603	-9.822810	-1.795463
1	4.315654	-8.479132	-2.055859
1	4.716731	-10.112065	-2.614902
8	-3.507464	2.824693	-3.350719
1	-6.741967	-0.071933	-2.389746
1	-6.279730	-0.709290	-4.041529
6	-3.476513	3.922120	-2.713049
6	-2.197178	4.261927	-1.970339
8	-4.443288	4.730871	-2.613775
6	-1.577115	5.575062	-2.008141
6	-1.614139	3.259105	-1.236842
7	-0.508550	3.400298	-0.454808
1	-2.042191	2.264346	-1.240772
6	-0.353465	5.698896	-1.193368
8	-1.988554	6.535988	-2.696519
6	0.166276	4.623611	-0.436508
6	0.027878	2.245667	0.249001
6	-0.906244	1.295339	0.949777
6	-0.007255	2.198126	1.757535
1	0.898058	1.816196	-0.243543
1	-0.477001	3.033253	2.269548
1	0.855083	1.774812	2.264947
1	-0.670677	0.237549	0.882067
1	-1.968219	1.521837	0.953080
6	0.337429	6.927458	-1.160348
6	1.481592	7.061101	-0.419822
6	2.052518	5.994901	0.324183
6	1.362399	4.778820	0.294037
1	-0.059856	7.772514	-1.712291
1	1.762011	3.932472	0.833023
9	2.081582	8.288965	-0.367853
7	3.213275	6.201124	1.084559
6	4.417666	6.647847	0.355024
6	3.551199	5.191870	2.091875
6	5.453257	7.217731	1.320501
1	4.146880	7.416604	-0.368001
1	4.853727	5.796016	-0.194235
6	4.577433	5.747834	3.081356
1	3.953120	4.275946	1.624716
1	2.648288	4.925905	2.648142
7	5.756338	6.249868	2.373780
1	4.876171	4.961381	3.771919
1	4.121507	6.565444	3.659716
1	5.067777	8.145054	1.770896
1	6.372940	7.450146	0.783708
6	7.040248	6.134035	2.833440
8	8.004144	6.691091	2.305488
8	7.110554	5.325581	3.913534
6	8.394441	4.989259	4.571851
6	7.947227	4.057736	5.702109
6	9.041918	6.254898	5.142343
6	9.311237	4.247782	3.594173
1	8.794309	3.381275	3.166132
1	10.193576	3.883980	4.133069
1	9.643446	4.899025	2.783393
1	8.336045	6.787181	5.790167
1	9.373177	6.928589	4.349787

1	9.911286	5.973306	5.747416
1	7.256701	4.571866	6.379442
1	8.818305	3.730641	6.279642
1	7.446213	3.170494	5.299931
8	-1.412942	1.315842	-4.251775
1	-1.722117	1.000132	-5.114441
1	-2.149649	1.884755	-3.903220
8	-6.786465	4.266366	-3.928494
1	-7.253729	5.111032	-3.837753
1	-5.912917	4.399605	-3.466073
9	-1.725163	-2.787480	-0.950271
9	-3.113157	-4.585566	-0.643245

Compound 5							
Min S_0 (implicit water)				Min S_1 (implicit water)			
6	-2.477169	0.095276	0.447544	6	-2.633277	-0.018345	0.382904
6	-2.446630	1.215920	-0.487608	6	-2.567215	1.116075	-0.496310
6	-3.179493	2.409007	-0.214966	6	-3.298085	2.310400	-0.211701
6	-2.938891	3.290466	-1.250360	6	-3.004034	3.230164	-1.188079
7	-1.785791	1.360526	-1.679311	7	-1.845193	1.313745	-1.652664
6	-2.077413	2.637063	-2.171456	6	-2.111255	2.601895	-2.101645
5	-0.856458	0.361010	-2.424966	5	-0.903807	0.342726	-2.386497
7	-0.509733	0.927165	-3.831378	7	-0.486468	0.952518	-3.736108
9	-1.496423	-0.885136	-2.553337	9	-1.544273	-0.893564	-2.589803
9	0.345310	0.206336	-1.681451	9	0.256087	0.124186	-1.592511
6	-1.607573	3.069672	-3.416273	6	-1.590138	3.091539	-3.310369
6	-0.852289	2.222096	-4.234577	6	-0.799618	2.252867	-4.112702
6	-1.923680	4.467632	-3.883787	6	-1.895702	4.481678	-3.754240
6	0.155060	0.332171	-4.871739	6	0.220257	0.376554	-4.768571
6	-0.379761	2.422437	-5.558991	6	-0.253805	2.500117	-5.403945
6	0.231992	1.250932	-5.960001	6	0.357968	1.341096	-5.813968
6	0.744767	-0.998969	-4.980844	6	0.806625	-0.929748	-4.886877
8	-0.878443	5.335248	-3.375710	8	-0.854961	5.360189	-3.255323
1	-2.887012	4.813587	-3.505825	1	-2.854334	4.832098	-3.369856
1	-1.945276	4.536606	-4.971913	1	-1.923125	4.565805	-4.841549
6	-0.972920	6.652127	-3.720234	6	-0.961304	6.664119	-3.589214
6	0.146924	7.450062	-3.178448	6	0.159315	7.469186	-3.065113
8	-1.895953	7.068395	-4.402228	8	-1.892039	7.079459	-4.253424
6	0.217268	8.899411	-3.351703	6	0.212635	8.913770	-3.224971
6	1.154834	6.794946	-2.493582	6	1.181738	6.820885	-2.411708
7	2.230328	7.391502	-1.944158	7	2.260378	7.418262	-1.883987
1	1.115045	5.722381	-2.365568	1	1.150254	5.746958	-2.292617
6	1.433997	9.517976	-2.785676	6	1.434024	9.537034	-2.682952
8	-0.641787	9.595605	-3.923184	8	-0.659980	9.605920	-3.765334
6	2.419545	8.774816	-2.102581	6	2.433163	8.799178	-2.034699
6	3.246325	6.577750	-1.286382	6	3.294835	6.612227	-1.260941
6	2.833522	5.439648	-0.391969	6	2.906155	5.482072	-0.356669
6	3.443526	6.683500	0.205603	6	3.528062	6.722517	0.218035
1	4.130689	6.436262	-1.903376	1	4.161030	6.470917	-1.901407
1	2.776821	7.347047	0.749078	1	2.876049	7.389804	0.772842
1	4.463459	6.651471	0.577878	1	4.555538	6.690456	0.565775
1	3.428680	4.533322	-0.449942	1	3.498841	4.576132	-0.423695
1	1.775072	5.273566	-0.215055	1	1.852384	5.318223	-0.156711
6	1.630999	10.905041	-2.926504	6	1.611896	10.922418	-2.817578
6	2.757646	11.499941	-2.421697	6	2.739910	11.518776	-2.335567
6	3.786988	10.779089	-1.761135	6	3.783383	10.801302	-1.707618
6	3.580270	9.401067	-1.614752	6	3.596583	9.429025	-1.568212

1	0.871623	11.501639	-3.420059	1	0.836430	11.514419	-3.289716
1	4.337680	8.803730	-1.129326	1	4.368876	8.834905	-1.104003
9	2.873939	12.855952	-2.527888	9	2.850924	12.868786	-2.432747
7	4.903504	11.443862	-1.242467	7	4.904413	11.474827	-1.216844
6	5.721594	12.231383	-2.188320	6	5.691977	12.238508	-2.195555
6	5.746378	10.718444	-0.287102	6	5.771079	10.750527	-0.293020
6	6.614212	13.216974	-1.439147	6	6.612984	13.221003	-1.491008
1	5.073093	12.784602	-2.866457	1	5.025686	12.788880	-2.857488
1	6.346702	11.549031	-2.788541	1	6.291180	11.545221	-2.807433
6	6.641474	11.692103	0.483094	6	6.692799	11.718862	0.437515
1	6.374756	9.967837	-0.796686	1	6.378088	9.996941	-0.821385
1	5.106706	10.200796	0.432641	1	5.154858	10.237305	0.448612
7	7.420419	12.517089	-0.440715	7	7.441386	12.526674	-0.516320
1	7.316250	11.129797	1.125813	1	7.385642	11.159719	1.061938
1	6.016465	12.340365	1.115391	1	6.093878	12.376108	1.083016
1	5.991534	13.977301	-0.943853	1	6.013706	13.990300	-0.984119
1	7.281922	13.718806	-2.139352	1	7.261819	13.709687	-2.216207
6	8.721357	12.890673	-0.238415	6	8.743763	12.890125	-0.359521
8	9.316240	13.696163	-0.956169	8	9.319633	13.682599	-1.098882
8	9.261597	12.255790	0.824526	8	9.313465	12.266812	0.683831
6	10.678916	12.433825	1.218572	6	10.730295	12.447182	1.027038
6	10.796663	11.514506	2.437634	6	10.890868	11.546472	2.246288
6	10.937354	13.890293	1.616743	6	11.000948	13.901421	1.398430
6	11.602259	11.957082	0.093152	6	11.613108	11.960679	-0.117373
1	11.349067	10.932276	-0.201695	1	11.348408	10.934799	-0.393089
1	12.638338	11.960388	0.450583	1	12.658583	11.965488	0.206601
1	11.535289	12.605207	-0.782907	1	11.518110	12.600189	-0.995610
1	10.220650	14.210736	2.381533	1	10.308472	14.229764	2.180209
1	10.863053	14.560407	0.758228	1	10.899882	14.560134	0.535371
1	11.944858	13.974673	2.039968	1	12.019658	13.989237	1.789073
1	10.103845	11.825272	3.227182	1	10.224686	11.865965	3.053295
1	11.815759	11.556243	2.836439	1	11.921466	11.593368	2.609615
1	10.573955	10.476961	2.165898	1	10.659755	10.507382	1.993274
1	-3.340495	4.289602	-1.355760	1	-3.384571	4.239094	-1.266669
1	-0.495652	3.323881	-6.145945	1	-0.325870	3.427900	-5.954437
6	-4.019347	2.537027	1.019654	6	-4.160740	2.414077	1.000780
6	-4.608257	1.159849	1.363103	6	-4.754814	1.039291	1.310043
1	-4.818078	3.272307	0.875775	1	-4.952431	3.154530	0.855435
1	-3.405462	2.892299	1.861447	1	-3.559062	2.754213	1.855717
6	-3.540165	0.083756	1.393874	6	-3.702470	-0.041988	1.326220
1	-5.358043	0.896384	0.601357	1	-5.494492	0.793621	0.534803
1	-5.132356	1.193128	2.323708	1	-5.289233	1.054267	2.263675
6	-1.516110	-0.938443	0.514013	6	-1.705216	-1.087374	0.411375
6	-1.606631	-1.951071	1.455732	6	-1.826666	-2.120354	1.312771
6	-2.669902	-1.966268	2.374077	6	-2.886991	-2.134743	2.230766
6	-3.627318	-0.943225	2.338090	6	-3.815609	-1.089528	2.229909
8	-2.679634	-2.998656	3.260418	8	-2.926582	-3.186217	3.076205
6	-3.731904	-3.071227	4.228784	6	-3.973257	-3.260743	4.040062
1	-3.530534	-3.969682	4.812802	1	-3.797065	-4.180155	4.596451
1	-4.708826	-3.160054	3.740475	1	-4.951157	-3.308074	3.551142
1	-3.721450	-2.194383	4.885902	1	-3.937371	-2.405362	4.721715
1	-4.450975	-0.931664	3.043428	1	-4.642012	-1.084674	2.930819
1	-0.675846	-0.937594	-0.165578	1	-0.865918	-1.086451	-0.267461
1	-0.856544	-2.735215	1.501948	1	-1.103256	-2.929082	1.334271
6	0.890627	0.872173	-7.252072	6	1.103892	1.021255	-7.065866
6	1.028795	-1.464638	-6.302360	6	1.210646	-1.340263	-6.198052
6	1.098609	-1.824308	-3.897878	6	1.053201	-1.814226	-3.816996
6	1.692481	-3.071561	-4.084342	6	1.661476	-3.043514	-4.007436
6	1.951587	-3.524479	-5.385319	6	2.046750	-3.429983	-5.295378

6	1.619038	-2.709635	-6.480632	6	1.816326	-2.566687	-6.375994
8	2.525721	-4.720681	-5.687950	8	2.646583	-4.601936	-5.593915
6	2.895578	-5.598200	-4.618472	6	2.911249	-5.527683	-4.543543
1	3.324873	-6.478679	-5.097361	1	3.385853	-6.385198	-5.018273
1	2.018870	-5.889324	-4.029142	1	1.982381	-5.842617	-4.058302
1	3.643472	-5.130540	-3.968348	1	3.590729	-5.093814	-3.803544
1	0.931190	-1.485384	-2.885396	1	0.789169	-1.524119	-2.811208
1	1.954214	-3.666811	-3.217301	1	1.840084	-3.683344	-3.152118
1	1.834461	-3.074098	-7.481699	1	2.121362	-2.889069	-7.367232
6	0.655151	-0.624812	-7.507981	6	0.922330	-0.462160	-7.390740
1	-0.410839	-0.779939	-7.734231	1	-0.118356	-0.628379	-7.702923
1	1.217122	-0.960639	-8.385395	1	1.556291	-0.755692	-8.231627
1	1.972414	1.068499	-7.199213	1	2.172536	1.238150	-6.926143
1	0.498841	1.471235	-8.080930	1	0.759457	1.645215	-7.895487
Min T_1 (implicit water)				TS T_1 (implicit water)			
6	-2.824750	-0.067727	0.372666	6	-2.943735	-0.237029	0.362506
6	-2.721684	1.072777	-0.502227	6	-3.078928	0.885215	-0.527012
6	-3.468819	2.270066	-0.249691	6	-4.094884	1.882063	-0.314380
6	-3.133634	3.192024	-1.214485	6	-3.947732	2.840853	-1.288727
7	-1.940768	1.280072	-1.641374	7	-2.342372	1.249938	-1.643245
6	-2.193679	2.564162	-2.094874	6	-2.866498	2.433802	-2.118829
5	-0.962474	0.310044	-2.343282	5	-1.148754	0.506722	-2.306849
7	-0.480264	0.937772	-3.671204	7	-0.802890	1.193788	-3.657937
9	-1.597135	-0.927687	-2.590932	9	-1.489885	-0.836219	-2.530616
9	0.164074	0.084126	-1.495039	9	-0.023694	0.583064	-1.449051
6	-1.619311	3.071291	-3.281059	6	-2.380773	3.057931	-3.319605
6	-0.784440	2.233932	-4.052229	6	-1.369850	2.376964	-4.081854
6	-1.913004	4.463287	-3.730487	6	-2.873630	4.285370	-3.735447
6	0.291625	0.368898	-4.686704	6	0.070154	0.770818	-4.648201
6	-0.175105	2.501341	-5.321281	6	-0.844600	2.725235	-5.357443
6	0.469563	1.351627	-5.715703	6	0.031732	1.730090	-5.720924
6	0.894496	-0.935851	-4.791387	6	0.937438	-0.374762	-4.709957
8	-0.886911	5.361672	-3.186170	8	-1.569210	5.871954	-2.784426
1	-2.884856	4.814769	-3.379902	1	-3.704808	4.750565	-3.225018
1	-1.897066	4.559130	-4.818100	1	-2.596670	4.718502	-4.685626
6	-0.987528	6.672633	-3.523478	6	-1.034119	6.674368	-3.629822
6	0.140249	7.473706	-2.992518	6	0.124723	7.494976	-3.088504
8	-1.914130	7.099773	-4.197405	8	-1.358135	6.800119	-4.833214
6	0.126828	8.933988	-3.003784	6	0.293905	8.909338	-3.374102
6	1.239469	6.805741	-2.486138	6	1.043521	6.849582	-2.298908
7	2.341421	7.398206	-1.983119	7	2.165955	7.417471	-1.777957
1	1.259435	5.724845	-2.477931	1	0.904453	5.805042	-2.049983
6	1.367860	9.554930	-2.496780	6	1.544108	9.493877	-2.852323
8	-0.822680	9.638815	-3.394160	8	-0.535799	9.613942	-3.991350
6	2.451946	8.798181	-2.003878	6	2.465089	8.748696	-2.080571
6	3.459016	6.576295	-1.534361	6	3.101790	6.598682	-1.022872
6	3.199599	5.323597	-0.741221	6	2.583023	5.613173	-0.009367
6	3.814255	6.526325	-0.068873	6	3.306268	6.854685	0.450618
1	4.276351	6.555524	-2.251635	1	3.972838	6.303239	-1.604540
1	3.181921	7.085553	0.614901	1	2.704888	7.636394	0.906165
1	4.869413	6.511987	0.188730	1	4.317404	6.768748	0.838423
1	3.825741	4.465545	-0.966488	1	3.090234	4.654577	0.046516
1	2.175760	5.077497	-0.475697	1	1.512625	5.568739	0.168291
6	1.487637	10.957980	-2.500129	6	1.847762	10.843081	-3.126122
6	2.634289	11.556905	-2.048288	6	3.012866	11.399017	-2.669019
6	3.758442	10.827462	-1.579370	6	3.980364	10.671504	-1.926606
6	3.629415	9.432527	-1.568112	6	3.670380	9.336881	-1.644930
1	0.654636	11.560858	-2.844821	1	1.138487	11.442001	-3.687246

1	4.459546	8.829429	-1.231365	1	4.377422	8.737118	-1.090808
9	2.679471	12.921083	-2.014077	9	3.236395	12.726559	-2.909742
7	4.893468	11.494746	-1.105052	7	5.143880	11.304587	-1.465255
6	5.571839	12.418959	-2.037446	6	6.028648	11.902159	-2.485990
6	5.863608	10.721269	-0.324296	6	5.923009	10.622319	-0.428572
6	6.493797	13.369862	-1.279223	6	6.998531	12.891769	-1.846710
1	4.831684	13.002405	-2.583521	1	5.431190	12.424140	-3.232666
1	6.159847	11.837336	-2.767292	1	6.596217	11.104449	-2.994830
6	6.791625	11.657497	0.453427	6	6.894259	11.598377	0.238921
1	6.467051	10.063432	-0.973174	1	6.488840	9.771147	-0.845794
1	5.326995	10.097210	0.395272	1	5.242436	10.240250	0.337087
7	7.430962	12.616074	-0.448437	7	7.740527	12.250923	-0.761591
1	7.555109	11.069729	0.959536	1	7.520486	11.057210	0.945825
1	6.209288	12.200844	1.212581	1	6.324069	12.360743	0.790787
1	5.893546	14.039389	-0.644774	1	6.440200	13.755081	-1.453744
1	7.061333	13.977277	-1.984106	1	7.708642	13.249695	-2.592191
6	8.728838	13.036256	-0.339904	6	9.056624	12.572459	-0.565814
8	9.208482	13.943708	-1.021384	8	9.712350	13.259513	-1.350583
8	9.406058	12.323495	0.586526	8	9.537503	12.028815	0.573528
6	10.851167	12.525047	0.843971	6	10.951924	12.178786	0.988454
6	11.135520	11.488222	1.934556	6	10.993418	11.387833	2.299111
6	11.102391	13.941708	1.369663	6	11.273201	13.655186	1.240461
6	11.659829	12.213835	-0.419086	6	11.878202	11.543293	-0.052923
1	11.412816	11.214747	-0.795968	1	11.580733	10.506657	-0.248335
1	12.728336	12.229590	-0.175739	1	12.903318	11.534177	0.334733
1	11.472360	12.946693	-1.206380	1	11.866927	12.098957	-0.992628
1	10.462543	14.148137	2.235247	1	10.555547	14.087862	1.946884
1	10.913649	14.693959	0.601521	1	11.252570	14.233717	0.314932
1	12.146552	14.026119	1.692048	1	12.273472	13.736330	1.681055
1	10.526043	11.682186	2.823876	1	10.299161	11.812868	3.032120
1	12.191100	11.532936	2.222736	1	12.003812	11.421263	2.720218
1	10.917705	10.476378	1.575822	1	10.724110	10.339617	2.129772
1	-3.510885	4.201108	-1.308392	1	-4.548193	3.730201	-1.419805
1	-0.228609	3.436029	-5.862550	1	-1.106769	3.603582	-5.930604
6	-4.390255	2.371044	0.924345	6	-5.055571	1.775910	0.824629
6	-4.997676	0.988496	1.207805	6	-5.333257	0.292297	1.112582
1	-5.176702	3.111163	0.743462	1	-5.984685	2.310494	0.603446
1	-3.828892	2.711905	1.807748	1	-4.620520	2.247077	1.718762
6	-3.940890	-0.094317	1.270983	6	-4.057058	-0.514009	1.223102
1	-5.704773	0.743813	0.400378	1	-5.938895	-0.119636	0.291475
1	-5.574248	1.004299	2.138074	1	-5.924472	0.182642	2.026575
6	-1.893241	-1.137582	0.444998	6	-1.786939	-1.053983	0.483641
6	-2.052076	-2.174652	1.344936	6	-1.730683	-2.089590	1.392227
6	-3.155580	-2.192254	2.219252	6	-2.836307	-2.361656	2.225752
6	-4.090166	-1.145510	2.173917	6	-3.989798	-1.564965	2.133358
8	-3.226260	-3.249216	3.067604	8	-2.688568	-3.395481	3.080613
6	-4.317347	-3.329374	3.993552	6	-3.762437	-3.735096	3.971766
1	-4.155189	-4.248982	4.556059	1	-3.401830	-4.587582	4.546836
1	-5.275266	-3.383519	3.464878	1	-4.657912	-4.018410	3.409190
1	-4.313712	-2.472744	4.676386	1	-3.986000	-2.900799	4.644443
1	-4.947716	-1.142782	2.837662	1	-4.846708	-1.760812	2.767790
1	-1.023639	-1.135360	-0.195360	1	-0.917132	-0.848617	-0.122415
1	-1.325451	-2.980129	1.397967	1	-0.837594	-2.699311	1.488172
6	1.276711	1.052652	-6.939444	6	0.873371	1.558219	-6.943685
6	1.365935	-1.328214	-6.092520	6	1.470331	-0.711558	-6.003611
6	1.100131	-1.835338	-3.718535	6	1.342347	-1.155387	-3.599752
6	1.732516	-3.060924	-3.895236	6	2.218331	-2.221441	-3.734396
6	2.186273	-3.429461	-5.171909	6	2.723302	-2.546397	-5.007327
6	1.996111	-2.551006	-6.255879	6	2.341516	-1.779688	-6.126139

8	2.817612	-4.595816	-5.460393	8	3.577881	-3.561268	-5.255430
6	3.048268	-5.539746	-4.406731	6	4.015577	-4.394945	-4.170763
1	3.556532	-6.382285	-4.875992	1	4.681834	-5.129800	-4.621965
1	2.101774	-5.875674	-3.969495	1	3.164772	-4.901743	-3.704099
1	3.688270	-5.108300	-3.629364	1	4.561388	-3.806919	-3.425879
1	0.785001	-1.561756	-2.722394	1	0.990725	-0.904398	-2.609926
1	1.876048	-3.709361	-3.038726	1	2.511371	-2.781190	-2.854262
1	2.350870	-2.857132	-7.236533	1	2.744987	-2.050057	-7.097906
6	1.125078	-0.435277	-7.291458	6	1.040299	0.058225	-7.233674
1	0.101278	-0.605722	-7.657902	1	0.076581	-0.343063	-7.581099
1	1.802486	-0.710741	-8.105826	1	1.759330	-0.099945	-8.042954
1	2.337160	1.277338	-6.747968	1	1.862031	2.011687	-6.777342
1	0.965257	1.684281	-7.777928	1	0.427189	2.073666	-7.799960
Products T_1 (implicit water)							
6	-2.717295	-1.299929	0.164760				
6	-3.022477	0.055496	-0.188282				
6	-4.222493	0.697616	0.293979				
6	-4.210570	1.992461	-0.163399				
7	-2.318029	0.970638	-0.948907				
6	-3.032466	2.149605	-0.942738				
5	-0.987665	0.765853	-1.735558				
7	-0.731992	2.007345	-2.638878				
9	-1.083199	-0.385877	-2.526623				
9	0.077059	0.641175	-0.814131				
6	-2.610641	3.304711	-1.699632				
6	-1.476007	3.166926	-2.581218				
6	-3.290641	4.498152	-1.614692				
6	0.221538	2.181226	-3.625316				
6	-0.991357	4.106487	-3.533459				
6	0.046635	3.496943	-4.195513				
6	1.268683	1.312666	-4.078688				
8	-3.113745	8.950511	-2.601058				
1	-4.144569	4.606382	-0.955878				
1	-3.000060	5.366903	-2.200135				
6	-2.233475	8.162894	-3.053464				
6	-0.777163	8.582614	-2.872908				
8	-2.444395	7.040830	-3.599597				
6	0.198613	8.543824	-3.946734				
6	-0.390970	9.013268	-1.629827				
7	0.878707	9.372711	-1.280030				
1	-1.118540	9.088743	-0.830913				
6	1.577673	8.871258	-3.539520				
8	-0.072875	8.276970	-5.140416				
6	1.904320	9.262512	-2.220089				
6	1.168422	9.735865	0.097730				
6	0.229018	10.647659	0.842361				
6	1.592343	11.145794	0.431133				
1	1.631239	8.929327	0.663352				
1	1.632010	11.858673	-0.387661				
1	2.362779	11.271706	1.186691				
1	0.044350	10.415062	1.886956				
1	-0.627742	11.051637	0.311206				
6	2.620916	8.792405	-4.485162				
6	3.911541	9.067667	-4.119945				
6	4.283668	9.423031	-2.796407				
6	3.246069	9.515530	-1.863800				
1	2.386539	8.528343	-5.510828				
1	3.478180	9.775000	-0.841213				

9	4.881373	9.032157	-5.084294
7	5.621911	9.716385	-2.491210
6	6.608430	8.643393	-2.729742
6	5.893066	10.408421	-1.228501
6	8.025482	9.209094	-2.755624
1	6.403393	8.159133	-3.684004
1	6.528032	7.883798	-1.933332
6	7.304482	10.999453	-1.236202
1	5.786558	9.728239	-0.365394
1	5.179186	11.228073	-1.109611
7	8.296187	9.964155	-1.532858
1	7.517905	11.437618	-0.262972
1	7.364044	11.792783	-1.996457
1	8.145190	9.866235	-3.630427
1	8.748092	8.396619	-2.831900
6	9.542041	9.905811	-0.969053
8	10.420736	9.126532	-1.341500
8	9.670878	10.788266	0.045628
6	10.902310	10.881764	0.864056
6	10.547660	11.987678	1.862146
6	12.086094	11.306110	-0.010673
6	11.152720	9.558371	1.593691
1	10.264566	9.260779	2.162814
1	11.980366	9.687486	2.300508
1	11.412290	8.758586	0.897300
1	11.847116	12.224830	-0.558496
1	12.355881	10.526866	-0.725952
1	12.952648	11.508641	0.629134
1	10.324009	12.924816	1.340906
1	11.391449	12.161332	2.538303
1	9.676026	11.705290	2.462530
1	-4.961526	2.749826	0.012598
1	-1.384843	5.106242	-3.690626
6	-5.198408	-0.033189	1.155267
6	-5.196182	-1.521580	0.773499
1	-6.201330	0.393260	1.056702
1	-4.907384	0.074285	2.210746
6	-3.795579	-2.087670	0.695193
1	-5.674826	-1.635979	-0.210359
1	-5.793183	-2.100260	1.484201
6	-1.429416	-1.899313	0.074117
6	-1.214974	-3.198535	0.473978
6	-2.285366	-3.969484	0.981991
6	-3.566998	-3.400829	1.089500
8	-1.978879	-5.227724	1.343256
6	-3.000420	-6.083241	1.884573
1	-2.502345	-7.029888	2.091071
1	-3.802300	-6.234888	1.155424
1	-3.402498	-5.663043	2.811612
1	-4.395786	-3.981955	1.476879
1	-0.590285	-1.320645	-0.282040
1	-0.227231	-3.645034	0.418636
6	0.937284	3.987681	-5.289686
6	1.885046	1.645178	-5.338028
6	1.770290	0.195499	-3.363094
6	2.816265	-0.571260	-3.845596
6	3.402102	-0.241931	-5.084661
6	2.925463	0.867966	-5.812078
8	4.420348	-0.916763	-5.648810

6	4.973930	-2.061176	-4.976495				
1	5.766108	-2.423240	-5.630988				
1	4.213882	-2.837778	-4.846824				
1	5.393883	-1.773548	-4.007627				
1	1.355911	-0.054415	-2.397738				
1	3.178511	-1.406121	-3.258057				
1	3.395169	1.098860	-6.763821				
6	1.365040	2.799702	-6.165699				
1	0.494711	2.454368	-6.742990				
1	2.123233	3.109476	-6.890848				
1	1.829710	4.460123	-4.852812				
1	0.433310	4.752808	-5.887718				
Min S_0 (explicit water)				Min S_1 (explicit water)			
6	-3.242655	-0.274296	0.029889	6	-3.260406	-0.265439	-0.014738
6	-3.078844	0.946026	-0.752862	6	-3.084411	0.939996	-0.775747
6	-3.944604	2.062089	-0.546995	6	-3.922272	2.076239	-0.556950
6	-3.534577	3.068979	-1.396641	6	-3.490833	3.086374	-1.380949
7	-2.168908	1.260826	-1.727440	7	-2.158411	1.262902	-1.743473
6	-2.431767	2.570738	-2.143671	6	-2.400158	2.573136	-2.138474
5	-1.013812	0.400469	-2.318292	5	-1.038080	0.391832	-2.341042
7	-0.392020	1.137773	-3.537710	7	-0.398207	1.124781	-3.533567
9	-1.507348	-0.854680	-2.715958	9	-1.557360	-0.847640	-2.755981
9	-0.013822	0.228210	-1.323462	9	-0.047078	0.157652	-1.348903
6	-1.718335	3.160303	-3.192703	6	-1.674791	3.178685	-3.178036
6	-0.733454	2.447585	-3.886274	6	-0.703448	2.435964	-3.870736
6	-2.018288	4.579951	-3.596572	6	-1.954014	4.584385	-3.581669
6	0.538015	0.698574	-4.443798	6	0.523021	0.662450	-4.447464
6	0.010560	2.819489	-5.036847	6	0.061449	2.808886	-5.010921
6	0.788285	1.734631	-5.391956	6	0.802580	1.711836	-5.376579
6	1.239588	-0.577812	-4.535575	6	1.192294	-0.604600	-4.540320
8	-1.005827	5.433698	-2.981672	8	-0.942990	5.446700	-2.973428
1	-3.000885	4.902917	-3.255201	1	-2.933777	4.921246	-3.246210
1	-1.968628	4.711935	-4.678599	1	-1.896143	4.721174	-4.662832
6	-1.046729	6.755353	-3.320032	6	-0.997587	6.758973	-3.286893
6	0.112516	7.505878	-2.811818	6	0.154331	7.516190	-2.778777
8	-1.960003	7.218309	-3.988576	8	-1.916102	7.224021	-3.939728
6	0.061792	8.955184	-2.632763	6	0.088724	8.955186	-2.581042
6	1.277974	6.816004	-2.532149	6	1.322677	6.839297	-2.515711
7	2.417305	7.383248	-2.093710	7	2.453134	7.410127	-2.077753
1	1.328895	5.745186	-2.674315	1	1.382713	5.770757	-2.670470
6	1.340497	9.553562	-2.205060	6	1.358696	9.560992	-2.148429
8	-0.952730	9.654698	-2.804742	8	-0.926953	9.644137	-2.739871
6	2.492326	8.779557	-1.947019	6	2.510836	8.799472	-1.909038
6	3.598826	6.553164	-1.884649	6	3.642828	6.598130	-1.889095
6	3.457320	5.204392	-1.230874	6	3.518436	5.246857	-1.252469
6	4.123579	6.335940	-0.487117	6	4.169257	6.373764	-0.501300
1	4.325398	6.653633	-2.687476	1	4.364179	6.718264	-2.692441
1	3.564801	6.785529	0.328959	1	3.605998	6.811017	0.317313
1	5.201884	6.328367	-0.356041	1	5.246576	6.376773	-0.370235
1	4.071951	4.404231	-1.632686	1	4.143993	4.460320	-1.661537
1	2.475099	4.896400	-0.882813	1	2.539084	4.923798	-0.911609
6	1.430191	10.949496	-2.043871	6	1.428214	10.950530	-1.965649
6	2.612088	11.527739	-1.661119	6	2.598889	11.532328	-1.576708
6	3.799772	10.785561	-1.426986	6	3.788363	10.800319	-1.357830
6	3.700665	9.395880	-1.577787	6	3.709743	9.421259	-1.531329
1	0.549178	11.561007	-2.205279	1	0.539507	11.552331	-2.116705
1	4.577653	8.785350	-1.422238	1	4.592973	8.818584	-1.384847
9	2.634358	12.877101	-1.458830	9	2.614055	12.871606	-1.354800

7	4.970367	11.426995	-1.010791	7	4.948581	11.452725	-0.936951
6	5.510871	12.487558	-1.886434	6	5.471541	12.503646	-1.821889
6	6.044531	10.598445	-0.455049	6	6.027473	10.628298	-0.402782
6	6.494214	13.369748	-1.122553	6	6.459245	13.386798	-1.077507
1	4.697797	13.106601	-2.263230	1	4.652390	13.118967	-2.189623
1	6.020721	12.025506	-2.748449	1	5.970922	12.040292	-2.687873
6	7.035284	11.463529	0.327123	6	7.022881	11.490877	0.362487
1	6.581473	10.052941	-1.249965	1	6.553932	10.088393	-1.206978
1	5.612624	9.867406	0.233504	1	5.608622	9.893228	0.288084
7	7.540425	12.553912	-0.508178	7	7.509828	12.576269	-0.479041
1	7.867296	10.846118	0.660436	1	7.861271	10.877973	0.684959
1	6.534258	11.881594	1.213116	1	6.533773	11.909148	1.253123
1	5.958241	13.932834	-0.343473	1	5.933556	13.948564	-0.292587
1	6.960369	14.080724	-1.804605	1	6.915218	14.097139	-1.765388
6	8.825717	13.023912	-0.469269	6	8.789652	13.040717	-0.464689
8	9.196157	14.038525	-1.061803	8	9.151008	14.049536	-1.062957
8	9.622688	12.228919	0.277093	8	9.596954	12.254223	0.263990
6	11.075028	12.479035	0.431394	6	11.037741	12.510594	0.390764
6	11.512156	11.318918	1.330393	6	11.499425	11.362368	1.280738
6	11.307165	13.820631	1.133313	6	11.274359	13.849915	1.080757
6	11.771982	12.397161	-0.930052	6	11.707846	12.429774	-0.976677
1	11.536615	11.447760	-1.424534	1	11.467157	11.479185	-1.463489
1	12.857086	12.442513	-0.782769	1	12.793743	12.479909	-0.849029
1	11.475449	13.220389	-1.582886	1	11.395003	13.249591	-1.624130
1	10.746102	13.862472	2.073885	1	10.729427	13.890990	2.029353
1	11.007045	14.660423	0.503741	1	10.958502	14.684180	0.453657
1	12.372438	13.924361	1.369311	1	12.341587	13.959433	1.297712
1	10.983369	11.349241	2.289248	1	10.988428	11.392838	2.247737
1	12.587431	11.386819	1.526541	1	12.576414	11.438184	1.455842
1	11.308699	10.355949	0.849518	1	11.292761	10.398148	0.806700
1	-3.977585	4.051341	-1.491773	1	-3.906634	4.081241	-1.459006
1	-0.041053	3.773675	-5.544641	1	0.042845	3.774885	-5.496601
6	-5.059548	2.004304	0.452385	6	-5.016093	2.043262	0.456497
6	-5.604931	0.568657	0.503741	6	-5.581032	0.624351	0.535616
1	-5.855537	2.709968	0.192330	1	-5.802850	2.760482	0.205978
1	-4.690596	2.291180	1.448921	1	-4.619482	2.335418	1.439302
6	-4.494521	-0.447930	0.685085	6	-4.493460	-0.410520	0.687151
1	-6.132023	0.356647	-0.439103	1	-6.135137	0.414240	-0.390325
1	-6.341091	0.464591	1.307234	1	-6.295683	0.537872	1.358367
6	-2.247506	-1.258963	0.223782	6	-2.296676	-1.293508	0.125269
6	-2.478872	-2.375629	1.010466	6	-2.536479	-2.400992	0.906022
6	-3.724149	-2.549908	1.638054	6	-3.756508	-2.534677	1.585453
6	-4.722095	-1.579427	1.473099	6	-4.724696	-1.532381	1.470780
8	-3.862356	-3.675599	2.388613	8	-3.903802	-3.652368	2.326778
6	-5.105269	-3.915182	3.058578	6	-5.116178	-3.850537	3.048994
1	-4.976560	-4.862145	3.583425	1	-5.000673	-4.803550	3.563093
1	-5.927758	-4.000629	2.339689	1	-5.971740	-3.900702	2.368528
1	-5.321288	-3.119866	3.780626	1	-5.268008	-3.052693	3.782357
1	-5.686759	-1.690547	1.955853	1	-5.673077	-1.619236	1.987637
1	-1.273667	-1.137518	-0.228516	1	-1.339921	-1.201786	-0.366138
1	-1.702845	-3.120735	1.159283	1	-1.786868	-3.177939	1.016456
6	1.752217	1.536613	-6.522475	6	1.788607	1.523128	-6.480101
6	1.854040	-0.879609	-5.790690	6	1.861158	-0.893279	-5.773441
6	1.399980	-1.495816	-3.481548	6	1.278770	-1.559385	-3.506203
6	2.116286	-2.681109	-3.638921	6	1.978637	-2.743883	-3.659609
6	2.700331	-2.974358	-4.879109	6	2.623093	-3.011642	-4.872268
6	2.564643	-2.063899	-5.940807	6	2.556077	-2.076168	-5.914876
8	3.419671	-4.097424	-5.148811	8	3.331968	-4.130656	-5.128953
6	3.602549	-5.065484	-4.109463	6	3.441911	-5.125740	-4.114623

1	4.194874	-5.865099	-4.555105	1	4.044153	-5.923062	-4.547566
1	2.639537	-5.464084	-3.771341	1	2.456142	-5.514854	-3.842244
1	4.145708	-4.632656	-3.261869	1	3.943588	-4.725124	-3.228428
1	0.979413	-1.278893	-2.509784	1	0.812286	-1.359759	-2.553201
1	2.218397	-3.352715	-2.794484	1	2.025707	-3.441637	-2.832759
1	3.031117	-2.304899	-6.892514	1	3.061926	-2.307404	-6.847695
6	1.701066	0.065903	-6.965873	6	1.756792	0.063440	-6.935467
1	0.731091	-0.122081	-7.451022	1	0.806128	-0.121604	-7.455094
1	2.473921	-0.139754	-7.713371	1	2.555297	-0.135702	-7.655035
1	2.774203	1.785637	-6.198257	1	2.797296	1.774063	-6.122209
1	1.513753	2.200194	-7.360403	1	1.572341	2.194923	-7.315627
8	-0.017683	4.713749	-0.182983	8	0.201950	4.586197	-0.385996
1	-0.372611	3.865953	0.128717	1	-0.123463	3.735090	-0.056932
1	-0.455041	4.864609	-1.040421	1	-0.305162	4.757408	-1.199217
8	-4.583312	6.915300	-5.103545	8	-4.423101	6.601558	-5.084138
1	-3.689806	7.005909	-4.716386	1	-3.558597	6.827222	-4.687726
1	-4.893917	7.824200	-5.237534	1	-4.834825	7.448102	-5.309767
Min T_1 (explicit water)				TS T_1 (explicit water)			
6	-3.320454	-0.305099	0.001474	6	-3.105537	-0.274838	0.031059
6	-3.120015	0.902570	-0.758998	6	-3.123539	0.881277	-0.825908
6	-3.939083	2.058714	-0.542592	6	-4.127009	1.899529	-0.676082
6	-3.487663	3.060938	-1.370415	6	-3.862910	2.886084	-1.598226
7	-2.176205	1.216049	-1.739181	7	-2.271316	1.262615	-1.854264
6	-2.398481	2.525741	-2.131483	6	-2.717121	2.474585	-2.337968
5	-1.067262	0.323221	-2.344207	5	-1.031852	0.515067	-2.418447
7	-0.408186	1.058432	-3.534613	7	-0.523184	1.246864	-3.690389
9	-1.612536	-0.906226	-2.774289	9	-1.376755	-0.809783	-2.734452
9	-0.078830	0.063449	-1.348010	9	-0.004159	0.522866	-1.440552
6	-1.660554	3.132716	-3.172475	6	-2.101083	3.121173	-3.458995
6	-0.696452	2.369270	-3.869109	6	-1.015809	2.460162	-4.122063
6	-1.929785	4.539757	-3.578635	6	-2.539114	4.380284	-3.888016
6	0.521011	0.581354	-4.461441	6	0.458571	0.848859	-4.589071
6	0.077862	2.741142	-5.014982	6	-0.329051	2.855328	-5.305833
6	0.810831	1.637634	-5.387407	6	0.569239	1.858350	-5.606776
6	1.177335	-0.696761	-4.560747	6	1.304384	-0.315482	-4.604245
8	-0.921109	5.423839	-2.949433	8	-1.447235	5.737926	-2.864809
1	-2.913177	4.882942	-3.258372	1	-3.472675	4.783773	-3.522499
1	-1.849576	4.686222	-4.657711	1	-2.218006	4.771916	-4.843157
6	-0.983337	6.742443	-3.266582	6	-1.205500	6.864518	-3.463220
6	0.172166	7.507775	-2.761654	6	-0.021494	7.621059	-2.931287
8	-1.907298	7.211255	-3.920292	8	-1.856982	7.301635	-4.433958
6	0.093400	8.947983	-2.532822	6	0.034609	9.075445	-2.889215
6	1.359981	6.838084	-2.537156	6	1.048506	6.883821	-2.477958
7	2.499155	7.417548	-2.110629	7	2.207459	7.403332	-2.005258
1	1.431173	5.774092	-2.716983	1	1.004306	5.802506	-2.491362
6	1.368657	9.562676	-2.117575	6	1.324364	9.619486	-2.420741
8	-0.941257	9.629240	-2.654386	8	-0.908328	9.833627	-3.196449
6	2.545075	8.808717	-1.916959	6	2.389523	8.792422	-1.999442
6	3.706224	6.610884	-1.968853	6	3.293876	6.511092	-1.625513
6	3.618365	5.235263	-1.363510	6	2.995637	5.260496	-0.841934
6	4.280168	6.354538	-0.597422	6	3.712886	6.410518	-0.179173
1	4.405140	6.759228	-2.788692	1	4.075989	6.454217	-2.379636
1	3.736966	6.758598	0.252307	1	3.148313	6.994019	0.542599
1	5.362001	6.369332	-0.499999	1	4.775825	6.326795	0.028660
1	4.239678	4.467006	-1.814412	1	3.557822	4.370730	-1.109339
1	2.655138	4.889037	-0.998718	1	1.971198	5.072402	-0.534550
6	1.429461	10.954164	-1.910010	6	1.516169	11.015032	-2.386256
6	2.606884	11.547898	-1.537590	6	2.710846	11.541396	-1.971372

6	3.817323	10.827402	-1.359257	6	3.816890	10.741662	-1.579423
6	3.747829	9.442105	-1.556950	6	3.617782	9.356205	-1.603262
1	0.530020	11.548705	-2.027288	1	0.700001	11.669657	-2.672203
1	4.642857	8.848384	-1.444935	1	4.430545	8.702412	-1.323482
9	2.602895	12.889939	-1.289147	9	2.827584	12.900857	-1.896758
7	4.982288	11.483474	-0.948522	7	5.005969	11.337060	-1.139161
6	5.477727	12.582715	-1.802574	6	5.686485	12.255337	-2.075440
6	6.087857	10.663980	-0.443569	6	5.971435	10.488613	-0.434515
6	6.457481	13.464466	-1.033679	6	6.692893	13.132140	-1.335125
1	4.641919	13.193463	-2.141458	1	4.952778	12.894119	-2.565463
1	5.978065	12.159826	-2.689948	1	6.207334	11.669660	-2.851781
6	7.075011	11.527985	0.344263	6	6.984338	11.348242	0.325242
1	6.619932	10.157072	-1.266904	1	6.507162	9.824024	-1.134353
1	5.688981	9.901110	0.230284	1	5.439014	9.867287	0.290524
7	7.535813	12.655754	-0.466926	7	7.628568	12.304207	-0.576120
1	7.928606	10.920889	0.639876	1	7.739616	10.705064	0.772932
1	6.584111	11.905936	1.253634	1	6.469107	11.893683	1.130064
1	5.926149	13.991173	-0.226425	1	6.159999	13.809628	-0.650828
1	6.891784	14.206423	-1.703639	1	7.256568	13.733538	-2.048278
6	8.808503	13.159692	-0.433437	6	8.949186	12.657643	-0.515529
8	9.141992	14.201015	-1.000992	8	9.440928	13.566422	-1.186623
8	9.638364	12.365397	0.276872	8	9.633254	11.878262	0.350254
6	11.085702	12.650263	0.416607	6	11.095274	12.008906	0.552013
6	11.567127	11.478035	1.276393	6	11.380777	10.915079	1.585128
6	11.293611	13.977674	1.152270	6	11.427720	13.389974	1.125201
6	11.763175	12.624706	-0.956846	6	11.836818	11.719905	-0.756780
1	11.545077	11.683432	-1.474246	1	11.529279	10.750504	-1.165383
1	12.848902	12.694921	-0.824596	1	12.913906	11.677613	-0.558631
1	11.434941	13.457555	-1.581771	1	11.651244	12.494710	-1.503263
1	10.745943	13.978851	2.101621	1	10.837102	13.581984	2.028274
1	10.962510	14.826356	0.550811	1	11.234664	14.182679	0.399958
1	12.359330	14.102506	1.375725	1	12.488092	13.419713	1.400905
1	11.052017	11.467515	2.243091	1	10.816373	11.093938	2.506763
1	12.642960	11.569841	1.459141	1	12.448138	10.905748	1.830017
1	11.382351	10.523530	0.771704	1	11.107212	9.929160	1.193863
1	-3.883005	4.064269	-1.449286	1	-4.427463	3.794856	-1.754750
1	0.069603	3.710505	-5.494488	1	-0.500695	3.764057	-5.865828
6	-5.040016	2.046350	0.469839	6	-5.195401	1.786169	0.362270
6	-5.635080	0.631975	0.548775	6	-5.539718	0.303211	0.569957
1	-5.813069	2.779653	0.217674	1	-6.084092	2.355813	0.072842
1	-4.640378	2.330686	1.455284	1	-4.835520	2.214554	1.309812
6	-4.564106	-0.427584	0.702564	6	-4.302361	-0.544626	0.773410
1	-6.194933	0.434594	-0.378257	1	-6.073999	-0.062815	-0.319666
1	-6.353010	0.561552	1.371950	1	-6.219514	0.181788	1.418622
6	-2.374703	-1.355021	0.145344	6	-1.990793	-1.133469	0.230278
6	-2.638562	-2.462850	0.928539	6	-2.050383	-2.198741	1.104696
6	-3.866882	-2.574955	1.607899	6	-3.235167	-2.459810	1.824040
6	-4.818485	-1.549476	1.489313	6	-4.351247	-1.624638	1.650754
8	-4.035184	-3.697113	2.351832	8	-3.197509	-3.523167	2.656471
6	-5.258971	-3.878441	3.075819	6	-4.357459	-3.849310	3.436985
1	-5.156023	-4.835954	3.586625	1	-4.077863	-4.728361	4.017283
1	-6.115024	-3.913702	2.393224	1	-5.207185	-4.087309	2.788795
1	-5.399074	-3.079752	3.812266	1	-4.615265	-3.025869	4.111035
1	-5.770469	-1.618172	2.003912	1	-5.269802	-1.812300	2.195116
1	-1.414358	-1.282575	-0.343332	1	-1.062650	-0.938741	-0.285945
1	-1.901655	-3.252923	1.039344	1	-1.188352	-2.840013	1.261036
6	1.794266	1.443694	-6.497883	6	1.555346	1.728798	-6.722416
6	1.843340	-0.987312	-5.802301	6	1.988662	-0.599894	-5.837728
6	1.258566	-1.661026	-3.527946	6	1.550300	-1.164739	-3.498294

6	1.950157	-2.855851	-3.689114	6	2.415342	-2.246036	-3.581492
6	2.592396	-3.126238	-4.908577	6	3.071561	-2.516386	-4.795971
6	2.530410	-2.180814	-5.950558	6	2.848025	-1.682643	-5.909238
8	3.295149	-4.255114	-5.176700	8	3.933371	-3.538858	-4.990875
6	3.401611	-5.265044	-4.164700	6	4.214305	-4.437045	-3.906645
1	3.996870	-6.062259	-4.610140	1	4.922646	-5.161851	-4.307404
1	2.412917	-5.649501	-3.891898	1	3.302997	-4.949400	-3.581308
1	3.910845	-4.875360	-3.276588	1	4.667354	-3.901300	-3.066069
1	0.796279	-1.462325	-2.572186	1	1.080592	-0.958739	-2.548014
1	1.992564	-3.557283	-2.864048	1	2.582220	-2.859458	-2.704066
1	3.031485	-2.411586	-6.886968	1	3.364843	-1.912204	-6.836923
6	1.746746	-0.020027	-6.963212	6	1.731075	0.242097	-7.068948
1	0.793120	-0.190636	-7.485583	1	0.811814	-0.117102	-7.555299
1	2.543700	-0.221430	-7.685812	1	2.543514	0.107862	-7.789450
1	2.807850	1.681596	-6.140547	1	2.523028	2.149124	-6.409479
1	1.583929	2.123286	-7.330249	1	1.230262	2.297729	-7.599223
8	0.187638	4.561603	-0.285586	8	-1.283965	5.224777	-0.095313
1	-0.093024	3.668187	-0.031493	1	-2.026843	4.622994	0.069965
1	-0.267173	4.734644	-1.130944	1	-1.323695	5.412629	-1.060418
8	-4.485088	6.825510	-5.085980	8	-4.566623	6.996415	-4.933708
1	-3.602249	6.937177	-4.678349	1	-3.600599	7.085533	-4.747449
1	-4.808192	7.726865	-5.239716	1	-4.892697	7.905269	-5.021711
Products T_1 (explicit water)							
6	-3.976302	-4.992583	1.349040				
6	-3.907512	-4.092217	0.235403				
6	-4.570659	-2.809539	0.271549				
6	-4.286334	-2.158414	-0.903964				
7	-3.249659	-4.204409	-0.975949				
6	-3.480142	-3.039057	-1.675989				
5	-2.405436	-5.392174	-1.523538				
7	-2.071317	-5.133478	-3.024238				
9	-3.129865	-6.584671	-1.404116				
9	-1.199298	-5.474857	-0.791738				
6	-2.995407	-2.844681	-3.021746				
6	-2.342180	-3.951525	-3.679358				
6	-3.187048	-1.646062	-3.669907				
6	-1.514093	-5.999782	-3.946805				
6	-1.948297	-4.056236	-5.041137				
6	-1.450760	-5.323358	-5.221424				
6	-1.016258	-7.335425	-3.795984				
8	-3.011816	1.841320	0.797526				
1	-3.701367	-0.816206	-3.195933				
1	-2.827952	-1.493432	-4.680983				
6	-2.522410	2.550587	-0.135208				
6	-1.344795	3.441861	0.209997				
8	-2.916053	2.539437	-1.337325				
6	-1.211080	4.808841	-0.263958				
6	-0.368224	2.906572	1.012141				
7	0.773895	3.543090	1.389437				
1	-0.471732	1.899147	1.395133				
6	0.061167	5.461855	0.100371				
8	-2.086355	5.424782	-0.912287				
6	1.035916	4.826676	0.903769				
6	1.758601	2.835278	2.192892				
6	1.301984	1.984588	3.348728				
6	2.030765	3.279911	3.609452				
1	2.604375	2.475792	1.610143				
1	1.442133	4.109842	3.990289				

1	3.060816	3.251991	3.953667
1	1.825620	1.045405	3.501329
1	0.241318	1.956351	3.581574
6	0.331840	6.765985	-0.361886
6	1.515310	7.381287	-0.051143
6	2.533369	6.760478	0.719931
6	2.256689	5.472125	1.188888
1	-0.416037	7.285460	-0.951249
1	3.001486	4.952262	1.773490
9	1.708155	8.667462	-0.474054
7	3.714156	7.452974	1.026320
6	4.531303	7.915527	-0.113980
6	4.559280	6.912696	2.094549
6	5.528408	8.980671	0.333533
1	3.885653	8.336336	-0.884059
1	5.074852	7.059720	-0.549490
6	5.558449	7.969053	2.571105
1	5.108144	6.015767	1.758460
1	3.928336	6.631733	2.942111
7	6.338805	8.486395	1.445805
1	6.229482	7.526228	3.304771
1	5.014213	8.796374	3.050901
1	4.986618	9.886767	0.644716
1	6.189909	9.239972	-0.492992
6	7.663336	8.824115	1.515802
8	8.266412	9.401564	0.609747
8	8.216203	8.429484	2.683536
6	9.654485	8.617960	2.984847
6	9.778425	8.001428	4.381174
6	9.993872	10.111169	3.023931
6	10.510975	7.845003	1.977188
1	10.200848	6.794535	1.936858
1	11.559105	7.876797	2.296023
1	10.439292	8.274857	0.976155
1	9.323108	10.638221	3.712075
1	9.916119	10.566365	2.034771
1	11.020132	10.238019	3.387156
1	9.132944	8.523895	5.095558
1	10.813557	8.078681	4.730238
1	9.496965	6.942892	4.365519
1	-4.608334	-1.169208	-1.209490
1	-2.045388	-3.284303	-5.791572
6	-5.364567	-2.385560	1.462953
6	-6.002721	-3.623090	2.112618
1	-6.128891	-1.654590	1.182344
1	-4.701384	-1.892249	2.189006
6	-5.000429	-4.736254	2.323514
1	-6.804270	-3.994163	1.456829
1	-6.471433	-3.358629	3.064886
6	-3.087688	-6.080240	1.580096
6	-3.203635	-6.874521	2.698149
6	-4.223395	-6.622456	3.643774
6	-5.110417	-5.549721	3.445510
8	-4.259012	-7.454042	4.700210
6	-5.255317	-7.268425	5.720535
1	-5.073340	-8.059775	6.446872
1	-6.260813	-7.371365	5.300920
1	-5.140029	-6.290407	6.197968
1	-5.895937	-5.345583	4.163883

	1	-2.282365	-6.274295	0.887576
	1	-2.512806	-7.692303	2.877267
	6	-0.889291	-5.997780	-6.429518
	6	-0.796706	-8.085266	-5.007188
	6	-0.677206	-7.945257	-2.560588
	6	-0.155297	-9.224732	-2.497326
	6	0.043899	-9.951297	-3.689236
	6	-0.279763	-9.364655	-4.930339
	8	0.542055	-11.198887	-3.745617
	6	0.904085	-11.876624	-2.529565
	1	1.267437	-12.854558	-2.843464
	1	0.031732	-11.993998	-1.879457
	1	1.698534	-11.333838	-2.008093
	1	-0.792201	-7.393198	-1.639605
	1	0.105516	-9.645196	-1.533654
	1	-0.116487	-9.947364	-5.832297
	6	-1.181626	-7.504410	-6.349756
	1	-2.258569	-7.664523	-6.506050
	1	-0.662336	-8.039453	-7.149942
	1	0.198430	-5.836881	-6.466251
	1	-1.305914	-5.566827	-7.345032
	8	-2.645267	2.065254	3.497279
	1	-3.525763	1.902234	3.868860
	1	-2.764738	2.016337	2.511419
	8	-4.891145	0.887528	-2.186587
	1	-4.188821	1.488290	-1.805839
	1	-5.723735	1.182686	-1.786804

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