

Supporting information

Research on Controllable Degradation of *N*-methylamido and dialkylamino Substituted at the 5th position of the Benzene Ring in Chlorsulfuron in Acidic Soil

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Crystal data of M03...	SI1
Crystal data of N03.....	SI2
The standard curves of target compounds.....	SI3
Characteristic data of target compounds and intermediates 18.....	SI4
Degradation curves of target compounds in pH 5.52 soil.....	SI5

SI.1. Crystal data of M03

Molecular formula	C ₁₇ H ₁₆ ClN ₆ O ₅ S
Formula weight	451.87
Temperature	113.15 K
Crystal system, Space group	triclinic system, P-1
Radiation	MoK α ($\lambda = 0.71073$ Å)
Unit cell dimensions	$a = 7.8939(16)$ Å, $b = 8.9985(18)$ Å, $c = 14.466(3)$ Å; $\alpha = 85.32(3)^\circ$, $\beta = 81.63(3)^\circ$, $\gamma = 72.73(3)^\circ$; cell ratio as $a/b = 0.8774$, $b/c = 0.6220$, $c/a = 1.8325$
calculated density	1.547 g/cm ³
Volume	970.0(4) Å ³
Z	2
Absorption coefficient	0.350 mm ⁻¹
F(000)	466.0
Crystal size	0.20 mm x 0.18 mm x 0.12 mm
2 θ range for data collection/ $^\circ$	4.744 $^\circ$ to 50.052 $^\circ$
Index ranges	-9 $\leq h \leq$ 9; -10 $\leq k \leq$ 10; -17 $\leq l \leq$ 17
Reflections collected	9370
Independent reflections	3424 [$R_{\text{int}} = 0.0315$, $R_{\text{sigma}} = 0.0346$]
Data/restraints/parameters	3424/3/274
Goodness-of-fit on F ²	1.058
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0570$, $wR_2 = 0.1506$
Final R indexes [all data]	$R_1 = 0.0676$, $wR_2 = 0.1597$
Largest difference peak and hole	1.67/-0.59 e/Å ⁻³

SI 2. Crystal data of N03

Molecular formula	C ₁₆ H ₁₉ ClN ₆ O ₄ S
Formula weight	426.88
Temperature	113(2) K
Crystal system, Space group	Monoclinic system, P2(1)/c
Radiation	MoK α ($\lambda = 0.71073$ Å)
Unit cell dimensions	$a = 10.2847(5)$ Å, $b = 17.1412(7)$ Å, $c = 11.2410(5)$ Å; $\alpha = 90^\circ$, $\beta =$ $102.533(5)^\circ$, $\gamma = 90^\circ$; cell ratio as $a/b = 0.6000$, $b/c = 1.5249$, $c/a =$ 1.0930
calculated density	1.466 g/cm ³
Volume	1934.48(15) Å ³
Z	4
Absorption coefficient	0.342 mm ⁻¹
F(000)	888
Crystal size	0.200 mm x 0.180 mm x 0.120 mm
θ range for data collection	2.028 $^\circ$ to 26.372 $^\circ$
Limiting indices	-12 $\leq h \leq$ 12; -21 $\leq k \leq$ 21; -14 $\leq l \leq$ 14
Reflections collected/unique	20402 / 3952 [$R_{\text{int}} = 0.0422$]
Completeness to $\theta = 25.242$	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1 and 0.51980
Refinement method	Full-matrix least-squares on F ²
Data/restraints/parameters	3952/2/262
Goodness-of-fit on F ²	1.040

Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0496$, $wR_2 = 0.1274$
R indices (all data)	$R_1 = 0.0589$, $wR_2 = 0.1345$
Extinction coefficient	n/a
Largest diff. peak and hole	0.621 and -0.548 e/Å ³

SI3. The standard curves of target compounds

Compud.	Standard curve	Correlation coefficient (R^2)
M01	Y=64660.8X-17.8837	$R^2 > 0.9999$
M02	Y=63086.9X-7391.33	$R^2 > 0.9999$
M03	Y=52581.4X+546.885	$R^2 > 0.9999$
M04	Y=49791.6X-349.667	$R^2 > 0.9999$
M05	Y=55169X+530.779	$R^2 > 0.9999$
N01	Y=59911.9X+10548.8	$R^2 > 0.9999$
N02	Y=55456.3X+8474.75	$R^2 > 0.9999$
N03	Y=66717X+626.688	$R^2 > 0.9999$
N04	Y=71978.9X+302.746	$R^2 > 0.9999$
N05	Y=50577.7X-2712.01	$R^2 > 0.9999$
N06	Y=47970.7X-1104.17	$R^2 > 0.9999$
N07	Y=50130.9X+1689.56	$R^2 > 0.9999$
N08	Y=49832.2X-395.95	$R^2 > 0.9999$
N09	Y=45583.9X+2775.24	$R^2 > 0.9999$
N10	Y=43188X+3159.8	$R^2 > 0.9999$
N11	Y=47694.5X+4134.51	$R^2 > 0.9999$
N12	Y=49563.8X+3671.63	$R^2 > 0.9999$
N13	Y=33761.4X+511.688	$R^2 > 0.9999$
Chlosulfuron	Y=41190.4X+7389.03	$R^2 > 0.9999$

SI4. Characteristic data of target compounds and intermediates 18

Sodium (4-methoxy-6-methyl-1,3,5-triazin-2-yl)(phenoxy-carbonyl)amide **18**: White solid, yield 92.5%; ¹H NMR (400 MHz, MeOD-*dd*) δ 7.07 (t, $J = 7.6$ Hz, 2H, Ph-**H**), 6.70 (d, $J = 7.8$ Hz, 2H, Ph-**H**), 6.59 (t, $J = 7.1$ Hz, 1H, Ph-**H**), 3.98 (s, 3H, OCH₃), 2.40 (s, 3H, CH₃). ¹³C NMR (101 MHz, DMSO-*dd*) δ : 175.89, 171.81, 171.08, 159.57, 153.97, 129.15, 122.52, 116.00, 53.48, 25.57. HRMS calcd for C₁₂H₁₁N₄NaO₃⁺[M+H] 283.0807, found 283.0801.

N-(4-chloro-3-(*N*-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)sulfamoyl)phenyl)-*N*-methylformamide **M01**: White solid, yield 89.3%, m.p. 181~183 °C; ¹H NMR (400 MHz, Acetone-*dd*) δ : 12.85 (s, 1H, SO₂NHCONH), 9.76 (s, 1H, NCOH), 7.43 (s, 1H, SO₂NHCONH), 7.32 (d, $J = 8.8$ Hz, 1H, Ph-**H**), 6.85 (d, $J = 6.5$ Hz, 1H, Ph-**H**), 5.76 (s, 1H, Ph-**H**), 4.03 (s, 3H, OCH₃), 2.85 (s, 3H, NCH₃), 2.51 (s, 3H, CH₃). ¹³C NMR (101 MHz, MeOD-*dd*) δ : 178.70, 172.16, 149.04, 147.48, 136.61, 133.61, 131.77, 116.91, 115.92, 114.65, 114.58, 54.74, 28.78, 23.81. HRMS calcd for C₁₄H₁₅ClN₆O₅S⁺[M+H] 415.0591,

found 415.0583.

N-(4-chloro-3-(*N*-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)sulfamoyl)phenyl)-*N*-methylacetamide **M02**: White solid, yield 83.5%, m.p 146-148 °C. ¹H NMR (400 MHz, CDCl₃) δ: 12.82 (s, 1H, SO₂NHCONH), 8.15 (s, 1H, Ph-H), 8.04 (s, 1H, SO₂NHCONH), 7.57 (d, *J* = 7.2 Hz, 1H, Ph-H), 7.43 (s, 1H, Ph-H), 4.06 (s, 3H, OCH₃), 3.30 (s, 3H, NCH₃), 2.59 (s, 3H, CH₃), 1.94 (s, 3H, COCH₃). ¹³C NMR (101 MHz, CDCl₃) δ: 179.20, 170.59, 170.20, 163.43, 148.02, 143.41, 137.11, 133.15, 132.89, 131.82, 130.72, 55.71, 37.20, 25.44, 22.57. HRMS calcd for C₁₅H₁₇ClN₆O₅S⁺[M+H] 429.0748, found 429.0741.

N-(4-chloro-3-(*N*-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)sulfamoyl)phenyl)-*N*-methylcyclopropanecarboxamide **M03**: White solid, yield 88.1%, m.p. 155~157 °C; ¹H NMR (400 MHz, CDCl₃) δ: 12.82 (s, 1H, SO₂NHCONH), 8.26 (d, *J* = 2.4 Hz, 1H, Ph-H), 7.71 (s, 1H, SO₂NHCONH), 7.56 (d, *J* = 8.4 Hz, 1H, Ph-H), 7.51 (dd, *J* = 8.5, 2.4 Hz, 1H, Ph-H), 4.06 (s, 3H, OCH₃), 3.35 (s, 3H, NCH₃), 2.59 (s, 3H, CH₃), 1.41 (s, 1H, Cyclopropyl-H), 1.15–0.99 (m, 2H, Cyclopropyl-H₂), 0.84–0.72 (m, 2H, Cyclopropyl-H₂). ¹³C NMR (101 MHz, CDCl₃) δ: 179.25, 173.44, 170.76, 163.41, 147.93, 143.32, 136.92, 133.15, 132.66, 131.55, 129.96, 55.77, 37.38, 25.49, 13.04, 9.08. HRMS calcd for C₁₇H₁₉ClN₆O₅S⁺[M+H] 455.0904, found 455.0900.

N-(4-chloro-3-(*N*-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)sulfamoyl)phenyl)-*N*-methylpivalamide **M04**: White solid, yield 87.2%, m.p. 154~156 °C; ¹H NMR (400 MHz, CDCl₃) δ: 12.81 (s, 1H, SO₂NHCONH), 8.19 (s, 1H, Ph-H), 7.81 (s, 1H, SO₂NHCONH), 7.56 (d, *J* = 8.3 Hz, 1H, Ph-H), 7.46 (d, *J* = 8.4 Hz, 1H, Ph-H), 4.07 (s, 3H, OCH₃), 3.27 (s, 3H, NCH₃), 2.60 (s, 3H, CH₃), 1.12 (s, 9H, C(CH₃)₃). ¹³C NMR (101 MHz, CDCl₃) δ: 179.30, 178.08, 170.64, 163.44, 147.87, 144.61, 136.91, 134.91, 132.86, 132.47, 130.72, 55.75, 41.12, 40.80, 29.37, 25.48. HRMS calcd for C₁₈H₂₃ClN₆O₅S⁺[M+H] 471.1217, found 471.1216.

N-(4-chloro-3-(*N*-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)sulfamoyl)phenyl)-*N*-methylbenzamide **M05**: White solid, yield 90.3%, m.p. 95~97 °C; ¹H NMR (400 MHz, CDCl₃) δ: 12.79 (s, 1H, SO₂NHCONH), 8.18 (d, *J* = 2.6 Hz, 1H, Ph-H), 7.47 (s, 1H, SO₂NHCONH), 7.32 (m, 2H, Ph-H), 7.30 – 7.21 (m, 4H, Ph-H), 7.11 – 7.05 (dd, *J* = 12.0, 2.0 Hz, 1H, Ph-H), 4.06 (s, 3H, OCH₃), 3.53 (s, 3H, NCH₃), 2.58 (s, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃) δ: 170.62, 163.38, 147.85, 143.99, 136.70, 134.82, 133.28, 132.07, 130.29, 129.11, 128.78, 128.53, 128.32, 128.29, 126.95, 55.77, 38.34, 25.48. HRMS calcd for C₂₀H₁₉ClN₆O₅S⁺[M+H] 491.0904, found 491.0899.

2-chloro-*N*-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)-5-(methyl(propyl)amino)benzenesulfonamide **N02**: White solid, yield 87.9%, m.p. 162~164 °C; ¹H NMR

(400 MHz, CDCl₃) δ 12.71 (s, 1H, SO₂NHCONH), 7.51 (d, *J* = 3.1 Hz, 1H, Ph-**H**), 7.30 (s, 1H, SO₂NHCONH), 7.25 (d, *J* = 10.1 Hz, 1H, Ph-**H**), 6.74 (dd, *J* = 9.0, 3.2 Hz, 1H, Ph-**H**), 4.05 (s, 3H, OCH₃), 3.32 (t, *J* = 7.6 Hz, 2H, NCH₂CH₂CH₃), 2.99 (s, 3H, NCH₃), 2.57 (s, 3H, CH₃), 1.66-1.59 (m, 2H, NCH₂CH₂CH₃), 0.93 (t, *J* = 7.4 Hz, 3H, NCH₂CH₂CH₃). ¹³C NMR (101 MHz, CDCl₃) δ 178.08, 170.70, 163.39, 147.93, 147.89, 135.81, 132.03, 116.96, 116.06, 115.14, 55.71, 54.30, 38.56, 25.46, 19.89, 11.44. HRMS calcd for C₁₆H₂₁ClN₆O₄S⁺[M+H] 429.1112, found 429.1108.

5-(allyl(methyl)amino)-2-chloro-N-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)benzenesulfonamide **N03**: White solid, yield 88.6%, m.p. 172~174 °C; ¹H NMR (400 MHz, CDCl₃) δ 12.67 (s, 1H, SO₂NHCONH), 7.55 (d, *J* = 3.0 Hz, 1H, Ph-**H**), 7.34 (s, 1H, SO₂NHCONH), 7.25 (d, *J* = 7.9 Hz, 1H, Ph-**H**), 6.76 (dd, *J* = 8.9, 3.1 Hz, 1H, Ph-**H**), 5.80 (ddd, *J* = 15.2, 9.9, 4.8 Hz, 1H, CH=CH₂), 5.17 (dd, *J* = 20.5, 13.7 Hz, 2H, CH=CH₂), 4.05 (s, 3H, OCH₃), 3.97 (d, *J* = 4.7 Hz, 2H, NCH₂), 3.02 (s, 3H, NCH₃), 2.57 (s, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃) δ 179.55, 170.50, 163.40, 148.00, 147.89, 135.85, 132.08, 132.02, 117.47, 116.92, 116.83, 115.51, 55.71, 54.98, 38.33, 25.46. HRMS calcd for C₁₆H₁₉ClN₆O₄S⁺[M+H] 427.0955, found 427.0951.

2-chloro-N-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)-5-(methyl(prop-2-yn-1-yl)amino)benzenesulfonamide **N04**: Yellow solid, yield 91.3%, m.p. 173~175 °C; ¹H NMR (400 MHz, CDCl₃) δ 12.69 (s, 1H, SO₂NHCONH), 7.66 (d, *J* = 3.1 Hz, 1H, Ph-**H**), 7.46 (s, 1H, SO₂NHCONH), 7.32 (d, *J* = 8.9 Hz, 1H, Ph-**H**), 6.92 (dd, *J* = 8.9, 3.1 Hz, 1H, Ph-**H**), 4.08 (d, *J* = 2.3 Hz, 2H, CH₂CCH), 4.05 (s, 3H, OCH₃), 3.05 (s, 3H, NCH₃), 2.57 (s, 3H, CH₃), 2.23 (t, *J* = 2.3 Hz, 1H, C≡CH). ¹³C NMR (101 MHz, CDCl₃) δ 179.12, 170.66, 163.40, 147.90, 147.61, 136.02, 132.09, 119.00, 118.88, 117.23, 77.97, 72.85, 55.72, 42.22, 38.70, 25.46. HRMS calcd for C₁₆H₁₇ClN₆O₄S⁺[M+H] 425.0799, found 425.0794.

5-(butyl(methyl)amino)-2-chloro-N-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)benzenesulfonamide **N06**: White solid, yield 86.3%, m.p. 109~111 °C; ¹H NMR (400 MHz, CDCl₃) δ 12.66 (s, 1H, SO₂NHCONH), 7.56 (s, 1H, Ph-**H**), 7.44 (s, 1H, SO₂NHCONH), 7.28 (d, *J* = 7.3 Hz, 1H, Ph-**H**), 6.81 (d, *J* = 7.9 Hz, 1H, Ph-**H**), 4.07 (s, 3H, OCH₃), 3.37 (t, *J* = 7.2 Hz, 2H, NCH₂CH₂CH₂CH₃), 3.01 (s, 3H, NCH₃), 2.59 (s, 3H, CH₃), 1.66-1.52 (m, 2H, NCH₂CH₂CH₂CH₃), 1.43-1.30 (m, 2H, NCH₂CH₂CH₂CH₃), 0.97 (t, *J* = 7.3 Hz, 3H, NCH₂CH₂CH₂CH₃). ¹³C NMR (101 MHz, CDCl₃) δ 178.78, 170.80, 163.39, 147.87, 147.64, 135.88, 132.06, 117.38, 116.59, 115.55, 55.69, 52.57, 38.70, 28.63, 25.43, 20.21, 13.90. HRMS calcd for C₁₇H₂₃ClN₆O₄S⁺[M+H] 443.1268, found 443.1266.

2-chloro-5-(isobutyl(methyl)amino)-N-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)benzenesulfonamide **N07**: White solid, yield 86.9%, m.p. 128~130 °C; ¹H NMR (400 MHz, CDCl₃) δ 12.64 (s, 1H, SO₂NHCONH), 7.51 (d, *J* = 3.2 Hz, 1H, Ph-**H**), 7.31 (s, 1H, SO₂NHCONH), 7.25 (d, *J* = 9.0 Hz, 1H, Ph-**H**), 6.73 (dd, *J* = 9.0, 3.2 Hz, 1H, Ph-**H**), 4.05 (s, 3H, OCH₃), 3.16 (d, *J* = 7.4 Hz,

2H, CH₂), 3.02 (s, 3H, NCH₃), 2.57 (s, 3H, CH₃), 2.05 (dt, *J* = 13.8, 6.8 Hz, 1H, CH), 0.93 (d, *J* = 6.6 Hz, 6H, CH(CH₃)₂). ¹³C NMR (101 MHz, CDCl₃) δ 179.54, 170.85, 163.39, 148.14, 147.88, 135.77, 131.96, 116.86, 115.99, 115.05, 60.54, 55.71, 39.60, 27.22, 25.46, 20.32. HRMS calcd for C₁₇H₂₃ClN₆O₄S⁺[M+H] 443.1268, found 443.1264.

2-chloro-5-(ethyl(propyl)amino)-N-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)benzenesulfonamide **N08**: White solid, yield 86.2%, m.p. 181~183 °C; ¹H NMR (400 MHz, CDCl₃) δ 12.66 (s, 1H, SO₂NHCONH), 7.56 (s, 1H, Ph-H), 7.37 (s, 1H, SO₂NHCONH), 7.28 (d, *J* = 3.1 Hz, 1H, Ph-H), 6.85 (d, *J* = 7.8 Hz, 1H, Ph-H), 4.07 (s, 3H, OCH₃), 3.43 (t, *J* = 4.0 Hz, 2H, NCH₂CH₃), 3.29 (t, *J* = 4.4 Hz, 2H, NCH₂CH₂CH₃), 2.59 (s, 3H, CH₃), 1.30-1.25 (m, 2H, NCH₂CH₂CH₃), 1.20 (t, *J* = 5.6 Hz, 3H, NCH₂CH₃), 0.97 (t, *J* = 6.8 Hz, 3H, NCH₂CH₂CH₃). ¹³C NMR (101 MHz, CDCl₃) δ 179.32, 171.00, 163.40, 147.87, 146.13, 136.04, 132.20, 117.72, 116.16, 115.86, 55.69, 52.69, 45.83, 25.43, 20.30, 11.84, 11.37. HRMS calcd for C₁₇H₂₃ClN₆O₄S⁺[M+H] 443.1268, found 443.1264.

2-chloro-5-(cyclopentyl(methyl)amino)-N-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)benzenesulfonamide **N09**: White solid, yield 91.1%, m.p. 81~83 °C; ¹H NMR (400 MHz, CDCl₃) δ 12.70 (s, 1H, SO₂NHCONH), 7.65 (d, *J* = 2.9 Hz, 1H, Ph-H), 7.41 (s, 1H, SO₂NHCONH), 7.26 (s, 1H, Ph-H), 6.88 (dd, *J* = 9.0, 3.1 Hz, 1H, Ph-H), 4.27 – 4.18 (m, 1H, Cyclopentyl-CH), 4.08 (s, 3H, OCH₃), 2.86 (s, 3H, NCH₃), 2.60 (s, 3H, CH₃), 2.02-1.89 (m, 2H, Cyclopentyl-CH₂), 1.70-1.83 (m, 2H, Cyclopentyl-CH₂), 1.54-1.70 (m, 4H, Cyclopentyl-CH₂CH₂). ¹³C NMR (101 MHz, CDCl₃) δ 179.18, 170.86, 149.24, 147.94, 135.78, 131.96, 129.63, 118.22, 116.71, 116.40, 59.99, 32.14, 28.77, 25.45, 24.25. HRMS calcd for C₁₈H₂₃ClN₆O₄S⁺[M+H] 455.1268, found 455.1265.

2-chloro-5-(dipropylamino)-N-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)benzenesulfonamide **N10**: White solid, yield 87.6%, m.p. 158~160 °C; ¹H NMR (400 MHz, CDCl₃) δ 12.64 (s, 1H, SO₂NHCONH), 7.50 (s, 1H, Ph-H), 7.42 (s, 1H, SO₂NHCONH), 7.23 (d, *J* = 8.8 Hz, 1H, Ph-H), 6.74 (s, 1H, Ph-H), 4.05 (s, 3H, OCH₃), 3.28 (t, *J* = 7.2 Hz, 4H, N(CH₂CH₂CH₃)₂), 2.57 (s, 3H, CH₃), 1.70-1.55 (m, 4H, N(CH₂CH₂CH₃)₂), 0.94 (t, *J* = 7.3 Hz, 6H, N(CH₂CH₂CH₃)₂). ¹³C NMR (101 MHz, CDCl₃) δ 179.79, 170.71, 163.41, 147.91, 146.70, 135.86, 132.09, 117.08, 115.74, 115.37, 55.72, 53.05, 25.45, 20.09, 11.38. HRMS calcd for C₁₈H₂₅ClN₆O₄S⁺[M+H] 457.1425, found 457.1423.

5-(butyl(propyl)amino)-2-chloro-N-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)benzenesulfonamide **N11**: White solid, yield 90.7%, m.p. 145~147 °C; ¹H NMR (400 MHz, CDCl₃) δ 12.62 (s, 1H, SO₂NHCONH), 7.50 (d, *J* = 2.7 Hz, 1H, Ph-H), 7.39 (s, 1H, SO₂NHCONH), 7.22 (d, *J* = 8.9 Hz, 1H, Ph-H), 6.72 (d, *J* = 6.8 Hz, 1H, Ph-H), 4.05 (s, 3H, OCH₃), 3.37-3.17 (m, 4H, NCH₂CH₂CH₃, NCH₂CH₂CH₂CH₃), 2.57 (s, 3H, CH₃), 1.69-1.52 (m, 4H, NCH₂CH₂CH₃, NCH₂CH₂CH₂CH₃), 1.44-1.30 (m, 2H, NCH₂CH₂CH₂CH₃), 0.90-1.00 (m, 6H, NCH₂CH₂CH₃,

NCH₂CH₂CH₂CH₃). ¹³C NMR (101 MHz, CDCl₃) δ 179.03, 171.12, 163.41, 147.89, 146.72, 135.84, 132.07, 116.91, 115.48, 115.30, 55.71, 52.94, 51.03, 28.98, 25.46, 20.23, 20.14, 13.93, 11.39. HRMS calcd for C₁₉H₂₇ClN₆O₄S⁺[M+H] 471.1581, found 471.1580.

5-(benzyl(methyl)amino)-2-chloro-N-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)benzenesulfonamide **N12**: White solid, yield 92.8%, m.p. 79~81 °C; ¹H NMR (400 MHz, CDCl₃) δ 12.63 (s, 1H, SO₂NHCONH), 7.66 (s, 1H, SO₂NHCONH), 7.63 (d, *J* = 2.6 Hz, 1H, Ph-H), 7.32 (t, *J* = 7.2 Hz, 2H, Ph-H), 7.27 (d, *J* = 6.0 Hz, 1H, Ph-H), 7.23 (s, 1H), 7.22-7.16 (m, 2H, Ph-H), 6.76 (dd, *J* = 8.8, 2.6 Hz, 1H, Ph-H), 4.57 (s, 2H, NCH₂), 4.05 (s, 3H, OCH₃), 3.09 (s, 3H, NCH₃), 2.57 (s, 3H, CH₃). ¹³C NMR (101 MHz, CDCl₃) δ 179.31, 170.62, 163.36, 148.20, 147.90, 137.20, 135.91, 132.05, 128.75, 127.29, 126.55, 117.54, 117.07, 115.38, 56.28, 55.63, 38.79, 25.37. HRMS calcd for C₂₀H₂₁ClN₆O₄S⁺[M+H] 477.1112, found 477.1110.

2-chloro-5-(dibutylamino)-N-((4-methoxy-6-methyl-1,3,5-triazin-2-yl)carbamoyl)benzenesulfonamide **N13**: White solid, yield 85.3%, m.p. 79~81 °C; ¹H NMR (400 MHz, CDCl₃) δ 12.59 (s, 1H, SO₂NHCONH), 7.84 (s, 1H, SO₂NHCONH), 7.49 (s, 1H, Ph-H), 7.22 (d, *J* = 8.9 Hz, 1H, Ph-H), 6.70 (d, *J* = 7.9 Hz, 1H, Ph-H), 4.05 (s, 3H, NCH₃), 3.30 (t, *J* = 7.6, 4H, N(CH₂CH₂CH₂CH₃)₂), 2.56 (s, 3H, CH₃), 1.57 (dd, *J* = 14.6, 7.4 Hz, 4H, N(CH₂CH₂CH₂CH₃)₂), 1.44 -1.28 (m, 4H, N(CH₂CH₂CH₂CH₃)₂), 0.96 (t, *J* = 7.3 Hz, 6H, N(CH₂CH₂CH₂CH₃)₂). ¹³C NMR (101 MHz, CDCl₃) δ 179.37, 170.62, 163.48, 147.97, 146.80, 135.84, 132.03, 116.80, 115.46, 115.28, 55.69, 50.87, 29.01, 25.42, 20.22, 13.91. HRMS calcd for C₂₀H₂₉ClN₆O₄S⁺[M+H] 485.1738, found 485.1736.

SI5. Degradation curves of target compounds in pH 5.52 soil







