Isolation and Bioactivity of Chlorinated Xanthones and Chromones from Solid Culture of the Fungus, *Alternaria sonchi*, a Potential Bioherbicide for Control of Sowthistles

Anna A. Dalinova¹, Leonid S. Chisty², Dmitry M. Kochura², Varvara V. Garnyuk², Maria O. Petrova¹, Darya S. Prokophyeva², Anton N. Yurchenko³, Vsevolod R. Dubovik¹, Alexander Y. Ivanov⁴, Sergey N. Smirnov⁴, Andrey A. Zolotarev⁴ and Alexander O. Berestetskiy¹

¹ All-Russian Institute of Plant Protection, Russian Academy of Agricultural Sciences, Pushkin, Saint-Petersburg 196608, Russian Federation

² Research Institute of Hygiene, Occupational Pathology and Human Ecology, Federal Medical Biological Agency, p/o Kuz'molovsky, Saint-Petersburg 188663, Russian Federation

³ G.B. Elyakov Pacific Institute of Bioorganic Chemistry, Far Eastern Branch of Russian Academy of Sciences, Vladivostok 690022, Russian Federation

⁴ St. Petersburg State University, Universitetsky Av. 26, St. Petersburg, 198504, Russian Federation

Figure S1 – ¹H NMR spectrum of compound 1

Figure S2 - ¹³C NMR spectrum of compound 1

- Figure S3 HSQC spectrum of compound 1
- Figure S4 HMBC spectrum of compound 1

Figure S5 – ESIMS of compound 1 recorded in positive ion mode

Figure S6 – UV spectrum of compound 1

Figure S7 - ¹H NMR spectrum of compound **2**

Figure $S8 - {}^{13}C$ NMR spectrum of compound 2

Figure S9 – HSQC spectrum of compound 2

Figure S10 – HMBC spectrum of compound 2

Figure S11 – HR ESIMS of compound 2 recorded in positive ion mode

Figure S12 – UV spectrum of compound 2

Figure S13 - ¹H NMR spectrum of compound **5**

Figure S14 - ¹³C NMR spectrum of compound 5

Figure S15 - ¹H NMR spectrum of compound 9

Figure $S16 - {}^{13}C$ NMR spectrum of compound 9

Table S1 – X-ray data of compound 1



Figure S3 – HSQC spectrum of compound 1



Figure S4 – HMBC spectrum of compound 1



Figure S5 – ESIMS of compound 1 recorded in positive ion mode



Figure $S8 - {}^{13}C$ NMR spectrum of compound 2



Figure S9 – HSQC spectrum of compound 2



Figure S10 - HMBC spectrum of compound 2



Figure S11 – HR ESIMS of compound 2 recorded in positive ion mode



Figure S15 - ¹H NMR spectrum of compound 9



Figure S16 - ¹³C NMR spectrum of compound 9

Table 31. Crystal data and structure refine	Table 51. Crystal data and structure remember for T	
Empirical formula	C ₁₆ H ₁₁ ClO ₅	
Formula weight	318.70	
Temperature, K	100(2)	
Crystal system	monoclinic	
Space group	$P2_{1}/c$	
a,Å	7.1243(5)	
b,Å	10.4999(7)	
c,Å	18.0434(13)	
β,°	92.221(6)	
Volume, Å ³	1348.71(16)	
Z	4	
$\rho_{calc}mg/mm^3$	1.570	
µ/mm ⁻¹	2.730	
F(000)	656.0	
Crystal size, mm ³	$0.21 \times 0.18 \times 0.13$	
Radiation	$CuK\alpha (\lambda = 1.54184)$	
2\to range, °	9.748 to 139.516	
Index ranges	$-8 \le h \le 5$, $-11 \le k \le 12$, $-21 \le 1 \le 21$	
Reflections collected	6007	
Independent reflections	2475 [$R_{int} = 0.0823$, $R_{sigma} = 0.0520$]	
Data/restraints/parameters	2475/0/205	
Goodness-of-fit on F ²	1.049	
Final R indexes [I>=2 σ (I)]	$R_1 = 0.0600, wR_2 = 0.1685$	
Final R indexes [all data]	$R_1 = 0.0674, wR_2 = 0.1835$	
Largest diff. peak/hole / e Å ⁻³	0.48/-0.58	
$R_{1} = \sigma F_{o} - F_{c} / \sigma F_{o} ; wR_{2} = \{ \sigma [w(F_{o}^{2} - F_{c}^{2})^{2}] / \sigma [w(F_{o}^{2})^{2}] \}^{1/2};$		
$w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, where $P = (F_o^2 + 2F_c^2)/3$; $s = \{\sigma[w(F_o^2 - F_c^2)]/(n-p)\}^{1/2}$		
where <i>n</i> is the number of reflections and <i>p</i> is the number of refinement parameters.		

Table S1. Crystal data and structure refinement for 1