Appendix A.Supplementary materials – manuscript bs5063:

During the investigation on the tetrazole crystal structures, a intermediate product of the (2) was determined. It was obtained as the result of next to the last synthesis step, according to the Scheme 1. The crystal structure of the compound (2a) was not discussed in the main text, since its molecule does not contain the tetrazole ring, most probably essential for the taste of the considered compounds.

Suitable crystals of the compounds (2a) were obtained by slow evaporation of ethanol solutions at room temperature. All non-hydrogen atoms were refined anisotropically. The positions of hydrogen atoms bonded to carbon atoms were calculated. The hydrogen atoms were refined with isotropic displacement parameter equal to 1.2 or 1.5 (methyl group) times that of the parent atom with the use of the riding model.

	(2a)
Crystal data	
Chemical formula	$C_9H_8ClNO_2S$
M_r	229.67
Cell setting, space group	Monoclinic, $P2_1/n$
Temperature (K)	293 (2)
a, b, c (Å)	7.0770 (6), 15.5895 (12), 9.3409 (7)
β (°)	98.114 (8)
V (Å ^{3})	1020.24 (14)
Z	4
D_x (Mg m^{-3})	1.495
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.55
Crystal form, colour	Prism, yellow
Crystal size (mm)	0.4 × 0.4 × 0.25
Data collection	
Diffractometer	Automatic single crystal diffractometer KM4
Data collection method	ω/2θ scan
Absorption correction	None
T_{min}	–
T_{max}	–
No. of measured, independent and observed reflections	5005, 2354, 2057
Criterion for observed reflections	$I > 2\sigma(I)$
R_{int}	0.029
θ_{max} (°)	27.6

Refinement

Refinement on	F^2
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.105, 1.05
No. of relections	2354 reflections
No. of parameters	127
H-atom treatment	Constrained refinement
Weighting scheme	Calculated $w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.3677P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$	0.001
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.31, −0.22

Figure 9 ORTEP III (Farrugia, 1997) view and atom numbering for (2a). The ellipsoids are drawn at 30% probability.

	(2a)
	mol R
S(1)-O(1)	1.429(2)
S(1)-O(2)	1.436(1)
S(1)-C(1)	1.755(2)
S(1)-C(7)	1.812(2)
C(7)-C(8)	1.472(3)
N(1)-C(8)	1.104(3)
C(1)-S(1)-C(7)-C(8)	61.1 (1)
C(1)-S(1)-C(7)-C(9)	-64.9(2)