

Table S1. X-ray diffraction and refinement parameters

Crystal Data			
Compound	KS25	KS33	KS51
Formula	2C ₃ H ₇ NO ₂ · HI ₃	3C ₂ H ₅ NO ₂ · LiI	4C ₆ H ₁₃ NO ₂ · 2HI · H ₂ O
Molecular Weight	559.91	359.05	798.54
Crystal System; Space group	Monoclinic, P2 ₁ /c	Monoclinic, P2 ₁	Monoclinic, C2
Lattice constants: a, b, c [Å]	8.1057(16); 8.9853(18); 10.541(2)	5.4692(11); 9.898(2); 11.193(2)	22.8411(7); 5.8290(2); 16.2238(5)
alpha, beta, gamma [deg]	90; 100.29(3); 90	90; 90.67(3); 90	90; 123.658(2); 90
V, [Å] ³ ; Z	755.4(3); 2	605.9(2); 2	1797.94(12); 2
D(calc)[g/cm ³]; F(000)	2.462; 512	1.968; 352	1.475; 812
Mu(MoKα) [mm ⁻¹]	6.205	2.662	1.796
Crystal Size [mm]	0.10 x 0.10 x 0.20	0.14 x 0.17 x 0.20	0.02 x 0.10 x 0.20
Data Collection			
T [⁰ K]; Radiation [Å]	200; MoKα; $\lambda=0.71073$	200; MoKα; $\lambda=0.71073$	100; MoKα; $\lambda=0.71073$
$\theta_{\min}, \theta_{\max}$, [deg]	2.6; 30.0	1.8; 30.0	3.2; 29.7
Dataset	0:11; 0:12; -14:14	0:7 ; -13:13 ; -15:15	-31:31; -8:8 ; -22:22
Tot., Uniq. Data, R(int)	2338, 2195, 0.023	4107, 3515, 0.022	9148, 4462, 0.029
Observed data, I > 2,0 sigma(I)	1737	3322	3726
Refinement			
Nref, Npa	2195; 102	3515; 157	4462; 185
R, wR ² , S	0.0351; 0.0859; 1.10	0.0377; 0.0955; 1.25	0.0458; 0.0684; 1.05
	w = 1/[s ² (Fo ²) + (0. 0374P) ² + 0.2440 P], where P=(Fo ² +2Fc ²)/3	w = 1/[s ² (Fo ²) + (0.037 4P) ² + 0.2440P], where	w = 1/[s ² (Fo ²) + (0.037 4P) ² + 0.2440P], где P=(Fo ² +2Fc ²)/3

		$P = (F_o^2 + 2F_c^2)/3$	
Max. and Av. Shift/Error	0.00; 0.00	0.00; 0.00	0.00; 0.00
Min. and Max. Resd. Dens. [e/Å³]	-1.03; 1.45	-1.56; 2.08	-0.94; 0.88