

Supplementary Information:

Structural investigation and compression of a co-crystal of indomethacin and saccharin.

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Table S1: Experimental details

For all structures: $C_{19}H_{16}ClNO_4 \cdot C_7H_5NO_3S$, $M_r = 540.96$, triclinic, $P\bar{1}$, $Z = 2$. Experiments were carried out with Mo $K\alpha$ radiation using a Bruker SMART APEX2 area detector. H-atom parameters were constrained.

	Ambient pressure, 297K	0.55 GPa, 297 K	1.66 GPa, 297 K
a, b, c (Å)	7.1314 (2), 10.4809 (2), 16.7109 (4)	7.0133 (6), 10.155 (2), 16.607 (3)	6.9301 (4), 9.9420 (7), 16.514 (3)
α, β, γ (°)	80.5779 (12), 86.4941 (12), 79.2821 (12)	79.683 (14), 85.829 (11), 79.844 (14)	79.013 (11), 85.441 (10), 80.339 (5)
V (Å ³)	1210.08 (5)	1144.3 (3)	1099.8 (2)
μ (mm ⁻¹)	0.30	0.31	0.33
Crystal size (mm)	0.25 × 0.30 × 0.05	0.25 × 0.05 × 0.04	0.24 × 0.04 × 0.04
Absorption correction	Multi-scan SADABS-2016/2 (Bruker,2016/2) was used for absorption correction. $wR2(int)$ was 0.0807 before and 0.0443 after correction. The Ratio of minimum to maximum transmission is 0.9327. The $\lambda/2$ correction factor is Not present.'	Multi-scan SADABS2016/2 (Bruker,2016/2) was used for absorption correction. $wR2(int)$ was 0.1025 before and 0.0509 after correction. The Ratio of minimum to maximum transmission is 0.8711. The $\lambda/2$ correction factor is Not present.	Multi-scan SADABS2016/2 (Bruker,2016/2) was used for absorption correction. $wR2(int)$ was 0.0861 before and 0.0545 after correction. The Ratio of minimum to maximum transmission is 0.7871. The $\lambda/2$ correction factor is Not present.
T_{min}, T_{max}	0.696, 0.746	0.649, 0.745	0.586, 0.745
No. of measured, independent and observed [$I > 2.0\sigma$ (I)] reflections	26677, 7292, 4554	3840, 1015, 682	5514, 1044, 761
R_{int}	0.034	0.073	0.081
θ_{max} (°)	30.5	23.2	23.3
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.714	0.555	0.556
$R[F^2 > 2\sigma(F^2)],$ $wR(F^2), S$	0.047, 0.125, 1.06	0.066, 0.166, 1.06	0.059, 0.149, 1.09
No. of reflections	7292	1015	1044
No. of parameters	337	126	126
No. of restraints	0	20	24
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.35, -0.55	0.28, -0.29	0.25, -0.22

Computer programs: SAINT v8.37A(Bruker AXS Inc., 2014) SHELXT(Sheldrick & IUCr, 2015) XL (Sheldrick, 2015) and Olex2(Dolomanov *et al.*, 2009)

Table S1 contd.: Experimental details

For all structures: $C_{19}H_{16}ClNO_4 \cdot C_7H_5NO_3S$, $M_r = 540.96$, triclinic, $P\bar{1}$, $Z = 2$. Experiments were carried out with Mo $K\alpha$ radiation using a Bruker SMART APEX2 area detector. H-atom parameters were constrained.

	3.33 GPa, 297K	4.06 GPa, 297 K
a, b, c (Å)	6.7888 (3), 9.6045 (11), 16.3703 (16)	7.0133 (6), 10.155 (2), 16.607 (3)
α, β, γ (°)	77.764 (8), 84.858 (6), 81.297 (8)	79.683 (14), 85.829 (11), 79.844 (14)
V (Å ³)	1029.30 (17)	1144.3 (3)
μ (mm ⁻¹)	0.35	0.31
Crystal size (mm)	0.25 × 0.05 × 0.04	0.25 × 0.05 × 0.04
Absorption correction	Multi-scan SADABS2014/5 (Bruker, 2014/5) was used for absorption correction. wR2(int) was 0.0729 before and 0.0488 after correction. The Ratio of minimum to maximum transmission is 0.9098. The l/2 correction factor is Not present.	Multi-scan SADABS2016/2 (Bruker, 2016/2) was used for absorption correction. wR2(int) was 0.1025 before and 0.0509 after correction. The Ratio of minimum to maximum transmission is 0.8711. The l/2 correction factor is Not present.
T_{\min}, T_{\max}	0.678, 0.745	0.649, 0.745
No. of measured, independent and observed [$I > 2.0\sigma(I)$] reflections	4793, 941, 747	3840, 1015, 682
R_{int}	0.050	0.073
θ_{\max} (°)	23.3	23.2
$(\sin \theta/\lambda)_{\max}$ (Å ⁻¹)	0.557	0.555
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.064, 0.163, 1.09	0.066, 0.166, 1.06
No. of reflections	941	1015
No. of parameters	126	126
No. of restraints	24	20
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å ⁻³)	0.27, -0.24	0.28, -0.29

Computer programs: SAINT v8.37A (Bruker AXS Inc., 2014) SHELXT (Sheldrick & IUCr, 2015) XL (Sheldrick, 2015) and Olex2 (Dolomanov *et al.*, 2009)

Table S1 contd.: Experimental details

For all structures: $C_{19}H_{16}ClNO_4 \cdot C_7H_5NO_3S$, $M_r = 540.96$, triclinic, $P\bar{1}$, $Z = 2$. Experiments were carried out with Mo $K\alpha$ radiation using a Bruker SMART APEX2 area detector. H-atom parameters were constrained.

	4.34 GPa, 297K	5.06 GPa, 297 K
a, b, c (Å)	6.7109 (4), 9.4367 (12), 16.2988 (17)	6.6623 (3), 9.3453 (11), 16.2637 (15)
α, β, γ (°)	77.132 (9), 84.534 (7), 81.962 (9)	76.764 (8), 84.331 (6), 82.375 (8)
V (Å ³)	994.17 (18)	974.52 (16)
μ (mm ⁻¹)	0.36	0.37
Crystal size (mm)	0.25 × 0.05 × 0.04	0.25 × 0.05 × 0.04
Absorption correction	Multi-scan <i>SADABS2014/5</i> (Bruker,2014/5) was used for absorption correction. $wR2(int)$ was 0.0702 before and 0.0505 after correction. The Ratio of minimum to maximum transmission is 0.9046. The $I/2$ correction factor is Not present.	Multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. $wR2(int)$ was 0.0674 before and 0.0484 after correction. The Ratio of minimum to maximum transmission is 0.8882. The $I/2$ correction factor is Not present.
T_{min}, T_{max}	0.674, 0.745	0.662, 0.745
No. of measured, independent and observed [$I > 2.0\sigma(I)$] reflections	4363, 898, 715	4517, 894, 694
R_{int}	0.050	0.053
θ_{max} (°)	23.2	23.4
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.555	0.559
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.065, 0.153, 1.05	0.067, 0.185, 1.08
No. of reflections	898	894
No. of parameters	126	126
No. of restraints	24	24
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.33, -0.25	0.33, -0.33

Computer programs: *SAINT* v8.37A(Bruker AXS Inc., 2014) *SHELXT*(Sheldrick & IUCr, 2015) *XL* (Sheldrick, 2015) and *Olex2*(Dolomanov *et al.*, 2009)

Table S2: Selected hydrogen-bond parameters of INSA at pressure

$D-H\cdots A$	$D-H$ (Å)	$H\cdots A$ (Å)	$D\cdots A$ (Å)	$D-H\cdots A$ (°)
Ambient Pressure				
O16—H161 \cdots O17 ⁽ⁱ⁾	0.84	1.84	2.6803(18)	176.2
N26—H261 \cdots O28 ⁽ⁱⁱ⁾	0.88	2.04	2.8855(19)	159.8
0.55GPa				
O16—H161 \cdots O17 ⁽ⁱ⁾	0.82	1.86	2.639(9)	158.2
N26—H261 \cdots O28 ⁽ⁱⁱ⁾	0.86	2.04	2.860(10)	159.4
1.66GPa				
O16—H161 \cdots O17 ⁽ⁱ⁾	0.82	1.79	2.609(16)	173.2
N26—H261 \cdots O28 ⁽ⁱⁱ⁾	0.86	1.96	2.796(13)	162.7
3.33GPa				
O16—H161 \cdots O17 ⁽ⁱ⁾	0.82	1.73	2.543(10)	172.4
N26—H261 \cdots O28 ⁽ⁱⁱ⁾	0.86	1.89	2.725(13)	161.9
4.06GPa				
O16—H161 \cdots O17 ⁽ⁱ⁾	0.82	1.73	2.527(10)	172.8
N26—H261 \cdots O28 ⁽ⁱⁱ⁾	0.86	1.87	2.708(9)	160.2
4.34GPa				
O16—H161 \cdots O17 ⁽ⁱ⁾	0.82	1.7	2.514(11)	172.2
N26—H261 \cdots O28 ⁽ⁱⁱ⁾	0.86	1.85	2.685(11)	162.0
5.06GPa				
O16—H161 \cdots O17 ⁽ⁱ⁾	0.82	1.68	2.496(12)	170.4
N26—H261 \cdots O28 ⁽ⁱⁱ⁾	0.86	1.82	2.655(12)	159.0

Symmetry code(s): (i) $-x-1, -y+2, -z+2$; (ii) $-x+1, -y+1, -z$; (iii) $-x, -y+2, -z+1$; (iv) $-x+2, -y+1, -z+1$.