

Supplementary Material (ESI) for Chemical Communications

This journal is © The Royal Society of Chemistry 2005

Electronic Supplementary Information for:

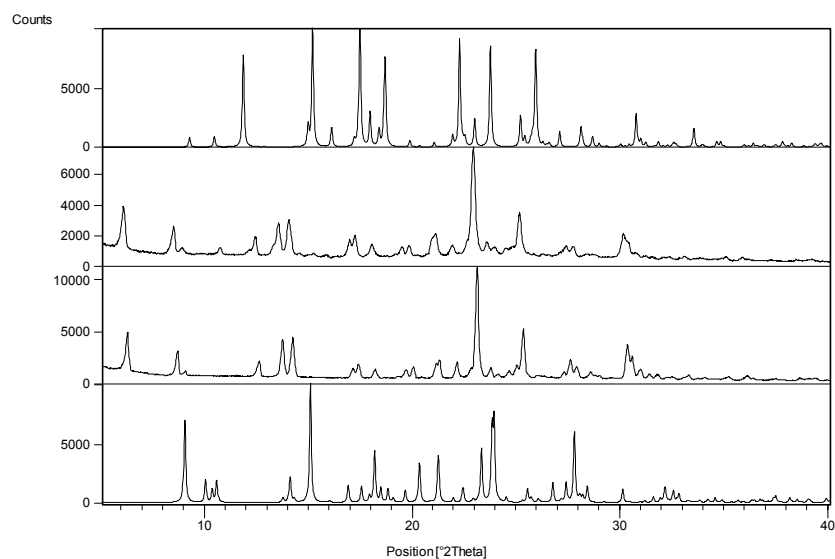
"Screening for Crystalline Salts via Mechanochemistry"

A. V. Trask, D. A. Haynes, W. D. S. Motherwell and W. Jones.

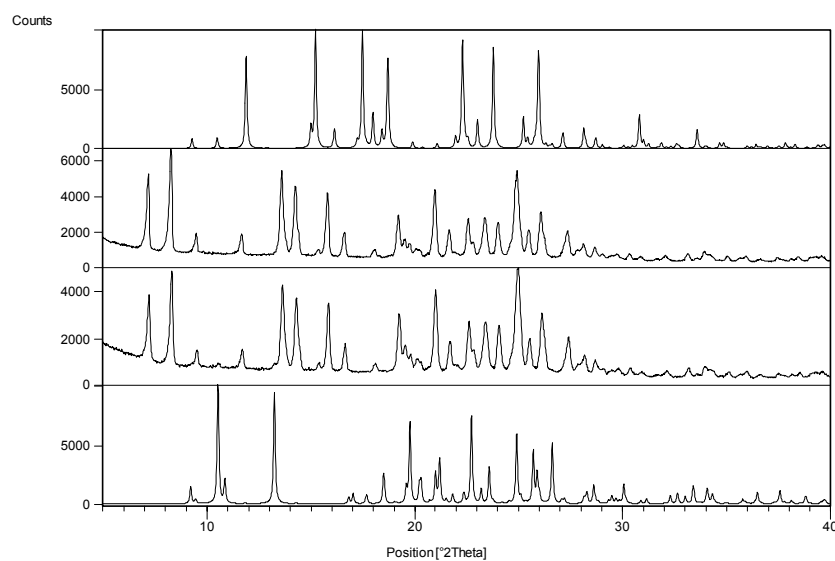
Literature references for all CSD crystal structures in manuscript text

CSD Reference Code	Description	Literature Reference
AMXBPM10	T free base	T. F. Koetzle and G. J. B. Williams. <i>J. Am. Chem. Soc.</i> , 1976, 98 , 2074.
MUFMAB	P free base	V. Sethuraman and P. T. Muthiah. <i>Acta Crystallogr.</i> , 2002, E58 , o817.
TMPFOR	T:formate	B. Umadevi, P. Prabakaran and P. T. Muthiah. <i>Acta Crystallogr.</i> , 2002, C58 , o510.
FUWVAU	T:acetate	R. F. Bryan, R. C. Haltiwanger and M. K. Woode. <i>Acta Crystallogr.</i> , 1987, C43 , 2412.
QIKDIX	T:maleate	P. Prabakaran, J. J. Robert, P. T. Muthiah, G. Bocelli and L. Righi. <i>Acta Crystallogr.</i> , 2001, C57 , 459.
CACBOY	T:glutarate	J. J. Robert, S. B. Raj and P. T. Muthiah. <i>Acta Crystallogr.</i> , 2001, E57 , o1206.
MIFWUT	T:salicylate (methanol solvate)	P. Panneerselvam, N. Stanley and P. T. Muthiah. <i>Acta Crystallogr.</i> , 2002, E58 , o180.
UHAYIL	P:formate	N. Stanley, V. Sethuraman, P. T. Muthiah, P. Luger and M. Weber. <i>Cryst. Growth Des.</i> , 2002, 2 , 631.
CIVDIU	P:acetate (monohydrate)	P. K. Bryant, J. Colby, R. G. Jenks, P. R. Lowe and C. H. Schwalbe. <i>Acta Crystallogr.</i> , 1984, A40 , C79.
ULAXOU	P:maleate	V. Sethuraman, N. Stanley, P. T. Muthiah, W. S. Sheldrick, M. Winter, P. Luger and M. Weber. <i>Cryst. Growth Des.</i> , 2003, 3 , 823.
ULAXIO	P:fumarate	V. Sethuraman, N. Stanley, P. T. Muthiah, W. S. Sheldrick, M. Winter, P. Luger and M. Weber. <i>Cryst. Growth Des.</i> , 2003, 3 , 823.
ULAYAH	P:succinate	V. Sethuraman, N. Stanley, P. T. Muthiah, W. S. Sheldrick, M. Winter, P. Luger and M. Weber. <i>Cryst. Growth Des.</i> , 2003, 3 , 823.
UHAYEH	P:glutarate	N. Stanley, V. Sethuraman, P. T. Muthiah, P. Luger and M. Weber. <i>Cryst. Growth Des.</i> , 2002, 2 , 631.
CIVDOA	P:salicylate	P. K. Bryant, J. Colby, R. G. Jenks, P. R. Lowe and C. H. Schwalbe. <i>Acta Crystallogr.</i> , 1984, A40 , C79.
MALIAC11	maleic acid	M. N. G. James and G. J. B. Williams. <i>Acta Crystallogr.</i> , 1974, B30 , 1249.
SUCACB06	succinic acid	I. M. Dodd, S. J. Maginn, M. M. Harding and R. J. Davey. Private Communication to CCDC. See www.ccdc.cam.ac.uk

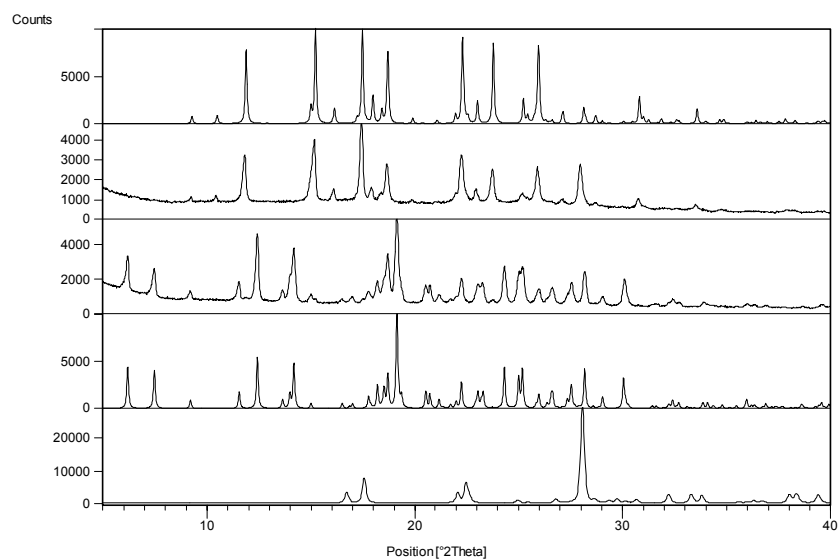
Overlays of all PXRD patterns from 'neat grinding' and 'solvent-drop grinding' experiments involving T and P.



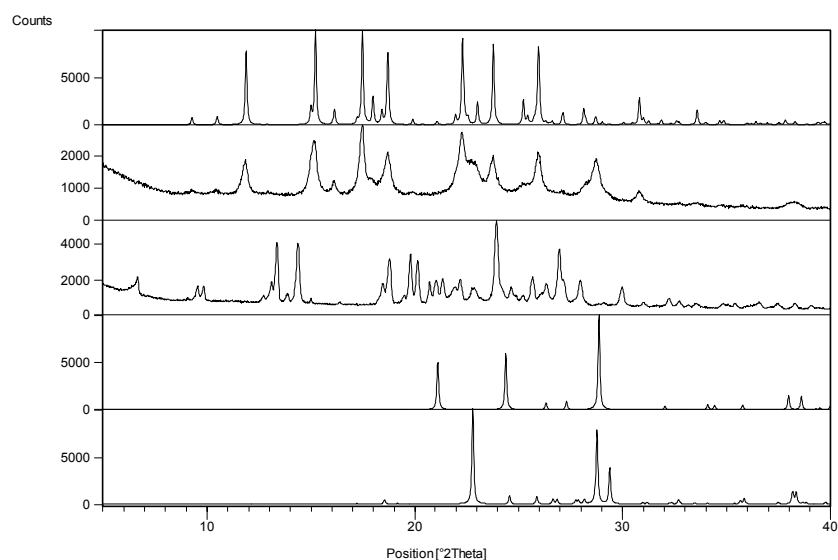
Top to bottom: T, simulated from CSD AMXBPM10; Neat grinding of T with formic acid; Methanol solvent-drop grinding of T with formic acid; T:formate simulated from CSD TMPFOR01



Top to bottom: T, simulated from CSD AMXBPM10; Neat grinding of T with acetic acid; Methanol solvent-drop grinding of T with acetic acid; T:acetate simulated from CSD FUWVAU



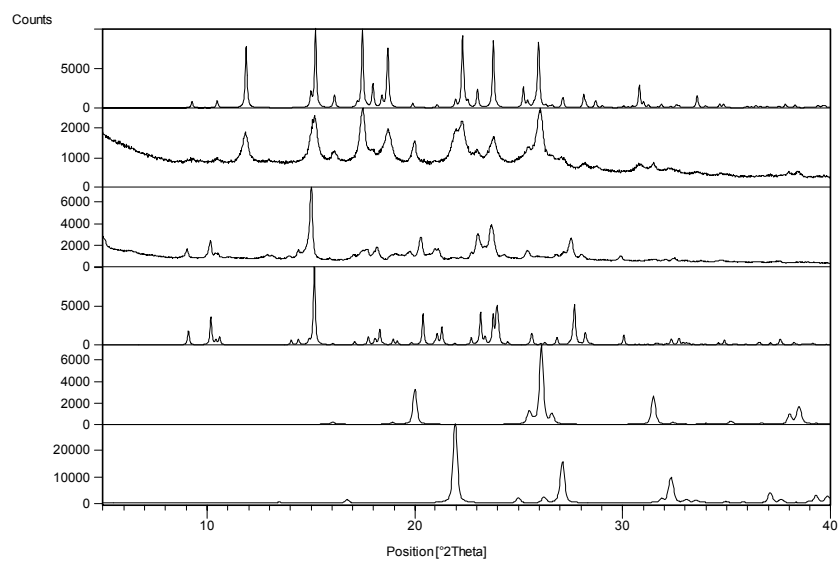
Top to bottom: **T**, simulated from CSD AMXBPM10; Neat grinding of **T** with maleic acid; Methanol solvent-drop grinding of **T** with maleic acid; **T**:maleate simulated from CSD QIKDIX; Maleic acid, simulated from CSD MALIAC11



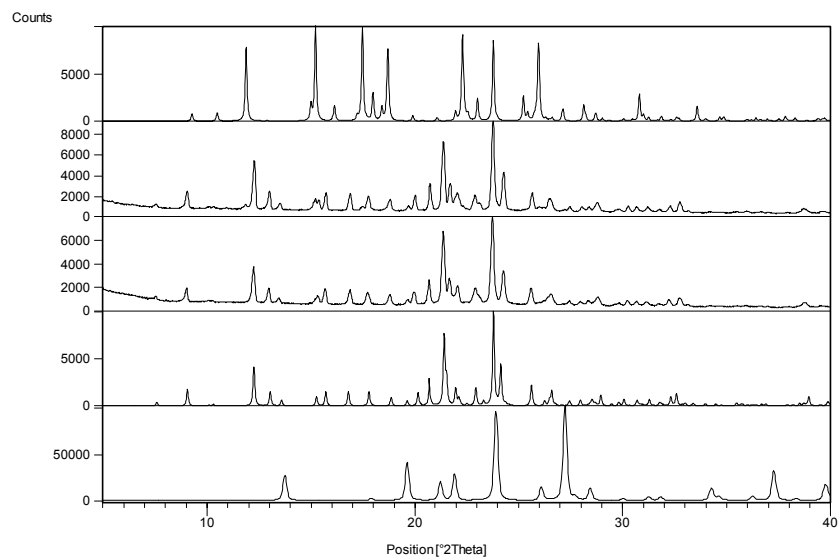
Top to bottom: **T**, simulated from CSD AMXBPM10; Neat grinding of **T** with fumaric acid; Methanol solvent-drop grinding of **T** with fumaric acid; fumaric acid beta polymorph, simulated from CSD FUMAAC01; Fumaric acid alpha polymorph, simulated from CSD FUMAAC

Supplementary Material (ESI) for Chemical Communications

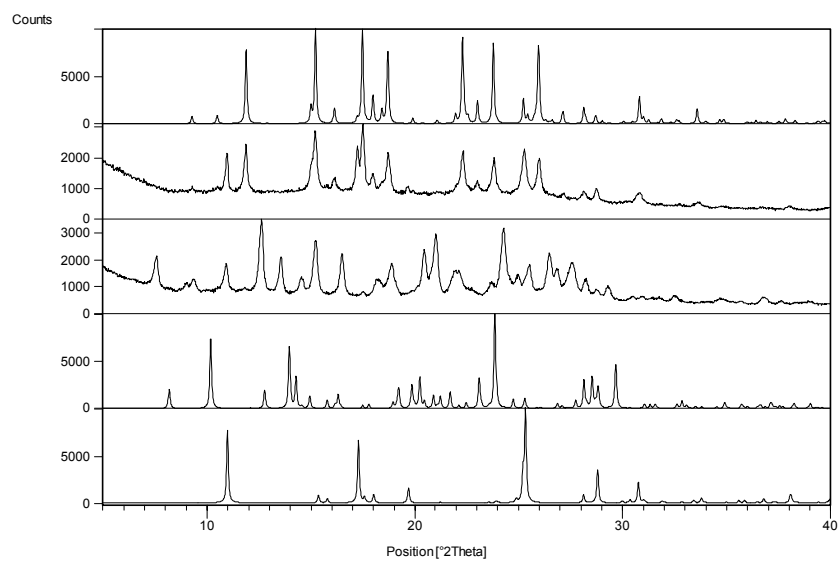
This journal is © The Royal Society of Chemistry 2005



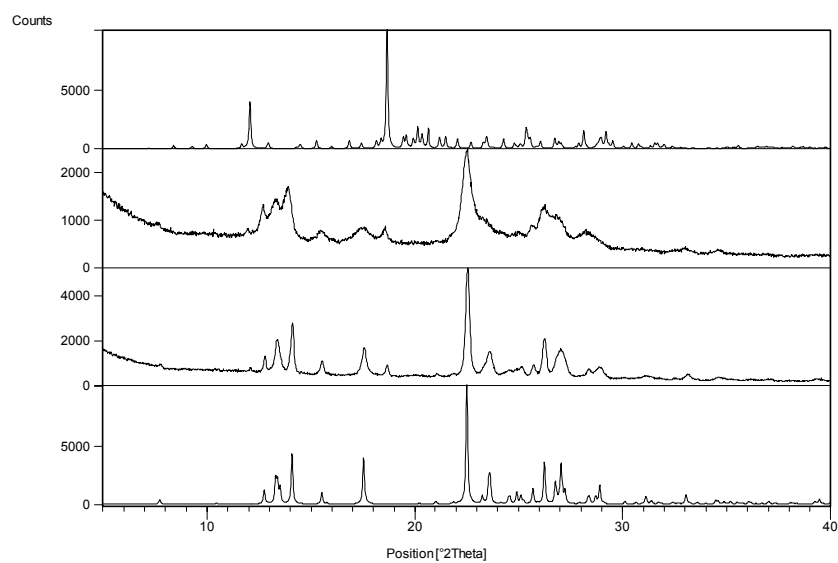
Top to bottom: **T**, simulated from CSD AMXBPM10; Neat grinding of **T** with succinic acid; Methanol solvent-drop grinding of **T** with succinic acid; **T**:succinate simulated from crystal structure data obtained in this study (CIF available as ESI); Succinic acid beta polymorph, simulated from CSD SUCACB06; Succinic acid alpha polymorph, simulated from CSD SUCACB07



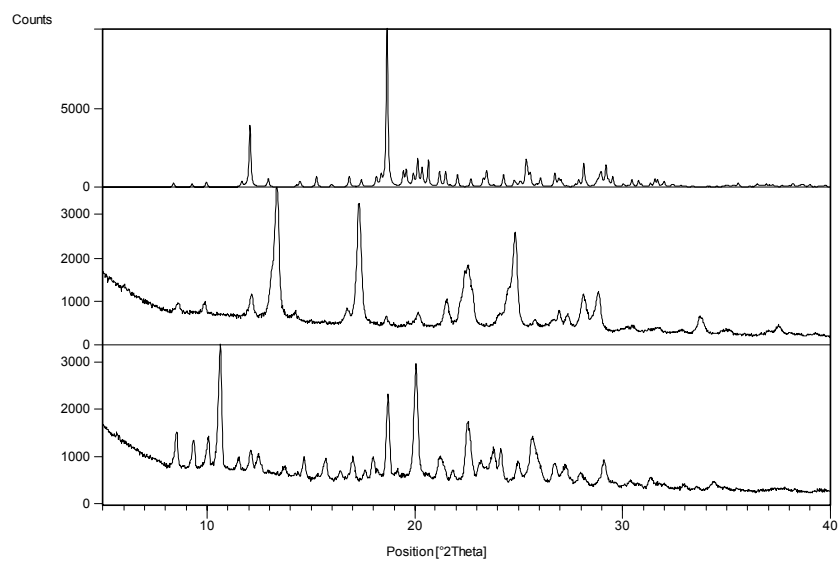
Top to bottom: **T**, simulated from CSD AMXBPM10; Neat grinding of **T** with glutaric acid; Methanol solvent-drop grinding of **T** with glutaric acid; **T**:glutarate simulated from CSD CACBOY; Glutaric acid beta polymorph, simulated from CSD GLURAC04



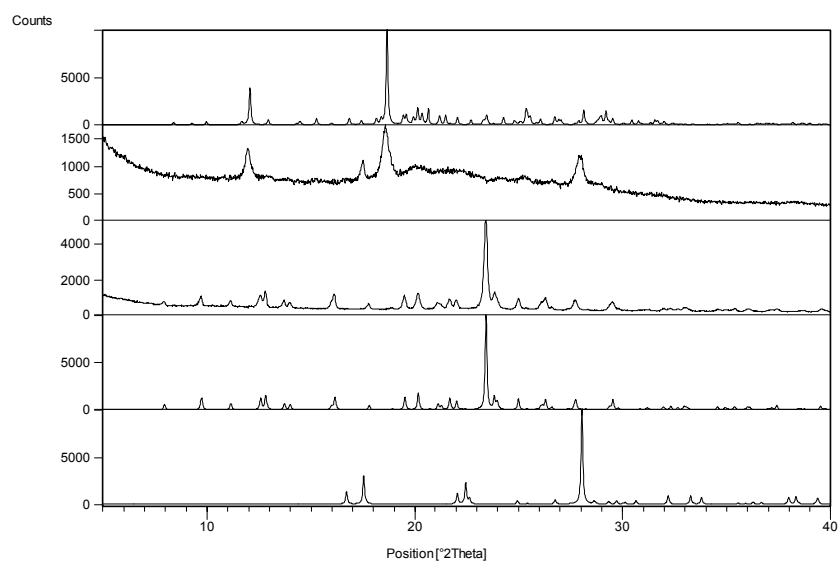
Top to bottom: **T**, simulated from CSD AMXBPM10; Neat grinding of **T** with salicylic acid; Methanol solvent-drop grinding of **T** with salicylic acid; **T**:salicylate simulated from CSD MIFWUT; Salicylic acid simulated from CSD SALIAC



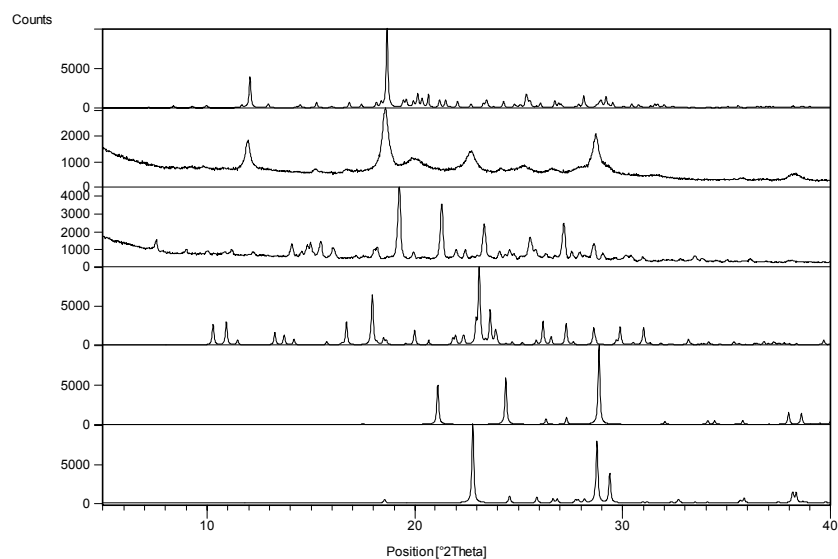
Top to bottom: **P**, simulated from CSD MUFMAB; Neat grinding of **P** with formic acid; Methanol solvent-drop grinding of **P** with formic acid; **P**:formate simulated from CSD UHAYIL



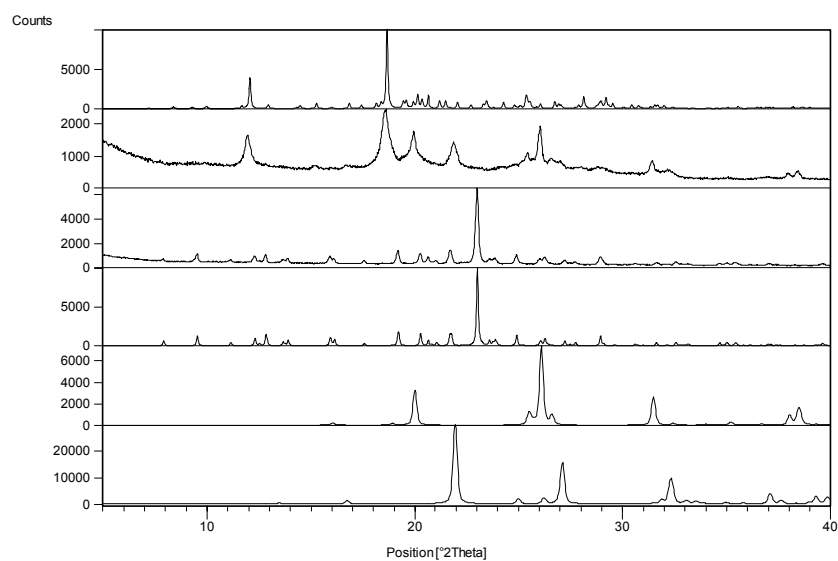
Top to bottom: **P**, simulated from CSD MUFMAB; Neat grinding of **P** with acetic acid; Methanol solvent-drop grinding of **P** with acetic acid



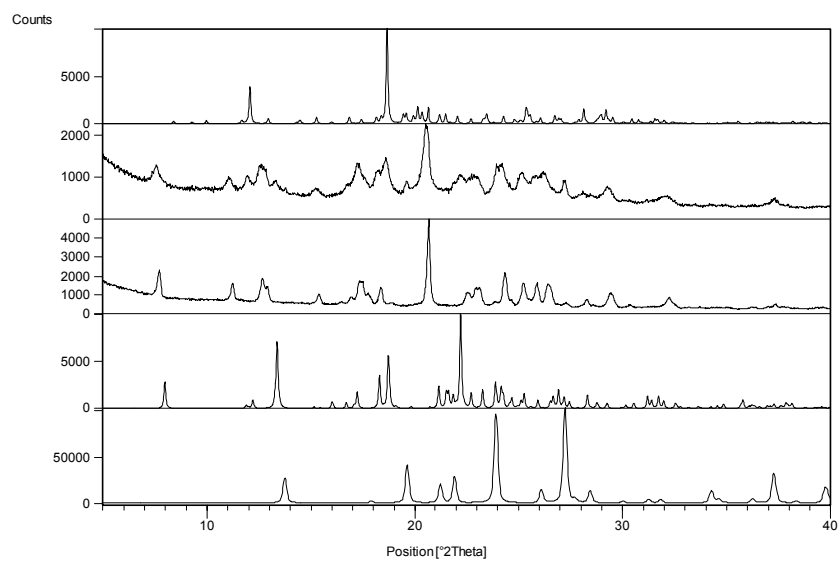
Top to bottom: **P**, simulated from CSD MUFMAB; Neat grinding of **P** with maleic acid; Methanol solvent-drop grinding of **P** with maleic acid; **P**:maleate simulated from CSD ULAXOU; Maleic acid simulated from CSD MALIAC11



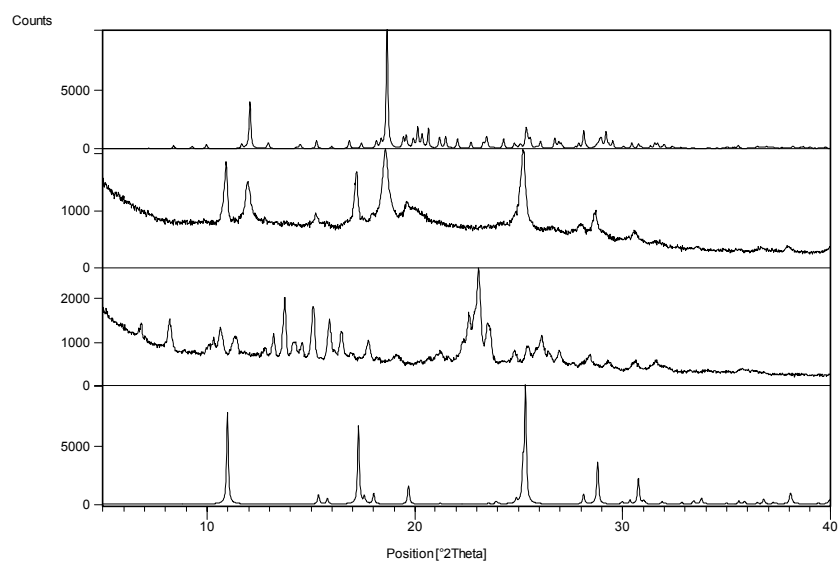
Top to bottom: **P**, simulated from CSD MUFMAB; Neat grinding of **P** with fumaric acid; Methanol solvent-drop grinding of **P** with fumaric acid; **P**:fumarate simulated from CSD ULAXIO; Fumaric acid beta polymorph simulated from CSD FUMAAC01; Fumaric acid alpha polymorph simulated from CSD FUMAAC



Top to bottom: **P**, simulated from CSD MUFMAB; Neat grinding of **P** with succinic acid; Methanol solvent-drop grinding of **P** with succinic acid; **P**:succinate simulated from CSD ULAYAH; Succinic acid beta polymorph simulated from CSD SUCACB06; Succinic acid alpha polymorph simulated from CSD SUCACB07



Top to bottom: **P**, simulated from CSD MUFMAB; Neat grinding of **P** with glutaric acid; Methanol solvent-drop grinding of **P** with glutaric acid; **P**:glutarate simulated from CSD UHAYEH; Glutaric acid simulated from CSD GLURAC04



Top to bottom: **P**, simulated from CSD MUFMAB; Neat grinding of **P** with salicylic acid; Methanol solvent-drop grinding of **P** with salicylic acid; Salicylic acid simulated from CSD SALIAC