Slow evaporation crystallization experiments for 3-oxauracil

The * symbol denotes a crystallization vial previously treated with $SiCl_2Me_2$. The plastic caps for the crystallization vials were generally punctured twice with a needle to allow slow evaporation. Where the † symbol is given below, the caps were punctured four times. Where the anhydrous (ANH) and monohydrate (MHY) forms were distinguished from their unit cells, this is noted in the final column.

Vial	Solvent	Co-solvent	Notes
A	Water	Ethanol	
B*	Water	Ethanol	
C	Water	THF	
D*	Water	THF	
E	Water	Acetone	
F*	Water	Acetone	
G	Water	Acetonitrile	
H*	Water	Acetonitrile	
I	Water	Propan-1-ol	
J*	Water	Propan-1-ol	Crystals – no cell obtained
K	Water	DMSO	
L*	Water	DMSO	
M	Methanol	Toluene	
N*	Methanol	Toluene	
O	Methanol	THF	
P*	Methanol	THF	
Q	Methanol	Acetonitrile	
R*	Methanol	Acetonitrile	Crystals – MHY cell
S	Methanol	Acetone	
T*	Methanol	Acetone	Crystals – MHY cell
U	Methanol	Propan-1-ol	
V*	Methanol	Propan-1-ol	
W	Methanol	DMSO	
X*	Methanol	DMSO	
Y	1,2-Dimethoxyethane	DMSO	
Z*	1,2-Dimethoxyethane	DMSO	
AA	1,2-Dimethoxyethane	Butan-1-ol	
AB*	1,2-Dimethoxyethane	Butan-1-ol	
AC	1,2-Dimethoxyethane	Propan-2-ol	
AD*	1,2-Dimethoxyethane	Propan-2-ol	
AE	1,2-Dimethoxyethane	Ethanol	
AF*	1,2-Dimethoxyethane	Ethanol	
AG	1,2-Dimethoxyethane	Toluene	Crystals – ANH data collection
AH*	1,2-Dimethoxyethane	Toluene	Crystals – ANH cell
AI	1,2-Dimethoxyethane	Acetonitrile	
AJ*	1,2-Dimethoxyethane	Acetonitrile	Crystals – MHY cell
AK	1,2-Dimethoxyethane	Ethyl acetate	
AL*	1,2-Dimethoxyethane	Ethyl acetate	
AM	1,2-Dimethoxyethane	THF	
AN*	1,2-Dimethoxyethane	THF	
AO	Methanol	Ethyl acetate	
AP*	Methanol	Ethyl acetate	Crystals – MHY data collection

AQ†	DMF	DMSO	
AR*†	DMF	DMSO	
AS†	Pyridine	DMSO	
AT*†	Pyridine	DMSO	
AU†	Pyridine	Butan-1-ol	
AV*†	Pyridine	Butan-1-ol	
AW†	DMF	Butan-1-ol	
AX*†	DMF	Butan-1-ol	
AY†	Pyridine	Propan-2-ol	
AZ*†	Pyridine	Propan-2-ol	
AAA†	DMF	Propan-2-ol	
AAB*†	DMF	Propan-2-ol	
AAC†	Pyridine	Toluene	
AAD*†	Pyridine	Toluene	
AAE†	DMF	Toluene	
AAF*†	DMF	Toluene	
AAG	Water	Propan-2-ol	
AAH*	Water	Propan-2-ol	
AAI	Methanol	Ethyl acetate	
AAJ*	Methanol	Ethyl acetate	
AAK	Methanol	Methyl acetate	
AAL*	Methanol	Methyl acetate	
AAM	Methanol	Propan-2-ol	
AAN*	Methanol	Propan-2-ol	Crystals – MHY cell
AAO	1,4-Dioxane	THF	
AAP*	1,4-Dioxane	THF	
AAQ	Methanol	Dichloromethane	
AAR*	Methanol	Dichloromethane	
AAS	1,2-Dimethoxyethane	Dichloromethane	
AAT*	1,2-Dimethoxyethane	Dichloromethane	
AAU	Pyridine	Dichloromethane	
AAV*	Pyridine	Dichloromethane	
AAW	DMF	Ethanol	
AAX*	DMF	Ethanol	
AAY	DMF	THF	
AAZ*	DMF	THF	
BA	DMF	Acetone	
BB*	DMF	Acetone	
BC	DMF	Acetonitrile	
BD*	DMF	Acetonitrile	
BE	DMF	Ethyl acetate	
BF*	DMF	Ethyl acetate	
BG	Pyridine	THF	
BH*	Pyridine	THF	
BI	Pyridine	Acetonitrile	
BJ*	Pyridine	Acetonitrile	
BK	Pyridine	Ethyl acetate	
BL*	Pyridine	Ethyl acetate	
BM	1,4-dioxane	Ethanol	
BN*	1,4-dioxane	Ethanol	

BO	1,4-dioxane	THF	
BP*	1,4-dioxane	THF	
BQ	1,4-dioxane	Acetone	
BR*	1,4-dioxane	Acetone	
BS	1,4-dioxane	Acetonitrile	
BT*	1,4-dioxane	Acetonitrile	
BU	1,4-dioxane	Propan-2-ol	
BV*	1,4-dioxane	Propan-2-ol	Crystals – MHY cell
BW	1,4-dioxane	Butan-1-ol	
BX*	1,4-dioxane	Butan-1-ol	
BY	1,4-dioxane	Toluene	
BZ*	1,4-dioxane	Toluene	
CA	1,4-dioxane	DMSO	
CB*	1,4-dioxane	DMSO	
CC	1,4-dioxane	Ethyl acetate	
CD*	1,4-dioxane	Ethyl acetate	
CE	1,4-dioxane	Ethyl acetate	
CF*	1,4-dioxane	Ethyl acetate	