Support Information

Design, screening, and properties of novel solvates of azoxystrobin based on isomorphism

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Table S1. Summary of the molecular size of the solvent in the reported AZO solvates.

Solvate (solvent)	Ratio	Solvent length (Å)	Solvent width (Å)	Solvent thickness (Å)
Diethyl oxalate	2:1	12.43	6.06	3.97
n-Heptane	2:1	11.71	4.37	3.97
Butyl acetate	2:1	11.41	5.36	3.97
Pyridine	1:1	6.52	6.49	3.0
1,4-Dioxane	1:1	6.29	4.93	4.19
DCE	1:1	6.76	6.25	3.99
DMF	1:1	6.70	6.37	4.35
THF	1:1	6.41	6.37	3.98
Acetone	1:1	6.49	5.10	3.96
Acetic acid	1:1	6.26	5.10	3.96
Dichloromethane	1:1	6.69	4.76	4.02
Chloroform	1:1	6.65	6.25	4.54

Table S2. Molecular sizes of 54 solvents

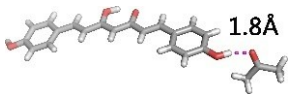
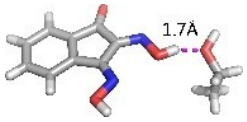
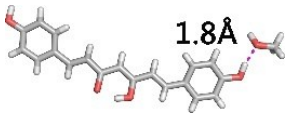
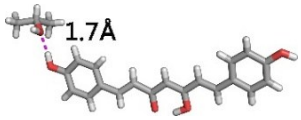
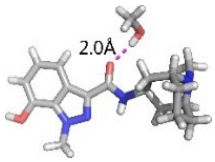
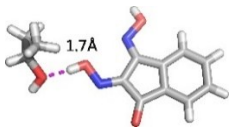
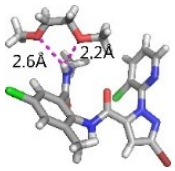
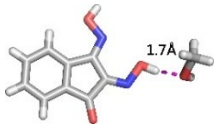
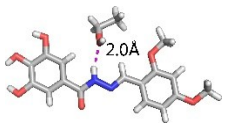
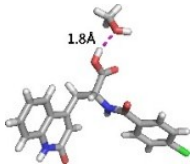
Solvent	**Length (Å)**	**Width (Å)**	**Thickness (Å)**
n-Octanol	14.05	4.37	3.96
Diethyl malonate	9.85	7.66	5.73
n-Butyl ether	14.01	4.38	3.97
n-Octane	13.00	4.43	3.97
1,2-Diethoxyethane	12.47	4.47	3.98
Dimethyl succinate	12.34	4.35	3.98
Ethyl butyrate	11.42	5.29	3.97
Isopropylbenzene	9.37	6.56	6.50
Ethyl lactate	10.09	6.21	5.27
4-Methyl-2-pentanone	9.08	5.27	5.70
Ethyl cyanoacetate	10.69	5.38	3.98
Paraxylene	8.88	6.50	3.97
n-Hexane	10.43	4.73	3.97
Anisole	9.30	6.49	4.42
Methyl tert-butyl ether	7.57	6.52	5.30
Cyclohexane	7.22	6.54	4.98
Toluene	8.15	6.50	3.97
Benzyl alcohol	9.22	6.51	3.97
Trifluorotoluene	8.40	6.51	4.93
Sulfolane	6.42	6.71	5.65
3-Methyl-1-butanol	8.90	5.96	4.96
2-Ethoxyethanol	9.92	4.46	3.98
N-methylpyrrolidone	7.26	7.03	4.47
N,N-dimethylacetamide	6.80	6.41	3.98
2-Methyltetrahydrofuran	7.52	5.84	5.05
Cyclohexanone	7.61	6.54	4.90
Chlorobenzene	8.59	6.51	3.60
tert-Butanol	6.52	5.80	5.65
Ether	8.89	4.46	3.98
n-butanol	8.91	4.36	3.96
Cyclopentanol	6.35	6.07	5.89
Ethylene glycol dimethyl ether	9.88	4.47	3.98
Diethylamine	8.99	4.42	3.97
2-Butanone	7.82	5.20	3.96
Ethyl acetate	8.84	5.34	3.97
2-Nitropropane	7.65	5.03	4.24
2-Butanol	7.84	5.21	4.60
Isobutanol	7.05	6.55	6.30
1,3-Propanediol	8.67	4.34	3.98
DMSO	6.89	5.59	5.41
Thiophene	6.82	6.39	3.70
1,2-Propanediol	7.38	5.98	5.27

Isopropanol	6.53	5.85	5.27
Ethyl formate	7.95	5.29	4.79
Ethylene glycol	7.39	4.56	3.98
1-Propanol	7.62	4.35	3.98
Trifluoroethanol	6.79	4.94	4.64
Furan	6.35	5.50	2.80
Ethanol	6.33	4.12	3.97
Nitromethane	5.04	4.98	3.99
Acetonitrile	5.62	3.97	3.74
Methanol	4.62	3.99	3.98
Formic acid	5.05	4.84	2.80
Water	3.78	3.07	2.80

Table S3. Interaction energies between AZO and solvent in AZO solvates.

Solvate (solvent)	**ΔE = E - (E1 + E2) kJ/mol**
Dimethyl succinate	13.73
Diethyl oxalate	10.65
n-Heptane	4.85
Acetic acid	13.87
DMF	9.10
Chloroform	8.64
Acetone	7.90
1,4-Dioxane	7.45
THF	6.37
Dichloromethane	3.81
Furan	3.56
1,2-Dichloroethane	3.59
Pyridine	3.19

Table S4. Interaction energies between API and solvent in selected solvates.

Solvate (CCDC)	Dimer structure	ΔE = E - (E1 + E2) kJ/mol
1867869		43.92
798077		42.92
1867871		41.67
1867870		40.02
768421		38.00
798083		34.60
1505332		32.91
798080		31.67
738267		30.91
1404894		30.89

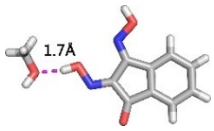
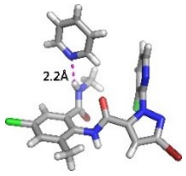
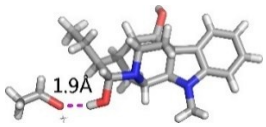
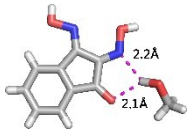
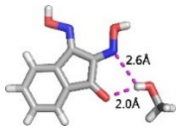
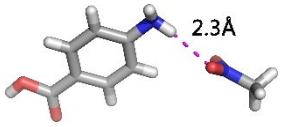
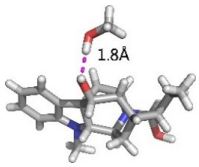
798079		30.12
1505333		27.48
774768		26.52
798082		24.66
798081		22.51
1539150		22.30
774767		22.21

Table S5. Hydrogen bonds for six solvates.

solvate	C-H…A	Distance(Å) H…A	Angle (°) C-H…A
AZO-DMS	C_{11}-H_{11}···O_5	2.61	122.6
	C_{20}-H_{20A}···O_4	2.65	159.7
	C_{22}-H_{22C}···O_4	2.49	164.7
	C_{4S}-H_{4S}···N1	2.55	135.1
AZO-FN	C_{11}-H_{11}···O_5	2.59	125.0
	C_{22}-H_{22B}···O_2	2.55	157.1
	C_{22}-H_{22C}···O_4	2.47	167.8
	C_{20}-H_{20A}···O_4	2.59	163.2
	C_{1S}-H_{1S}···O_4	2.51	157.6
AZO-BAC	C_{20}-H_{20}···O_4	2.51	85.7
	C_{13}-H_{13}···N_2	2.78	138.3
	C_{14}-H_{14}···O2S	2.34	148.9
AZO-DCE	C_{20}-H_{20C}···O_4	2.40	91.3
	C_{13}-H_{13}···N_2	2.78	138.2
	C_{1S}-H_{1AS}···N_1	2.56	103.3
	C_{1S}-H_{1BS}···N_1	2.48	119.3
AZO-DCM	C_{20}-H_{20C}···O_4	2.36	94.1
	C_{13}-H_{13}···N_2	2.71	137.9
	C_S-H_S···N_1	2.79	157.6
AZO-TCM	C_{20}-H_{20C}···O_4	2.52	84.6
	C_{13}-H_{13}···N_2	2.87	143.3
	C_S-H_S···N_1	2.45	137.2

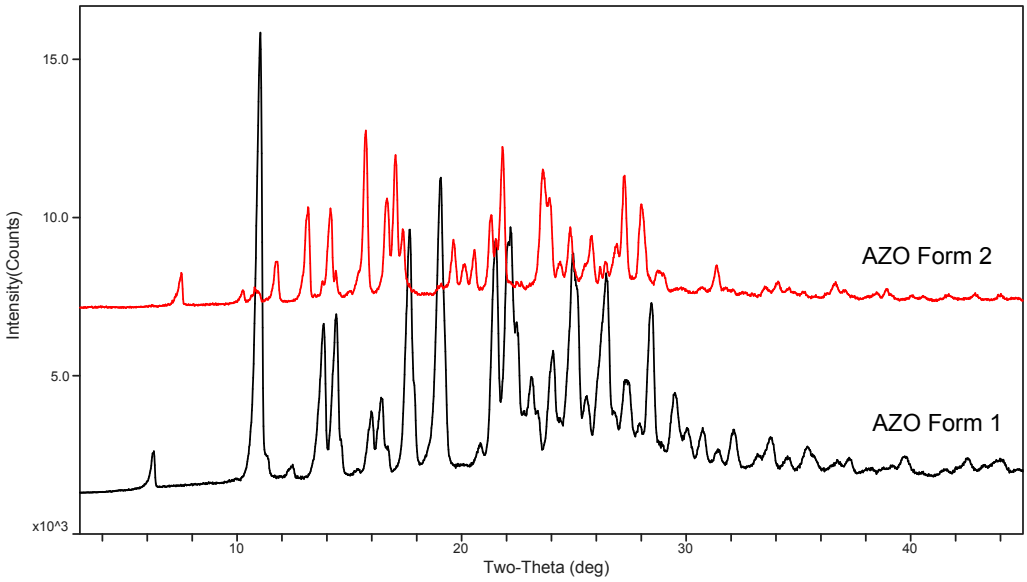


Fig. S1. PXRD patterns of AZO Form 1 and Form 2.

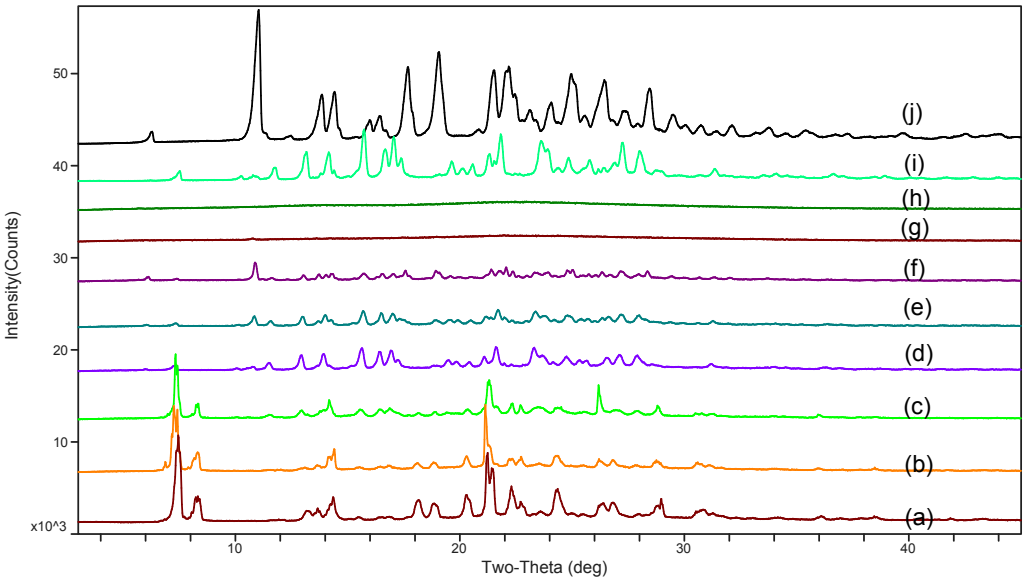


Fig. S2. Crystal form of (a) AZO-DEE, and AZO-DEE solvate heated to different temperatures: (b) 60 °C, (c) 70 °C, (d) 80 °C, (e) 90 °C, (f) 100 °C, (g) 110 °C, (h) 120 °C, (i) AZO form 2, and (j) AZO form 1.

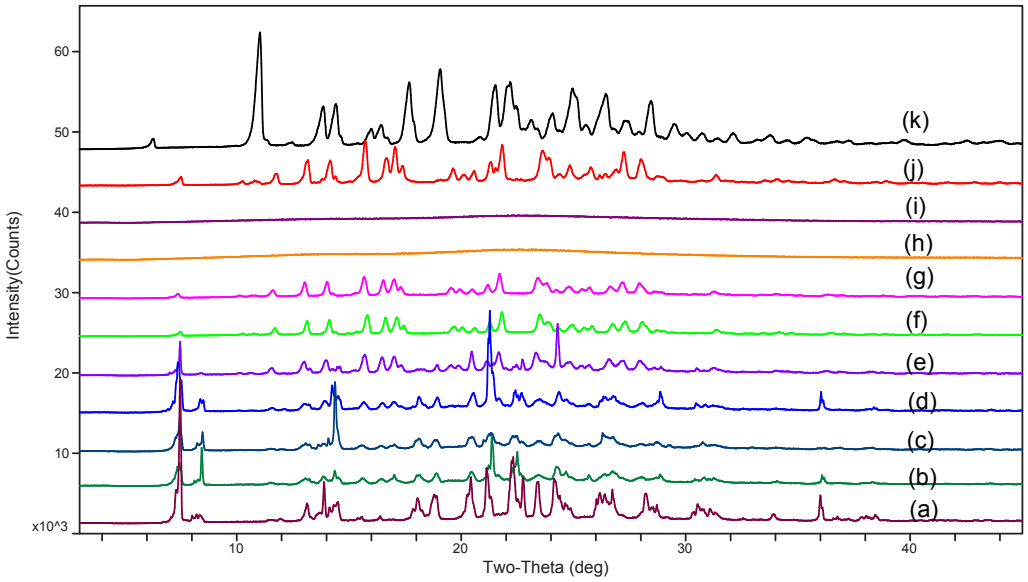


Fig. S3. Crystal form of (a) AZO-EB, and AZO-EB solvate heated to different temperatures: (b) 50 °C, (c) 60 °C, (d) 70 °C, (e) 80 °C, (f) 90 °C, (g) 100 °C (h) 110 °C, (i) 120 °C, (j) AZO form 2, and (k) AZO form 1.

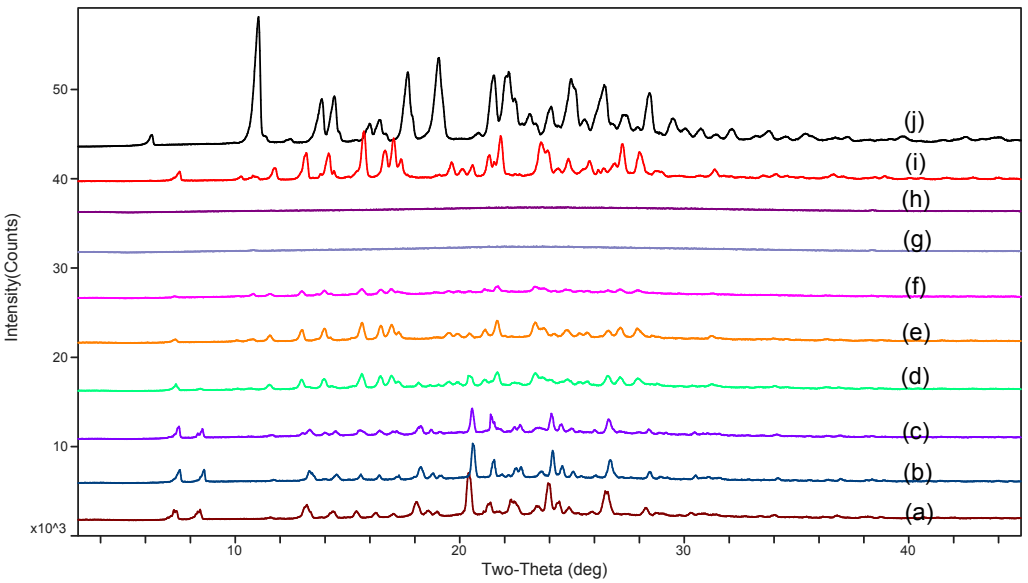


Fig. S4. Crystal form of (a) AZO-FN, and AZO-FN solvate heated to different temperatures: (b) 60 °C, (c) 70 °C, (d) 80 °C, (e) 90 °C, (f) 100 °C, (g) 110 °C, (h) 120 °C, (i) AZO form 2, and (j) AZO form 1.

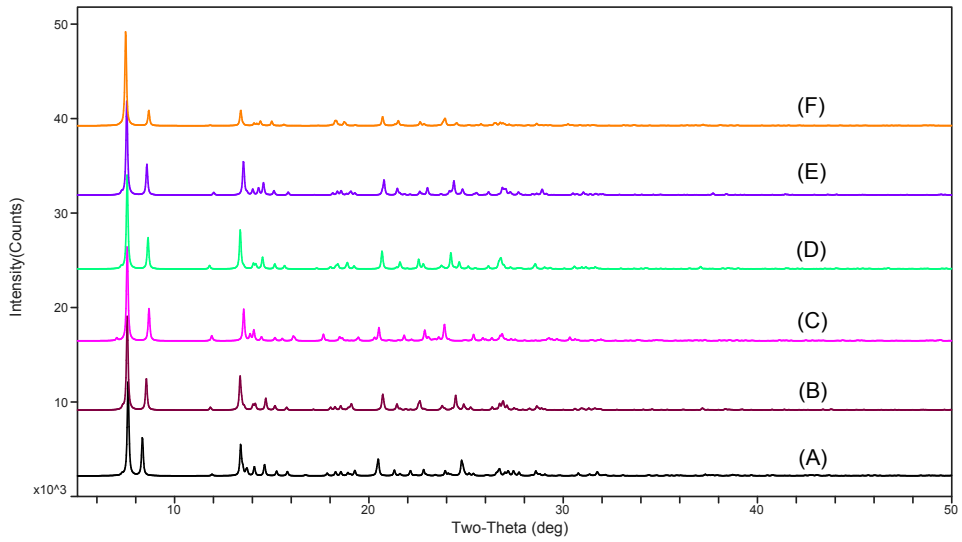


Fig. S5. Hypothetical powder X-ray diffractometric patterns of AZO solvates with (A) Dimethyl succinate, (B) butyl acetate, (C) chloroform, (D) furan, (E) dichloromethane, and (F) 1,2-dichloroethane, calculated from the unit cell structure, from which the solvent molecules had been removed using *Mercury 3.3* software.