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Supporting information for article:

Improved performance of crystal structure solution from powder diffraction data through parameter tuning of a simulated annealing algorithm

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Table S1: Compound names and corresponding CSD reference codes of the 101 crystal structures, together with the code names used throughout this work.

Code	Compound Name	CSD refcode	Reference
A1	Alaptide	KUTBEH	(Rohlicek *et al.*, 2010)
A2	Hydrochlorothiazide	HCSBTZ	(Dupont & Dideberg, 1972)
A3	Dapsone	DAPSUO10	(Alleaume, 1967)
A4	2-(Phenylsulfonyl)acetamide	Not deposited	(Florence *et al.*, 2005)
A5	Captopril	MCPRPL	(Fujinaga & James, 1980)
A6	Methyl 4-[(4-aminophenyl)ethynyl]-benzoate	Not deposited	(Florence *et al.*, 2005)
A7	Zopiclone	CUHNEY10	(Borea *et al.*, 1987)
A8	2-(4-Hydroxy-2-oxo-2,3-dihydro-1,3-benzothiazol-7-yl) ethylammonium chloride	BIFRAK	(Florence *et al.*, 2005)
A9	Salbutamol	BHHPHE	(Beale & Stephens, 1972)
A10	Dopamine hydrobromide	QQQAEJ01	(Shankland *et al.*, 1996)
A11	Chlorpropamide	BEDMIG	(Koo *et al.*, 1980)
A12	Creatine monohydrate	CREATH03	(Kato *et al.*, 1979)
A13	2,5-dioxopyrrolidin-1-yl 2-(benzoylsulfanyl) acetate	OQUPOG	(Rukiah & Al-Ktaifani, 2011)
A14	α-Lactose monohydrate	LACTOS10	(Fries *et al.*, 1971)
A15	Promazine hydrochloride	PROMZC01	(David *et al.*, 1998)
A16	Tolbutamide	ZZZPUS02	(Donaldson *et al.*, 1981)
A17	Carbamazepine dihydrate	FEFNOT01	(Florence *et al.*, 2005)
A18	Pigment orange 36 (PO 36)	HOYVOH	(van de Streek *et al.*, 2009)
A19	(4'-(2-(p-Tosylamino)benzylideneamino)-2,3-benzo-15-crown-5)-isothiocyanato-lithium	RIFVEI	(Dorokhov *et al.*, 2007)
A20	Famotidine	FOGVIG03	(Florence *et al.*, 2003)
A21	Sotalol hydrochloride	SOTALC	(Gadret *et al.*, 1976)
A22	Glipizide	SAXFED	(Burley, 2005)
A23	Diltiazem hydrochloride	CEYHUJ01	(Kojicprodic *et al.*, 1984)
A24	Zopiclone dihydrate	UCUVET	(Shankland *et al.*, 2001)
A25	Capsaicin	FABVAF01	(David *et al.*, 1998)
A26	Pigment yellow (PY 181 polymorph β)	GITWUC	(van de Streek *et al.*, 2009)
A27	Clarithromycin monohydrate	LAQSON	(Noguchi, Fujiki, *et al.*, 2012)
A28	Sodium 4-[(E)-(4-hydroxyphenyl)diazenyl] benzene sulfonate dihydrate	YAYWUQ	(Kennedy *et al.*, 2001)
A29	Indomethacin:nicotinamide 1:1	SESKUY	(Majumder *et al.*, 2013)
A30	Carbamazepine:indomethacin 1:1	LEZKEI	(Majumder *et al.*, 2013)
A31	2-[3-(2-Phenylethoxy)propyl sulfonyl] ethyl benzoate	BIFREO	(Florence *et al.*, 2005)
A32	S-Ibuprofen	JEKNOC10	(Freer *et al.*, 1993)
A33	Ampicilline trihydrate	AMPCIH01	(Burley *et al.*, 2006)
A34	Verapamil hydrochloride	CURHOM	(Carpy *et al.*, 1985)
A35	Amodiaquinium dichloride dihydrate	SENJIF	(Llinas *et al.*, 2006)
A36	Nifedipine (polymorph C)	BICCIZ01	(Bortolotti *et al.*, 2011)
A37	N-(2-(4-Hydroxy-2-oxo-2,3-dihydro-1,3-benzothiazol-7-yl)ethyl)-3-(2-(2-naphthalen-1-ylethoxy) ethylsulfonyl) propylaminium benzoate	PAHFIO	(Johnston *et al.*, 2004)

Code	Compound Name	CSD refcode	Reference
A38	Carbamazepine (polymorph γ)	CBMZPN13	(Fernandes, Shankland, *et al.*, 2007)
A39	Cyheptamide	TEVSOD01	(Florence *et al.*, 2008)
A40	Ornidazole	NETRUZ	(Shin *et al.*, 1995)
B1	Tetraformaltrisazine	UDALIV	(Albov *et al.*, 2006)
B2	Decalin	POVZUW	(Eibl *et al.*, 2009)
B3	Pigment violet	QAMQOL	(Schmidt *et al.*, 2005)
B4	N,N'-Bis[1-pyridin-4-yl-meth-(E)-ylidene]hydrazine	LIZCUS	(Shanmuga Sundara Raj *et al.*, 2000)
B5	β- Phenazepam	BCHBZP01	(Sergeev *et al.*, 2010)
B6	2-Mercaptobenzoic acid	ZZZLWW01	(Steiner, 2000)
B7	Carbamazepine (polymorph β)	CBMZPN10	(Himes *et al.*, 1981)
B8	Hydroflumethiazide	EWUHAF	(Florence *et al.*, 2003)
B9	Paracetamol (polymorph I)	HXACAN07	(Nichols & Frampton, 1998)
B10	Paracetamol (polymorph II)	HXACAN08	(Nichols & Frampton, 1998)
B11	Phenylacetic acid	ZZZMLY01	(Hodgson & Asplund, 1991)
B12	5-anilinomethylene-2,2-dimethyl-1,3-dioxane-4,6-dione	MENMOI01	(Smrcok *et al.*, 2007)
B13	2,2,2-Trifluoro-N-(1a,2,7,7a-tetrahydronaphtho[2,3-b]oxiren-3-yl) acetamide	FAFQAG	(Rukiah & Assaad, 2010)
B14	Ethyl 1',2',3',4',4a',5',6',7'-octahydrodispiro[cyclohexane-1,2'-quinazoline-4',1''-cyclohexane]-8'-carbodithioate	RUJSOF	(Avila *et al.*, 2009)
B15	5-amino-3-[4-(3-methoxyphenyl)piperazin-1-yl]-1,2,3,4-tetrahydronaphthalen-2-ol	CALJOQ	(Assaad & Rukiah, 2011)
B16	(Z)-3-Methyl-N-(7-nitroacridin-3-yl)-2,3-dihydro-1,3-benzothiazol-2-imine	CALDOK	(Vallcorba *et al.*, 2011)
B17	trans-Dichlorobis(triphenylphosphine)nickel(II)	CLTPNI03	(Brammer & Stevens, 1989)
B18	Pamoic acid	DEGDAV	(Haynes *et al.*, 2006)
B19	4-(4’ -Dimethylaminostyryl)pyridine N-oxide	IJEKAJ	(Ivashevskaja *et al.*, 2003)
B20	2-(Benzoylsulfanyl)acetic acid	OQUPIA	(Rukiah & Al-Ktaifani, 2011)
B21	bis(4'-(2-(p-Tosylamino)benzylideneamino)-2,3-benzo-15-crown-5-N,N',O)-copper(ii)	RIFVAE	(Dorokhov *et al.*, 2007)
B22	trans-Di-isothiocyanato-bis(triphenylphosphine)-nickel	GEBZUI	(Bamgboye & Sowerby, 1986)
B23	Methyl 4-[4-(dimethylamino)phenyl]ethynyl benzoate	Not Deposited	(Marder, 2004)
B24	cis-Thiothixene	THTHXN01	(David *et al.*, 1998)
B25	Tetracycline hydrochloride	XAYCAB	(Clegg & Teat, 2000)
B26	Ezetimibe anhydrate	QUWYIR	(Bruning *et al.*, 2010)
B27	4-(Phenyldiazenyl)naphthalen-1-amine hydrochloride	QIJCAN	(Yatsenko *et al.*, 2001)
B28	3-azabicyclo[3.3.1]nonane-2,4-dione (form 2)	BOQQUT01	(Hulme *et al.*, 2006)
B29	1,4-Bis(2-phenethyloxyethanesulfonyl) piperazine	BIFRIS	(Florence *et al.*, 2005)
B30	3,5-Bis[(N,N-dimethylamino)methyl-eneamino]-1-methyl-4-nitropyrazole	WOCVUF	(Chernyshev *et al.*, 2000)
B31	Telmisartan (polymorph A)	XUYHOO01	(Dinnebier *et al.*, 2000)
B32	Telmisartan (polymorph B)	XUYHOO	(Dinnebier *et al.*, 2000)
B33	Clomipramine hydrochloride	CIMPRA	(Post & Horn, 1977)
B34	Clarithromycin (polymorph I)	NAVSUY02	(Noguchi, Miura, *et al.*, 2012)

Code	Compound Name	CSD refcode	Reference
B35	Pigment orange 62(PO 62)	HOYVUN	(van de Streek *et al.*, 2009)
B36	Pigment yellow (PY 151)	HOYWAU	(van de Streek *et al.*, 2009)
B37	Pigment yellow (PY 154 polymorph α)	HOYWEY	(van de Streek *et al.*, 2009)
B38	Pigment yellow 194 (PY 194)	HOYWIC	(van de Streek *et al.*, 2009)
B39	2,4-dinitro-N-phenyl-6-(phenylazo)-benzamide	IHESUJ	(Chernyshev *et al.*, 2002)
B40	N-methyl-2,4-dinitro-N-phenyl-6-(phenylazo)benzamide	IHETEU	(Chernyshev *et al.*, 2002)
B41	chlorothiazide N,N-dimethylformamide solvate	WEJHAV	(Fernandes *et al.*, 2006)
B42	Trihexyphenidyl hydrochloride	KUZDIT	(Maccaroni *et al.*, 2010)
B43	N-(2-methoxyphenyl)-2-(2-methoxyphenylazo)-4,6-dinitrobenzamide	IHETAQ	(Chernyshev *et al.*, 2002)
B44	Nimustine hydrochloride	WAWZAX	(Beko *et al.*, 2012)
B45	(R)-1-phenylethylammonium (R)-2-phenylbutyrate (polymorph II)	PBUPEA01	(Fernandes, Florence, *et al.*, 2007a)
B46	(R)-1-phenylethylammonium (R)-2-phenylbutyrate (polymorph III)	PBUPEA02	(Fernandes, Florence, *et al.*, 2007b)
B47	Tetracaine hydrochloride	XISVOK	(Nowell *et al.*, 2002)
B48	α/β-lactose	LAKKEO	(Lefebvre *et al.*, 2005)
B49	N-(6-Phenylhexanoyl)glycyltryptophanamide	FEFNOV	(Bushmarinov *et al.*, 2012)
B50	Pigment yellow 183 (PY183 polymorph α)	HOMMEC01	(Ivashevskaya *et al.*, 2009)
B51	Pigment yellow 191 (PY191 polymorph α)	HOMMIG01	(Ivashevskaya *et al.*, 2009)
B52	Pigment yellow 191 (PY191 polymorph β)	HOMMOM01	(Ivashevskaya *et al.*, 2009)
B53	Lisinopril dihydrate	GERWUX01	(Sorrenti *et al.*, 2013)
B54	Prednisolone succinate	KIXDEB01	(Nishibori *et al.*, 2008)
B55	Cytenamide (polymorph II)	SODNOP	(Florence *et al.*, 2008)
B56	Carvedilol dihydrogen phosphate propan-2-ol solvate	PUJTOE	(Chernyshev *et al.*, 2010)
B57	Ritonavir	YIGPIO01	(Bauer *et al.*, 2001)
B58	Crystal Violet Anhydrous	Not Deposited	Shankland, Private communication
B59	d-sorbitol	GLUCIT03	(Rukiah *et al.*, 2004)
B60	Chlorothiazide N,N-dimethylformamide solvate	NILSEH	(Fernandes, Shankland, *et al.*, 2007)
B61	1,2,3,-tris(nonadecanoyl)glycerol (polymorph β)	MEZNAG	(Helmholdt *et al.*, 2002)

Table S2: Full molecular and crystallographic details for each structure in the dataset λ = wavelength of radiation used in data collection; PO = preferred orientation direction. A-codes represent the training set and B-codes the test (validation) set.

No	Space Group	a (Å)	b (Å)	c (Å)	α (^{0})	β (^{0})	γ (^{0})	Volume (Å^3)	Z'	Total DoF	DoF Position	DoF Orient	DOF Torsion	λ (Å)	PO
A1	*P* $2_12_12_1$	21.14	7.22	6.15	90	90	90	938.41	1	6	3	3	0	0.79984	
A2	*P* 2_1	10.01	8.51	7.40	90	111.74	90	587.47	1	7	3	3	1	1.54056	
A3	*P* $2_12_12_1$	25.54	8.06	5.76	90	90	90	1190.64	1	8	3	3	2	1.54056	
A4	*P* $2_1/c$	8.88	5.41	19.47	90	101.66	90	916.25	1	9	3	3	3	1.54056	
A5	*P* $2_12_12_1$	8.81	17.98	6.84	90	90	90	1083.37	1	10	3	3	4	1.54056	
A6	*P* 2_1	7.57	5.91	14.15	90	95.33	90	630.45	1	10	3	3	4	1.54056	
A7	*P* $2_12_12_1$	5.57	8.85	35.68	90	90	90	1758.13	1	10	3	3	4	0.8000	
A8	*P* $2_1/a$	7.55	14.42	10.25	90	109.60	90	1051.59	1	11	6	3	2	1.54056	
A9	*P b c a*	21.65	8.80	14.56	90	90	90	2774.81	1	11	3	3	5	1.54056	
A10	*P b c* 2_1	10.67	11.48	7.94	90	90	90	972.28	1	11	6	3	2	1.54056	
A11	*P* $2_12_12_1$	9.07	5.22	26.60	90	90	90	1258.54	1	12	3	3	6	1.54056	
A12	*P* $2_1/c$	12.51	5.05	12.19	90	108.90	90	728.36	1	12	6	3	3	1.54056	
A13	*P* $\bar{1}$	6.52	8.53	12.92	84.33	80.58	69.19	661.22	1	12	3	3	6	1.54056	
A14	*P* 2_1	7.98	21.56	4.82	90	109.57	90	782.29	1	13	6	3	4	1.54056	
A15	*P* $2_1/c$	11.81	11.49	13.43	90	111.72	90	1692.28	1	13	6	3	4	1.54056	
A16	*P n a* 2_1	20.22	7.83	9.09	90	90	90	1439.55	1	13	3	3	7	1.54056	
A17	*C m c a*	19.63	4.84	28.80	90	90	90	2738.11	0.5	13	9	3	2	1.54056	
A18	*P* $\bar{1}$	8.65	9.12	11.38	74.72	81.60	88.98	856.78	1	14	3	3	8	0.5200	
A19	*P* $2_1/c$	9.29	23.01	15.28	90	108.06	90	3106.11	1	14	3	3	8	1.54056	
A20	*P* $2_1/c$	17.65	5.29	18.26	90	123.55	90	1421.84	1	15	3	3	9	1.54056	
A21	*C* 2/*c*	15.35	13.48	15.30	90	91.45	90	3164.83	1	15	6	3	6	0.85075	
A22	*P* $\bar{1}$	9.15	24.29	5.18	93.12	101.15	83.48	1121.18	1	16	3	3	10	1.7900	
A23	*P* $2_12_12_1$	12.83	13.06	13.83	90	102.68	90	2262.19	1	16	6	3	7	1.54056	
A24	*P* $2_1/c$	16.37	7.03	17.18	90	108.62	90	1874.61	1	16	9	3	4	1.54056	
A25	*P* $2_1/c$	12.22	14.79	9.47	90	93.98	90	1707.74	1	17	3	3	11	1.54056	
A26	*P* $2_1/c$	22.55	4.96	21.28	90	109.45	90	2246.15	1	17	3	3	11	1.54056	

No	Space Group	a (Å)	b (Å)	c (Å)	α (^{0})	β (^{0})	γ (^{0})	Volume (Å^3)	Z'	Total DoF	DoF Position	DoF Orient	DOF Torsion	λ (Å)	PO
A27	*P* $2_12_12_1$	15.7	18.88	15.03	90	90	90	4454.53	1	17	6	3	8	1.30000	
A28	*P b c n*	14.38	5.81	32.89	90	90	90	2750.03	1	18	12	3	3	1.54056	
A29	*P* $2_1/c$	17.20	5.02	27.38	90	97.31	90	2342.68	1	18	6	6	6	1.54056	
A30	*P* $2_1/c$	10.24	29.15	10.21	90	106.64	90	2921.62	1	18	6	6	6	1.54056	
A31	*P* $2_1/n$	5.07	37.85	9.64	90	97.86	90	1833.22	1	18	3	3	12	1.54056	
A32	*P* 2_1	12.46	8.03	13.54	90	112.89	90	1248.93	2	20	6	6	8	1.54056	
A33	*P* $2_12_12_1$	15.52	18.93	6.67	90	90	90	1960.60	1	20	12	3	5	0.70030	
A34	*P* $\bar{1}$	7.09	10.59	19.20	100.10	93.73	101.55	1382.06	1	22	6	3	13	1.54056	
A35	*P* $2_1/c$	7.84	26.99	10.81	90	92.96	90	2283.7	1	24	15	3	6	1.79000	
A36	*P* $\bar{1}$	9.864	13.89	14.29	61.23	79.83	81.78	1685.37	2	24	6	6	12	0.50000	
A37	*P* $\bar{1}$	7.63	13.67	15.81	84.39	87.47	75.71	1589.52	1	25	6	6	13	1.54056	
A38	*P* $\bar{1}$	5.186	20.58	22.24	84.19	87.98	85.11	2351.44	4	28	12	12	4	0.51561	
A39	*P* $\bar{1}$	5.649	19.56	22.07	84.22	88.41	83.60	2411.72	4	28	12	12	4	1.54056	
A40	*P* $\bar{1}$	13.60	14.05	8.913	71.59	78.73	64.86	1460.09	3	30	9	9	12	0.65278	
B1	*P* $2_1/n$	6.32	4.86	11.33	90	92.04	90	348.32	0.5	6	3	3	0	1.54056	
B2	*P* $2_1/n$	7.81	10.47	5.26	90	90.99	90	430.32	0.5	6	3	3	0	0.69400	
B3	*P* $\bar{1}$	4.28	8.31	14.09	107.23	93.53	97.17	471.94	0.5	6	3	3	0	1.54056	
B4	*P* $2_1/c$	3.85	11.02	12.73	90	92.31	90	539.88	0.5	7	3	3	1	1.54056	
B5	*P* $2_1/c$	14.80	11.68	8.48	90	93.68	90	1461.84	1	7	3	3	1	1.54056	
B6	*P* $2_1/c$	12.83	13.06	13.83	90	100.48	90	687.72	1	7	3	3	1	1.54056	
B7	*P* $2_1/n$	7.54	11.16	13.91	90	92.86	90	1168.30	1	7	3	3	1	1.54056	
B8	*P* 2_1	7.52	8.62	9.74	90	110.36	90	592.15	1	8	3	3	2	1.54056	
B9	*P* $2_1/n$	7.09	9.23	11.62	90	97.82	90	753.94	1	8	3	3	2	1.54056	
B10	*P b c a*	17.17	11.78	7.21	90	90	90	1458.02	1	8	3	3	2	1.54056	[001]
B11	*P* $2_1/c$	10.20	4.96	14.44	90	99.17	90	720.67	1	8	3	3	2	1.54056	
B12	*P* $\bar{1}$	10.60	11.60	5.50	97.88	103.89	71.46	621.43	1	9	3	3	3	1.79000	[121]
B13	*P* $2_1/c$	8.06	8.81	16	90	99.45	90	1120.66	1	9	3	3	3	1.54060	
B14	*P* $2_1/n$	21.74	10.06	9.45	90	99.96	90	2034.72	1	9	3	3	3	0.80098	
B15	*P* $2_1/c$	12.62	8.91	17.27	90	102.85	90	1894.18	1	9	3	3	3	1.54060	[100]

No	Space Group	a (Å)	b (Å)	c (Å)	α (^{0})	β (^{0})	γ (^{0})	Volume (Å^3)	Z'	Total DoF	DoF Position	DoF Orient	DOF Torsion	λ (Å)	PO
B16	*P b c a*	36.63	12.51	7.58	90	90	90	3470.96	1	9	3	3	3	1.54059	
B17	*P* $2_1/c$	11.58	8.09	17.22	90	107.20	90	1541.82	0.5	10	3	3	4	1.54056	
B18	*C* 2/*c*	19.73	4.79	19.25	90	108.96	90	1720.51	0.5	10	3	3	4	1.79000	
B19	*P* $2_1/n$	26.82	7.76	6.08	90	94.03	90	1261.82	1	10	3	3	4	1.54056	
B20	*P* $2_1/n$	13.39	5.14	14.66	90	112.65	90	931.81	1	10	3	3	4	1.54060	
B21	*P* $2_1/c$	19.04	17.43	17.42	90	113.82	90	5287.66	1	10	3	3	4	0.51966	[100]
B22	*P* $\bar{1}$	7.94	10.46	11.47	111.08	74.56	92.25	855.04	0.5	11	3	3	5	1.54056	
B23	*P n a* 2_1	6.12	7.47	32.99	90	90	90	1507.84	1	11	3	3	5	1.54056	
B24	*P* 2_1	10.15	8.70	13.69	90	110.65	90	1130.59	1	11	3	3	5	1.54056	[010]
B25	*P* $2_12_12_1$	10.93	12.72	15.71	90	90	90	2183.29	1	11	6	3	2	0.69200	
B26	*P* $2_12_12_1$	5.95	15.89	21.38	90	90	90	2019.69	1	12	3	3	6	1.54060	
B27	*P* $2_1/c$	7.43	13.31	14.03	90	95.32	90	1379.94	1	12	6	3	3	1.54056	
B28	*P* $2_1/c$	7.67	10.55	18.89	90	95.58	90	1521.00	2	12	6	6	0	1.54056	
B29	*P* $2_1/a$	13.23	5.11	19.66	90	107.67	90	1267.06	0.5	13	3	3	7	1.54056	
B30	*P* $\bar{1}$	9.58	9.97	7.60	106.11	95.12	78.22	682.40	1	13	3	3	7	1.54056	[511]
B31	*P* $2_1/c$	18.78	18.10	8.01	90	97.06	90	2701.25	1	13	3	3	7	1.14981	
B32	*P* $2_1/a$	16.06	13.09	13.32	90	99.40	90	2764.21	1	13	3	3	7	1.14981	
B33	*P* $2_1/c$	15.51	8.61	14.03	90	96.69	90	1859.40	1	13	6	3	4	1.54056	
B34	*P* $2_12_12_1$	14.45	34.69	8.711	90	90	90	4367.52	1	14	3	3	8	1.30000	[010]
B35	*P* $\bar{1}$	7.27	10.32	12.18	96.46	95.87	109.85	843.78	1	14	3	3	8	1.54056	[100]
B36	*P* $\bar{1}$	5.13	9.23	17.41	95.86	95.51	91.80	815.42	1	14	3	3	8	1.54056	[100]
B37	*P* $2_1/c$	14.58	8.54	13.78	90	96.07	90	1707.63	1	14	3	3	8	1.54056	[010]
B38	*P* $2_1/c$	14.72	5.99	20.79	90	114.82	90	1662.32	1	14	3	3	8	1.54056	
B39	*P* 2_1	11.72	6.83	11.05	90	94.38	90	881.67	1	14	3	3	8	1.54056	[010]
B40	*P* $2_1/c$	8.68	18.56	12.10	90	90.38	90	1948.06	1	14	3	3	8	1.54056	[100]
B41	*P* $\bar{1}$	7.98	8.88	11.10	86.69	75.08	73.20	728.41	1	14	6	6	2	1.54056	
B42	*P* $2_12_12_1$	30.03	11.23	5.89	90	90	90	1987.09	1	14	6	3	5	1.54056	[100]
B43	*P* $2_12_12_1$	22.79	13.02	6.920	90	90	90	2052.85	1	16	6	3	7	1.54056	[001]
B44	*P* $2_1/c$	5.25	12.24	21.41	90	93.24	90	1374.05	1	16	6	3	7	1.54056	

No	Space Group	a (Å)	b (Å)	c (Å)	α (^{0})	β (^{0})	γ (^{0})	Volume (Å^3)	Z'	Total DoF	DoF Position	DoF Orient	DOF Torsion	λ (Å)	PO
B45	$P\,2_12_12_1$	6.06	16.78	16.89	90	90	90	1717.80	1	16	6	6	4	1.54056	
B46	$P\,2_1$	11.88	5.98	13.08	90	113.51	90	851.42	1	16	6	6	4	1.54056	
B47	$P\bar{1}$	7.40	8.57	13.69	106.21	90.85	98.78	822.26	1	18	6	3	9	1.00045	[001]
B48	$P\,1$	7.63	19.66	5.06	95.65	105.43	81.00	721.01	2	20	6	6	8	1.54056	
B49	$P\,2_12_12_1$	35.94	12.92	5.00	90	90	90	2319.37	1	20	3	3	14	1.54056	[100]
B50	$P\,\bar{1}$	5.69	10.59	18.53	73.32	87.84	76.13	1037.86	0.5	21	12	3	6	1.54056	
B51	$P\,\bar{1}$	5.69	10.61	18.56	72.83	88.27	76.42	1039.37	0.5	21	12	3	6	1.54056	
B52	$P\bar{1}$	6.01	10.82	18.09	85.68	86.39	75.78	1136.55	1	24	15	3	6	0.64980	
B53	$P\,2_1$	14.55	5.90	14.24	90	112.83	90	1124.84	1	25	9	3	13	1.54056	
B54	$I\,2$	21.03	9.11	24.38	90	98.34	90	4622.43	2	26	6	6	14	1.00140	
B55	$P\,\bar{1}$	5.65	19.56	22.07	84.22	88.41	83.60	2411.72	4	28	12	12	4	1.54056	
B56	$P\,\bar{1}$	11.55	16.65	7.86	95.40	94.64	71.25	1424.06	1	28	9	9	10	1.54059	[001]
B57	$P\,2_12_12_1$	13.44	50.29	27.06	90	103.15	90	1872.12	1	28	3	3	22	1.54056	
B58	$P\,2_1/c$	9.55	22.29	22.07	90	93.75	90	4686.28	2	30	12	6	12	0.79977	
B59	$P\,2_12_12_1$	24.30	20.57	4.87	90	90	90	2433.30	3	33	9	9	15	0.49957	
B60	$P\,2_1/c$	12.36	8.56	37.30	90	92.88	90	3942.30	2	42	18	18	6	1.54056	
B61	$P\,\bar{1}$	11.67	56.51	5.43	73.06	100.02	120.08	301.82	1	49	3	3	43	0.85005	

Table S3: A summary of the baseline DASH performance against the dataset based on the 50 and 100 SA runs (1×10^7 moves), together with information of the Pawley refinement and best SA solution quality. * indicates the SR was achieved with 100 SA runs

No	Total DoF	Resolution (Å)	No. of Reflections	Pawley χ^2	Best Profile χ^2	χ^2 ratio	Success Rate (%)	RMSD (Å)
A1	6	1.17	389	13.85	28.41	2.05	100	0.034
A2	7	1.75	136	3.88	9.35	2.41	100	0.024
A3	8	1.57	214	3.68	6.27	1.70	100	0.021
A4	9	1.83	153	8.45	32.67	3.87	100	NA
A5	10	1.66	168	3.26	8.41	2.58	100	0.029
A6	10	2.03	96	3.41	9.10	2.67	100	NA
A7	10	2.10	143	1.99	3.18	1.60	48	0.032
A8	11	1.75	208	2.63	4.77	1.81	100	0.037
A9	11	1.76	263	4.40	30.09	6.84	100	0.083
A10	11	1.82	103	8.20	62.01	7.56	100	0.119
A11	12	1.86	148	8.52	23.92	2.81	100	0.0541
A12	12	1.52	219	5.57	22.92	4.11	100	0.059
A13	12	2.20	124	4.21	35.89	8.52	78	0.155
A14	13	1.85	140	3.21	18.51	5.77	96	0.066
A15	13	1.77	318	3.48	10.57	3.04	100	0.120
A16	13	1.54	228	8.89	22.91	2.58	42	0.147
A17	13	2.08	164	12.16	95.34	7.84	100	0.141
A18	14	2.29	148	3.40	13.44	3.95	4	0.645
A19	14	1.86	499	0.56	2.75	4.91	14	0.104
A20	15	1.86	228	5.25	11.44	2.18	34	0.095
A21	15	2.13	174	2.01	4.40	2.19	56	0.022
A22	16	3.18	72	2.71	11.23	4.14	28	0.085
A23	16	2.19	161	5.23	14.35	2.74	54	0.087
A24	16	1.81	336	3.70	12.79	3.46	50	0.136
A25	17	1.76	338	7.87	38.05*	4.83	2*	0.266
A26	17	2.62	126	2.14	15.29*	7.14	1*	0.099
A27	17	2.00	369	3.39	23.70	6.99	78	0.053
A28	18	1.63	341	3.81	18.04	4.73	8	0.139
A29	18	2.37	182	2.41	12.51	5.19	60	0.045
A30	18	2.31	252	0.81	10.65	13.15	34	0.376
A31	18	1.97	262	4.07	11.37	2.79	16	0.081
A32	20	1.68	320	3.63	9.47	2.61	18	0.048
A33	20	1.99	180	29.09	144.57	4.97	14	0.127
A34	22	1.76	518	4.04	10.90	2.70	4	0.087
A35	24	2.65	123	2.68	8.25	3.08	14	0.126
A36	24	3.13	111	3.44	5.89	1.71	46	0.180
A37	25	1.80	567	0.34	4.86	14.29	0	NA
A38	28	2.80	218	3.47	7.81	2.25	98	0.118
A39	28	2.92	195	7.93	107.29*	13.53	1*	0.263
A40	30	2.04	362	11.32	207.38*	18.32	0*	NA
B1	6	1.67	76	6.48	15.02	2.32	92	0.070
B2	6	1.41	165	0.50	4.37	8.74	100	0.067
B3	6	3.64	19	1.45	2.67	1.84	100	0.281
B4	7	1.68	120	4.56	9.02	1.98	100	0.031
B5	7	2.60	87	4.37	36.07	8.25	100	0.117
B6	7	1.44	243	2.76	5.28	1.91	100	0.031
B7	7	1.64	276	3.74	9.16	2.45	100	0.011
B8	8	1.98	94	5.15	16.4	3.18	100	0.098
B9	8	1.44	267	3.48	8.62	2.48	100	0.123
B10	8	1.52	223	5.87	18.4	3.13	100	0.130
B11	8	1.62	173	11.00	26.03	2.37	100	0.083
B12	9	1.74	245	6.47	19.65	18.05	96	0.118
B13	9	1.52	331	2.01	67.14	33.40	100	0.109

No	Total DoF	Resolution (Å)	No. of Reflections	Pawley χ^2	Best Profile χ^2	χ^2 ratio	Success Rate (%)	RMSD (Å)
B14	9	1.86	327	5.75	12.27	2.13	100	0.012
B15	9	2.13	204	6.93	20.78	3.00	66	0.045
B16	9	2.49	113	4.34	13.03	3.00	100	0.042
B17	10	1.80	288	5.61	14.20	2.53	100	0.079
B18	10	1.82	154	1.11	2.13	1.92	70	0.102
B19	10	2.055	148	1.70	3.92	2.31	100	0.188
B20	10	2.25	87	8.60	46.94	5.46	100	0.264
B21	10	2.03	280	0.47	0.84	1.79	44	0.331
B22	11	1.90	264	5.45	12.62	2.32	100	0.057
B23	11	2.04	98	1.60	3.64	2.28	98	NA
B24	11	1.86	214	4.44	19.69	4.43	96	0.217
B25	11	2.01	188	4.62	17.83	3.86	100	0.075
B26	12	2.24	133	1.43	3.18	2.22	84	0.014
B27	12	1.97	188	5.77	10.34	1.79	44	0.026
B28	12	2.17	156	1.07	3.93	3.67	100	0.075
B29	13	1.83	220	7.99	16.87	2.11	92	0.171
B30	13	2.06	165	4.89	10.49	2.15	64	0.065
B31	13	2.22	260	1.49	3.15	2.11	58	0.160
B32	13	2.60	160	4.88	10.69	2.19	100	0.142
B33	13	1.85	306	5.18	16.55	3.19	100	0.067
B34	14	1.90	427	28.99	47.97	1.65	50	0.052
B35	14	2.64	95	5.57	13.25	2.38	14	0.182
B36	14	2.40	123	4.79	24.17	5.05	4	0.060
B37	14	2.13	184	2.83	7.05	2.49	12	0.039
B38	14	2.66	93	2.43	15.26	6.28	36	0.233
B39	14	2.17	111	87.65	149.48	1.71	4	0.175
B40	14	2.24	184	63.03	124.28	1.97	8	0.126
B41	14	2.16	150	1.00	2.24	2.24	98	0.765
B42	14	2.52	100	229.92	1252.69	5.45	20	0.280
B43	16	2.22	135	55.26	220.77	4.00	12	0.158
B44	16	1.76	256	2.00	13.05	6.53	8	0.103
B45	16	1.55	311	8.58	13.81	1.61	14	0.079
B46	16	1.55	289	3.16	5.61	1.78	4	0.068
B47	18	2.53	103	27.61	61.01	2.21	14	0.017
B48	20	2.39	110	9.20	36.09*	3.92	4*	0.130
B49	20	1.86	260	52.10	373.79*	7.17	0*	NA
B50	21	2.87	88	1.25	60.04*	48.03	0*	NA
B51	21	2.59	121	4.04	37.71*	9.33	1*	0.197
B52	24	2.03	280	1.09	7.36*	6.75	0*	NA
B53	25	1.75	237	3.51	13.50	3.85	2	0.077
B54	26	2.32	230	0.04	0.27*	6.75	0*	NA
B55	28	2.92	196	3.79	25.29	6.67	4	0.081
B56	28	2.71	148	43.42	381.91*	8.80	0*	NA
B57	28	2.17	257	4.69	221.32*	47.18	0*	NA
B58	30	2.62	276	9.09	29.26	3.22	78	NA
B59	33	1.67	358	16.74	523.34*	31.26	0*	NA
B60	42	2.45	280	1.77	26.75*	13.53	0*	NA
B61	49	2.64	332	22.52	602.88*	18.32	0*	NA

Table S4: A summary of the SRs achieved with the six best performing SA parameter configurations, against the dataset, based on the 50 and 100 SA runs. * indicates SR was achieved with 100 SA runs

No	0.02/ 20/25	0.27/ 73/56	0.27/ 73/61	0.27/ 73/51	0.27/ 60/ 63	0.25/ 35/ 86	0.25/ 46/ 62
A1	100	100	100	100	100	100	100
A2	100	100	100	100	100	100	100
A3	100	100	100	100	100	100	100
A4	100	100	100	100	100	100	100
A5	100	100	100	100	100	100	100
A6	100	100	100	100	100	100	100
A7	48	78	78	70	62	58	74
A8	100	100	100	100	100	100	100
A9	100	100	100	100	100	100	98
A10	100	100	100	100	100	100	100
A11	100	100	100	100	100	100	100
A12	100	100	100	100	100	100	100
A13	78	98	98	96	94	94	92
A14	96	100	100	100	100	100	100
A15	100	100	100	100	100	100	100
A16	42	74	96	82	86	82	90
A17	100	100	100	100	100	100	100
A18	4	6	8	4	2	6	2
A19	14	12	10	14	14	12	24
A20	34	88	92	90	66	82	72
A21	56	78	98	92	86	74	78
A22	28	74	86	70	62	64	52
A23	54	92	88	70	72	82	76
A24	50	84	92	78	80	86	80
A25	2*	24	12	18	10	16	26
A26	1*	10	6	12	4	12	2
A27	78	96	98	100	98	100	98
A28	8	40	44	32	32	44	30
A29	60	96	90	92	94	94	82
A30	34	56	50	36	41	32	26
A31	16	20	28	18	16	22	20
A32	18	54	42	56	48	46	48
A33	14	40	32	60	52	38	38
A34	4	36	34	44	26	22	24
A35	14	48	36	24	44	20	12
A36	46	72	76	68	66	62	62
A37	0*	1*	0*	1*	0*	0*	1*
A38	98	100	100	100	100	98	98
A39	1*	4	2	4	2	2	2
A40	0*	4	2	2	2	2	0
B1	92	100	100	100	100	100	100
B2	100	100	100	100	100	100	100
B3	100	100	100	100	100	100	100
B4	100	100	100	100	100	100	100
B5	100	100	100	100	100	100	100
B6	100	100	100	100	100	100	100
B7	100	100	100	100	100	100	100
B8	100	100	100	100	100	100	100
B9	100	100	100	100	100	100	100
B10	100	100	100	100	100	100	100
B11	100	100	100	100	100	100	100

No	0.02/ 20/25	0.27/ 73/56	0.27/ 73/61	0.27/ 73/51	0.27/ 60/ 63	0.25/ 35/ 86	0.25/ 46/ 62
B12	96	100	78	100	78	96	100
B13	100	100	100	100	100	100	100
B14	100	100	100	100	100	100	100
B15	66	98	96	86	86	88	78
B16	100	100	100	100	100	100	100
B17	100	100	100	100	100	100	100
B18	70	100	98	98	96	94	92
B19	100	100	100	100	92	100	100
B20	100	100	100	100	100	100	100
B21	44	60	74	84	56	52	56
B22	100	100	100	100	100	100	100
B23	98	100	100	100	100	100	100
B24	96	98	98	96	98	100	98
B25	100	100	100	100	100	100	100
B26	84	98	98	100	96	90	90
B27	44	78	82	66	74	78	70
B28	100	100	100	100	100	100	100
B29	92	100	100	100	100	100	100
B30	64	98	96	92	100	88	90
B31	58	50	74	66	66	54	54
B32	100	100	100	100	100	100	100
B33	100	100	100	100	100	100	100
B34	50	100	100	98	96	98	96
B35	14	48	54	44	40	30	48
B36	4	12	6	12	4	6	6
B37	12	30	38	22	16	26	20
B38	36	76	60	56	66	70	60
B39	4	14	24	22	12	14	14
B40	8	26	18	26	30	18	16
B41	98	100	100	98	100	100	98
B42	20	44	56	42	46	34	34
B43	12	32	28	16	22	22	32
B44	8	48	52	26	36	32	26
B45	14	54	40	52	68	48	56
B46	4	70	60	50	60	58	50
B47	14	54	64	58	64	62	62
B48	4*	12	8	14	4	4	8
B49	0*	1*	0*	0*	0*	0*	0*
B50	0*	0*	0*	1*	2	1*	0*
B51	1*	6	6	20	10	14	10
B52	0*	18	18	10	8	12	16
B53	2	22	38	44	46	36	26
B54	0*	1*	14	2	2	8	2
B55	4	90	64	96	96	96	90
B56	0*	0*	0*	0*	0*	0*	0*
B57	0*	0*	0*	0*	0*	0*	0*
B58	78	100	96	100	100	100	96
B59	0*	0*	0*	0*	0*	0*	0*
B60	0*	1*	0*	1	1*	6	1*
B61	0*	0*	0*	0*	0*	0*	0*

Table S5: A summary of the SRs achieved with the six best performing SA parameter configurations, against the FDS, based on the 500 SA runs. The SRs given in brackets are based on the 100 SA runs as given in Table S4. * indicates the SR was achieved with 100 SA runs (500 SA runs not required)

No	0.02/ 20/25	0.27; 73;56	0.27; 73;61	0.27; 73;51	0.27; 60; 63	0.25; 35; 86	0.25; 46; 62
A37	0	1*	1.6	1*	0.8	0.4	1*
A40	0.2	4*	2*	2*	2*	2*	0.2
B49	0	1*	0.6	0	0.4	0.4	0.2
B50	0.2	0.4	0.6	1*	2*	1*	0.2
B52	9.4	18*	18*	10*	8*	12*	16*
B54	2	1*	14*	2*	2*	8*	2*
B56	0	0	0	0	0	0	0
B57	0	0.4	0	0.2	0.4	0	0
B59	0	0.2	0.4	0.2	0.2	0.6	0
B60	0.4	1*	3.4	1*	1*	6*	1*
B61	0	0	0	0	0	0	0

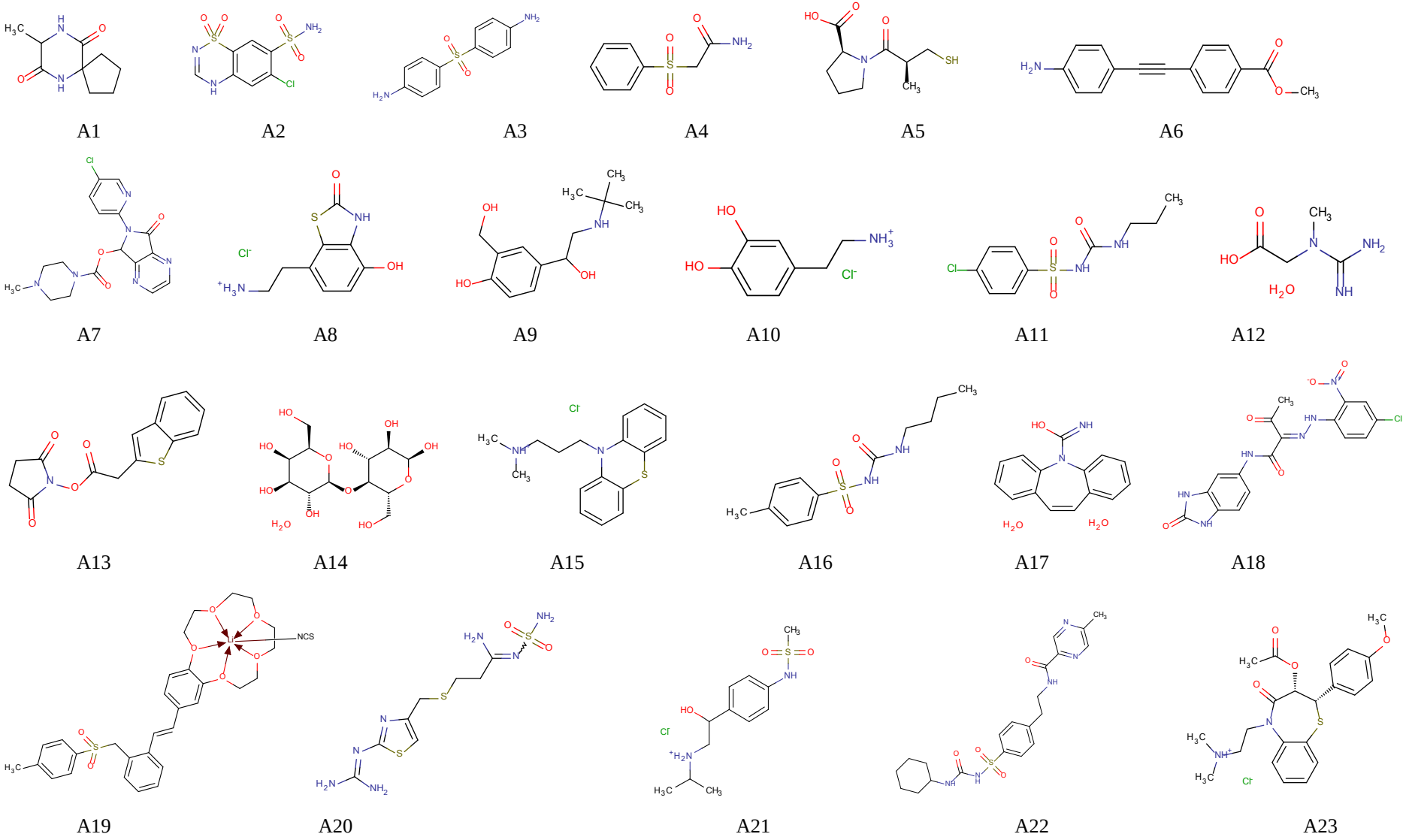
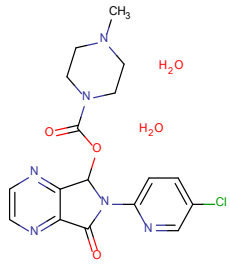
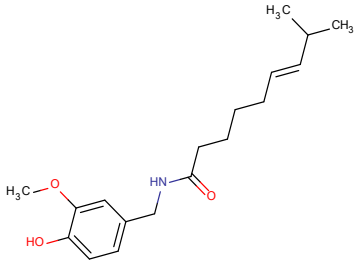


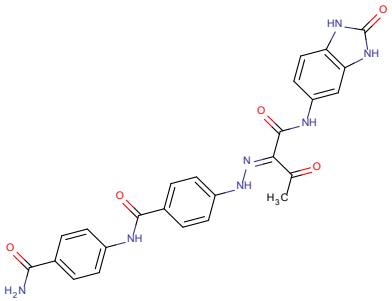
Figure S1: Molecular structures of the 101 compounds listed in Table S1



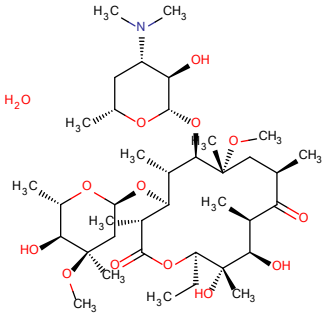
A24



A25



A26



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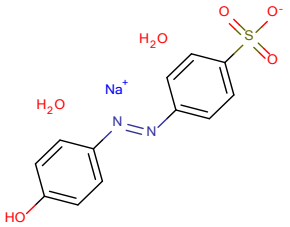

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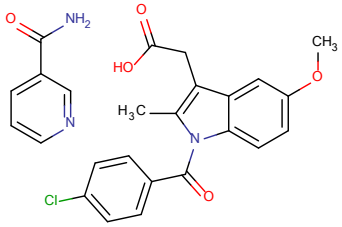

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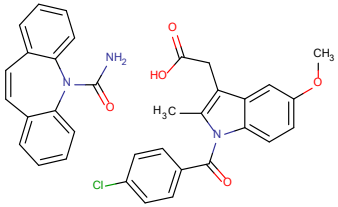

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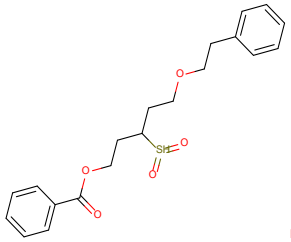

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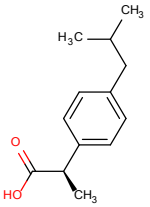

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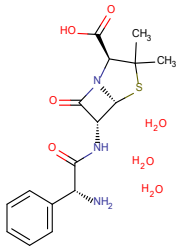

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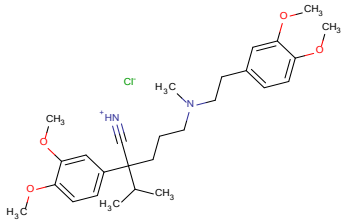

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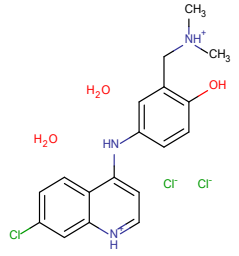

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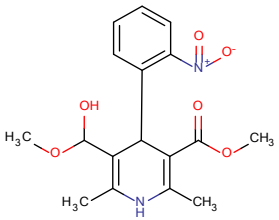

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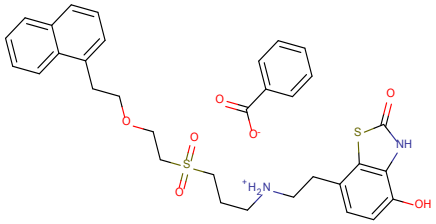

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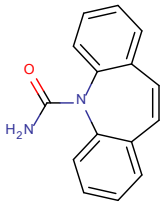

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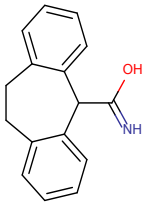

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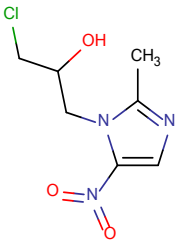

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Figure S1: Molecular structures of the 101 compounds listed in Table S1 (continued)

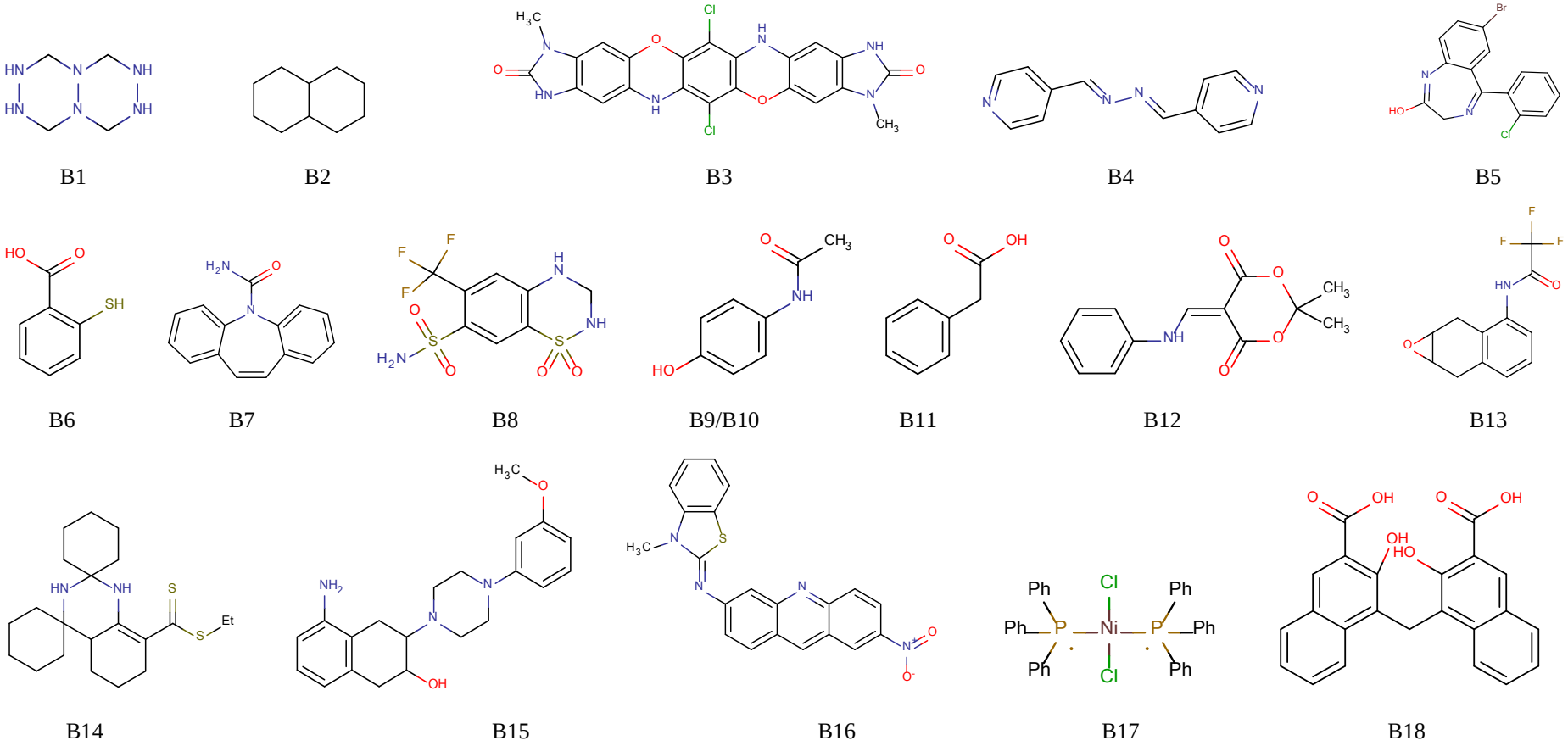
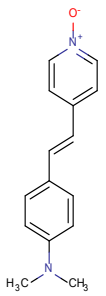


Figure S1: Molecular structures of the 101 compounds listed in Table S1 (continued)



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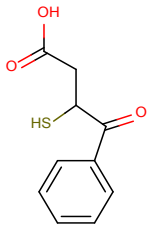

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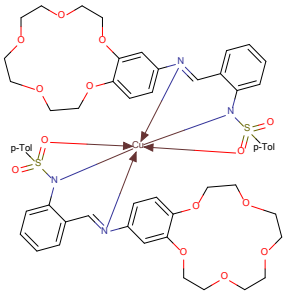

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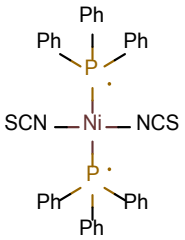

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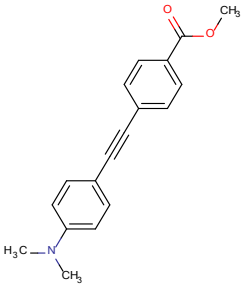

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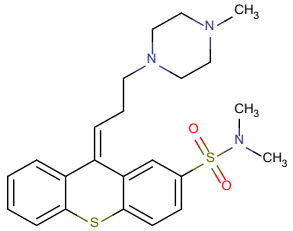

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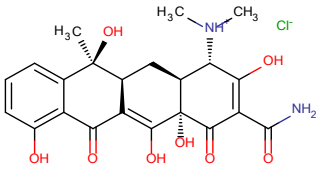

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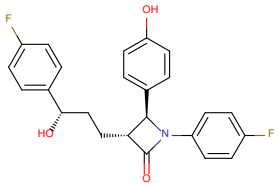

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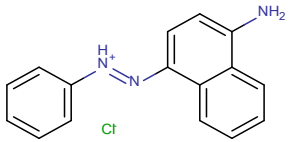

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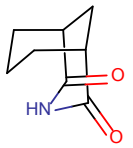

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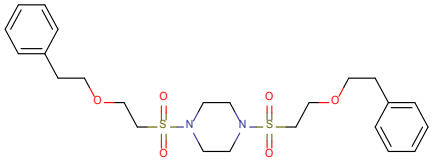

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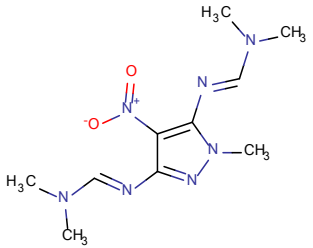

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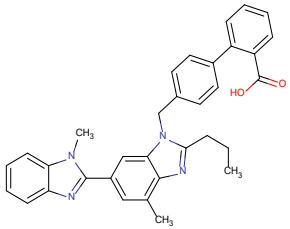

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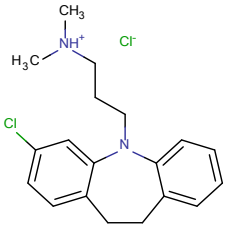

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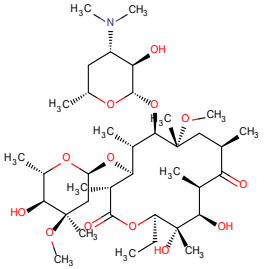

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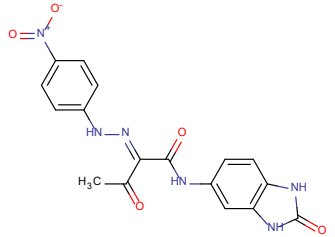

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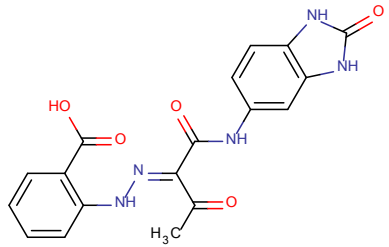
Figure S1: Molecular structures of the 101 compounds listed in Table S1 (continued)



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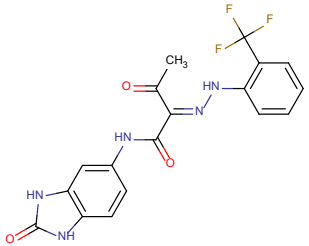

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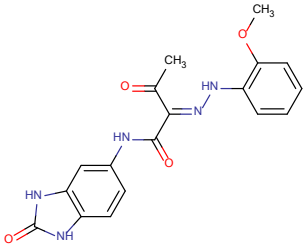

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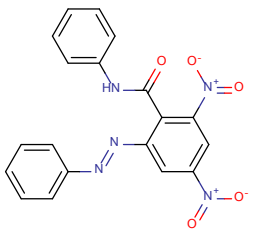

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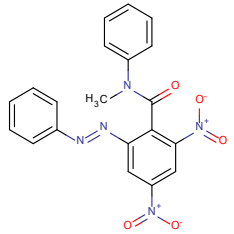

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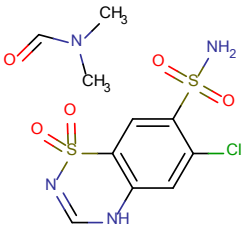

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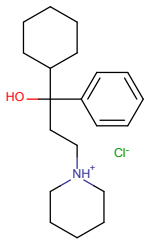

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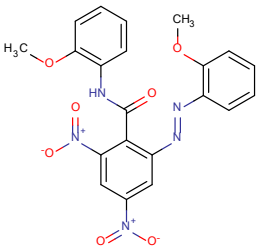

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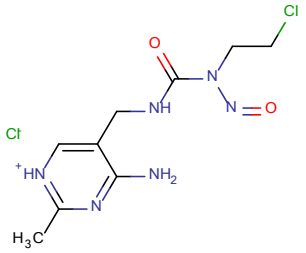

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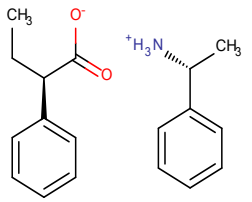

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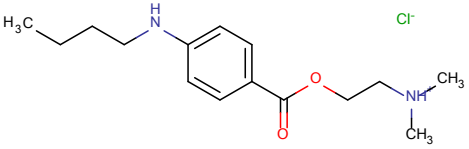

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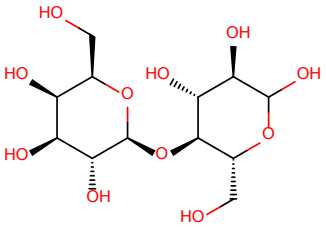

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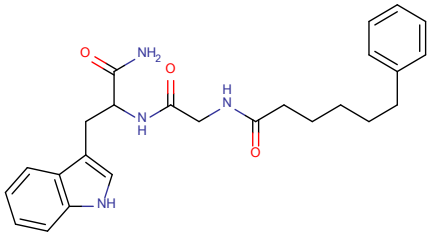

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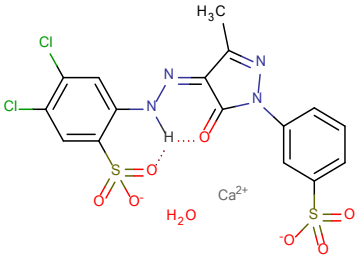

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Figure S1: Molecular structures of the 101 compounds listed in Table S1 (continued)

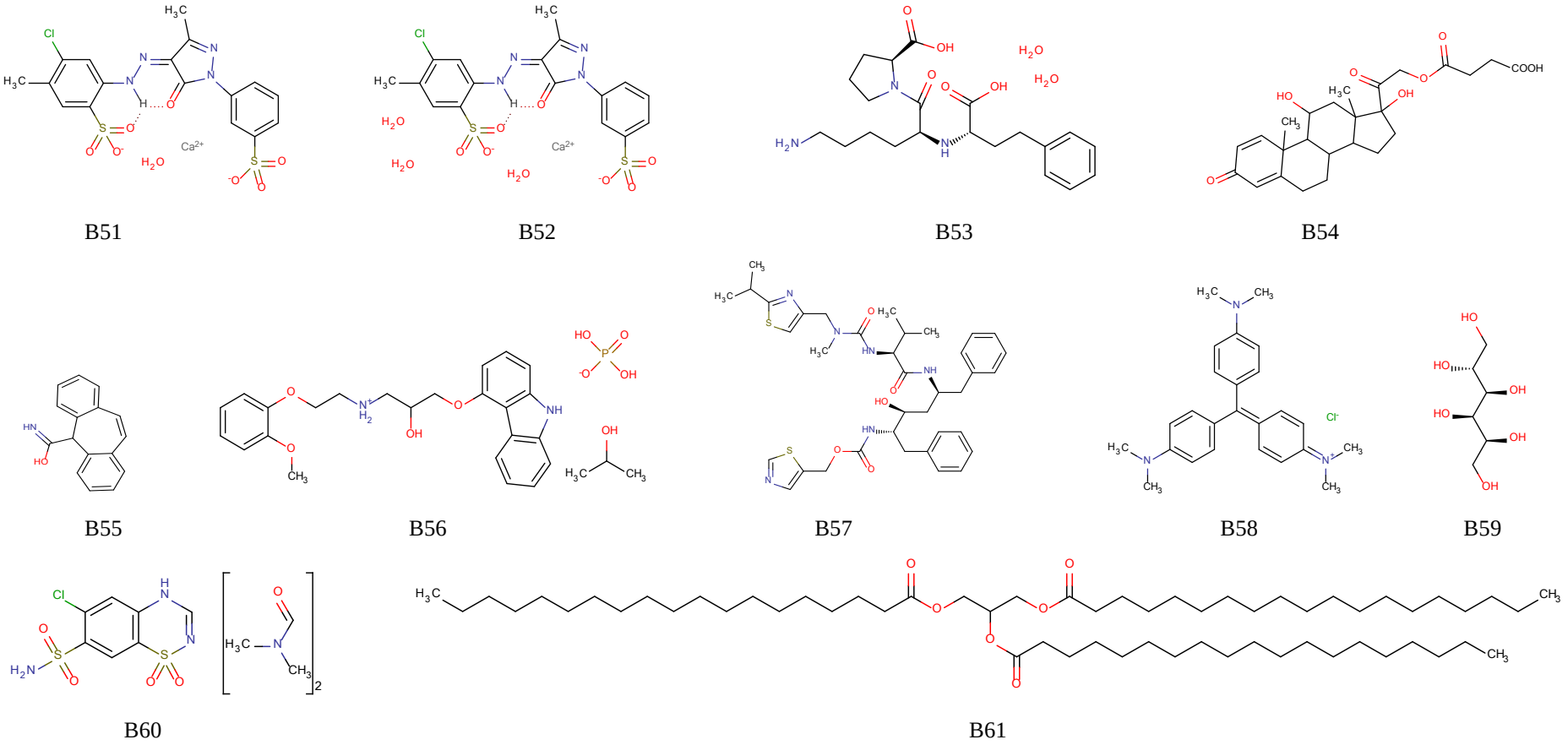
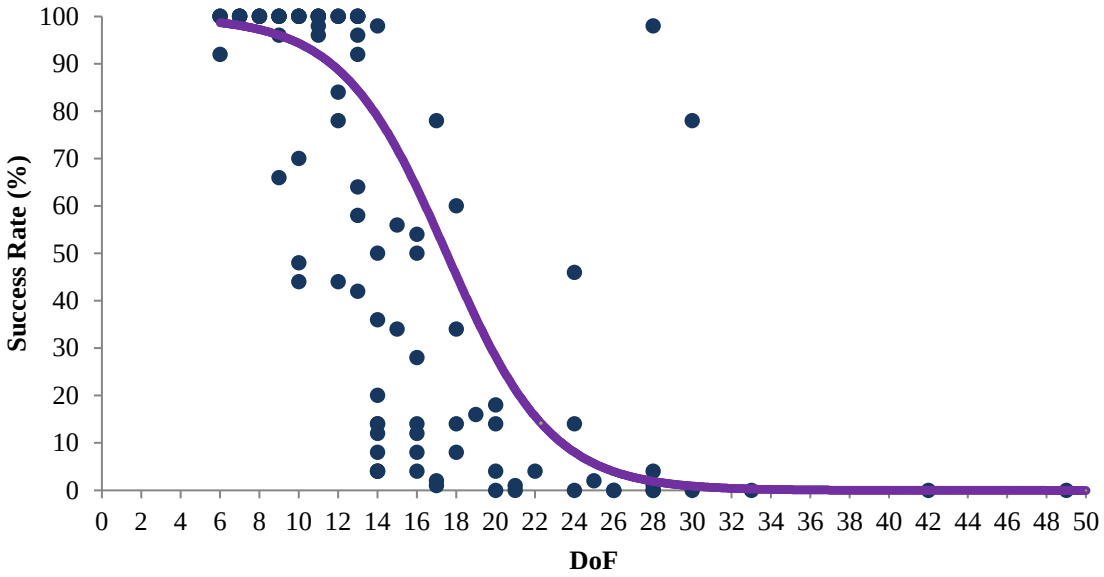
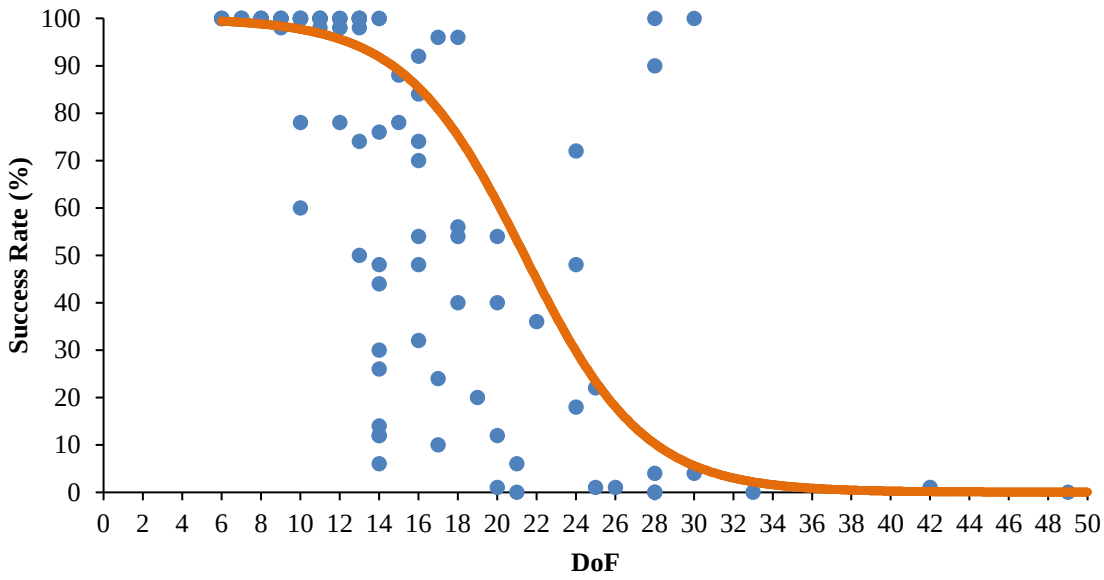


Figure S1: Molecular structures of the 101 compounds listed in Table S1 (continued)

Figure S2 Graphical representation of (a) the baseline DASH success rate as a function of the total degrees of freedom (SA parameters used: T_0=0; CR = 0.02; N_1=20; and N_2=25) and (b) the optimised DASH success rate as a function of the total degrees of freedom (SA parameters used: T_0=0; CR = 0.27; N_1=73; and N_2=56). The purple and orange lines show the ELO fit to the experimental data based on total DoF..



a)



b)

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