Article:
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SUPPLEMENTARY DATA SET 1

An *in vivo* platform for identifying inhibitors of protein aggregation

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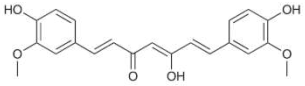
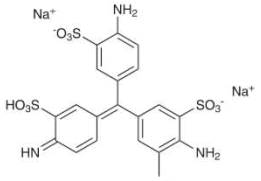
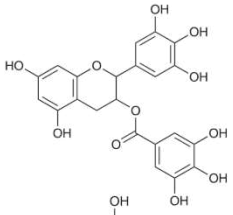
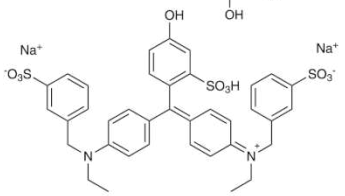
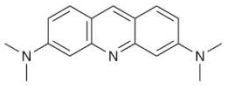
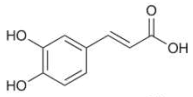
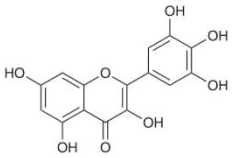
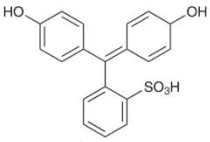
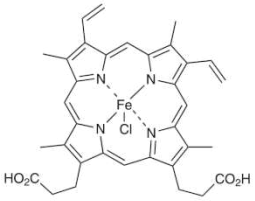
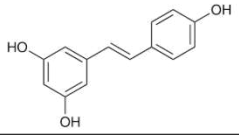
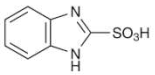
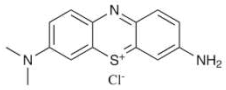
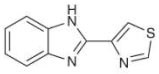
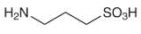
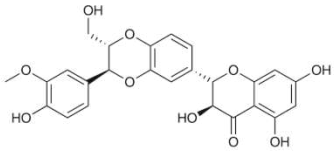
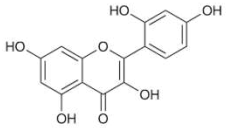
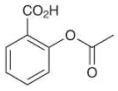
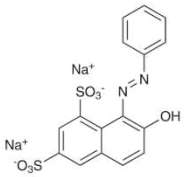
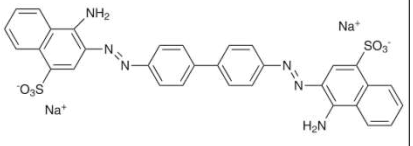
Supplementary Dataset 1 contains a full list of all small molecules used in this study and their structures and chemical properties.

SUPPLEMENTARY DATA SET 1

N°	Compound name	IUPAC Name	MW (Da)	LogP	PAINS	Structure
1	Curcumin	1(*E*,6*E*)-1,7-Bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione	368.4	3.0	[Michael acceptor] protein reactivity, membrane disruptor	
2	Acid fuchsin	2-Amino-5-({4-amino-3-methyl-5-[(sodiooxy)sulfonyl]phenyl}-[(1*E*)-4-imino-3-[(sodiooxy)sulfonyl]-cyclohexa-2,5-dien-1-ylidene]-methyl)benzene-1-sulfonic acid	585.5	-3.9	Dye [Michael acceptor] protein reactive	
3	EGCG	[(2*R*,3*R*)-5,7-Dihydroxy-2-(3,4,5-trihydroxyphenyl)chroman-3-yl] 3,4,5-trihydroxybenzoate	458.4	2.2	[Catechol] protein reactivity, redox	
4	Fast green FCF	Disodium 2-[(*E*)-{4-[ethyl(3-sulfonato-benzyl)-amino]phenyl}-{(4*E*)-4-[ethyl-(3-sulfonatobenzyl)-iminio]-2,5-cyclohexadien-1-ylidene}methyl]-5-hydroxybenzenesulfonate	809.9	-4.4	Dye [Michael acceptor] possibly protein reactive	
5	Acridine orange	*N,N,N',N'*-Tetramethylacridine-3,6-diamine	265.4	3.3	Dye	
6	Caffeic acid	3-(3,4-Dihydroxyphenyl)-2-propenoic acid-3,4-dihydroxy-cinnamic-acid trans-caffeate	180.2	0.9	[Michael acceptor] protein reactive, [Catechol] protein reactivity, redox	
7	Myricetin	3,5,7-Trihydroxy-2-(3,4,5-trihydroxyphenyl)-4-chromenone	318.2	1.4	Potential PAINS [Catechol] protein reactivity, redox	
8	Phenol red	4,4'-(1,1-Dioxido-3*H*-2,1-benzoxathiole-3,3-diyl)diphenol	356.4	-0.6	Dye	
9	Hemin	Chloro[3,7,12,17-tetramethyl-8,13-divinylporphyrin-2,18-dipropanoato(2−)]iron(III)	651.9	6.8	Metal complexer	
10	Resveratrol	5-[(*E*)-2-(4-Hydroxyphenyl)-vinyl]-1,3-benzenediol	228.2	3.0	No	

Supplementary Data Set 1. Structure and properties of small molecules. Hit compounds from the *in vivo* screen are highlighted in pink. LogP values (the log of the aqueous/hydrophobic partition coefficient) were calculated using www.molinspiration.com software, which determines the hydrophobic properties of the substituents. Molecules with high positive LogP values have high hydrophobicity. PAINS key: [functional group or substructure] followed by possible mechanism of action of PAINS (determined by historical analysis of PAINS filters[21, 22]). No = molecule with absence of PAINS substructure. Note: it is not always possible to allocate a specific functional group or substructure to the PAINS.

SUPPLEMENTARY DATA SET 1

N°	Compound name	IUPAC Name	MW (Da)	LogP	PAINS	Structure
11	1*H*-B-SA	1*H*-Benzimidazole-2-sulfonic acid	198.2	-1.1	No	
12	Azure A	*N*',*N*-dimethylphenothiazin-5-ium-3,7-diamine chloride	291.8	0.0	Dye	
13	Benzimidazole	1*H*-Benzimidazole	118.1	1.4	No	
14	Thiabendazole	2-(1,3-Thiazol-4-yl)-1*H*-benzimidazole	201.2	2.3	No	
15	Tramiprosate	3-Amino-1-propanesulfonic acid	139.2	-3.5	No	
16	Silibinin	(2*R*,3*R*)-3,5,7-Trihydroxy-2-[(2*R*,3*R*)-3-(4-hydroxy-3-metho-xyphenyl)-2-(hydroxymethyl)-2,3-dihydro-1,4-benzodioxin-6-yl]-2,3-dihydro-4*H*-chromen-4-one	482.4	1.5	Potential PAINS: metal complexer	
17	Morin hydrate	2-(2,4-Dihydroxyphenyl)-3,5,7-trihydroxychromen-4-one	302.2	1.9	Potential PAINS: [Michael accpetor] protein reactive	
18	Aspirin	2-Acetoxybenzoic acid	180.2	-2.1	No	
19	Orange G	Disodium 7-hydroxy-8-[(*E*)-phenyldiazenyl]-1,3-naphthalenedisulfonate	452.4	-0.3	[Azo] dye and singlet oxygen quencher	
20	Congo red	Disodium 4-amino-3-[4-[4-(1-amino-4-sulfonato-naphthalen-2-yl)diazenylphenyl]phenyl]diazenyl-naphthalene-1-sulfonate	696.7	3.1	[Azo] dye and singlet oxygen quencher	

Supplementary Data Set 1 continued. **Structure and properties of small molecules.** Hit compounds from the *in vivo* screen are highlighted in pink. LogP values (the log of the aqueous/hydrophobic partition coefficient) were calculated using www.molinspiration.com software, which determines the hydrophobic properties of the substituents. Molecules with high positive LogP values have high hydrophobicity. PAINS key: [functional group or substructure] followed by possible mechanism of action of PAINS (determined by historical analysis of PAINS filters[21, 22]). No = molecule with absence of PAINS substructure. Note: it is not always possible to allocate a specific functional group or substructure to the PAINS.

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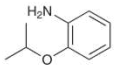
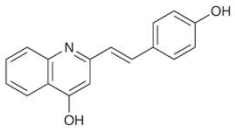
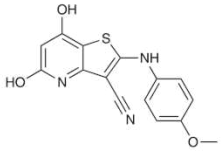
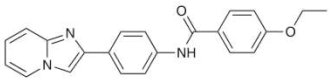
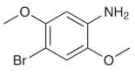
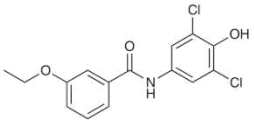
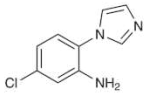
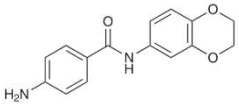
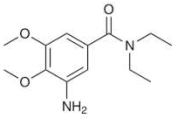
N°	Compound name	IUPAC Name	MW (Da)	LogP	PAINS	Structure
21		(2-isopropoxyphenyl) amine	151.2	2.2	No	
22		2-[2-(4-hydroxyphenyl) vinyl]-4-quinolinol	263.3	4.3	No	
23		5,7-dihydroxy-2-[(4-methoxyphenyl)amino] thieno[3,2-b]pyridine-3-carbonitrile	313.3	3.7	Potential PAINS [masked 2-amino-3-cyanothiophene]	
24		4-ethoxy-N-(4-imidazo [1,2-a]pyridin-2-ylphenyl) benzamide	357.4	4.3	No	
25		(4-bromo-2,5-dimethoxyphenyl)a mine	232.1	2.2	No	
26		N-(3,5-dichloro-4-hydroxyphenyl)-3-ethoxybenzamide	326.2	4.2	No	
27		[1,2,4]triazolo[1,5-a] [1,3,5]triazin-7-amine	136.1	-1.0	No	
28		5-Chloro-2-(1*H*-imidazol-1-yl)aniline	193.6	1.6	No	
29		4-amino-N-(2,3-dihydro-1,4-benzodioxin-6-yl)benzamide	270.3	1.4	No	
30		3-amino-N,N-diethyl-4,5-dimethoxybenzam ide	252.3	0.9	No	

Supplementary Data Set 1 continued. **Structure and properties of small molecules.** Hit compounds from the *in vivo* screen are highlighted in pink. LogP values (the log of the aqueous/hydrophobic partition coefficient) were calculated using www.molinspiration.com software, which determines the hydrophobic properties of the substituents. Molecules with high positive LogP values have high hydrophobicity. PAINS key: [functional group or substructure] followed by possible mechanism of action of PAINS (determined by historical analysis of PAINS filters[21, 22]). No = molecule with absence of PAINS substructure. Note: it is not always possible to allocate a specific functional group or substructure to the PAINS.

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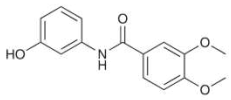
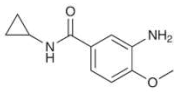
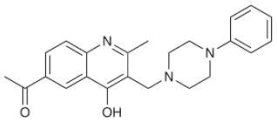
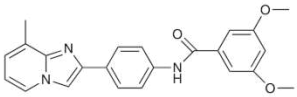
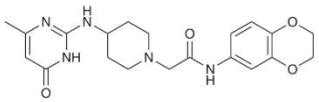
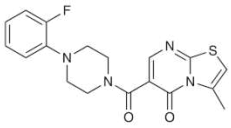
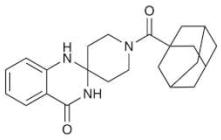
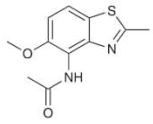
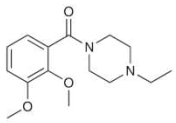
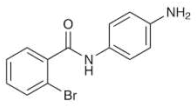
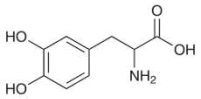
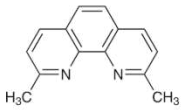
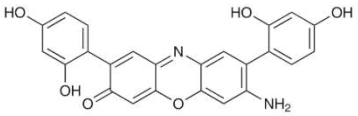
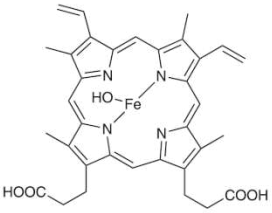
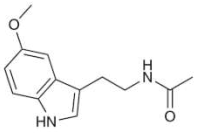
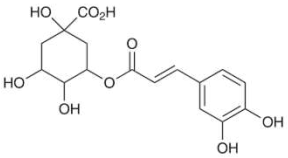
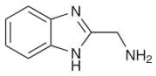
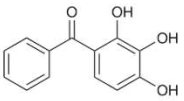
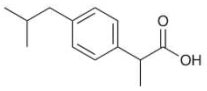
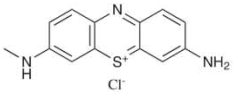
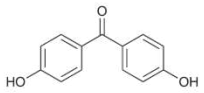
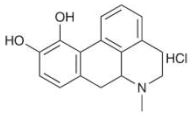
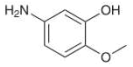
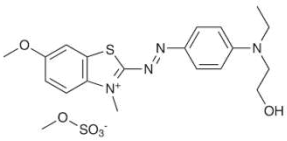
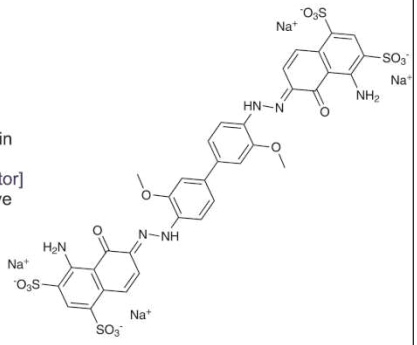
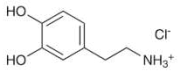
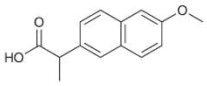
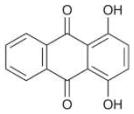
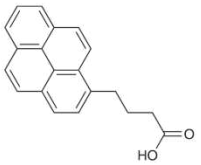
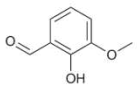
N°	Compound name	IUPAC Name	MW (Da)	LogP	PAINS	Structure
31		*N*-(3-Hydroxyphenyl)-3,4-dimethoxybenzamide	273.3	2.0	No	
32		3-Amino-*N*-cyclopropyl-4-methoxybenzamide	206.1	1.0	Potential PAINS [anisidine]	
33		1-{4-Hydroxy-2-methyl-3-[(4-phenyl-1-piperazinyl)methyl]-6-quinolinyl}ethanone	375.2	3.6	No	
34		3,5-Dimethoxy-*N*-[4-(8-methylimidazo[1,2-a]pyridin-2-yl)phenyl]benzamide	387.4	4.3	No	
35		*N*-(2,3-Dihydro-1,4-benzodioxin-6-yl)-2-[4-{(4-methyl-6-oxo-1,6-dihydropyrimidin-2-yl)amino}piperidin-1-yl]acetamide	399.4	1.6	No	
36	JCS-1	6-{[4-(2-Fluorophenyl)-1-piperazinyl]carbonyl}-3-methyl-5H-[1,3]thiazolo[3,2-a]pyrimidin-5-one	372.4	1.4	No	
37		1-(Adamantan-1-ylcarbonyl)-1'*H*-spiro[piperidine-4,2'-quinazolin]-4'(3'*H*)-one	379.5	3.5	No	
38		*N*-(5-Methoxy-2-methyl-1,3-benzothiazol-4-yl)acetamide	236.3	1.3	No	
39		1-(2,3-Dimethoxybenzoyl)-4-ethylpiperazineylphenyl)benzamide	278.4	1.5	No	
40		*N*-(4-Aminophenyl)-2-bromobenzamide	291.1	2.7	No	

Supplementary Data Set 1 continued. **Structure and properties of small molecules.** Hit compounds from the *in vivo* screen are highlighted in pink. LogP values (the log of the aqueous/hydrophobic partition coefficient) were calculated using www.molinspiration.com software, which determines the hydrophobic properties of the substituents. Molecules with high positive LogP values have high hydrophobicity. PAINS key: [functional group or substructure] followed by possible mechanism of action of PAINS (determined by historical analysis of PAINS filters[21, 22]). No = molecule with absence of PAINS substructure. JCS-1 contains a sub-structural class (carboxypyrimidinone) which although is not specified as problematic by the Baell 2010 PAINS filters[21], is structurally related to the cyanopyridone group, which is a PAINS.

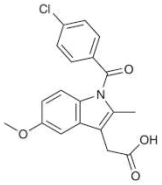
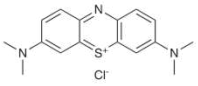
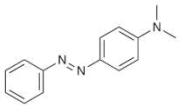
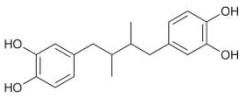
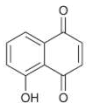
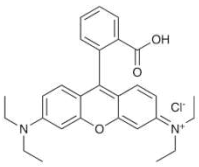
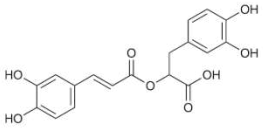
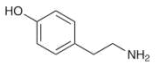
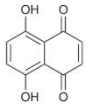
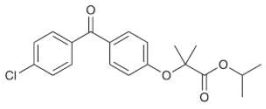
N°	Compound name	IUPAC Name	MW (Da)	LogP	PAINS	Structure
41	L-DOPA	*L*-3,4-Dihydroxyphenyl-alanine	214.2	-2.2	[Catechol] redox and protein reactive	
42	Neocuprione	2,9-Dimethyl-1,10-Phenanthroline	303.8	2.0	Potential PAINS: possible metal complexer	
43	Lacmoid	7-Amino-2,8-bis(2,4-dihydroxyphenyl)-phenoxazin-3-one	189.6	4.0	[Azaquinone] protein reactive	
44	Hematin	(Hydroxy[3,7,12,17-tetramethyl-8,13-divinylporphyrin-2,18-dipropanoato(2-)(iron III))	482.6	5.9	Potential PAINS: possible metal complexer	
45	Melatonin	(*N*-{2-(5-methoxy-14-ind-3-yl)ethyl}acetaminde)	232.3	1.4	No	
46	Chloragenic acid	((1*S*,3*R*,4*R*,5*R*)-3-{[(2*Z*)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy}-1,4,5-trihydroxycyclohexane-carboxylic acid	139.2	-0.5	[Michael acceptor] protein reactive, [Catechol] protein reactive, redox	
47		2-Amino-methyl-benzimidazole	230.3	0.7	No	
48		2,3,4-Trihydroxy-benzophenone	240.2	2.4	[Catechol] protein reactive, redox	
49	Ibuprofen	((*RS*)-2-(4-(2-Methylpropyl)phenyl) -propanoic acid)	288.3	3.5	No	
50	Azure C	(3-Amino-7-(methylamino)phen o-thiazin-5-ium chloride)	152.1	-0.2	Dye	

Supplementary Data Set 1 continued. **Structure and properties of small molecules.** Hit compounds from the *in vivo* screen are highlighted in pink. LogP values (the log of the aqueous/hydrophobic partition coefficient) were calculated using www.molinspiration.com software, which determines the hydrophobic properties of the substituents. Molecules with high positive LogP values have high hydrophobicity. PAINS key: [functional group or substructure] followed by possible mechanism of action of PAINS (determined by historical analysis of PAINS filters[21, 22]). No = molecule with absence of PAINS substructure. Note: it is not always possible to allocate a specific functional group or substructure to the PAINS.

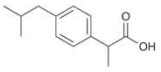
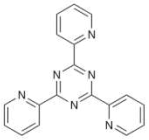
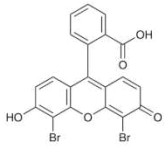
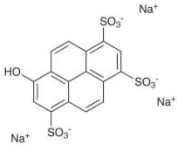
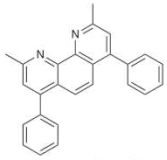
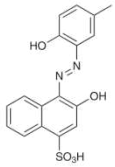
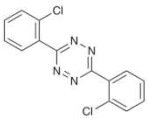
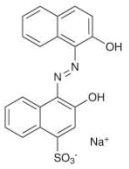
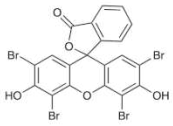
N°	Compound name	IUPAC Name	MW (Da)	LogP	PAINS	Structure
51	4,4′-Dihydroxy-benzophenone	Bis(4-hydroxyphenyl)-methanone	214.2	2.4	No	
52	Apomorphine hydrochloride hemihydrate	6-Methyl-5,6,6a,7-tetrahydro-4*H*-dibenzo-[de,g]-quinoline-1-0,11-diol hydrochloride	303.8	2.9	[Catechol] redox and protein reactive	
53	5-Amino-2-methoxyphenol	5-Amino-2-methoxyphenol	139.2	0.4	Potential PAINS [anisidine]	
54	Basic Blue 41	2-[(*E*)-{4-[Ethyl(2-hydroxyethyl)-amino]phenyl}diazenyl]-6-methoxy-3-methyl-1,3-benzothiazol-3-ium methyl sulfate	482.6	0.9	[Azo] dye and protein reactive	
55	Chicago Sky Blue	Tetrasodium (6Z)-4-amino-6-({4′-[(2*E*)-2-(8-amino-1-oxo-5,7-disulfonato-2(1*H*)-naphthalenylidene)hydrazino]-3,3'-dimethoxy-4-biphenylyl}-hydrazono)-5-oxo-5,6-dihydro-1,3-naphthalenedisulfonate	992.8	-5.1	[Azo] dye and protein reactive, [Michael acceptor] protein reactive	
56	Dopamine hydrochloride	4-(2-Aminoethyl)-1,2-benzenediol hydrochloride	189.6	0.0	[Catechol] redox and protein reactive	
57	DL-naproxen	2-(6-Methoxy-2-naphthyl)propanoic acid	230.3	3.4	No	
58	1,4-Dihydroxy-anthraquinone	1,4-Dihydroxy-9,10-anthraquinone	240.2	3.1	[Quinone] redox and protein reactive	
59	1-Pyrenebutyric acid	4-(1-Pyrenyl)-butanoic acid	288.3	5.0	Potential PAINS: dye (fluorescent)	
60	Ortho-vanillin	2-Hydroxy-3-methoxy-benzaldehyde	152.1	1.3	Potential PAINS: metal chelation	

Supplementary Data Set 1 continued. **Structure and properties of small molecules.** Hit compounds from the *in vivo* screen are highlighted in pink. LogP values (the log of the aqueous/hydrophobic partition coefficient) were calculated using www.molinspiration.com software, which determines the hydrophobic properties of the substituents. Molecules with high positive LogP values have high hydrophobicity. PAINS key: [functional group or substructure] followed by possible mechanism of action of PAINS (determined by historical analysis of PAINS filters[21, 22]). No = molecule with absence of PAINS substructure. Note: it is not always possible to allocate a specific functional group or substructure to the PAINS.

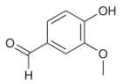
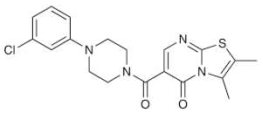
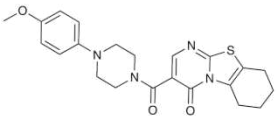
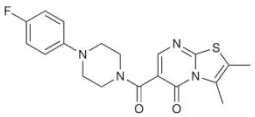
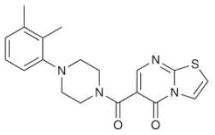
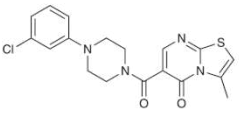
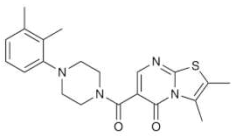
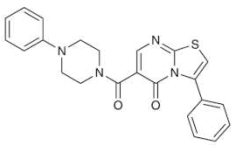
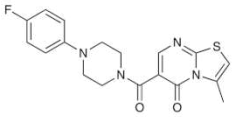
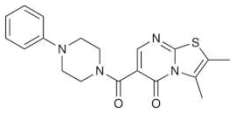
SUPPLEMENTARY DATA SET 1

N°	Compound name	IUPAC Name	MW (Da)	LogP	PAINS	Structure
61	Indomethacin	[1-(4-Chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl]acetic acid	357.8	4.0	Potential PAINS [indole-3-acetamide-like]	
62	Methylene blue	3,7-Bis(dimethyl-amino)phenothiazin-5-ium chloride	319.9	1.0	Dye	
63	Methyl yellow	*N,N*-Dimethyl-4-[(*E*)-phenyldiazenyl]aniline	225.3	4.2	[Azo] dye and singlet oxygen quencher	
64	Nordihydro-guaiaretic acid	4,4'-(2,3-Dimethyl-1,4-butanediyl)-di(1,2-benzenediol)	302.4	3.5	[Quinone] protein reactive, [Catechol] redox and protein reactive	
65	Juglone	5-Hydroxy-1,4-naphthoquinone	174.2	1.4	[Quinone] protein reactive	
66	Rhodamine B	9-(2-Carboxyphenyl)-6-(diethylamino)-*N,N*-diethyl-3*H*-xanthen-3-iminium chloride	479.0	2.7	[Michael acceptor] protein reactive, dye	
67	Rosmarinic acid	3-(3,4-Dihydroxyphenyl)-2-{[(2*E*)-3-(3,4-dihydroxyphenyl)-2-propenoyl]oxy}propanoic-acid	360.3	1.6	[Michael acceptor] protein reactive, [Catechol] redox and protein reactive	
68	Tyramine	4-(2-Aminoethyl)phenol	137.2	0.4	No	
69	5,8-Dihydroxy-1,4-naphthoquinone	5,8-Dihydroxy-1,4-naphthoquinone	190.2	1.3	[Quinone] protein reactive	
70	Fenofibrate	Isopropyl 2-[4-(4-chlorobenzoyl)phenoxy]-2-methylpropanoate	360.8	5.5	No	

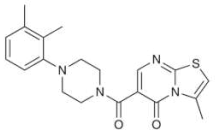
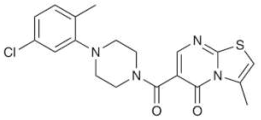
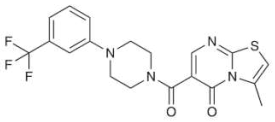
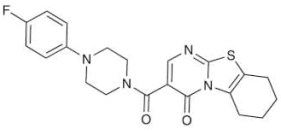
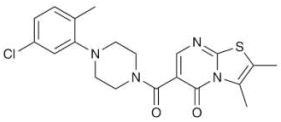
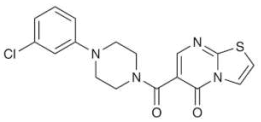
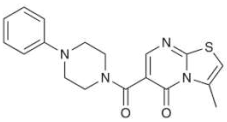
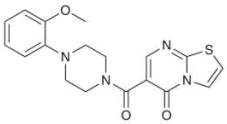
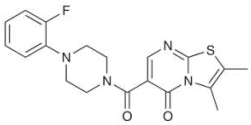
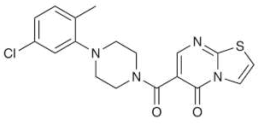
Supplementary Data Set 1 continued. **Structure and properties of small molecules.** Hit compounds from the *in vivo* screen are highlighted in pink. LogP values (the log of the aqueous/hydrophobic partition coefficient) were calculated using www.molinspiration.com software, which determines the hydrophobic properties of the substituents. Molecules with high positive LogP values have high hydrophobicity. PAINS key: [functional group or substructure] followed by possible mechanism of action of PAINS (determined by historical analysis of PAINS filters[21, 22]). No = molecule with absence of PAINS substructure. Note: it is not always possible to allocate a specific functional group or substructure to the PAINS.

N°	Compound name	IUPAC Name	MW (Da)	LogP	PAINS	Structure
71	Ibuprofen	2-(4-Isobutylphenyl)-propanoic acid	206.3	3.5	No	
72	2,4,6-Tris(2-pyridyl)-s-triazine	2,4,6-Tri(2-pyridinyl)-1,3,5-triazine	312.3	2.2	Metal chelator	
73	4',5'-Dibromo-fluorescein	2-(4,5-Dibromo-6-hydroxy-3-oxo-3*H*-xanthen-9-yl)benzoic acid	490.1	5.7	Dye	
74	4,5-Dihydroxy-2,7-naphthalenedi-sulfonic acid	4,5-Dihydroxy-2,7-naphthalenedisulfonic acid	320.3	-3.5	[Quinone] protein reactive	
75	HPTS	Trisodium 8-hydroxy-1,3,6-pyrenetrisulfonate	524.4	-2.0	Dye (fluorometric indicator)	
76	Bathocuproine	2,9-Dimethyl-4,7-diphenyl-1,10-phenanthroline	360.5	6.8	Dye, possible metal complexer	
77	Calmagite	3-Hydroxy-4-[(*E*)-(2-hydroxy-5-methylphenyl)diazenyl]-1-naphthalenesulfonic acid	358.4	2.1	[Azo] protein reactive, possible metal complexer	
78	Clofentezine	3,6-Bis(2-chlorophenyl)-1,2,4,5-tetrazine	303.2	4.7	No	
79	Eriochrome® blue black	Sodium 3-hydroxy-4-[(*E*)-(2-hydroxy-1-naphthyl)-diazenyl]--1-naphthalenesulfonate	416.4	1.8	[Azo] protein reactive, metal complexer	
80	Eosin Y	2',4',5',7'-Tetrabromo-3',6'-dihydroxy-3*H*-spiro[2-benzofuran-1,9'-xanthen]-3-one	647.9	7.2	Dye	

Supplementary Data Set 1 continued. **Structure and properties of small molecules.** Hit compounds from the *in vivo* screen are highlighted in pink. LogP values (the log of the aqueous/hydrophobic partition coefficient) were calculated using www.molinspiration.com software, which determines the hydrophobic properties of the substituents. Molecules with high positive LogP values have high hydrophobicity. PAINS key: [functional group or substructure] followed by possible mechanism of action of PAINS (determined by historical analysis of PAINS filters[21, 22]). No = molecule with absence of PAINS substructure. Note: it is not always possible to allocate a specific functional group or substructure to the PAINS.

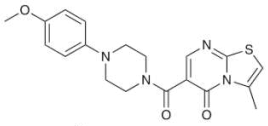
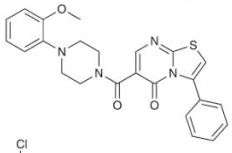
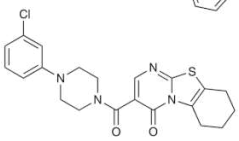
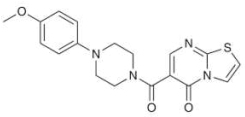
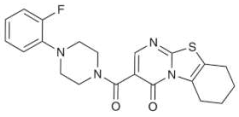
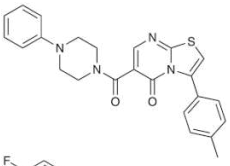
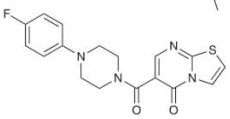
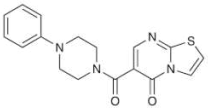
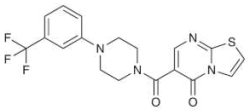
N°	Compound name	IUPAC Name	MW (Da)	LogP	PAINS	Structure
81		(Vanillin) 4-hydroxy-3-methoxy-benzaldehyde	152.1	1.1	Potential PAINS: metal chelation	
82		6-{[4-(3-Chlorophenyl)-1-piperazinyl]-carbonyl}-2,3-dimethyl-5*H*-[1,3]thiazolo-[3,2-a]pyrimidin-5-one	402.9	2.2	No	
83		3-{[4-(4-Methoxyphenyl)-1-piperazinyl]-carbonyl}-6,7,8,9-tetrahydro-4*H*-pyrimido[2,1-b][1,3]benzothiazol-4-one	424.5	2.4	No	
84	JCS-2	6-{[4-(4-Fluorophenyl)-1-piperazinyl]-carbonyl}-2,3-dimethyl-5*H*-[1,3]-thiazolo[3,2-a]pyrimidin-5-one	386.4	1.7	No	
85		6-{[4-(2,3-Dimethylphenyl)-1-piperazinyl]-carbonyl}-5*H*-[1,3]thiazolo-[3,2-a]pyrimidin-5-one	368.5	1.9	No	
86		6-{[4-(3-Chlorophenyl)-1-piperazinyl-]carbonyl}-3-methyl-5*H*-[1,3]-thiazolo[3,2-a]pyrimidin-5-one	388.9	2.0	No	
87		6-{[4-(2,3-Dimethylphenyl)-1-piperazinyl]carbonyl}-2,3-dimethyl-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	396.5	2.4	No	
88		3-Phenyl-6-[(4-phenyl-1-piperazinyl)carbonyl]-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	416.5	2.8	No	
89		6-{[4-(4-Fluorophenyl)-1-piperazinyl]carbonyl}-3-methyl-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	372.4	1.5	No	
90		2,3-Dimethyl-6-[(4-phenyl-1-piperazinyl)-carbonyl]-5*H*-[1,3]thiazolo-[3,2-a]pyrimidin-5-one	368.5	1.5	No	

Supplementary Data Set 1 continued. **Structure and properties of small molecules.** Hit compounds from the *in vivo* screen are highlighted in pink. LogP values (the log of the aqueous/hydrophobic partition coefficient) were calculated using www.molinspiration.com software, which determines the hydrophobic properties of the substituents. Molecules with high positive LogP values have high hydrophobicity. PAINS key: [functional group or substructure] followed by possible mechanism of action of PAINS (determined by historical analysis of PAINS filters[21, 22]). No = molecule with absence of PAINS substructure. Note: it is not always possible to allocate a specific functional group or substructure to the PAINS. Compounds 82 – 109 contain a sub-structural class (carboxypyrimidinone) which although is not specified as problematic by the Baell 2010 PAINS filters[21], is structurally related to the cyanopyridone group, which is a PAINS.

N°	Compound name	IUPAC Name	MW (Da)	LogP	PAINS	Structure
91		6-{[4-(2,3-Dimethylphenyl)-1-piperazinyl]carbonyl}-3-methyl-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	382.5	2.1	No	
92		6-{[4-(5-Chloro-2-methylphenyl)-1-piperazinyl]-carbonyl}-3-methyl-5*H*-[1,3]thiazolo-[3,2-a]pyrimidin-5-one	402.9	2.4	No	
93		3-Methyl-6-({4-[3-(trifluoromethyl)-phenyl]-1-piperazinyl}carbonyl)-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	422.4	2.2	No	
94	JCS-3	3-{[4-(4-Fluorophenyl)-1-piperazinyl]-carbonyl}-6,7,8,9-tetrahydro-4*H*-pyrimido[2,1-b][1,3]benzothiazol-4-one	412.5	2.5	No	
95		6-{[4-(5-Chloro-2-methylphenyl)-1-piperazinyl]carbonyl}-2,3-dimethyl-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	416.9	2.6	No	
96		6-{[4-(3-Chlorophenyl)-1-piperazinyl]carbonyl}-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	374.8	1.8	No	
97		3-Methyl-6-[(4-phenyl-1-piperazinyl)carbonyl]-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	354.4	1.3	No	
98		6-{[4-(2-Methoxyphenyl)-1-piperazinyl]carbonyl}-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	370.4	1.1	No	
99		6-{[4-(2-Fluorophenyl)-1-piperazinyl]carbonyl}-2,3-dimethyl-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	386.4	1.7	No	
100	JCS-4	6-{[4-(5-Chloro-2-methylphenyl)-1-piperazinyl]carbonyl}-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	388.9	2.2	No	

Supplementary Data Set 1 continued. Structure and properties of small molecules. Hit compounds from the *in vivo* screen are highlighted in pink. LogP values (the log of the aqueous/hydrophobic partition coefficient) were calculated using www.molinspiration.com software, which determines the hydrophobic properties of the substituents. Molecules with high positive LogP values have high hydrophobicity. PAINS key: [functional group or substructure] followed by possible mechanism of action of PAINS (determined by historical analysis of PAINS filters[21, 22]). No = molecule with absence of PAINS substructure. Note: it is not always possible to allocate a specific functional group or substructure to the PAINS. Compounds 82 – 109 contain a sub-structural class (carboxypyrimidinone) which although is not specified as problematic by the Baell 2010 PAINS filters[21], is structurally related to the cyanopyridone group, which is a PAINS.

SUPPLEMENTARY DATA SET 1

N°	Compound name	IUPAC Name	MW (Da)	LogP	PAINS	Structure
101		6-{[4-(4-Methoxyphenyl)-1-piperazinyl]carbonyl}-3-methyl-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	384.5	1.4	No	
102		6-{[4-(2-Methoxyphenyl)-1-piperazinyl]-carbonyl}-3-phenyl-5*H*-[1,3]thiazolo-[3,2-a]pyrimidin-5-one	446.5	2.8	No	
103	JCS-5	3-{[4-(3-Chlorophenyl)-1-piperazinyl]-carbonyl}-6,7,8,9-tetrahydro-4*H*-pyrimido[2,1-b][1,3]benzothiazol-4-one	428.9	3.0	No	
104		6-{[4-(4-Methoxyphenyl)-1-piperazinyl]-carbonyl}-5*H*-[1,3]thiazolo-[3,2-a]pyrimidin-5-one	370.4	1.2	No	
105		3-{[4-(2-Fluorophenyl)-1-piperazinyl]-carbonyl}-6,7,8,9-tetrahydro-4*H*-pyrimido[2,1-b][1,3]benzothiazol-4-one	412.5	2.5	No	
106		3-(4-Methylphenyl)-6-[(4-phenyl-1-piperazinyl)-carbonyl]-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	430.5	3.2	No	
107		6-{[4-(4-Fluorophenyl)-1-piperazinyl]carbonyl}-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	358.4	1.3	No	
108		6-[(4-Phenyl-1-piperazinyl)carbonyl]-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	340.4	1.1	No	
109		6-({4-[3-(Trifluoromethyl)phenyl]-1-piperazinyl}carbonyl)-5*H*-[1,3]thiazolo[3,2-a]pyrimidin-5-one	408.4	2.0	No	

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