Critical Review

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Biogenic colourants in the textile industry – a promising and sustainable alternative to synthetic dyes

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Supplement

Table S1: Acute toxicity, bioactivity and predicted biodegradability of selected microbial dyes. Data was obtained from EPA CompTox database.

Class/Name	CAS no.	Toxicity test type	Value acute toxicity	Test species	Ref	Predicted biodegradability half-life (days)	Confidence level in OPERA model	Bioassay activity	Colour index no.
Polyenes									
β-Carotene (**9**)	7235-40-7	LD_{50}	>5000 mg·kg^{-1}	rat (oral)	[1]	74.4	0.517	binding solute carrier transporter, antiviral, antioxidant	C.I. Food Orange 5
Astaxanthin (**10**)	472-61-7	LD_{50}	>20000 mg·kg^{-1}	rat (oral)	[2]	44.4	0.514		
Azulene	275-51-4	LD_{50}	108 mg·kg^{-1}	mouse (intra-peritoneal)	[3]	8.58	0.553		
Azulene	275-51-4	LD_{50}	>3000 mg·kg^{-1}	mouse (oral)	[3]				
Guaiazulene (**11**)	489-84-9	LD_{50}	525 mg·kg^{-1}	mouse (intra-peritoneal)	[4]	2.5	0.73	binding nuclear receptors and histone enzymes	
Guaiazulene (**11**)	489-84-9	LD_{50}	1220 mg·kg^{-1}	mouse (oral)	[4]				
Quinones									
Actinorhodin (**14**)	1397-77-9					153	0.441		
Emodin (**15**)	518-82-1	LD_{50}	1000 mg·kg^{-1}	rat (oral)	[5]	44.6	0.481	ser-thr kinase, cyp1a2+2c9, microtubule assoc. protein, aldehyde dehydrogenase	C.I. Natural Yellow 14
Monascin (**20**)	21516-68-7					4.74	0.514		
Indoles									

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Violacein (**26**)	548-54-9	LD_{50}	100 mg·kg^{-1}	mouse (intra-peritoneal)	MSDS, [6]				
Violacein (**26**)	548-54-9	EC_{50}	560 mg·L^{-1}	*P. capsici* (fungus)	[7]				
Oxyviolacein		EC_{50}	460 mg·L^{-1}	*P. capsici* (fungus)	[7]				
Oxyviolacein		EC_{50}	2010 mg·L^{-1}	*R. solani* (fungus)	[7]				
Deoxyviolacein	5839-61-2	EC_{50}	1730 mg·L^{-1}	*R. solani* (fungus)	[7]				
Other N-heterocycles									
Rubrolone (**41**)	65445-21-8	LD_{50}	930 mg·kg^{-1}	mouse (intra-peritoneal)	[8]	142	0.449		
Rubrolone (**41**)	65445-21-8	LD_{50}	>4000 mg·kg^{-1}	mouse (oral)	[8]				
Pyrroles									
Prodigiosin (**31**)	82-89-3	LD_{50}	18 mg·kg^{-1}	mouse (intra-peritoneal)	[9]	3.35	0.595	x	x
Undecyl-prodigiosin	52340-48-4	LD_{50}	26.7 mg·kg^{-1}	mouse (intravenous)	[6]				
Prodigiosin-25C	14960-80-6	LD_{50}	7.1 mg·kg^{-1}	mouse (intra-peritoneal)	[10]				
Phenazines									
Pyocyanin (**35**)	85-66-5		acute toxicity		MSDS	3.35	0.623		
Lavandu-cyanin	122228-60-8	LD_{50}	>100 mg·kg^{-1}	mouse (intra-peritoneal)	[11]	47.8	0.459		
Flavins									
Riboflavin	83-88-5	LD_{50}	560 mg·kg^{-1}	rat (intra-peritoneal)	[12]	6.73	0.501	binding G-protein subunit and various enzymes (as a cofactor)	C.I. Food Yellow 15
Riboflavin	83-88-5	LD_{50}	>10000 mg·kg^{-1}	rat (oral)	[12]				

[a] Predicted biodegradability half-life comes with a confidence level index (ranging from 0 to 1) to decide about the reliability of this prediction.

Table S2: Acute toxicity, bioactivity and predicted biodegradability of selected synthetic dyes. Data was obtained from EPA CompTox database.

Class/Name/ Colour index no.	CAS no.	Toxicity test type	Value acute toxicity	Test species	Ref	Predicted biodegradability half-life (days)	Confidence level in OPERA model[a]	Bioassay activity
Azo								
Reactive Red 1	17752-85-1					15.3	0.398	
Direct Black 80 (Na+ salt or free acid)	8003-69-8	LC_{50}	180 mg·L^{-1}	fathead minnow (fish)		113	0.443	predicted androgen receptor binding
Polycyclics								
Cu-phthalocyanine	147-14-8	LD_{50}	10000 mg·kg^{-1}	mouse (oral)	[13]	153	0.519	predicted androgen receptor binding
Cu-phthalocyanine	147-14-8	LC_{50}	100 mg·L^{-1}	zebrafish	[13]			
Oxazines								
Basic Blue 12 (Nile Blue) (**8**)	2381-85-3	LD_{50}	18 mg·kg^{-1}	mouse (intravenous)	[14]	45.3	0.495	
Anthraquinones								
Mordant Red 3 (Na+ salt or free acid) (**3**)	130-22-3	LD_{50}	70 mg·kg^{-1}	mouse (intravenous)	[15]	8.83	0.569	human phosphoglycerate-mutase inhibitor
Mordant Red 3 (Na+ salt or free acid) (**3**)	130-22-3	LC_{50}	250 mg·L^{-1}	japanese medaka (fish)	[16]			
Pigment Yellow 108 (**4**)	4216-01-7					149	0.459	

Triaryl-carbonium								
Basic Green 4 (Malachite green) (**7**)	569-64-2	LD_{50}	80 $mg \cdot kg^{-1}$	mouse (oral)	[17]	4.04	0.774	binding to many human receptors
Basic Green 4 (**7**)	569-64-2	LC_{50}	0.6 $mg \cdot L^{-1}$	japanese medaka (fish)	[18]			
Indoles								
Acid Blue 74 (Indigo Carmine)	860-22-0	LD_{50}	2500 $mg \cdot kg^{-1}$	mouse (oral)	[19]	15.4	0.429	binding oestrogen receptor1 and inhibitor of several enzymes

[a] Predicted biodegradability half-life comes with a confidence level index (ranging from 0 to 1) to decide about the reliability of this prediction.

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