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Solubility and Toxicity Level of *Monascus* Pigments

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Abstract

Research on *Monascus* pigments (MPs) has been progressing very rapidly. The progresses include the discovery of new pigments and methods used for isolating and identifying the new pigments. Currently, nearly fifty-seven new pigments have been found as derivations of the six main pigments existed. The process of new pigments discovery is unable to separate from that of fermentation or isolation process. In several new pigments, there was no complete information relating to solubility and level of toxicity. This research covers data of all fifty-seven new pigments including color, molecular weight, water solubility, log Kow (octanol-water partition coefficient), and baseline toxicity level by Ecological Structure Activity Relationships (ECOSAR) Program. These results are expected to give more comprehensive data about *Monascus* pigments.

Keywords: *Monascus* pigments; Solubility; Toxicity; Ecosar

Introduction

Monascus Pigments (MPs) has long been used as a natural food colorant, especially in some Asian countries such as South China. *Monascus* produces red yeast rice, which is rice covered with a red *Monascus* sp. Angkak can be used as a dye for yoghurt, bacon, and sausage and also for the preservative of fruits, vegetables, and fish products [1].

The Ecological Structure Activity Relationships (ECOSAR) is a computerized predictive system that estimates aquatic toxicity. The program estimates a chemical's acute (short-term) toxicity and chronic (long-term or delayed) toxicity to aquatic organisms, such as fish, aquatic invertebrates, and aquatic plants, by using computerized Structure Activity Relationships (SARs) [2].

Materials and Methods

Data collected from various studies that have been done before [3-5] and added with some of the data from ECOSAR results. This toxicity test on ECOSAR program was used to determine the toxicity against water organisms.

Result

Table 1: Solubility and Toxicity Level of Monascus Pigments.

No	Pigments	Color	MW (g/mol)	Water Solubility (mg/L)	Log Kow	Neutral organic SAR (Baseline Toxicity) (mg/L)		
						Fish LC_{50}, 96h	Daphnid LC_{50}, 48h	Green Algae EC_{50}, 96h
1	Glycyl Rubropuctamin	Red	413.18	18.68	0.071	18328.39	6725.24	6168.59
2	Isolate from MPs 1	Red	510.25	4.793	0.043	24022.46	8766.53	8039.59
3	Isolate from MPs 2	Red	538.28	5.417	2.2	292.25	160.59	149.11
4	Isolate from MPs 3	Red	439.20	0.6096	1.621	790.75	389.32	360.29
5	Isolate from MPs 4	Red	439.24	0.2773	2.021	345.60	183.58	170.28
6	N-glutaryl Monascorubramine	Red	511.22	0.4876	1.197	2209.66	1003.9	926.80
7	N-glutaril Rubropuctamine	Red	483.19	5.089	0.215	15920.09	6003.13	5510.82
8	N-glucosyl rubropunctamine	Red	557.64	0.2901	3.536	19.1	13.53	12.66
9	N-glucosyl monascorubramine	Red	585.69	0.02759	4.519	2.63	2.25	2.11
10	Compound R3	Red	374.17	336.5	1.905	374.68	194.67	180.45

11	Red Derivative 1	Red	453.22	0.2188	2.039	344.06	183.36	170.1
12	Red Derivative 2	Red	425.18	2.266	1.056	2460.49	1088.33	1003.93
13	Red Derivative 3	Red	497.20	1.576	0.706	5933.47	2455.88	2260.86
14	Red Derivative 4	Red	437.54	0.5376	4.586	1.71	1.48	1.39
15	Red Derivative 5	Red	453.22	0.2188	2.039	344.06	183.36	170.1
16	Red Derivative 6	Red	425.18	2.266	1.056	2460.49	1088.33	1003.93
17	Red Derivative 7	Red	497.20	1.576	0.706	5933.47	2455.88	2260.86
18	Red Derivative 8	Red	469.17	16.42	-0.276	42679.29	14661.65	13421.26
19	Un Named	Red	375.20	1636	1.676	602.53	299.78	277.52
20	Manascopyridine A	Red	355.18	231.1	1.634	622.53	307.25	284.37
21	Manascopyridine B	Red	383.21	22.58	2.616	88.11	52.40	48.77
22	Manascopyridine C	Red	357.19	795.3	1.588	687.97	336.62	311.47
23	Monascopyridine D	Red	343.21	25.02	3.446	14.17	9.87	9.23
24	New red pigment	Red	375.20	1636	1.676	602.53	299.78	277.52
25	Red Shandong 1	Red	303.40	1973	2.087	208.25	112.01	103.93
26	Red Shandong 2	Red	331.46	195.2	3.069	29.85	19.34	18.05
27	PP-V	Purple red	411.17	2612	0.46	8164.14	3224.95	2964.64
28	Monaphilol A	Orange	384.19	11.23	3.562	12.51	8.90	8.33
29	Monaphilol B	Orange	356.16	114.9	2.579	88.37	52.18	48.56
30	Monaphilol C	Orange	440.22	16.81	2.947	51.01	32.3	30.12
31	Monaphilol D	Orange	412.48	173.8	1.965	364.07	191.34	177.43
32	Monascusone A	Yellow	254.12	2608	1.094	1361.60	606.53	559.61
33	Monascusone B	Yellow	302.12	1972	0.914	2346.48	1010.26	931.14
34	Xanthomonascin A	Yellow	388.15	383.3	1.738	548.76	276.24	255.81
35	Xanthomonascin B	Yellow	414.20	18.8	3.082	36.36	23.62	22.04
36	Yellow II	Yellow	372.19	6.886	3.299	20.84	14.1	13.18
37	FK17-P2B2	Yellow	236.10	242.9	2.417	81.98	46.94	43.64
38	Monaphilones A	Yellow	360.49	5.540	4.192	3.06	2.45	2.31
39	Monaphilones B	Yellow	332.20	56.21	3.21	21.44	14.27	13.33
40	Monaphilones C	Yellow	336.23	97.28	2.903	40.95	25.71	23.97
41	Y3	Yellow	448.21	897.6	0.731	5085.16	2114.57	1946.93
42	Monashexenone (Y)	Yellow	320.20	86.53	2.976	34.95	22.25	20.76
43	Rubropunctin	Yellow	358.21	0.3022	5.486	0.23	0.23	0.22
44	Monarubrin (Y,BF)	Yellow	330.18	29.06	3.559	10.34	7.35	6.88
45	Purpureusone	Yellow	390.24	12.92	2.849	55.40	34.43	32.09
46	Monapurones A	Yellow oil	330.18	3.322	4.466	1.73	1.46	1.37
47	Monapurones B	Yellow oil	344.20	0.02141	6.434	0.03	0.04	0.03
48	Monapurones C	Yellow oil	344.20	0.02141	6.434	0.03	0.04	0.03
49	Monascuspiloin	Yellowish oil	360.45	22.07	3.39	16.72	11.52	10.77
50	Monankarin A-B	Yellow needles	358.14	2754	1.629	633.97	312.61	289.32
51	Monankarin C-D	Yellow needles	372.16	771.2	2.176	212.43	116.21	107.89
52	Monankarin E	Yellow needles	344.13	7610	1.212	1444.69	658.11	607.62
53	Monankarin F	Yellow needles	356.16	80.15	3.442	14.85	10.33	9.66

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54	Monasfluor A	Blue fluorescent	354.18	0.08076	5.688	0.14	0.15	0.14
55	Monasfluor B	Blue fluorescent	384.19	0.9693	4.21	3.27	2.63	2.47
56	Monascuskaodione A	Colorless oil	356.42	9.922	3.228	23.11	15.43	14.42
57	Monascuskaodione B	Colorles oil	384.47	4.210	0,969	3.27	2.63	2.47

As shown in Table 1, data showed that the lower log Kow of a compound, the lower of toxicity. And from the toxicity point of view, those of compounds to categorize having lower toxicity than others were LC50 and EC50 values>100mg/L. This was because the lower binding energy of a compound, the stronger bond between the receptor and that compound. It made the compound attach to biological membranes longer and more toxicable [2].

Conclusion

Based on log Kow value of fifty-seven pigments of *Monascus* were determined, Red Pigment 8 has the lowest toxicity while Monapurones (B and C) have the highest toxicity.

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