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Research Article

Druglikeness of Flowerophoric Model

Kavita Bisht [1], Alok maithani[2], Luv Kush*[3]

[1]M.Sc. Pharmaceutical Chemistry, Sardar Bhagwan Singh University, Balawala Dehradun-248161, Uttarakhand, India
[2]Assistant Professor, Dept. of Applied Chemistry, SBS, Balawala Dehradun-248161, Uttarakhand, India
[3]Academic Advisor Cum Educator, Deptt of Applied Chemistry, SBS University, Balawala Dehradun-248161, Uttarakhand, India

ABSTRACT

Angiospermic biodiversity is composed of extraordinary versatile flowers of different shapes, colors and aromas. Recently flowers have emerged as the complementary medicine. The druglikeness of commonly occurring terpenoids, flavonoids and pigments in the flowers was rationalized to suggest flowerophoric model at naturotherapeutical level.

Keywords- Druglikeness, Flowerophoric, Lipinski's rule, Natural product, Naturotherapeutical.

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***Address for Correspondence:**

Luv Kush, Academic Advisor Cum Educator, Deptt of Applied Chemistry, SBS University, Balawala Dehradun-248161, Uttarakhand, India

INTRODUCTION

The medicinal relevance of flowers[1-9] is authenticated by multiple bioactivities of naturotherapeutical significance,. The natural product chemistry of medicinal flowers[10-14] have organic structures of terpenoids, flavonoids and pigments as well as functional nutrients (vitamins, minerals). The pollen garins[15-17] are the rich source of nutraceuticals and novel chemical entities. Recently flower therapy[18] is found to be quite effective for the emotional and social welfares of the people. The druglikeness is the focal point to be rationalized for their value as the naturotherapeuticals.

Theoretical Methodology

Lipinski's rule[19] and veber's[20] rule ascertain the druglikeness for the pharmacokinetic compliance. We selected total ten compounds of different organic structures which commonly occur in almost every flower. The data of both the rules is given in tables 1 & 2.

RESULT AND DISCUSSION

The Flowers therapeutics is based on chromogenic and perfumogenic chemical entitles for the naturopathy. The flowerophoric model is analogues to pharmacophore[21] and ayurvedicophore[22,23] because druglikeness of chemical structures of terpenoids, flavonoids, and pigments was rationalized for the pharmacokinetic compliance. The molecular mass, H-bond acceptors and donors showed satisfactory compliance with Lipinski's rule except pigments, therefore terpenoids and flavonoids have better druglikeness than pigments. Veber's modification data suggested violation of the rule of molecular flexibility by Lycopene. The flowerophoric model for binding at site of action should be composed of optimal hydrophobic surface

to accommodate alkyl, acyclic and aryl structural moieties. The dominance of oxygen functions may act both as H-bond acceptor and donor. Interestingly profound unsaturation due to πbonds impart high degree of planarity, for intercalative action.

Table 1: Lipinski's rule related data

Pharmac Ophoric properties	Anthocyanin	B- carotone	Caryop hyllene	Delphinidin	Kaempf erol	Lycopene	Linalool	Nerolidol	Quercetin	Zeaxanthin
Molecular formula	$C_{15}H_{11}O$	$C_{40}H_{56}$	$C_{15}H_{24}$	$C_{15}H_{11}O_7$	$C_{15}H_{10}O_6$	$C_{40}H_{56}$	$C_{10}H_{18}O$	$C_{15}H_{26}O$	$C_{15}H_{10}O_7$	$C_{40}H_{56}O_2$
Molecular weight	207.252 g/mol	536.8 g/mol	204.357 g/mol	303.24 3g/mol	286.236 g/mol	536.87 3g/mol	154.25 3g/mol	222.3 6g/mol	302.23 8g/mol	568.8 7g/mol
No. of Chiral atom	0	0	2	0	0	0	1	1	0	0
H-bond acceptors	0	0	0	6	6	0	1	1	7	2
H-bond Donors	0	0	0	6	4	0	1	1	5	2
Log-p value	4.47	9.72	4.52	2.07	1.99	9.16	2.68	4.55	2.16	8.3

Table 2: Veber's rule related data

Pharmac Ophoric properties	Anthocyanin	B- carotone	Caryop hyllene	Delphinidin	Kaempferol	Lycopene	Linalool	Nerolidol	Quercetin	Zeaxan thin
No. of Aryl rings	3	2	0	3	3	0	0	0	3	2
Sum of H-Bond donors & acceptors	0	0	0	12	10	0	2	2	12	4
Rotable bond count	1	10	0	1	1	16	4	7	1	10

CONCLUSION

Flower therapeutics is the future of naturotherapeutics. Flowers are integral part of human love, romance, friendship, respect and worship. They have remarkable chemical entities of druglikeness, gifted by nature. The druglikeness of ten compounds was theoretically evaluated fo the pharmacokinetic compliance. A flowerophoric model was suggested, composed of hydrophobic, H-bond acceptor and donor binding sites for bioaction. The flowerophoric model may innovate rational use for emotional and social welfares of human life.

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