Druglikeness of Flowerophoric Model

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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 naturomerapeutic level.

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

INTRODUCTION

The medicinal relevance of flowers1-9 is authenticated by multiple bioactivities of naturomerapeutic significance. The natural product chemistry of medicinal flowers10-14 have organic structures of terpenoids, flavonoids and pigments as well as functional nutrients (vitamins, minerals). The pollen garins15-17 are the rich source of nutraceuticals and novel chemical entities. Recently flower therapy18 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 naturomerapeutics.

Theoretical Methodology

Lipinski’s rule19 and veber’s20 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 pharmacophore21 and ayurvedicophore22,23 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 π bonds impart high degree of planarity, for intercalative action.

Table 1: Lipinski’s rule related data

<table>
<thead>
<tr>
<th>Pharmacophoric properties</th>
<th>Anthocyanin</th>
<th>B- carotene</th>
<th>Caryophyllene</th>
<th>Delphinidin</th>
<th>Kaempferol</th>
<th>Lycopene</th>
<th>Linalool</th>
<th>Nerolidol</th>
<th>Quercetin</th>
<th>Zeaxanthin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular formula</td>
<td>C_{13}H_{17}O</td>
<td>C_{48}H_{50}</td>
<td>C_{31}H_{34}</td>
<td>C_{13}H_{17}O_{7}</td>
<td>C_{31}H_{29}O_{3}</td>
<td>C_{29}H_{58}</td>
<td>C_{13}H_{29}O</td>
<td>C_{13}H_{29}O_{7}</td>
<td>C_{29}H_{58}</td>
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<tr>
<td>Molecular weight</td>
<td>207.252 g/mol</td>
<td>536.8 g/mol</td>
<td>204.357 g/mol</td>
<td>303.24 g/mol</td>
<td>266.236 g/mol</td>
<td>536.87 g/mol</td>
<td>154.25 g/mol</td>
<td>222.3 g/mol</td>
<td>302.23 g/mol</td>
<td>568.8 g/mol</td>
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<tr>
<td>No. of Chiral atom</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>H-bond acceptors</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>6</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>7</td>
<td>2</td>
</tr>
<tr>
<td>H-bond Donors</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>6</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>5</td>
<td>2</td>
</tr>
<tr>
<td>Log-p value</td>
<td>4.47</td>
<td>9.72</td>
<td>4.52</td>
<td>2.07</td>
<td>1.99</td>
<td>9.16</td>
<td>2.68</td>
<td>4.55</td>
<td>2.16</td>
<td>8.3</td>
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</tbody>
</table>

Table 2: Veber’s rule related data

<table>
<thead>
<tr>
<th>Pharmacophoric properties</th>
<th>Anthocyanin</th>
<th>B- carotene</th>
<th>Caryophyllene</th>
<th>Delphinidin</th>
<th>Kaempferol</th>
<th>Lycopene</th>
<th>Linalool</th>
<th>Nerolidol</th>
<th>Quercetin</th>
<th>Zeaxanthin</th>
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<tbody>
<tr>
<td>No. of Aryl rings</td>
<td>3</td>
<td>2</td>
<td>0</td>
<td>3</td>
<td>3</td>
<td>0</td>
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<td>0</td>
<td>3</td>
<td>2</td>
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<tr>
<td>Sum of H-bond donors &amp; acceptors</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>12</td>
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<td>0</td>
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<td>4</td>
</tr>
<tr>
<td>Rotable bond count</td>
<td>1</td>
<td>10</td>
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<td>1</td>
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<td>16</td>
<td>4</td>
<td>7</td>
<td>1</td>
<td>10</td>
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</tbody>
</table>

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 drug likeness, gifted by nature. The drug likeness of ten compounds was theoretically evaluated to 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 welfare of human life.

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REFERENCES

5. Therapeutic uses of flowers leads from traditional system of medicine, International journal of herbal medicine, www.florajournal.com
11. Essentials oils: www.bojeneen.net
19. Ashutosh kar, Medicinal chemistry. 2010; 90.
23. AkshayNegi & Dr. Luv kush “Tricophoric Ayurvedicophore”. IJIRD 2013; (2)7:127-131