2017.2.16

Carotenoid DB Chemical Fingerprint Description

Carotenoid DB Chemical Fingerprints represent the chemical modification patterns in carotenoids.
Chemical modification patterns can be classified into 23 categories as follows in descending order of frequency.

Categories	Notation	Description
1. Hydroxylation	Cn-OH	Hydroxylation at carbon n
2. Saturation	Cn, Cn+1 +H	Saturation between carbon n and n+1
3. Cyclization	beta,beta, psi,psi, beta,psi, beta,epsilon, kappa,chi, etc.	Cyclization (end group)
4. Ketolation	Cn =O	Ketolation at carbon n
5. Desaturation	Cn, Cn+1 --H	Desaturation between carbon n and n+1
6. Stereoisomer (RS)	(CmR,CnS), etc.	Stereoisomer (RS)
7. Apo	Cn -apo	All of the molecule beyond the carbon n has been replaced by hydrogen atoms
8. Epoxidation	Cm, Cn-Epoxy	Epoxidation between carbon m and carbon n
9. Esterification	Cn -ester	Esterification at carbon n
10. Cis/trans isomerization	CnZ / CnE	Cis or trans isomerization at carbon n
11. Glycosidation	Cn -b-Glc, Cn -a-Lrha, etc	Glycosidation, rhamnosylation, etc. at carbon n
12. Aldehyde addition	Cn -al	Aldehyde addition at carbon n
13. Carbonylation	Cn -COOH, Cn -COOCH3 etc.	Carbonylation at carbon n
14. Alkoxylation	Cn -Methoxy, Cn -Ethanoyloxy, etc.	Methoxylation, ethanoyloxylation, etc. at carbon n
15. Isoprene polymerization	Cn -isoprene	Isoprene polymerization at carbon n
16. Nor	Cn -nor	Elimination of carbon n
17. Complex polymerization	Complex derivative	Complex polymerization
18. Olide	Cm, Cn-olide	Lactone formation between carbon m and n
19. Sulfation	Cn -SO4-Na	Sodium sulfation at carbon n
20. Seco	Cm,Cn -seco	Fission of the bond between carbon m and n
21. Retro	Cm, Cn-retro	All single and double bonds are shifted by one position from carbon m to carbon n
22. Cycloaddition	Cm,Cn-cyclo	Cycloaddition between carbon m and carbon n
23. Geranylgeranylation	Cn -geranylgeranyl	Geranylgeranylation at carbon n

C_m, and/or C_n represent the chemically modified carbons' numbers. Numbering of carbons is indicated below as is well defined by the "Rule Carotenoid 4." in the Nomenclature of Carotenoids issued by the IUPAC Commission on the Nomenclature of Organic Chemistry and the IUPAC-IUB Commission on Biochemical Nomenclature.
(See also http://pac.iupac.org/publications/pac/pdf/1975/pdf/4103x0405.pdf)

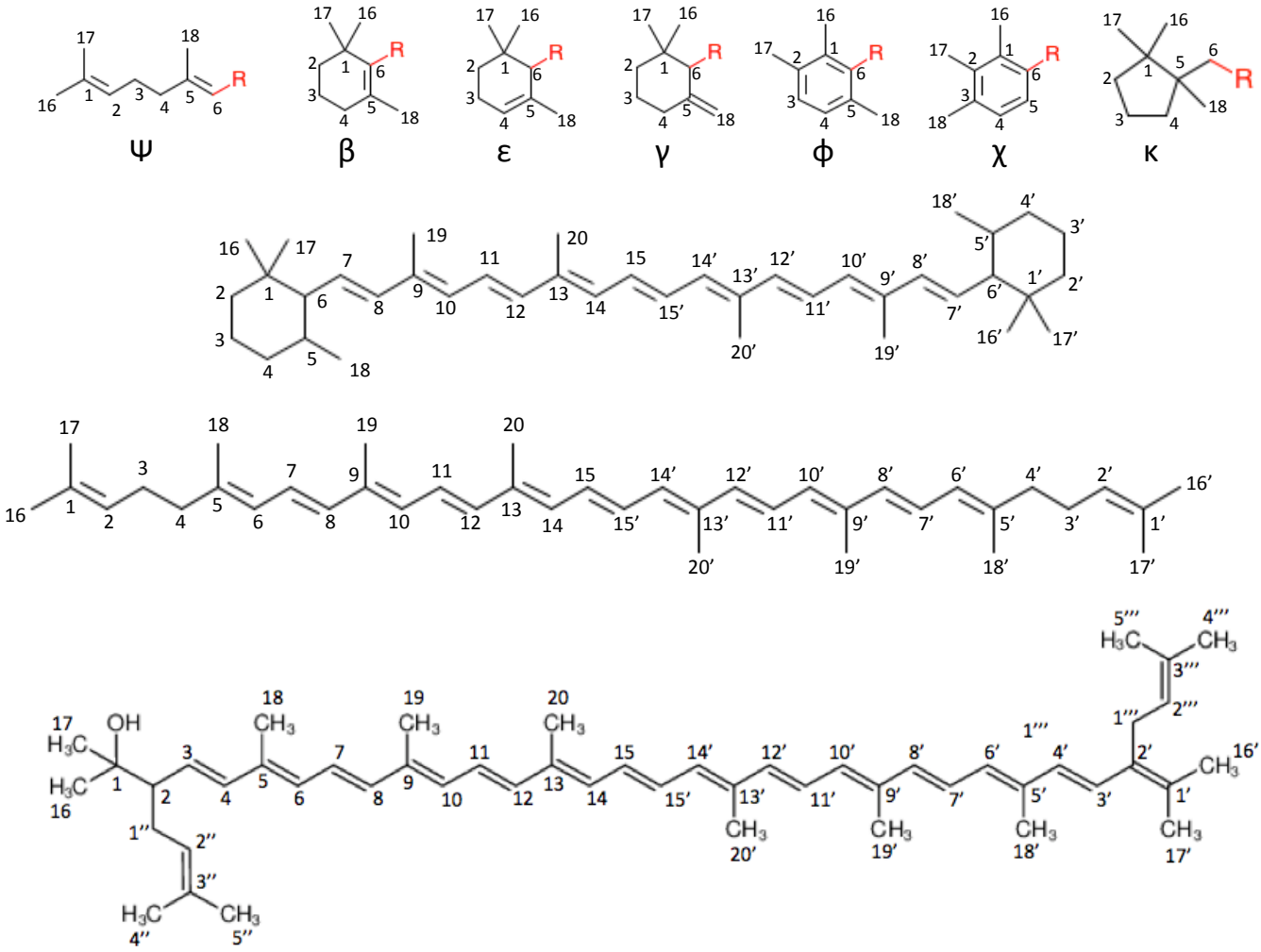

Figure: Numbering of carbon positions.