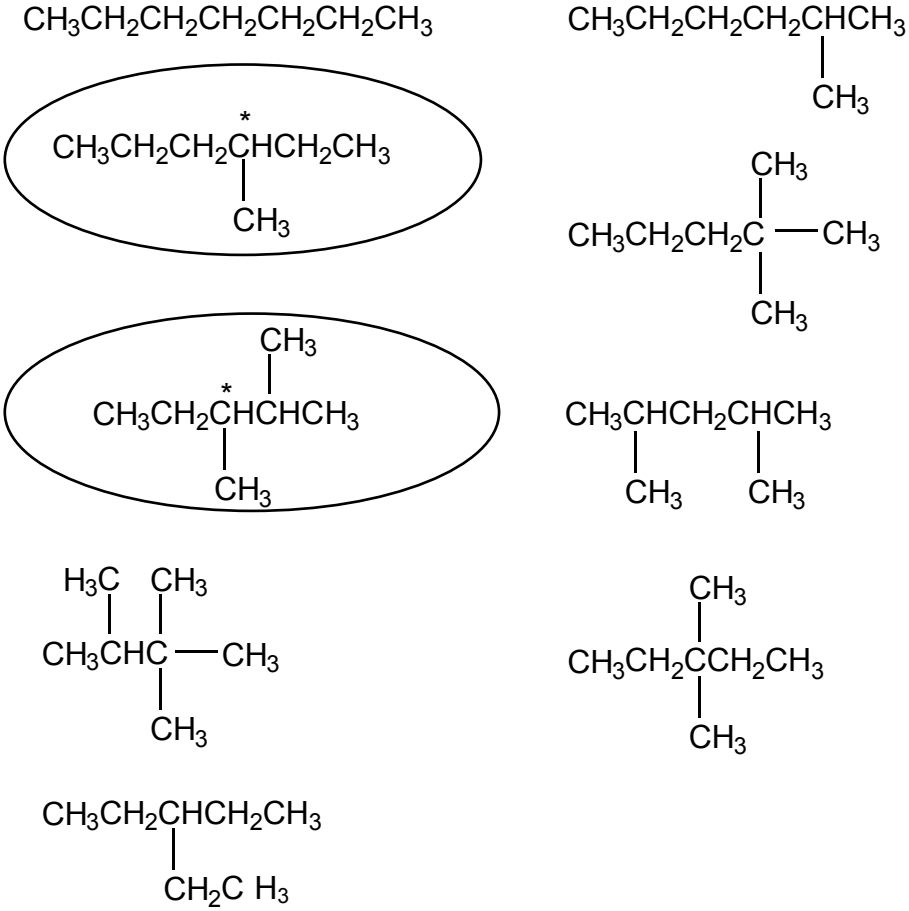
Problem Set 7: Stereochemistry-ANSWER KEY

Chemistry 260 **Organic Chemistry**

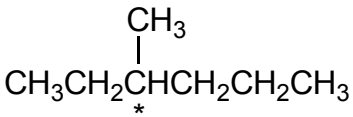
1. The answer is (2).

Circled isomers have a stereogenic carbon (*) and hence a stereogenic centre.

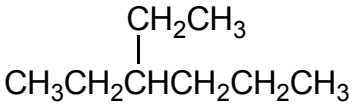


2. Note: a star (*) is used to denote a stereogenic centre (tetrahedral geometry, bonded to 4 different groups) in the structures in this question.

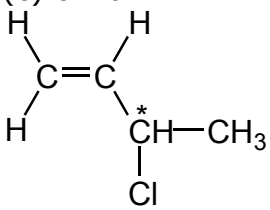
(a) chiral



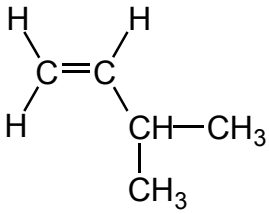
(b) not chiral - no stereogenic centre



(c) chiral



(d) not chiral - no stereogenic centre



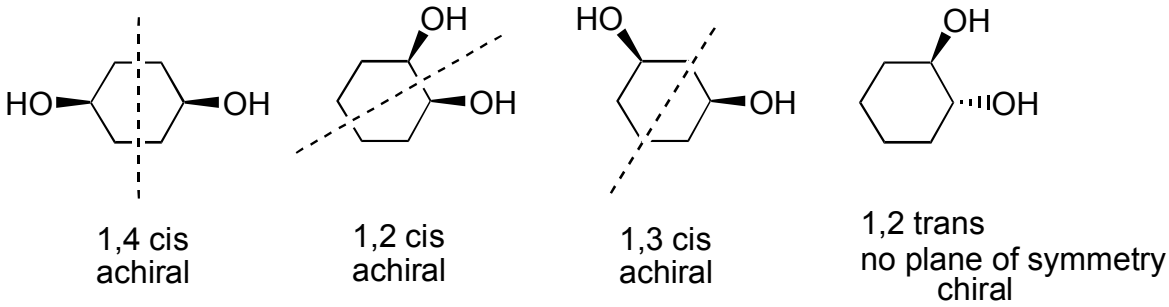
3. (1S, 3R)-1-chloro-3-methylcyclopentane

NOTE: (cis)-1-chloro-3-methylcyclopentane does not include enough information about the absolute configuration of the stereogenic centers)

4. The answers are (2), (3) and (4).

The pairs in (2), (3) and (4) all have a stereogenic carbon and are enantiomers (nonsuperimposable mirror images). The structures in choice (1) do not have a stereogenic carbon and therefore cannot have optical isomers.

5. Structure (4) is chiral.
To see this clearly redraw the cyclohexane rings in a planer representation and look for a plane of symmetry.



6. The answer is (4).
Both of these structures represent cis-1,2-dihydroxycyclohexane and they are identical (again there is no possibility of enantiomers since the molecule is achiral).

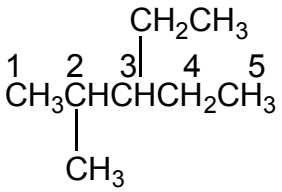
7. The answer is (4).
Both of these structures represent cis-1,2-dihydroxycyclohexane and they are identical (again there is no possibility of enantiomers since the molecule is achiral).

8. The answer is 4.

Both molecules have the formula C_8H_{18}, but differ in the placement of the bonds. Therefore, they are constitutional isomers:

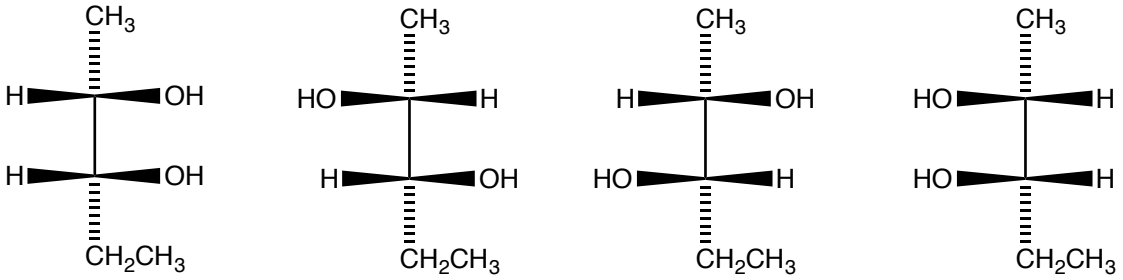
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$

n-octane

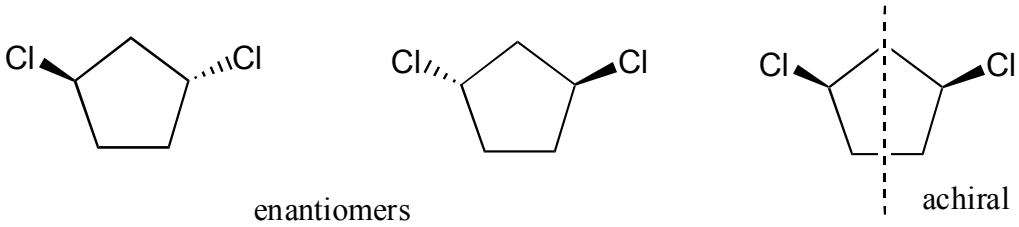


3-ethyl-2-methylpentane

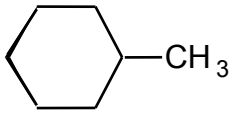
9. Total 4 stereoisomers.



10. Total 3 stereoisomers.

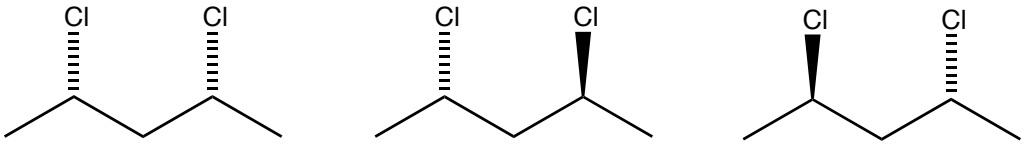


11. Only 1 stereoisomer.

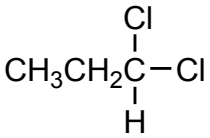


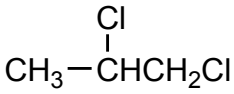
only one isomer possible (of course it exists as two rapidly interconverting conformers, axial and equatorial)

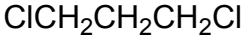
12. Total 3 stereoisomers.

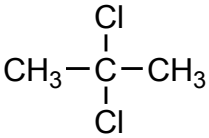


13. There are four isomers with formula $C_3H_6Cl_2$ are:

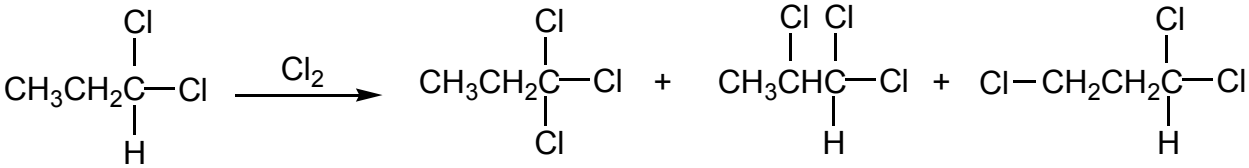

1,1-dichloropropane

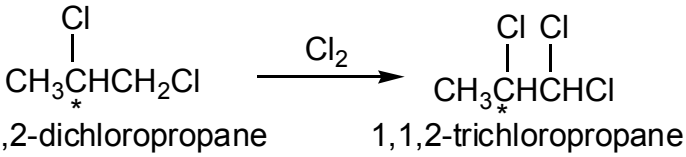

1,2-dichloropropane


1,3-dichloropropane

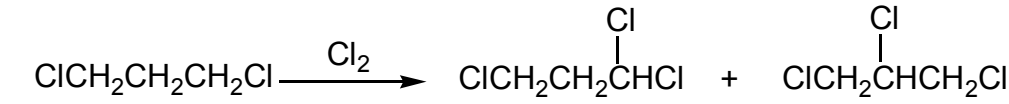

2,2-dichloropropane

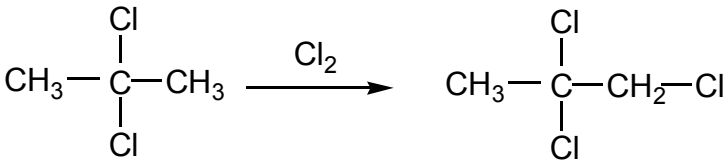
These must be A, B, C, and D, but we still have to determine which particular isomer is A, which is B, etc. We do this by considering how many trichloroproducts we get from the chlorination of each one. Note: in this question we consider only the chlorination to produce a trichloro product (i.e. we do not consider tetra-, penta-, etc. chlorinated products that could result from extensive chlorination reactions).


1,1-dichloropropane
(D)


1,2-dichloropropane
(C)

1,1,2-trichloropropane
(E)


1,3-dichloropropane
(B)


2,2-dichloropropane
(A)

Since 2,2-dichloropropane gives one trichloro product, it must be A. Similarly,

1,3-dichloropropane gives two trichloro products and so must be B. Both 1,1-dichloropropane and 1,2-dichloropropane give three products, but only 1,2-dichloropropane is chiral (it has a chiral carbon, designated by a *), so it must be C. Of the three products of C, the only optically active one is 1,1,2-trichloropropane, so it must be E.

14. (*R*)-Epinephrine has a specific rotation of -51°. A sample that contains a mixture of R- and S-isomers was found to have a rotation of +11.2°. What is the percentage of R and S isomers in this sample?

Rotation of sample = [mole fraction of R in the sample · rotation of sample of pure R isomer] + [mole fraction of S in the sample · rotation of sample pure S isomer]

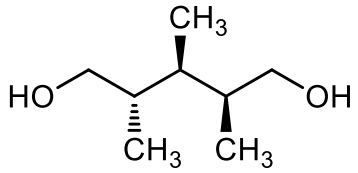
Rotation of sample = +11.2
Rotation of sample of pure R isomer = -51
Rotation of sample of pure S isomer = +51

So, let x = mole fraction of R and 1-x = mole fraction of S

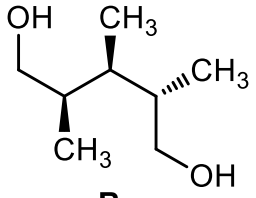
$$
\begin{aligned}
11.2 &= [x \cdot (-51)] + [1-x \cdot (+51)] \\
11.2 &= -51x + 51 - 51x \\
-39.8 &= -102x \\
x &= 0.39
\end{aligned}
$$

Thus, there is 39% of the R-isomer and 61% of the S-isomer in the sample.

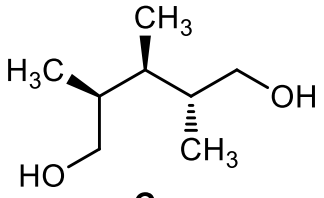
15. This is a modified version of question #8 from the Stereochemistry-1 problem set. Given the following five structures, indicate for each pair listed below whether the structures are identical, enantiomers or diastereomers.



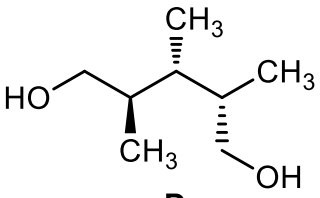
A



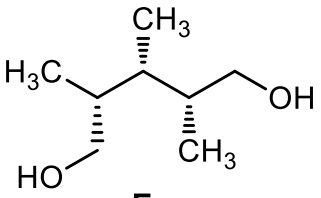
B



C



D



E

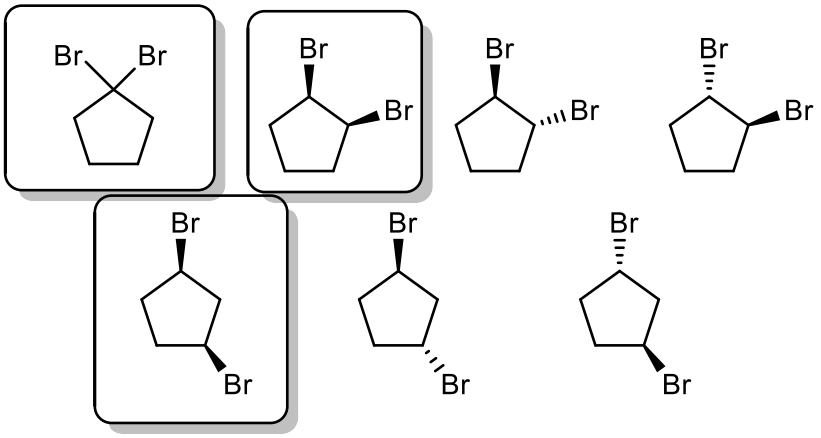
(a) A and B are diastereomers

(b) A and E are enantiomers

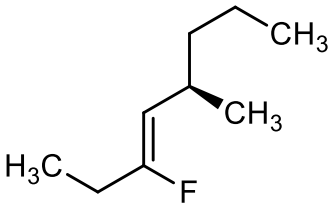
(c) B and E are diastereomers

(d) C and D are identical (meso)

16. Circle all the achiral compounds.

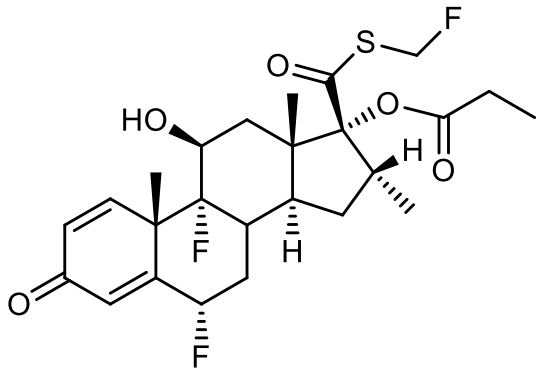


17. Provide a name for the following compound



(3Z,5R)-3-fluoro-5-methyl-3-octene

18. Fluticasone propionate (marketed under the tradename Flovent™) is a steroid based drug that is used in many inhalers as a treatment during an asthma attack.

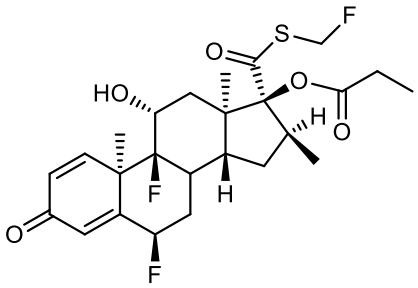


Fluticasone propionate (Flovent™)

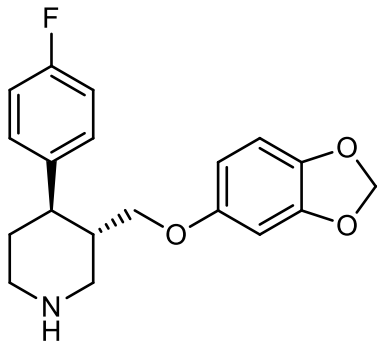
(a) How many asymmetric centres are located in Flovent?

8

(b) Draw the enantiomer of Flovent

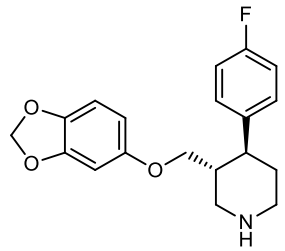


19. (-) – Paroxetine, also known as Paxil (shown below) is a selective serotonin re-uptake inhibitor that is used as an antidepressant. (-) – Paroxetine has affinity for various protein receptors.



(-) - Paroxetine

(a) Draw the enantiomer of (-) – Paroxetine.



(b) Would you expect (-) – Paroxetine and its enantiomer to have the same biological effect? (In other words, would (-) – Paroxetine and its enantiomer have the same interaction with the same protein target?) Briefly justify your answer.

No: enantiomers have different shapes and fit into the enzyme site/ biological receptor (which are chiral) in a different manner. Hence their interaction with the same protein target will probably be different

(c) Would you expect (-) – Paroxetine and its enantiomer to have the same boiling point? Briefly justify your answer.

Yes, enantiomers have the same chemical and physical properties except optical activity.

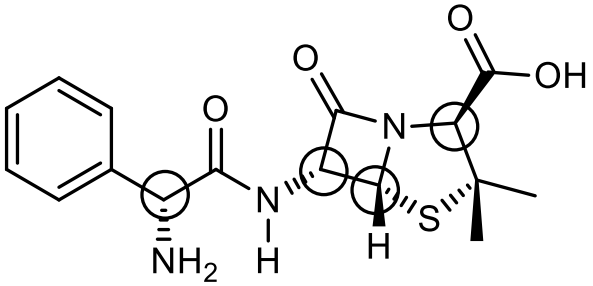
(d) (-) – Paroxetine has a specific rotation of -24.3 at 298K. What is the specific rotation of its enantiomer under the same conditions?

+24.3

(e) What would be the specific rotation of a sample that contains 39% of (-) – Paroxetine and 61% of its enantiomer?

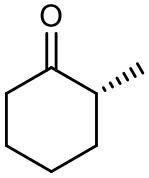
Observed specific rotation = (0.39) x (-24.3) + (0.61) x (24.3) = +5.346

20. Ampicillin has been one of the most widely prescribed antibiotics. In the structure of ampicillin below, clearly circle all the carbon asymmetric centers.



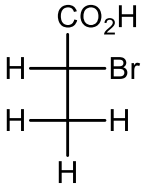
21. Name the following compounds. Be sure to indicate stereochemistry where appropriate.

(a)



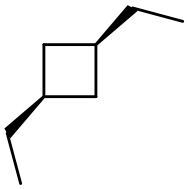
(R)-2-methylcyclohexanone

(b)



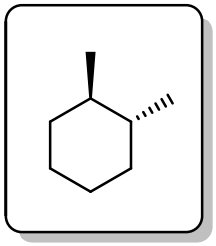
(R)-2-bromopropanoic acid

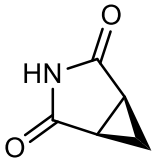
(c)

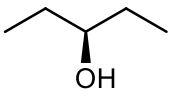


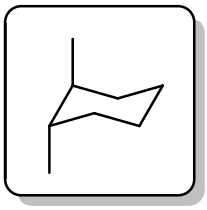
1,3-cis-diethylcyclobutane

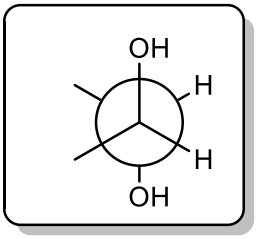
22. Circle all the **chiral** compounds

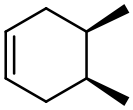


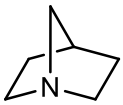


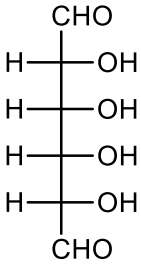






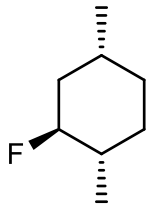


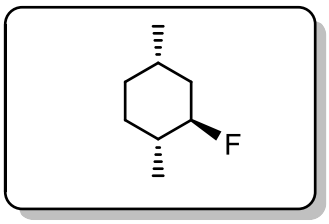




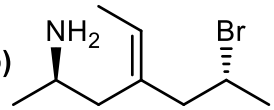
23. Draw the enantiomer of each of the following molecules.

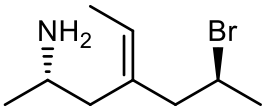
(a)



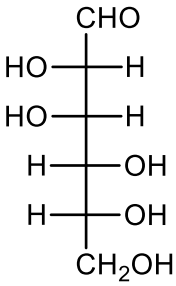


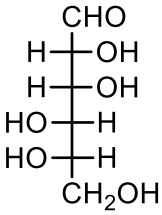
(b)



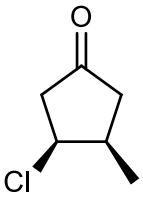


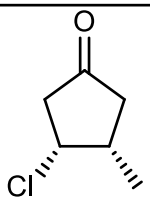
(c)



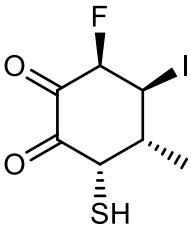


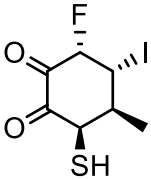
(d)





(e)





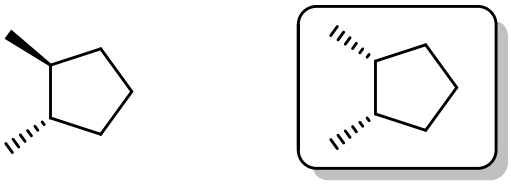
24. Below are eight pairs of structural formulas. In the box to the right of each pair, place the number (from the six terms listed below) that BEST describes the relationship between the two structures. NOTE: Each term may be used more than once and not all terms need be used. **ALSO, CIRCLE ALL THE MESO COMPOUNDS.**

1. Identical
2. Diastereomeers
3. Conformers
4. Constitutional Isomers
5. Enantiomers
6. None of the above

(a)

1

(b)

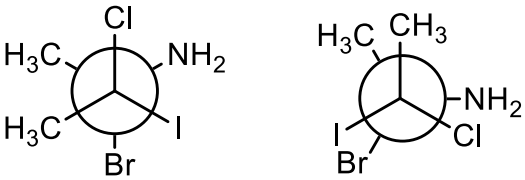


2

(c)

1

(d)

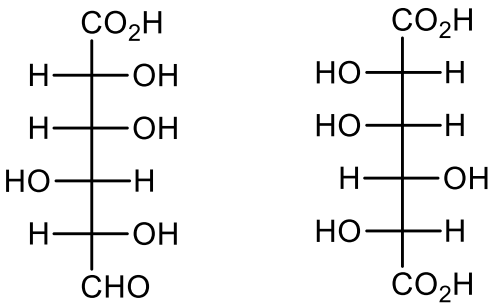


3

(e)

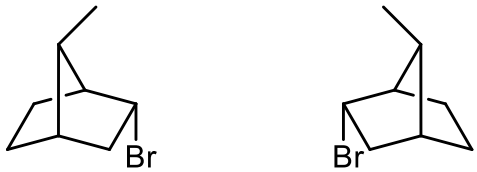
2

(f)



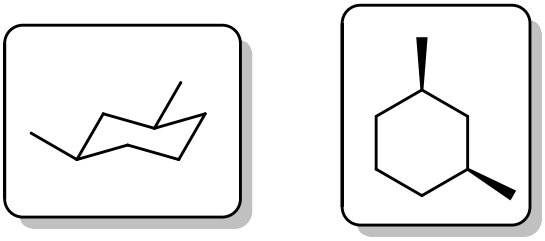
6

(g)



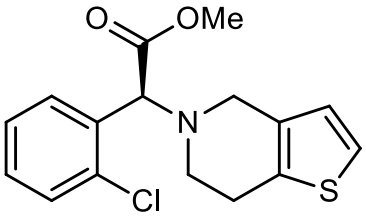
5

(h)



1

25. In the pharmaceutical business, a blockbuster drug is one which achieves sales up to and exceeding a billion dollars a year. Clopidogrel, marketed under the trade name Plavix™, is a blockbuster drug that is a potent anti-clotting agent. Studies suggest that the compound below is the active compound; the opposite enantiomer has been shown to have no biological effect.



Clopidogrel (Plavix™)

(a) Assign the assymetric centre as either *R* or *S*

S

(b) Draw the biologically inactive enantiomer of Clopidogrel