

Post Graduate Diploma in Chemoinformatics
Annual Examinations – 2006

Paper: PGDC – 103
Modern Combinational Chemistry

Time allowed: Three hours

Maximum Marks: 100

SECTION – I

Marks

Q 1. Attempt all the objective type questions given below.

1X20=20

I. Fill in the blanks:

- i) Tanimato coefficient has a value between _____ and _____.
- ii) Captoril is an _____ antagonist.
- iii) HTS is usually the _____ stage after target identification.
- iv) pka affects _____, _____, permeability and _____ of a drug.
- v) SURF is _____.
- vi) FSPE is used for the purification of _____ combinatorial libraries.
- vii) Deconvolution means _____.

II. State whether True or False.

- viii) In solid phase synthesis excess reagents can be used to drive reactions to completion.
- ix) In DCR method the quantities of the compounds produced can be very large.
- x) Safety catch linkers involve a functional gp which is reactive during synthesis but becomes inactive prior to cleavage.
- xi) Solution phase methods always apply smoothly to solid phase.
- xii) In positional scanning most effective residue is determined independently for each position.

III. Answer Briefly.

- xiii) What is topological index?
- xiv) Mention four main approaches to select diverse set of compounds.
- xv) What does MCSS stands for?
- xvi) Technically, site map is the union of three separately computed maps. Name them.
- xvii) Name two photo labile linkers used in SPS.
- xviii) Which are the major issues to be taken care of during assay miniaturization?
- xix) What is nanocan technique?
- xx) What is the use of sphere exclusion algorithm?

SECTION – II

Attempt any six questions. All questions carry equal marks.

5X6=30

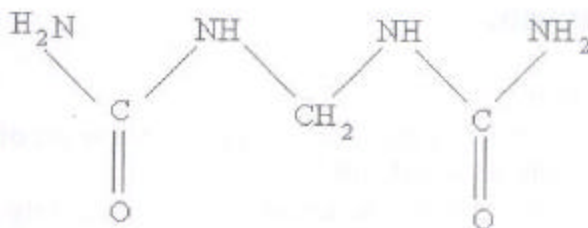
- Q2. What are the advantages and disadvantages of using solid phase synthesis (SPS) over solution phase synthesis?
- Q3. Discuss photo lithography as a spatially addressed method of synthesis. What are the applications and advantages of using this method?
- Q4. Write a short note on chemical encoding.
- Q5. Explain how ladder synthesis approach via MALDI - TOFMS can be used for identifying a library member.
- Q6. What is clustering and what are the uses of structural clustering?
- Q7. How are radio frequency tags used for deconvolution in combinatorial synthesis?
- Q8. How can we use 'Ugi rxn' for solution phase synthesis of combinatorial libraries?
- Q9. Which are the different types of scavenger resins that can be used in solution phase synthesis? Give examples.

SECTION – III

Answer any three. All questions carry equal marks.

10 x 3 = 30

- Q10. Discuss how divide-couple-recombine (DCR) method allows for sequential reaction of compound. List the advantages and disadvantages of using this method.
- Q11. What is optical barcoding?
- Q12. a) What are the desirable properties of a linker used in SPS? Which are the different linkers commonly used.
b) Discuss cyclative cleavage and traceless linkers, giving examples.
- Q13. a) What are connection tables? Mention different types of connection tables used.
b) Draw a redundant and non redundant connection table for the following molecule.



- Q14. a) What is similarity searching and what is the rationale behind using similarity searching?
b) How is the similarity coefficient of a set of compound determined?