

## STRUCTURE – ACTIVITY RELATIONSHIP

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| Module designation  | <i>Structure – Activity Relationship</i>   |
| Semester(s) in which the module is taught                     | 2  |
| Person responsible for the module                             | 1. Prof. Dr. Siswandono, MS., Apt. ( <b>Course Coordinator</b> )<br>2. Prof. Dr. Bambang Tri Purwanto, MS., Apt.<br>3. Dr. Nuzul WD  |
| Language  | <i>Bahasa Indonesia</i>  |
| Relation to curriculum  | <i><del>Compulsory</del> / <del>elective</del> / specialisation</i>  |
| Teaching methods  | <i>lecture, discussion, assignment</i>   |
| Workload (incl. contact hours, self-study hours)              | <i>(Estimated) Total workload:<br/>Contact hours (structured activities.): 90,67 hours<br/>Private study including independent learning activities: 90,67 hours</i>  |
| Credit points   | <i>2 SCU / 6 ECTS</i>  |
| Required and recommended prerequisites for joining the module | NA   |
| Module objectives/intended learning outcomes                  | <p>Students are:</p> <p>LO1: Able to realize excellence based on religious morals (excellence with morality), able to work together, and show a responsible attitude to work in their field of expertise independently.</p> <p>LO2: Able to internalize the spirit of independence, struggle, and entrepreneurship.</p> <p>LO4: Able to develop a pharmaceutical professional performance with analytical acumen in solving pharmaceutical problems and managing research in the pharmaceutical field related to national and global systems and policies, both inter and inter-disciplinary approaches.</p> <p>LO5: Able to access and review information through an Information and Communication Technology (ICT) system, decide on a specific subject of study, maintain the feasibility of implementing research designs, conduct research, analyze data, conclude research results comprehensively, and create strategic issues based on the study that reflect the latest updates in the field of pharmaceutical sciences, and communicate them in the media and scientific forums at the national and international level through an interdisciplinary or multidisciplinary approach in the form of a thesis or other equivalent forms.</p> <p>LO8: Able to carry out drug designs through the synthesis of bioactive compounds based on the structure-activity relationship.</p> <p>LO13: Able to design drug development both from natural products and/or synthetic compounds by considering the biological mimicry system.</p> |

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| Content                            | The Advanced Structure-Activity Relationship (SAR) course describes introductory material for SAR, the relationship between structural changes and drug development, qualitative and quantitative relationships between structure-activity of drug derivatives, methods of determining and techniques for obtaining parameter values for physicochemical properties, analysis of QSAR models, structure-activity relationships on the drug-receptor interaction process, a computational program to determine parameter values of physicochemical properties, QSAR (2D and 3D) analysis, activity prediction, Absorption, Distribution, Metabolism, and Elimination (ADME) profile and drug toxicity prediction.   |
| Exams and assessment formats       | <i>Take-home written assignments</i>   |
| Study and examination requirements | <i>the final grade in the module is composed of 30% discussion, 30% presentation, 30% take-home assignments, 10% in-class participation and soft-skills assessment. Students must have a final grade of 70% or higher to pass</i>  |
| Reading list                       | <ol style="list-style-type: none"> <li>1. Siswandono, ed., 2016. <i>Kimia Medisinal I. Edisi Kedua</i>, Sura-baya: Airlangga University Press</li> <li>2. Lemke, T.L., Williams, D.A., Roche, V.F. and Zito, S.W. eds., 2013. <i>Foye's Principles of Medicinal Chemistry. 7th ed.</i>, Baltimore: Lippincott Williams &amp; Wilkins.</li> <li>3. Li, J.J., 2021. <i>Medicinal Chemistry for Practitioners</i>, New Jork: John Wiley &amp; Sons, Inc.</li> <li>4. Duchowicz, P.R., Mercader, A.G., Sivakumar, P.M., 2016. <i>Chemometrics Applications and Research, QSAR in Medicinal Chemistry</i>, Boca Raton: Apple Academic Press, Inc.</li> <li>5. Puzyn, T., Leszczynski, J. and Cronin, M.T.D., eds., 2010. <i>Recent Advances in QSAR Studies, Methods and Applications</i>, Dordrecht: Springer Science+Business Media B.V.</li> <li>6. Roy K, Kar S, Das RN, 2015. <i>A Primer on QSAR-QSPR Modeling, Fundamental Concepts</i>, Heidelberg: Springer International Publishing.</li> <li>7. <i>Tutorial dalam Program Komputer SPSS 25, ChemOffice 2020, dan Molegro 5.5.</i></li> </ol> |