Literature discussion

Please look through the following paper before coming to the class: Origins of Enantioselectivity during Allylic Substitution Reactions Catalyzed by Metallacyclic Iridium Complexes and answer the following questions.

J. Am. Chem. Soc., 2012, 134 (19), pp 8136–8147

 DOI: 10.1021/ja212217j

In the Supporting Information (SI), the researchers identified the positions of allylic protons, including the *syn* and *anti* protons for the terminal allylic position for the allyliridium compound **2c**.



1. Please find the structure of complex **2c** in the paper (the simplified structure of this compound is given above). Give a short description of gCOSY NMR spectroscopy (This can be found in section 6.2 of the book on Organic structural spectroscopy by Lambert) and Nuclear Overhauser effect (NOE, section 5.4 of the book on Organic structural spectroscopy by Lambert).
2. Crystal structure gave indications that through space coupling could be used to identify the positions of Hanti and Hsyn. How can gCOSY and NOE be used to find chemical shifts corresponding to Hanti, Hsyn Ha and Hb? Please describe briefly.
3. NOESY and ROESY are two methods that are used to measure through space correlation spectra. In this paper ROESY spectroscopy was used, please describe why (this information is not provided in the article, so don’t hesitate to use web resources)