C–H activation is a vibrant area of research due to high atom, step and redox economy, offering new opportunities for synthesis. Despite extensive progress over the last two decades, significant challenges remain. Selective activation of C–H bonds within a substrate that contains multiple C–H bonds is a grand challenge for synthetic chemistry. The primary objective of my Ph.D. research was to develop of various transition metal-catalyzed strategies for site selective C–H functionalization.

The contents of this thesis have been divided into six chapters based on the results of experimental works performed during the complete course of the research period. The first chapter of the thesis presents an outline on different aspects of C–H functionalization processes, its challenges and solutions to address these problems. Chapter II illustrates Pd-catalyzed regioselective o-hydroxylation and o-acetoxylation of 2-arylbenzothiazole and 3,5-diarylisoxazole. Chapter III describes o-arylation strategies of various directing arenes such as 2-arylbenzothiazole, 2-arylbenzoxazole and 3,5-diarylisoxazole using aldehyde as the arylating source in presence of Pd-catalyst. Chapter IV demonstrates the use of ceric ammonium nitrate (CAN) as an efficient and mild oxidant for Pd(II)-catalyzed substrate directed decarboxylative o-arylation of directing arenes. Chapter V illustrates ruthenium catalyzed regiospecific C–H/O–H annulations of directing arenes via weak coordination. Chapter VI discusses protocols for the regioselective cycloalkylation-peroxidation and cycloalkylation across C3-C4 conjugated double bond of 3-substituted coumarins. The use of Cu(I)/TBHP catalytic system provides C4 cycloalkylation-C3 peroxidation whereas the use of Fe(III) / DTBP system affords C3-cycloalkylation product exclusively. Each of these chapters comprises introduction, previous works, present work, experimental section, references, spectral data and some selected spectra.