This thesis deals with the study of novel aspects of quantum computational resources, and the experimental implementations of various quantum computing protocols on three-qubit, single-qutrit and hybrid qubit-qudit NMR quantum computers. The study is conducted in two main parts. The first part focuses on different aspects of multipartite entanglement to gain insights about a three-qubit system. GHZ and W-classes are the two inequivalent entanglement classes in a system of three qubits. While threeparty correlations inW-class of states can be uniquely and completely determined from its reduced two-party correlations, GHZ class exhibits non-decomposable three-party correlations. An NMR experimental implementation is carried out that supports a recently exposed fact about a three-qubit W-superposition state that belongs to GHZ class but does not possess any non-decomposable three-party correlations. This exercise reveals various hidden aspects of multipartite entanglement in a system of three qubits. The second part is aimed at the study of contextuality, which is a purely quantum concept and is exhibited by even the indivisible single-qutrit system. The intrinsic quantumness and hence the computational speedup in a single qutrit is attributed to contextuality. This thesis focuses on developing the machinery for a single-qutrit NMR quantum computer using a geometrical representation, followed by a singlequtrit algorithmic implementation exploiting contextuality. Computational protocols on hybrid-qudit systems are also discussed and implemented experimentally. A part of the study is focused on NMR methodology development with an emphasis on the applications of numerically optimized radio-frequency pulses for biomolecular NMR and quantum gate optimizations. The contents of the present thesis have been divided into seven chapters and an appendix whose brief account is sketched below: Chapter 1 This chapter describes an introduction to the field of NMR quantum computation and quantum information as well as the motivation behind the present thesis. In addition to the basics of NMR, and quantum computation, recent developments in the field of quantum computation and quantum information are discussed. Chapter 2 In this chapter, a general pulse sequence to create a five-parameter based, three-qubit generic pure state is proposed and experimentally implemented for various three-qubit states with a non-trivial set of parameters. Experimental evidence is provided in support of a recently proposed idea that three-qubit correlations can be completely and uniquely obtained from a pair of its reduced two-party states (with a few exceptions). The experimental tests are performed for arbitrarily weighted generic-three qubits states, maximally entangled GHZ and W-states, and a recently proposed Wsuperposition state that is a coherent superposition of W-state and its obverse. Chapter 3 This chapter describes the geometrical realization and dynamics of a single-qutrit, represented by a pair of points on the Majorana sphere in three-dimensional real space (R3). This geometrical realization is used to develop an intuitive picture of a singlequtrit magnetization vector. Single-qutrit dynamics is studied under SO(3) and SU(3) transformations, which in the context of Majorana sphere leads to the development of several interesting features. Close analysis of the single-qutrit dynamics on the Majorana sphere leads to the development of NMR pulse sequences implementing singlequtrit quantum gates. Thus using the insights gained via the Majorana representation, basic operations such as the SWAP operations, phase gates and the 3-dimensional analogue of the Hadamard gate are performed. Experimental implementations of these basic computing elements are carried out on spin-1 oriented in a liquid crystal. Chapter 4 This chapter focuses on exploring single-qutrit contextuality, which is an intrinsic feature providing speed up in quantum computational tasks. Contextuality refers to the context of a measurement, which states that the measurement of an observable may bear different outcomes when measured in different contexts. In this chapter, various theoretical protocols revealing single-qutrit contextuality are studied. An NMR experimental test is proposed and implemented on a single-qutrit NMR quantum information processor that provides evidence in support of the contextual nature of a single-qutrit, using a set of four experiments. The quantum features of the single-qutrit are further exploited by implementing a black-box based algorithm, that determines the parity of a permutation among three objects by a single oracle call whereas its classical counterpart requires two oracle calls. The NMR experiments on a single-qutrit are carried out on a spin-1 oriented in a liquid crystalline matrix. Chapter 5 This chapter describes the design and implementation of quantum gates for quditcomputing using NMR, and the emulation of qubit-qubit-qutrit (QQT) QFT algorithm on a four-qubit (QQQQ) NMR quantum information processor. The QQQQ system used in this chapter possesses a peculiar coupling pattern giving rise to a spectrum that resembles that of a QQT system. A non-trivial correspondence is described between the QQQQ and the QQT systems. A general QQT tomography protocol is proposed and implemented on the QQQQ emulator to reconstruct the resultant QQT state. Chapter 6 This chapter deals with NMR methodology development, focused on the design and implementation of GRAPE optimized numerical pulses. These numerical pulses are optimized for the uniform and precise band-selective excitations in SOFAST-HMQC experiments for biomolecular NMR, quantum gate optimizations for qudit QFT implementation on a qubit-qutrit system and in the simulation of low-temperature protein dynamics. Chapter 7 This chapter contains a brief summary of the main results of the present thesis, their applications as well as their possible future extensions. Appendix A1 This appendix contains a brief description of the lyotropic liquid crystal sample preparation that provides an anisotropic environment to a spin-1 system. This sample is used to perform qutrit quantum computing using NMR (as described in Chapters 3 and 4).