

## Table of the contents

	Page No
<b>Abstract</b>	<b>i</b>
<b>Preface</b>	<b>iii</b>
<b>Acknowledgments</b>	<b>iv</b>
<b>Table of the contents</b>	<b>v</b>
<b>List of figures</b>	<b>viii</b>
<b>List of tables</b>	<b>xvi</b>
<b>List of appendices</b>	<b>xvii</b>
<b>Chapter I: General Introduction</b>	<b>1-18</b>
1.1. Target analyte	1
1.1.1. Metal ions	1
1.1.2. Anions	2
1.1.3. Molecules or compounds	3
1.2. Chemosensor	4
1.3. Photophysical analysis	7
1.4. Signaling mechanisms for optical chemosensors	8
1.5. Density functional theory (DFT)	12
1.6. Literature survey	13
1.7. Aim and objectives of the present thesis work	14
References	15
<b>Chapter II: A Ratiometric, Turn-on Chromo-fluorogenic Sensor for Sequential Detection of Aluminium Ions and Picric acid</b>	<b>19-47</b>
2.1. Introduction	19
2.2. Experimental section	21
2.2.1 Chemicals and instrumentations	21
2.2.2. Fluorescence quantum yield measurement	22
2.2.3. Metals solution preparation for photophysical studies	22
2.3. Results and discussion	22
2.3.1. Design and synthesis of HBAN	22
2.3.2. Spectrophotometric analysis	24
2.3.3. Fluorimetric investigation	25
2.3.4. Experimental study on metal ions selectivity	30
2.3.5. Interference studies	31
2.3.6. Stoichiometry and the binding mechanism	32
2.4. Application of Al <sup>3+</sup> chelated HBAN complex for the sensing of picric acid	36

2.5. Construction of molecular logic gate	39
2.6. Fabrication of a test kit	40
2.7. Conclusion	41
References	42
<b>Chapter III: A Phthalimide Scaffold Smart Molecule for Visualization of Acid-Base Equilibrium and Determination of Acid Dissociation Constants in the Non-Aqueous Medium</b>	<b>48-68</b>
3.1. Introduction	48
3.2. Experimental sections	50
3.2.1. Reagents and solvents	50
3.2.2. Solutions preparation	50
3.2.3. Instrumentations	50
3.2.4. Computational details	50
3.3. Results and discussions	51
3.3.1. Synthesis and characterizations of Z1	51
3.3.2. Colorimetric and UV–visible spectral analysis	53
3.3.3. Test strips for the detection of acid in solution and vapor phase	58
3.3.4. Estimation of $pK_a$ values of several acids in a non-aqueous medium	59
3.3.5. Reversibility and construction of the molecular logic gates	63
3.4. Conclusion	65
References	66
<b>Chapter IV: A Chromogenic Probe for Detection of Biologically Important Anions and Its Implications for Designing Molecular Logic Gates</b>	<b>69-87</b>
4.1. Introduction	69
4.2. Experimental section	70
4.2.1 Chemicals and instruments	70
4.2.2. Preparation of stock solution for spectral study	71
4.3. Results and discussion	71
4.3.1. Synthesis procedure and characterizations of BEN	71
4.3.2. Spectrophotometric analysis	73
4.3.3. Anion selectivity study	75
4.3.4. Interference investigations	76
4.3.5. Determination of stoichiometric ratio, binding constant, and detection limit	77
4.3.6. Proton NMR titration of BEN by $F^-$ , $CN^-$ and $AcO^-$ ions	78
4.3.7. Reversibility of BEN- $F^-$ system by $HSO_4^-$ ions	80
4.3.8. Practical use of paper-based test kit for identification of anions ( $F^-$ , $CN^-$ and	81

AcO <sup>-</sup> )	
4.4. Designing of INHIBIT logic gate	82
4.5. Developing the memory device	83
4.6. Smartphone-based assay analysis	84
4.7. Conclusion	85
References	85
<b>Chapter V: An ESIPT-based Chromone-coumarin Coupled Fluorogenic Dyad for Specific Recognition of Sarin Gas Surrogate, Diethylchlorophosphate</b>	<b>88-110</b>
5.1. Introduction	88
5.2. Experimental sections	90
5.2.1. Chemicals and instrumentation	90
5.2.2. Synthesis process of MATC	91
5.2.3. Estimation of fluorescence quantum yields	93
5.3. Results and discussions	94
5.3.1. Spectrophotometric study	94
5.3.2. Fluorimetric titration investigation	95
5.3.3. Organophosphate selectivity experiment	97
5.3.4. Detection mechanism	98
5.3.5. Estimation limit of detection (LOD) and limit of quantification (LOQ)	100
5.3.6. Practical utility of MATC as a solid phase sensor	101
5.3.7. Dip-stick method for the identification of DCP in the vapor phase	102
5.4. Conclusion	106
References	106
<b>Chapter VI: Summary and Scope for Further Work</b>	<b>111</b>
<b>6.1. Summary</b>	<b>111</b>
<b>6.2. Scope for further work</b>	<b>111</b>
<b>Appendices</b>	<b>112-113</b>
<b>Bibliography</b>	<b>114-128</b>