

Index

Chapter 1 – Introduction.....	p.3
1.1 Particulate Matter: Dimensional Characterization.....	p.6
1.2 Particulate Matter: Sources.....	p.8
1.3 Particulate Matter: Evolution.....	p.10
1.4 The lignin.....	p.11
1.5 The atmospheric products of Polycyclic Aromatic Hydrocarbons: Oxygenated and Nitrated Polycyclic Aromatic Hydrocarbons.....	p.21
1.5.1 Polycyclic Aromatic Hydrocarbons (PAHs).....	p.21
1.5.2 Oxygenated Polycyclic Aromatic Hydrocarbons (Oxi-PAHs).....	p.26
1.5.3 Nitrated Polycyclic Aromatic Hydrocarbons.....	p.31
1.6 The Bisphenol A.....	p.34
1.6.1 Human Exposure and Toxic Effect on Human Health.....	p.35
1.6.2 The Concentration of Bisphenol A in the Particulate Matter.....	p.36
Chapter 2 – Characterisation of Residual Lignin Polymers in Particulate Matter.....	p.38
2.1 Materials and Methods.....	p.39
2.1.1 Gel permeation chromatography (GPC).....	p.39
2.1.2 Zeisel Technique by Gas chromatography – Electron Capture Detector (GC-ECD).....	p.41
2.1.3 Analysis of Monolignols by Gas Chromatography – Mass Spectrometry (GC-MS).....	p.47
2.1.4 Structural Investigation by Liquid Chromatography – Mass Spectrometry (LC-MS).....	p.52
2.1.5 Structural Investigation by Nuclear magnetic resonance Spectroscopy (NMR).....	p.55
2.1.6 Structural Investigation by Ultraviolet –Visible Spectrometry (UV-VIS) and Infrared Spectrometry (IR).....	p.56
2.1.7 Samples collecting system.....	p.56
2.2 Experimental Part: Result and Discussion.....	p.57
2.2.1 Gel permeation chromatography (GPC) Results.....	p.58
2.2.2 Zeisel Results.....	p.60
2.2.3 Gas Chromatography – Mass Spectrometry (GC-MS) Results.....	p.61
2.2.4 Liquid Chromatography – Mass Spectrometry (LC-MS) Results.....	p.63
2.2.5 Nuclear magnetic resonance Spectroscopy (NMR) Results.....	p.65
2.2.6 Ultraviolet –Visible Spectrometry (UV-VIS) Results.....	p.67
2.2.7 Infrared Spectrometry (IR) Results.....	p.67
2.2.8 Compared Analysis Results.....	p.69
Chapter 3 – Analysis of trace toxic pollutants in the particulate matter.....	p.73
3.1 Materials and Methods.....	p.73
3.1.1 Sampling and Collecting System.....	p.73
3.1.2 Analysis of PAHs and Oxy-PAHs in the PM10 samples by HPLC-FLD and HPLC-MS.....	p.75

3.1.3 Analysis of PAHs; Oxy-PAHs and Nitro-PAHs in the PM1 and PM2 Samples by GC-MS...	p.78
3.1.4 Analysis of Bisphenol A by LC-MS-MS system.....	p.81
3.2 Analysis Results.....	p.85
3.2.1 Oxy-PAHS in the PM10 samples.....	p.85
3.2.2 Oxy-PAHs, Nitro-PAHs in Outdoor/Indoor PM1 and PM2.5 samples for Urban, Rural and Remote Sites.....	p.89
3.2.3 Bisphenol A in summer and winter; Indoor and Outdoor PM2,5.....	p.96
Chapter 4 – Analysis of Particulate Matter Pollutants Biological Mechanism of Action.....	p.100
4.1 Molecular Docking.....	p.100
4.2 Docking Protocol.....	p.103
4.2.1 Conformations Generations.....	p.103
4.3 Analysis Results.....	p.104
4.3.1 Investigation of the interaction between Bisphenol A and the Coagulation Pathway Proteins.....	p.105
4.3.2 Redocking.....	p.108
4.3.3 Binding Mode between BPA and the Serine Protease Alpha Thrombin and the Blood Factor Xa.....	p.110
Chapter 5 – Conclusions.....	p.116
Acknowledgements.....	p.117
Bibliography.....	p.118
Appendix 1 – Puntual Data	p.124