

List of Figures

Number and Name of Figures	Page No.
1. Figure 1.1- General Structure of drug Acridine-4-carboxamide.	7
2. Figure 1.2- General Structure of drug Azaacridine-4-carboxamide. N of the ring A is attached to location 5, 6, 7 or 8 for forming different aza derivatives. X= -CO, -NH ₂ , -Cl.	7
3. Figure 3.1 – The optimum stacked structure of 9-aminoacridine and Adenine (AD-A) corresponding to MNDO method of calculation.	23
4. Figure 3.2a – The optimum stacked structure of 9-aminoacridine and Cytosine (AD-C1) corresponding to MNDO method of calculation.	23
5. Figure 3.2b – The optimum stacked structure of 9-aminoacridine and Cytosine (AD-C2) corresponding to MNDO method of calculation.	23
6. Figure 3.3a – The optimum stacked structure of 9-aminoacridine and Guanine (AD-G1) corresponding to MNDO method of calculation.	24
7. Figure 3.3b – The optimum stacked structure of 9-aminoacridine and Guanine (AD-G2) corresponding to MNDO method of calculation.	24
8. Figure 3.4a – The optimum stacked structure of 9-aminoacridine and Uracil (AD-U1) corresponding to MNDO method of calculation.	24
9. Figure 3.4b – The optimum stacked structure of 9-aminoacridine and Uracil (AD-U2) corresponding to MNDO method of calculation.	25
10. Figure 3.5a – The optimum stacked structure of 9-aminoacridine and AU base pair (AT-AD2) corresponding to MNDO method of calculation.	25
11. Figure 3.5b– The optimum stacked structure of 9-aminoacridine and AU base pair (AT-AD3) corresponding to MNDO method of calculation.	25
12. Figure 3.6a– The optimum stacked structure of 9-aminoacridine and GC base pair (GC-AD6) corresponding to MNDO method of calculation.	26
13. Figure 3.6b– The optimum stacked structure of 9-aminoacridine and GC base pair (GC-AD7) corresponding to MNDO method of calculation.	26
14. Figure 3.7 – Plot of stacking models versus Interaction energies of π - π interaction of AT base pair and 9-aminoacridine in different levels of theory.	26
15. Figure 3.8- Plot of stacking models versus Interaction energies of π - π interaction of GC base pair and 9-aminoacridine in different levels of theory.	27
16. Figure 3.9: Optimum stacked structure of 9-aminoacridine and GC corresponding to HF/6-31G** calculation. (GC-acri-12)	27
17. Figure 3.10: Optimum stacked structure of 9-aminoacridine and AT corresponding to HF/6-31G** calculation. (AT-acri-7)	27
18. Figure 4.1 a-b – The configuration of sugar and carboxamide side chain with respect to methyl group of base pair.	38
19. Figure 4.2 – Model of DNA base pair and drug stacking.	38
20. Figure 4.3 - Structure of Azaacridine-4-carboxamide. N at the ring A is attached to location 5, 6, 7 or 8 for forming different aza derivatives. X= -CO, -NH ₂ , -Cl.	38
21. Figure 4.4 - GC Base pair.	39
22. Figure 4.5 - AT Base pair.	39

Number and Name of Figures	Page No.
23. Figure 4.6a – Plot of angle of rotation of two stacked Benzene versus Interaction energies using HF/6-31G.	39
24. Figure 4.6b – Plot of angle of rotation of two stacked Benzene versus Interaction energies using HF/6-31G*.	40
25. Figure 4.6c – Plot of angle of rotation of two stacked Benzene versus Interaction energies using HF/6-31G**.	40
26. Figure 4.6d – Plot of angle of rotation of two stacked Benzene versus Interaction energies using MP2/6-31G**.	40
27. Figure 4.6e – Plot of angle of rotation of stacked Benzene and Pyridine versus Interaction energies using HF/6-31G.	41
28. Figure 4.6f – Plot of angle of rotation of stacked Benzene and Pyridine versus Interaction energies using HF/6-31G*.	41
29. Figure 4.6g – Plot of angle of rotation of stacked Benzene and Pyridine versus Interaction energies using HF/6-31G**.	41
30. Figure 4.6h – Plot of angle of rotation of stacked Benzene and Pyridine versus Interaction energies using MP2/6-31G**.	42
31. Figure 4.7a - Optimum AZN5-GC Stacking.	42
32. Figure 4.7b - Optimum AZN6-GC Stacking.	42
33. Figure 4.7c - Optimum AZN7-GC Stacking.	42
34. Figure 4.7d - Optimum AZN8-GC Stacking.	42
35. Figure 4.8a - Optimum AZN5-AT Stacking.	43
36. Figure 4.8b - Optimum AZN6-AT Stacking.	43
37. Figure 4.8c - Optimum AZN7-AT Stacking.	43
38. Figure 4.8d - Optimum AZN8-AT Stacking.	43
39. Figure 4.9a - Plot for stacking models versus variation of Interaction energies of 9-aminoazaacridine-4-carboxamide (AZN) with different position of Nx and AT.	44
40. Figure 4.9b - Plot for stacking models versus variation of Interaction energies of 9-aminoazaacridine-4-carboxamide (AZN) with different position of Nx and GC.	44
41. Figure 4.10a - Net charge on Nx and N10 versus Interaction energy variation of AZN and AT base pair stacking. (HF/6-31g**)	45
42. Figure 4.10b - Net charge on Nx and N10 versus Interaction energy variation of AZN and AT base pair stacking. (B3LYP/6-31g**)	45
43. Figure 4.10c - Net charge on Nx and N10 versus Interaction energy variation of AZN and GC base pair stacking. (HF/6-31g**)	45
44. Figure 4.10d - Net charge on Nx and N10 versus Interaction energy variation of AZN and GC base pair stacking. (B3LYP/6-31g**)	46
45. Figure 5.1 – Model of DNA base pair and drug stacking.	59
46. Figure 5.2 – General Structure of drug Azaacridine-4-carboxamide. AZA derivatives are formed by substituting N in to location 5, 6, 7 or 8. X= -CO, -NH ₂ , -Cl.	59
47. Figure 5.3 – GC Base pair.	59
48. Figure 5.4 – AT Base pair.	59

Number and Name of Figures	Page No.
49. Figure 5.5a – Optimum AZO5-AT Stacking.	60
50. Figure 5.5b – Optimum AZO6-AT Stacking.	60
51. Figure 5.5c – Optimum AZO7-AT Stacking.	60
52. Figure 5.5d – Optimum AZO8-AT Stacking.	60
53. Figure 5.5e – Optimum AZN5-AT Stacking.	60
54. Figure 5.5f – Optimum AZN6-AT Stacking.	60
55. Figure 5.5g – Optimum AZN7-AT Stacking.	61
56. Figure 5.5h – Optimum AZN8-AT Stacking.	61
57. Figure 5.5i – Optimum AZC5-AT Stacking.	61
58. Figure 5.5j – Optimum AZC6-AT Stacking.	61
59. Figure 5.5k – Optimum AZC7-AT Stacking.	61
60. Figure 5.5l – Optimum AZC8-AT Stacking.	61
61. Figure 5.6a – Optimum AZO5-GC Stacking.	62
62. Figure 5.6b – Optimum AZO6-GC Stacking.	62
63. Figure 5.6c – Optimum AZO7-GC Stacking.	62
64. Figure 5.6d – Optimum AZO8-GC Stacking.	62
65. Figure 5.6e – Optimum AZN5-GC Stacking.	62
66. Figure 5.6f – Optimum AZN6-GC Stacking.	62
67. Figure 5.6g – Optimum AZN7-GC Stacking.	63
68. Figure 5.6h – Optimum AZN8-GC Stacking.	63
69. Figure 5.6i – Optimum AZC5-AT Stacking.	63
70. Figure 5.6j – Optimum AZC6-AT Stacking.	63
71. Figure 5.6k – Optimum AZC7-AT Stacking.	63
72. Figure 5.6l – Optimum AZC8-AT Stacking.	63
73. Figure 5.7a – Optimum AZC7-AT Stacking.	64
74. Figure 5.7b – Optimum AZN7-AT Stacking.	64
75. Figure 5.7c – Optimum AZO7-AT Stacking.	64
76. Figure 5.8a – Optimum AZC7-GC Stacking.	64
77. Figure 5.8b – Optimum AZN7-GC Stacking.	64
78. Figure 5.8c – Optimum AZO7-GC Stacking.	65
79. Figure 5.9a – Plot of stacking models versus variation of interaction energies with different position of Nx for 9-oxoazaacridone-4-carboxamide (AZO) and AT stacking. (HF/6-31G)	65
80. Figure 5.9b – Plot of stacking models versus variation of interaction energies with different position of Nx for 9-aminoazaacridine-4-carboxamide (AZN) and AT stacking. (HF/6-31G)	66
81. Figure 5.9c – Plot of stacking models versus variation of interaction energies with different position of Nx for 9-chloroazaacridine-4-carboxamide (AZC) and AT stacking. (HF/6-31G)	66
82. Figure 5.10a – Plot of stacking models versus variation of interaction energies with different position of Nx for 9-oxoazaacridone-4-carboxamide (AZO) and GC stacking. (HF/6-31G)	66
83. Figure 5.10b – Plot of stacking models versus variation of interaction energies with different position of Nx for 9-aminoazaacridine-4-carboxamide (AZN) and GC stacking. (HF/6-31G)	67

Number and Name of Figures	Page No.
84. Figure 5.10c – Plot of stacking models versus variation of Interaction energies with different position of Nx for 9-chloroazaacridine-4-carboxamide (AZCl) and GC stacking. (HF/6-31G)	67
85. Figure 6.1a- Optimum stacking (AT-AZNL-8).	80
86. Figure 6.1b- Optimum stacking (AT-AZNL-10).	80
87. Figure 6.1c- Optimum stacking (AT-AZNL-11).	80
88. Figure 6.2a- Optimum stacking (GC-AZNL-8).	80
89. Figure 6.2b- Optimum stacking (GC-AZNL-10).	80
90. Figure 6.2c- Optimum stacking (GC-AZNL-11).	81
91. Figure 6.3- Plot of stacking models versus variation of Interaction Energies AT and 9-anilinoacridine (AZNL). (HF/6-31G)	81
92. Figure 6.4- Plot of stacking models versus variation of Interaction Energies GC and 9-anilinoacridine (AZNL). (HF/6-31G)	81
93. Figure 7.1a- Intercalation model of AT-AZCl7-AT (Top view)	88
94. Figure 7.1b- Intercalation model of AT-AZCl7-AT (Side view)	88
95. Figure 7.1c- Intercalation model of GC-AZCl5-GC (Top view)	88
96. Figure 7.1d- Intercalation model of GC-AZCl5-GC (Side view)	88
97. Figure 7.1e- Intercalation model of GC-AZN5-GC (Top view)	88
98. Figure 7.1f- Intercalation model of GC-AZN5-GC (Side view)	88
99. Figure 7.1g- Intercalation model of AT-AZN7-AT (Top view)	89
100. Figure 7.1h- Intercalation model of AT-AZN7-AT (Side view)	89
101. Figure 7.1i- Intercalation model of GC-AZO8-GC (Top view)	89
102. Figure 7.1j- Intercalation model of GC-AZO8-GC (Side view)	89
103. Figure 7.1k- Intercalation model of AT-AZO5-AT (Top view)	89
104. Figure 7.1l- Intercalation model of AT-AZO5-AT (Side view)	89
105. Figure 7.2a - Plot of stacking distance versus Interaction energies of AZO5 and AT-AT stacking.	90
106. Figure 7.2b - Plot of stacking distance versus Interaction energies of AZO8 and GC-GC stacking.	90
107. Figure 7.2c - Plot of stacking distance versus Interaction energies of AZN7 and AT-AT stacking.	90
108. Figure 7.2d - Plot of stacking distance versus Interaction energies of AZN5 and GC-GC stacking.	91
109. Figure 7.2e - Plot of stacking distance versus Interaction energies of AZCl7 and AT-AT stacking.	91
110. Figure 7.2f - Plot of stacking distance versus Interaction energies of AZCl5 and GC-GC stacking.	91
111. Figure 7.3 - Plot of orientation versus Interaction energies of AZO8 and two GC stacking.	92
112. Figure 8.1a – Unprotonated AZCL5.	102
113. Figure 8.1b – Unprotonated AZCL6.	102
114. Figure 8.1c – Unprotonated AZCL7.	102
115. Figure 8.1d – Unprotonated AZCL8.	102

Number and Name of Figures	Page No.
116. Figure 8.2a – Unprotonated AZO5.	102
117. Figure 8.2b – Unprotonated AZO6.	102
118. Figure 8.2c – Unprotonated AZO7.	103
119. Figure 8.2d – Unprotonated AZO8.	103
120. Figure 8.3a – Unprotonated AZN5.	103
121. Figure 8.3b – Unprotonated AZN6.	103
122. Figure 8.3c – Unprotonated AZN7.	103
123. Figure 8.3d – Unprotonated AZN8.	103
124. Figure 8.4a – Optimised AZCL5-19+	104
125. Figure 8.4b – Optimised AZCL6-19+	104
126. Figure 8.4c – Optimised AZCL7-19+	104
127. Figure 8.4d – Optimised AZCL8-19+	104
128. Figure 8.4e – Optimised AZO5-19+	104
129. Figure 8.4f – Optimised AZO6-19+	104
130. Figure 8.4g – Optimised AZO7-19+	105
131. Figure 8.4h – Optimised AZO8-19+	105
132. Figure 8.4i – Optimised AZN5-20+	105
133. Figure 8.4j – Optimised AZN6-20+	105
134. Figure 8.4k – Optimised AZN7-20+	105
135. Figure 8.4l – Optimised AZN8-20+	105
136. Figure 9.1- Structure of 9-aminoacridine.	113
137. Figure 9.2- Structure of 9-aminoazaacridine.	113
138. Figure 9.3a- Structure of 9-aminoacridine protonated at N10.	113
139. Figure 9.3b- Structure of 9-aminoazaacridine protonated at N10.	113
140. Figure 9.3c- Structure of 9-aminoazaacridine protonated at N7.	114
141. Figure 9.4a: Optimum stacked structure of GC and unprotonated 9-aminoacridine.	114
142. Figure 9.4b: Optimum stacked structure of AT and unprotonated 9-aminoacridine.	114
143. Figure 9.4c: Optimum stacked structure of GC and unprotonated 9-aminoaza(6)acridine.	114
144. Figure 9.4d: Optimum stacked structure of AT and unprotonated 9-aminoaza(6)acridine.	115
145. Figure 9.5a: Optimum stacked structure of GC and 9-aminoaza(6)acridine (protonated at N10).	115
146. Figure 9.5b: Optimum stacked structure of GC and 9-aminoaza(6)acridine (protonated at N7).	115
147. Figure 9.5c: Optimum stacked structure of AT and 9-aminoaza(6)acridine (protonated at N10).	115
148. Figure 9.5d: Optimum stacked structure of AT and 9-aminoaza(6)acridine (protonated at N7).	116