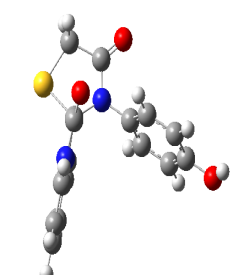
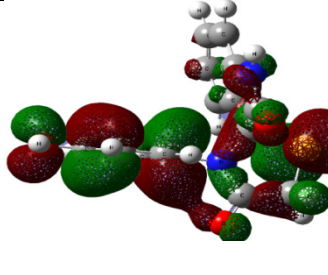
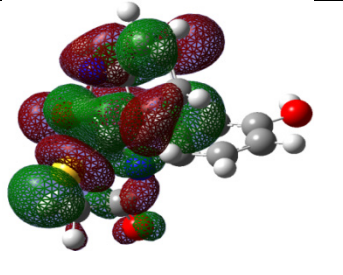
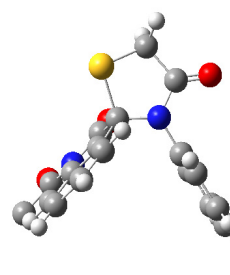
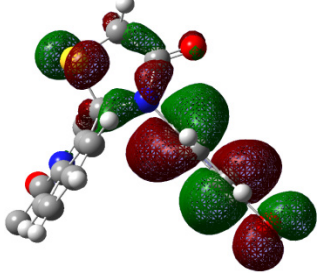
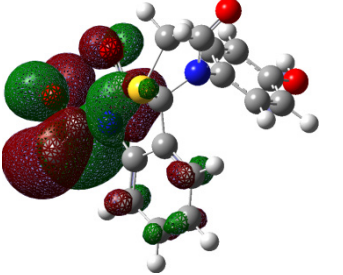
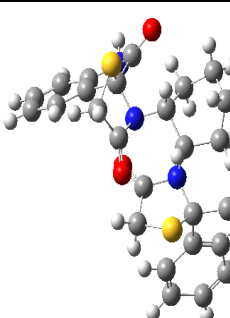
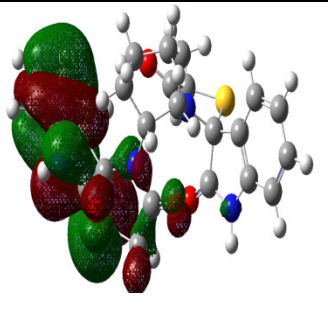
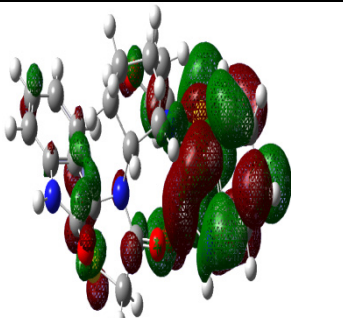


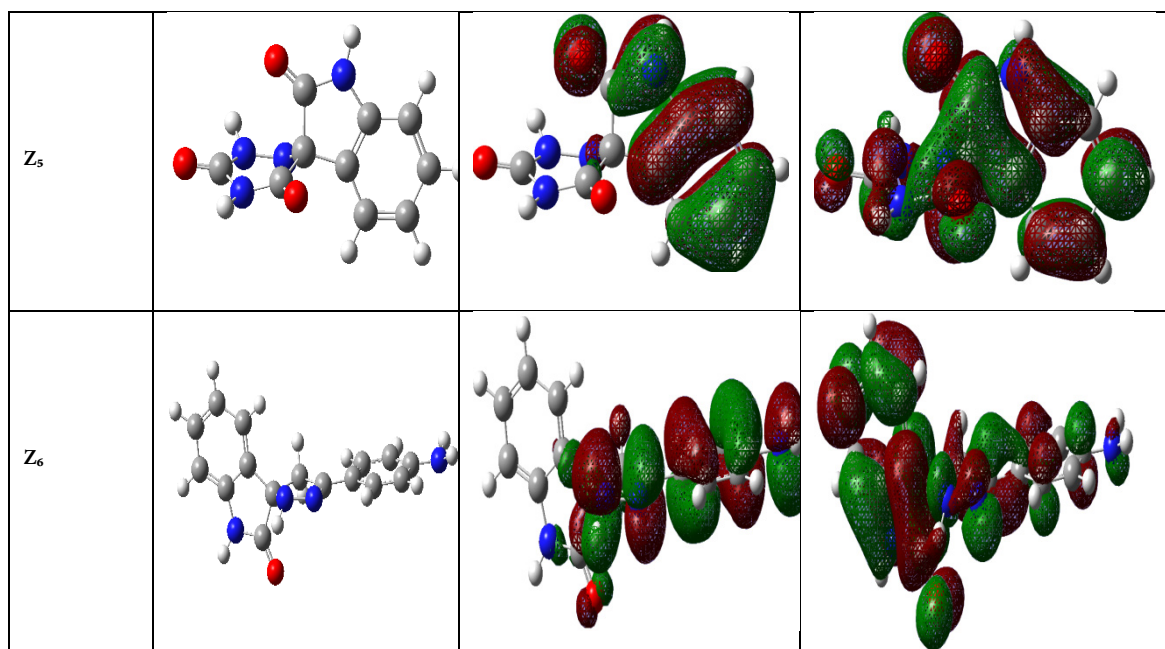
Synthesis, Characterization, and Antimicrobial Activity of Spiro Heterocyclic Compounds from Statin

Zubaida Amir Al-Heety ¹, Ali Kareem Al-Nasseri ^{2*}

Supplementary Information

Supp. Table 1. Humo and Lumo of spiroheterocyclic [Z₁-Z₆]

		HUMO	LUMO
Z ₁			
Z ₂			
Z ₄			

Supp. Table 2. Bond length, Angel and 2nd Angel (Z₁)

Bond length		Angel (°)		2nd Angel (°)	
C(2)C(1)	1.403				
C(15)C(2)	1.51	C(15)C(2)C(1)	108.708		
C(3)C(2)	1.388	C(3)C(2)C(1)	120.142	C(3)C(2)C(1)C(15)	131.077
C(6)C(1)	1.39	C(6)C(1)C(2)	121.806	C(6)C(1)C(2)C(3)	0.917
N(12)C(1)	1.406	N(12)C(1)C(2)	109.644	N(12)C(1)C(2)C(6)	128.549
C(4)C(3)	1.402	C(4)C(3)C(2)	118.936	C(4)C(3)C(2)C(1)	-1.366
C(5)C(6)	1.402	C(5)C(6)C(1)	117.553	C(5)C(6)C(1)C(2)	0.037
C(7)C(15)	1.568	C(7)C(15)C(2)	102.489	C(7)C(15)C(2)C(1)	3.973
S(20)C(15)	1.863	S(20)C(15)C(2)	110.501	S(20)C(15)C(2)C(7)	109.585
N(21)C(15)	1.459	N(21)C(15)C(2)	117.692	N(21)C(15)C(2)C(7)	111.644
C(17)N(21)	1.385	C(17)N(21)C(15)	117.215	C(17)N(21)C(15)C(2)	146.838
C(24)N(21)	1.441	C(24)N(21)C(15)	120.228	C(24)N(21)C(15)C(17)	119.898
C(23)C(24)	1.399	C(23)C(24)N(21)	120.056	C(23)C(24)N(21)C(15)	95.359
C(25)C(24)	1.398	C(25)C(24)N(21)	120.253	C(25)C(24)N(21)C(23)	119.669
C(26)C(25)	1.395	C(26)C(25)C(24)	120.111	C(26)C(25)C(24)N(21)	-179.089
C(27)C(26)	1.399	C(27)C(26)C(25)	119.905	C(27)C(26)C(25)C(24)	0.226
C(28)C(23)	1.392	C(28)C(23)C(24)	120.53	C(28)C(23)C(24)N(21)	179.194
C(16)S(20)	1.826	C(16)S(20)C(15)	91.288	C(16)S(20)C(15)C(2)	-152.57
O(33)C(27)	1.369	O(33)C(27)C(26)	122.59	O(33)C(27)C(26)C(28)	117.238
O(14)C(7)	1.217	O(14)C(7)N(12)	126.775	O(14)C(7)N(12)C(15)	126.603
O(22)C(17)	1.218	O(22)C(17)C(16)	123.215	O(22)C(17)C(16)N(21)	124.624
H(8)C(3)	1.086	H(8)C(3)C(2)	120.3	H(8)C(3)C(2)C(4)	120.764
H(9)C(4)	1.085	H(9)C(4)C(3)	119.857	H(9)C(4)C(3)C(5)	119.868
H(10)C(5)	1.086	H(10)C(5)C(4)	119.625	H(10)C(5)C(4)C(6)	119.097
H(11)C(6)	1.086	H(11)C(6)C(1)	121.451	H(11)C(6)C(1)C(5)	120.996

H(29)C(23)	1.084	H(29)C(23)C(24)	119.481	H(29)C(23)C(24)C(28)	119.987
H(30)C(25)	1.085	H(30)C(25)C(24)	119.689	H(30)C(25)C(24)C(26)	120.197
H(31)C(26)	1.088	H(31)C(26)C(25)	119.854	H(31)C(26)C(25)C(27)	120.239
H(32)C(28)	1.085	H(32)C(28)C(23)	121.184	H(32)C(28)C(23)C(27)	119.206
H(13)N(12)	1.01	H(13)N(12)C(1)	125.383	H(13)N(12)C(1)C(7)	122.12
H(18)C(16)	1.091	H(18)C(16)C(17)	109.371	H(18)C(16)C(17)S(20)	110.14
H(19)C(16)	1.093	H(19)C(16)C(17)	108.775	H(19)C(16)C(17)S(20)	111.926
H(34)O(33)	0.966	H(34)O(33)C(27)	110.088	H(34)O(33)C(27)C(26)	-1.523

Supp. Table 3. Bond length , Angel and 2nd Angel (Z₂)

Bond length		Angel (°)		2nd Angel (°)	
C(2)C(1)	1.397				
C(16)C(1)	1.506	C(16)C(1)C(2)	109.916		
C(6)C(1)	1.391	C(6)C(1)C(2)	119.792	C(6)C(1)C(2)C(16)	130.22
C(3)C(2)	1.39	C(3)C(2)C(1)	122.539	C(3)C(2)C(1)C(6)	-0.902
N(12)C(2)	1.428	N(12)C(2)C(1)	109.818	N(12)C(2)C(1)C(3)	127.642
C(4)C(3)	1.4	C(4)C(3)C(2)	117.085	C(4)C(3)C(2)C(1)	0.013
C(5)C(6)	1.399	C(5)C(6)C(1)	118.825	C(5)C(6)C(1)C(2)	1.27
C(7)C(16)	1.558	C(7)C(16)C(1)	102.931	C(7)C(16)C(1)C(2)	-3.971
N(21)C(16)	1.457	N(21)C(16)C(1)	117.675	N(21)C(16)C(1)C(7)	111.27
S(23)C(16)	1.863	S(23)C(16)C(1)	110.517	S(23)C(16)C(1)C(7)	109.2
C(17)N(21)	1.387	C(17)N(21)C(16)	117.215	C(17)N(21)C(16)C(1)	-146.225
C(24)N(21)	1.442	C(24)N(21)C(16)	120.258	C(24)N(21)C(16)C(17)	120.142
C(25)C(24)	1.398	C(25)C(24)N(21)	120.31	C(25)C(24)N(21)C(16)	86.525
C(26)C(24)	1.399	C(26)C(24)N(21)	119.968	C(26)C(24)N(21)C(25)	119.705
C(27)C(25)	1.395	C(27)C(25)C(24)	120.107	C(27)C(25)C(24)N(21)	179.462
C(29)C(26)	1.392	C(29)C(26)C(24)	120.492	C(29)C(26)C(24)N(21)	-179.495
C(31)C(27)	1.4	C(31)C(27)C(25)	119.901	C(31)C(27)C(25)C(24)	-0.316
C(18)S(23)	1.827	C(18)S(23)C(16)	91.286	C(18)S(23)C(16)C(1)	152.23
O(34)C(31)	1.367	O(34)C(31)C(27)	122.675	O(34)C(31)C(27)C(29)	117.17
C(13)N(12)	1.353	C(13)N(12)C(2)	123.938	C(13)N(12)C(2)C(7)	125.685
O(22)C(17)	1.216	O(22)C(17)C(18)	123.303	O(22)C(17)C(18)N(21)	124.521
O(36)C(7)	1.204	O(36)C(7)N(12)	125.712	O(36)C(7)N(12)C(16)	127.496
C(15)C(13)	1.378	C(15)C(13)N(12)	147.355	C(15)C(13)N(12)C(2)	1.245
O(14)C(13)	1.291	O(14)C(13)N(12)	131.553	O(14)C(13)N(12)C(15)	81.091
H(8)C(3)	1.084	H(8)C(3)C(2)	121.834	H(8)C(3)C(2)C(4)	121.081
H(9)C(4)	1.085	H(9)C(4)C(3)	119.03	H(9)C(4)C(3)C(5)	119.709
H(10)C(5)	1.085	H(10)C(5)C(4)	119.747	H(10)C(5)C(4)C(6)	119.763
H(11)C(6)	1.085	H(11)C(6)C(1)	120.244	H(11)C(6)C(1)C(5)	120.929
H(28)C(25)	1.085	H(28)C(25)C(24)	119.896	H(28)C(25)C(24)C(27)	119.994
H(30)C(26)	1.084	H(30)C(26)C(24)	119.551	H(30)C(26)C(24)C(29)	119.953
H(32)C(27)	1.087	H(32)C(27)C(25)	119.826	H(32)C(27)C(25)C(31)	120.272

H(33)C(29)	1.085	H(33)C(29)C(26)	121.192	H(33)C(29)C(26)C(31)	119.172
H(19)C(18)	1.091	H(19)C(18)C(17)	109.428	H(19)C(18)C(17)S(23)	110.018
H(20)C(18)	1.093	H(20)C(18)C(17)	108.896	H(20)C(18)C(17)S(23)	111.866
H(35)O(34)	0.966	H(35)O(34)C(31)	110.282	H(35)O(34)C(31)C(27)	0.706
H(37)C(15)	1.113	H(37)C(15)C(13)	109.5	H(37)C(15)C(13)N(12)	0
H(38)C(15)	1.113	H(38)C(15)C(13)	109.442	H(38)C(15)C(13)H(37)	109.442
H(39)C(15)	1.113	H(39)C(15)C(13)	109.462	H(39)C(15)C(13)H(37)	109.462

Supp. Table 4. Bond length , Angel and 2nd Angel (Z₄)

Bond length		Angel (°)		2nd Angel(°)	
C(14)C(13)	1.406				
C(15)C(13)	1.512	C(15)C(13)C(14)	108.069	C(15)C(13)C(14)	
C(12)C(13)	1.388	C(12)C(13)C(14)	119.824	C(12)C(13)C(14)C(15)	131.772
C(9)C(14)	1.39	C(9)C(14)C(13)	122.072	C(9)C(14)C(13)C(12)	-1.372
N(17)C(14)	1.406	N(17)C(14)C(9)	128.033	N(17)C(14)C(9)C(13)	109.895
C(10)C(9)	1.402	C(10)C(9)C(14)	117.524	C(10)C(9)C(14)C(13)	0.156
C(11)C(12)	1.402	C(11)C(12)C(13)	118.907	C(11)C(12)C(13)C(14)	1.896
C(16)C(15)	1.564	C(16)C(15)C(13)	102.605	C(16)C(15)C(13)C(12)	178.984
N(7)C(15)	1.467	N(7)C(15)C(13)	123.462	N(7)C(15)C(13)C(16)	111.499
S(29)C(15)	1.867	S(29)C(15)N(7)	104.356	S(29)C(15)N(7)C(13)	107.046
C(31)N(7)	1.382	C(31)N(7)C(15)	112.97	C(31)N(7)C(15)C(13)	-156.349
C(3)N(7)	1.489	C(3)N(7)C(15)	123.867	C(3)N(7)C(15)C(31)	114.541
C(2)C(3)	1.535	C(2)C(3)N(7)	115.096	C(2)C(3)N(7)C(15)	-17.119
C(4)C(3)	1.59	C(4)C(3)C(2)	111.619	C(4)C(3)C(2)N(7)	113.903
C(1)C(2)	1.546	C(1)C(2)C(3)	109.983	C(1)C(2)C(3)C(4)	-63.798
C(5)C(4)	1.547	C(5)C(4)C(3)	110.151	C(5)C(4)C(3)C(2)	23.564
N(8)C(4)	1.486	N(8)C(4)C(3)	118.616	N(8)C(4)C(3)C(5)	110.118
C(22)N(8)	1.47	C(22)N(8)C(4)	121.507	C(22)N(8)C(4)C(3)	-123.365
C(21)C(22)	1.51	C(21)C(22)N(8)	118.886	C(21)C(22)N(8)C(4)	-28.303
C(20)C(21)	1.405	C(20)C(21)C(22)	108.461	C(20)C(21)C(22)N(8)	127.619
C(26)C(21)	1.39	C(26)C(21)C(20)	119.935	C(26)C(21)C(20)C(22)	131.435
N(19)C(20)	1.401	N(19)C(20)C(21)	109.879	N(19)C(20)C(21)C(22)	0.272
C(23)C(20)	1.391	C(23)C(20)N(19)	128.323	C(23)C(20)N(19)C(21)	121.766
C(24)C(23)	1.401	C(24)C(23)C(20)	117.692	C(24)C(23)C(20)N(19)	177.153
C(25)C(26)	1.402	C(25)C(26)C(21)	119.064	C(25)C(26)C(21)C(20)	-2.811
C(18)C(22)	1.567	C(18)C(22)N(8)	112.577	C(18)C(22)N(8)C(21)	102.45
S(33)C(22)	1.866	S(33)C(22)N(8)	105.228	S(33)C(22)N(8)C(18)	107.334
C(35)N(8)	1.369	C(35)N(8)C(4)	122.437	C(35)N(8)C(4)C(22)	115.74
C(6)C(1)	1.547	C(6)C(1)C(2)	112.518	C(6)C(1)C(2)C(3)	37.718
C(30)S(29)	1.821	C(30)S(29)C(15)	90.79	C(30)S(29)C(15)N(7)	29.922
C(34)S(33)	1.825	C(34)S(33)C(22)	89.633	C(34)S(33)C(22)N(8)	-28.805
O(27)C(16)	1.218	O(27)C(16)C(15)	126.334	O(27)C(16)C(15)N(17)	127.045
O(28)C(18)	1.217	O(28)C(18)N(19)	126.713	O(28)C(18)N(19)C(22)	126.553
O(32)C(31)	1.226	O(32)C(31)N(7)	123.565	O(32)C(31)N(7)C(30)	122.243
O(36)C(35)	1.227	O(36)C(35)N(8)	124.816	O(36)C(35)N(8)C(34)	122.333

H(47)C(9)	1.086	H(47)C(9)C(10)	121.114	H(47)C(9)C(10)C(14)	121.362
H(48)C(10)	1.086	H(48)C(10)C(9)	119.186	H(48)C(10)C(9)C(11)	119.755
H(49)C(11)	1.085	H(49)C(11)C(10)	119.892	H(49)C(11)C(10)C(12)	119.517
H(50)C(12)	1.082	H(50)C(12)C(11)	120.59	H(50)C(12)C(11)C(13)	120.472
H(53)C(23)	1.086	H(53)C(23)C(20)	121.276	H(53)C(23)C(20)C(24)	121.032
H(54)C(24)	1.086	H(54)C(24)C(23)	119.138	H(54)C(24)C(23)C(25)	119.626
H(55)C(25)	1.085	H(55)C(25)C(24)	119.934	H(55)C(25)C(24)C(26)	119.816
H(56)C(26)	1.085	H(56)C(26)C(21)	120.427	H(56)C(26)C(21)C(25)	120.505
H(37)C(1)	1.096	H(37)C(1)C(2)	108.207	H(37)C(1)C(2)C(6)	110.08
H(38)C(1)	1.097	H(38)C(1)C(2)	109.773	H(38)C(1)C(2)C(6)	109.601
H(39)C(2)	1.092	H(39)C(2)C(1)	107.881	H(39)C(2)C(1)C(3)	110.71
H(40)C(2)	1.091	H(40)C(2)C(1)	110.938	H(40)C(2)C(1)C(3)	109.788
H(41)C(3)	1.098	H(41)C(3)C(2)	106.912	H(41)C(3)C(2)C(4)	103.257
H(42)C(4)	1.089	H(42)C(4)C(3)	104.901	H(42)C(4)C(3)C(5)	108.284
H(43)C(5)	1.094	H(43)C(5)C(4)	108.382	H(43)C(5)C(4)C(6)	110.479
H(44)C(5)	1.094	H(44)C(5)C(4)	109.727	H(44)C(5)C(4)C(6)	109.804
H(45)C(6)	1.098	H(45)C(6)C(1)	110.287	H(45)C(6)C(1)C(5)	109.12
H(46)C(6)	1.095	H(46)C(6)C(1)	110.429	H(46)C(6)C(1)C(5)	109.929
H(51)N(17)	1.01	H(51)N(17)C(14)	125.433	H(51)N(17)C(14)C(16)	122.333
H(52)N(19)	1.01	H(52)N(19)C(18)	121.404	H(52)N(19)C(18)C(20)	124.771
H(57)C(30)	1.093	H(57)C(30)S(29)	112.544	H(57)C(30)S(29)C(31)	108.878
H(58)C(30)	1.091	H(58)C(30)S(29)	109.821	H(58)C(30)S(29)C(31)	108.593
H(59)C(34)	1.09	H(59)C(34)S(33)	110.52	H(59)C(34)S(33)C(35)	109.274
H(60)C(34)	1.094	H(60)C(34)S(33)	111.563	H(60)C(34)S(33)C(35)	109.728

Supp. Table 5. Bond length , Angel and 2nd Angel (Z_s)

Bond length		Angel (°)		2nd Angel(°)	
C(2)C(1)	1.402				
C(15)C(2)	1.512	C(15)C(2)C(1)	108.873	C(15)C(2)C(1)	
C(3)C(2)	1.387	C(3)C(2)C(1)	120.257	C(3)C(2)C(1)C(15)	130.869
C(6)C(1)	1.389	C(6)C(1)C(2)	121.788	C(6)C(1)C(2)C(3)	0.703
N(12)C(1)	1.403	N(12)C(1)C(2)	109.466	N(12)C(1)C(2)C(6)	128.744
C(4)C(3)	1.403	C(4)C(3)C(2)	118.848	C(4)C(3)C(2)C(1)	-0.897
C(5)C(6)	1.402	C(5)C(6)C(1)	117.526	C(5)C(6)C(1)C(2)	-0.066
C(7)C(15)	1.568	C(7)C(15)C(2)	102.365	C(7)C(15)C(2)C(1)	-2.5
N(16)C(15)	1.477	N(16)C(15)C(2)	110.163	N(16)C(15)C(2)C(7)	107.962
C(17)C(15)	1.541	C(17)C(15)C(2)	113.663	C(17)C(15)C(2)C(7)	110.112
N(18)N(16)	1.408	N(18)N(16)C(15)	114.427	N(18)N(16)C(15)C(2)	172.21
C(19)N(18)	1.374	C(19)N(18)N(16)	122.742	C(19)N(18)N(16)C(15)	-32.861
N(24)C(17)	1.386	N(24)C(17)C(15)	113.664	N(24)C(17)C(15)C(2)	-149.129
O(14)C(7)	1.215	O(14)C(7)N(12)	127.02	O(14)C(7)N(12)C(15)	126.347
O(22)C(19)	1.218	O(22)C(19)N(18)	124.185	O(22)C(19)N(18)N(24)	122
O(23)C(17)	1.216	O(23)C(17)C(15)	123.954	O(23)C(17)C(15)N(24)	122.381
H(8)C(3)	1.087	H(8)C(3)C(2)	121.022	H(8)C(3)C(2)C(4)	120.12
H(9)C(4)	1.085	H(9)C(4)C(3)	119.803	H(9)C(4)C(3)C(5)	119.94
H(10)C(5)	1.086	H(10)C(5)C(4)	119.602	H(10)C(5)C(4)C(6)	119.077
H(11)C(6)	1.085	H(11)C(6)C(1)	121.504	H(11)C(6)C(1)C(5)	120.97
H(13)N(12)	1.01	H(13)N(12)C(1)	125.652	H(13)N(12)C(1)C(7)	121.734
H(20)N(16)	1.018	H(20)N(16)C(15)	109.462	H(20)N(16)C(15)N(18)	108.806
H(21)N(18)	1.012	H(21)N(18)N(16)	115.526	H(21)N(18)N(16)C(19)	115.702

H(25)N(24)	1.015	H(25)N(24)C(17)	116.111	H(25)N(24)C(17)C(19)	114.638
------------	-------	-----------------	---------	----------------------	---------

Supp. Table 6. Bond length, Angel and 2nd Angel (Z_6)

Bond length		Angel (°)		2nd Angel (°)	
C(24)C(22)	1.403				
C(21)C(22)	1.515	C(21)C(22)C(24)	109.264	C(21)C(22)C(24)	
C(25)C(22)	1.388	C(25)C(22)C(21)	130.817	C(25)C(22)C(21)C(24)	119.919
C(26)C(24)	1.391	C(26)C(24)C(22)	122.067	C(26)C(24)C(22)C(21)	-179.161
N(33)C(24)	1.406	N(33)C(24)C(22)	109.141	N(33)C(24)C(22)C(26)	128.789
C(27)C(25)	1.404	C(27)C(25)C(22)	119.011	C(27)C(25)C(22)C(21)	179.33
C(29)C(26)	1.402	C(29)C(26)C(24)	117.48	C(29)C(26)C(24)C(22)	-0.414
C(23)C(21)	1.56	C(23)C(21)C(22)	102.079	C(23)C(21)C(22)C(24)	-3.475
C(15)C(21)	1.556	C(15)C(21)C(22)	115.737	C(15)C(21)C(22)C(23)	110.999
N(19)C(21)	1.485	N(19)C(21)C(15)	101.781	N(19)C(21)C(15)C(22)	113.809
C(14)C(15)	1.52	C(14)C(15)C(21)	101.97	C(14)C(15)C(21)N(19)	12.922
C(1)C(14)	1.464	C(1)C(14)C(15)	124.205	C(1)C(14)C(15)C(21)	175.295
N(18)N(19)	1.394	N(18)N(19)C(21)	110.75	N(18)N(19)C(21)C(15)	-16.526
C(2)C(1)	1.405	C(2)C(1)C(14)	121.303	C(2)C(1)C(14)C(15)	-2.028
C(6)C(1)	1.41	C(6)C(1)C(2)	117.606	C(6)C(1)C(2)C(14)	121.091
C(3)C(2)	1.393	C(3)C(2)C(1)	121.463	C(3)C(2)C(1)C(6)	0.066
C(4)C(3)	1.404	C(4)C(3)C(2)	120.567	C(4)C(3)C(2)C(1)	0.034
C(5)C(6)	1.387	C(5)C(6)C(1)	121.241	C(5)C(6)C(1)C(2)	-0.207
N(11)C(4)	1.395	N(11)C(4)C(3)	121.023	N(11)C(4)C(3)C(5)	120.646
O(35)C(23)	1.218	O(35)C(23)C(21)	127.067	O(35)C(23)C(21)N(33)	125.918
H(7)C(2)	1.086	H(7)C(2)C(1)	120.098	H(7)C(2)C(1)C(3)	118.439
H(8)C(3)	1.087	H(8)C(3)C(2)	119.728	H(8)C(3)C(2)C(4)	119.704
H(9)C(5)	1.087	H(9)C(5)C(4)	119.456	H(9)C(5)C(4)C(6)	119.697
H(10)C(6)	1.085	H(10)C(6)C(1)	118.793	H(10)C(6)C(1)C(5)	119.967
H(28)C(25)	1.086	H(28)C(25)C(22)	120.328	H(28)C(25)C(22)C(27)	120.655
H(30)C(26)	1.086	H(30)C(26)C(24)	121.532	H(30)C(26)C(24)C(29)	120.987
H(31)C(27)	1.085	H(31)C(27)C(25)	119.83	H(31)C(27)C(25)C(29)	119.822
H(32)C(29)	1.086	H(32)C(29)C(26)	119.134	H(32)C(29)C(26)C(27)	119.696
H(16)C(15)	1.096	H(16)C(15)C(14)	111.596	H(16)C(15)C(14)C(21)	111
H(17)C(15)	1.094	H(17)C(15)C(14)	112.158	H(17)C(15)C(14)C(21)	112.286
H(20)N(19)	1.016	H(20)N(19)N(18)	109.888	H(20)N(19)N(18)C(21)	115.081
H(34)N(33)	1.011	H(34)N(33)C(23)	121.912	H(34)N(33)C(23)C(24)	125.487
H(12)N(11)	1.01	H(12)N(11)C(4)	116.33	H(12)N(11)C(4)C(3)	23.095
H(13)N(11)	1.01	H(13)N(11)C(4)	116.262	H(13)N(11)C(4)H(12)	112.78

Supp. Table 7. The HOMO-LUMO energies and E_g , ΔS , ΔH , ΔG , 0 PPINT of spiroheterocyclic [Z_1 - Z_6]

Code No.	EHOMO	ELUMO	ΔE (Egap)(Hartree/Particle)	ΔG (Hartree/Particle)	ΔS (Hartree/Particle)	ΔH (Hartree/Particle)	Zero (Hartree/Particle)
Z_1	-0.23963	-0.06097	0.17866	0.206316	0.220653	0.272104	0.253226
Z_2	-0.25032	-0.08747	0.161573	0.201397	0.247790	0.275276	0.253336
Z_4	-0.23221	-0.05770	0.17451	0.409571	0.304470	0.500349	0.469507
Z_5	-0.24916	-0.05988	0.18928	0.144049	0.181072	0.198036	0.183994
Z_6	-0.19313	-0.04257	0.15056	0.226395	0.201724	0.286540	0.269757

Supp. Table 8. The quantum chemical parameters of spiroheterocyclic [Z₁-Z₆]

Code No.	X	η	δ	Pi	Δ	ω	ΔN_{\max}	EA	IP	D.M. (μ) (Debye)
Z ₁	0.1503	0.08933	11.19444	0.001774	5.597223	0.321403	1.68252	0.06097	0.057422	5.1058
Z ₂	0.168895	0.081425	12.2812	0.012405	6.140620	0.384771	2.07424	0.08747	0.062660	5.3399
Z ₄	0.144955	0.087255	11.46066	0.001889	5.730330	0.308985	1.66128	0.05770	0.053921	4.9727
Z ₅	0.15452	0.096586	10.35346	-0.0011	6.984605	0.321371	1.59981	0.05988	0.062080	9.0700
Z ₆	0.11785	0.07528	13.28374	0.002635	6.641870	0.247735	1.56548	0.04257	0.037299	3.7990