

Table S1. The DFT dihedral angle data of the investigated compounds.

	4c		6c		11c
C(28)-C(29)-C(30)-C(20)	0.005	C(26)-C(27)-C(28)-C(18)	0.26	C(29)-C(30)-C(31)-C(26)	-0.01
C(27)-C(28)-C(29)-C(30)	0.028	C(25)-C(26)-C(27)-C(28)	0.137	C(28)-C(29)-C(30)-C(31)	-0.024
Cl(31)-C(28)-C(29)-C(30)	179.999	Cl(29)-C(26)-C(27)-C(28)	179.836	Cl(32)-C(29)-C(30)-C(31)	179.992
C(26)-C(27)-C(28)-C(29)	-0.02	C(24)-C(25)-C(26)-C(27)	-0.186	C(27)-C(28)-C(29)-C(30)	0.013
C(26)-C(27)-C(28)-Cl(31)	-179.991	C(24)-C(25)-C(26)-Cl(29)	-179.884	C(27)-C(28)-C(29)-Cl(32)	179.997
C(20)-C(26)-C(27)-C(28)	-0.022	C(18)-C(24)-C(25)-C(26)	-0.162	C(26)-C(27)-C(28)-C(29)	0.032
C(23)-C(24)-N(25)-C(8)	0.024	C(21)-C(22)-N(23)-C(8)	-0.005	N(25)-C(26)-C(31)-C(30)	-179.926
N(22)-C(23)-C(24)-N(25)	-0.039	N(20)-C(21)-C(22)-N(23)	-0.042	C(27)-C(26)-C(31)-C(30)	0.054
C(21)-N(22)-C(23)-C(24)	0.009	C(19)-N(20)-C(21)-C(22)	0.034	N(25)-C(26)-C(27)-C(28)	179.917
C(8)-C(21)-N(22)-C(23)	0.032	C(8)-C(19)-N(20)-C(21)	0.018	C(31)-C(26)-C(27)-C(28)	-0.065
C(19)-C(20)-C(30)-C(29)	179.945	C(16)-C(18)-C(28)-C(27)	179.325	N(24)-N(25)-C(26)-C(27)	-179.574
C(26)-C(20)-C(30)-C(29)	-0.044	C(24)-C(18)-C(28)-C(27)	-0.591	N(24)-N(25)-C(26)-C(31)	0.407
C(19)-C(20)-C(26)-C(27)	-179.937	C(16)-C(18)-C(24)-C(25)	-179.377	C(15)-N(24)-N(25)-C(26)	-179.861
C(30)-C(20)-C(26)-C(27)	0.053	C(28)-C(18)-C(24)-C(25)	0.541	C(21)-C(22)-N(23)-C(8)	0.006
C(15)-C(19)-C(20)-C(26)	179.516	C(15)-C(16)-C(18)-C(24)	163.998	N(20)-C(21)-C(22)-N(23)	-0.035
C(15)-C(19)-C(20)-C(30)	-0.473	C(15)-C(16)-C(18)-C(28)	-15.916	C(19)-N(20)-C(21)-C(22)	0.023
C(15)-C(16)-N(17)-C(13)	0.193	N(17)-C(16)-C(18)-C(24)	-14.814	C(8)-C(19)-N(20)-C(21)	0.014
O(18)-C(16)-N(17)-C(13)	-179.795	N(17)-C(16)-C(18)-C(28)	165.272	C(15)-C(16)-N(17)-C(13)	-0.316
S(14)-C(15)-C(19)-C(20)	0.088	C(15)-C(16)-N(17)-C(13)	0.238	C(18)-C(16)-N(17)-C(13)	179.373
C(16)-C(15)-C(19)-C(20)	-179.99	C(18)-C(16)-N(17)-C(13)	179.179	S(14)-C(15)-N(24)-N(25)	-179.255
S(14)-C(15)-C(16)-N(17)	-0.609	S(14)-C(15)-C(16)-N(17)	-0.702	C(16)-C(15)-N(24)-N(25)	0.641
S(14)-C(15)-C(16)-O(18)	179.379	S(14)-C(15)-C(16)-C(18)	-179.554	S(14)-C(15)-C(16)-N(17)	0.081
C(19)-C(15)-C(16)-N(17)	179.454	C(13)-S(14)-C(15)-C(16)	0.71	S(14)-C(15)-C(16)-C(18)	-179.583
C(19)-C(15)-C(16)-O(18)	-0.558	N(12)-C(13)-N(17)-C(16)	177.233	N(24)-C(15)-C(16)-N(17)	-179.819
C(13)-S(14)-C(15)-C(16)	0.614	S(14)-C(13)-N(17)-C(16)	0.344	N(24)-C(15)-C(16)-C(18)	0.516
C(13)-S(14)-C(15)-C(19)	-179.457	N(12)-C(13)-S(14)-C(15)	-177.752	C(13)-S(14)-C(15)-C(16)	0.118
N(12)-C(13)-N(17)-C(16)	178.658	N(17)-C(13)-S(14)-C(15)	-0.621	C(13)-S(14)-C(15)-N(24)	-179.961
S(14)-C(13)-N(17)-C(16)	0.322	N(10)-N(12)-C(13)-S(14)	-161.42	N(12)-C(13)-N(17)-C(16)	178.332
N(12)-C(13)-S(14)-C(15)	-179.082	N(10)-N(12)-C(13)-N(17)	21.806	S(14)-C(13)-N(17)-C(16)	0.416
N(17)-C(13)-S(14)-C(15)	-0.586	H(38)-N(12)-C(13)-S(14)	-33.527	N(12)-C(13)-S(14)-C(15)	-178.334
N(10)-N(12)-C(13)-S(14)	-161.526	H(38)-N(12)-C(13)-N(17)	149.698	N(17)-C(13)-S(14)-C(15)	-0.312
N(10)-N(12)-C(13)-N(17)	20.11	C(9)-N(10)-N(12)-C(13)	-74.325	N(10)-N(12)-C(13)-S(14)	-158.688
H(40)-N(12)-C(13)-S(14)	-21.44	C(9)-N(10)-N(12)-H(38)	155.898	N(10)-N(12)-C(13)-N(17)	23.481
H(40)-N(12)-C(13)-N(17)	160.196	C(5)-C(9)-N(10)-N(12)	179.195	H(41)-N(12)-C(13)-S(14)	-26.929
C(9)-N(10)-N(12)-C(13)	-70.318	C(11)-C(9)-N(10)-N(12)	-2.482	H(41)-N(12)-C(13)-N(17)	155.24
C(9)-N(10)-N(12)-H(40)	147.98	N(7)-C(8)-N(23)-C(22)	-179.903	C(9)-N(10)-N(12)-C(13)	-74.72
C(5)-C(9)-N(10)-N(12)	178.151	C(19)-C(8)-N(23)-C(22)	0.057	C(9)-N(10)-N(12)-H(41)	151.684
C(11)-C(9)-N(10)-N(12)	-3.48	N(7)-C(8)-C(19)-N(20)	179.895	C(5)-C(9)-N(10)-N(12)	178.757
N(7)-C(8)-N(25)-C(24)	-179.879	N(23)-C(8)-C(19)-N(20)	-0.066	C(11)-C(9)-N(10)-N(12)	-3.04
C(21)-C(8)-N(25)-C(24)	0.016	C(2)-N(7)-C(8)-C(19)	-179.8	N(7)-C(8)-N(23)-C(22)	-179.932
N(7)-C(8)-C(21)-N(22)	179.852	C(2)-N(7)-C(8)-N(23)	0.161	C(19)-C(8)-N(23)-C(22)	0.032

N(25)-C(8)-C(21)-N(22)	-0.046	H(34)-N(7)-C(8)-C(19)	-0.238	N(7)-C(8)-C(19)-N(20)	179.921
C(2)-N(7)-C(8)-C(21)	179.755	H(34)-N(7)-C(8)-N(23)	179.723	N(23)-C(8)-C(19)-N(20)	-0.043
C(2)-N(7)-C(8)-N(25)	-0.347	C(4)-C(5)-C(9)-N(10)	10.21	C(2)-N(7)-C(8)-C(19)	-179.801
H(36)-N(7)-C(8)-C(21)	-0.33	C(4)-C(5)-C(9)-C(11)	-168.215	C(2)-N(7)-C(8)-N(23)	0.163
H(36)-N(7)-C(8)-N(25)	179.567	C(6)-C(5)-C(9)-N(10)	-169.202	H(37)-N(7)-C(8)-C(19)	-0.037
C(4)-C(5)-C(9)-N(10)	9.527	C(6)-C(5)-C(9)-C(11)	12.373	H(37)-N(7)-C(8)-N(23)	179.927
C(4)-C(5)-C(9)-C(11)	-168.944	C(4)-C(5)-C(6)-C(1)	0.131	C(4)-C(5)-C(9)-N(10)	8.502
C(6)-C(5)-C(9)-N(10)	-169.67	C(9)-C(5)-C(6)-C(1)	179.564	C(4)-C(5)-C(9)-C(11)	-169.812
C(6)-C(5)-C(9)-C(11)	11.859	C(3)-C(4)-C(5)-C(6)	-0.641	C(6)-C(5)-C(9)-N(10)	-170.839
C(4)-C(5)-C(6)-C(1)	0.185	C(3)-C(4)-C(5)-C(9)	179.923	C(6)-C(5)-C(9)-C(11)	10.846
C(9)-C(5)-C(6)-C(1)	179.409	C(2)-C(3)-C(4)-C(5)	0.623	C(4)-C(5)-C(6)-C(1)	0.193
C(3)-C(4)-C(5)-C(6)	-0.665	C(1)-C(2)-N(7)-C(8)	-1.09	C(9)-C(5)-C(6)-C(1)	179.558
C(3)-C(4)-C(5)-C(9)	-179.894	C(1)-C(2)-N(7)-H(34)	179.348	C(3)-C(4)-C(5)-C(6)	-0.652
C(2)-C(3)-C(4)-C(5)	0.643	C(3)-C(2)-N(7)-C(8)	179.104	C(3)-C(4)-C(5)-C(9)	179.98
C(1)-C(2)-N(7)-C(8)	-1.429	C(3)-C(2)-N(7)-H(34)	-0.458	C(2)-C(3)-C(4)-C(5)	0.599
C(1)-C(2)-N(7)-H(36)	178.657	C(1)-C(2)-C(3)-C(4)	-0.074	C(1)-C(2)-N(7)-C(8)	-0.594
C(3)-C(2)-N(7)-C(8)	178.855	N(7)-C(2)-C(3)-C(4)	179.744	C(1)-C(2)-N(7)-H(37)	179.642
C(3)-C(2)-N(7)-H(36)	-1.059	C(2)-C(1)-C(6)-C(5)	0.402	C(3)-C(2)-N(7)-C(8)	179.554
C(1)-C(2)-C(3)-C(4)	-0.118	C(6)-C(1)-C(2)-C(3)	-0.428	C(3)-C(2)-N(7)-H(37)	-0.211
N(7)-C(2)-C(3)-C(4)	179.617	C(6)-C(1)-C(2)-N(7)	179.769	C(1)-C(2)-C(3)-C(4)	-0.064
C(2)-C(1)-C(6)-C(5)	0.323			N(7)-C(2)-C(3)-C(4)	179.798
C(6)-C(1)-C(2)-C(3)	-0.357			C(2)-C(1)-C(6)-C(5)	0.324
C(6)-C(1)-C(2)-N(7)	179.931			C(6)-C(1)-C(2)-C(3)	-0.388
				C(6)-C(1)-C(2)-N(7)	179.762