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SUPPLEMENTARY MATERIAL TO

Microwave assisted synthesis of novel spiro diarylidenes and their antimicrobial assay

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*4-Methyl-2,6,10-triphenyl-2,3-diaza-spiro[4.5]dec-3-ene-1,8-dione (**3**)*

Yield: 285 mg, 70 % (Conventional) and 334 mg, 82 % (MW). M.p. 166––168 °C. ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.12 (*s*, 3H, CH_3), 2.60 (*dd*, 2H, J = 14.0 Hz, 3.6 Hz, 7H/9H-equatorial), 3.53 (*dd*, 2H, J = 14.0 Hz, 3.6 Hz, 7H/9H-axial), 4.01–4.08 (*m*, 2H, 2×CH of C-6 & C-10), 7.2–7.3 (*m*, 11H, H-20, H-12, H-13, H14, H-15, H-16, H-12', H-13', H14', H-15', H-16',), 7.34–7.38 (*m*, 2H, H-19 & H-21), 7.42 (*d*, 2H, J = 8.0 Hz, H-18 & H-22). ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 207.64, 186.52, 160.63, 139.58, 137.97, 129.53, 128.61, 128.11, 127.44, 127.09, 121.29, 63.36, 48.95, 42.96, 16.33. (+) LCMS (*m*/*z*): calculated for $[C_{27}H_{24}N_2O_2 + H]^+$ 408.4, observed 409.1.

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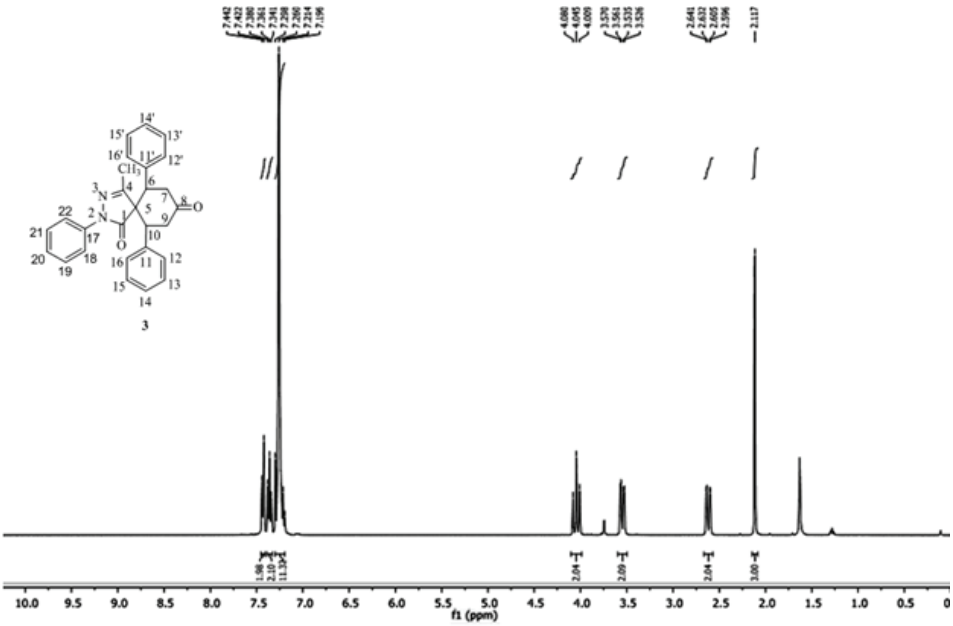

Figure S-1. ^{1}H NMR spectrum of 4-methyl-2,6,10-triphenyl-2,3-diaza-spiro [4.5] dec-3-ene--1,8-dione (**3**) ($CDCl_3$, 400 MHz)

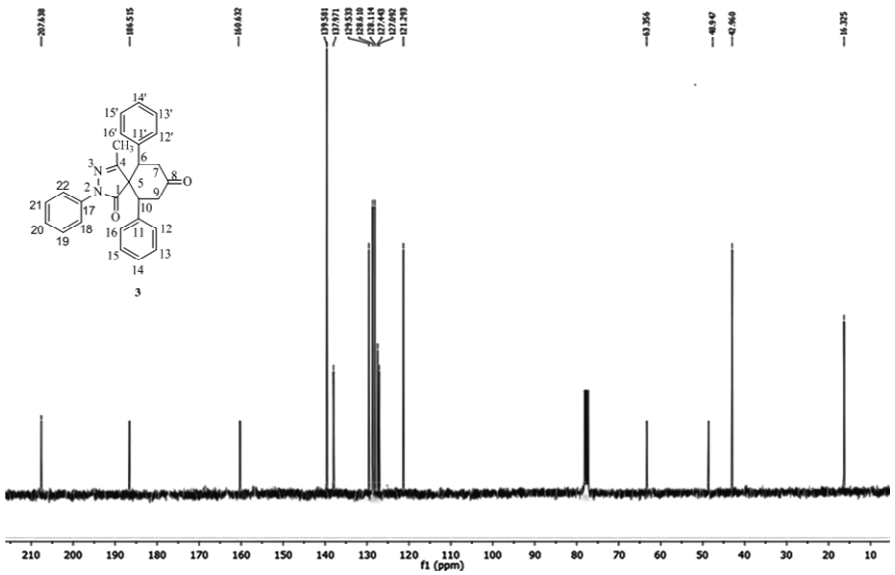

Figure S-2. ^{13}C NMR spectrum of 4-methyl-2,6,10-triphenyl-2,3-diaza-spiro [4.5] dec-3-ene--1,8-dione (**3**) ($CDCl_3$, 100 MHz)

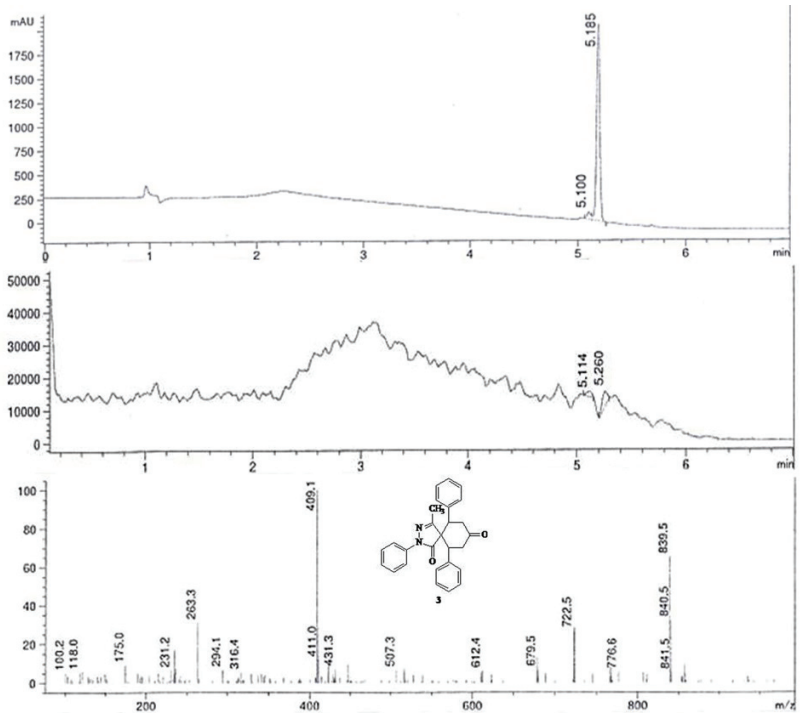

Figure S-3. Mass spectrum of 4-methyl-2,6,10-triphenyl-2,3-diaza-spiro [4.5] dec-3-ene-1,8-dione (**3**)

*4-Methyl-7,9-bis-(4-nitro-benzylidene)-2,6,10-triphenyl-2,3-diaza-spiro[4.5] dec-3-ene-1,8-dione(**5a**)*

Dark brown solid. Yield: 512 mg, 76 % (Conventional) and 566 mg, 84 % (MW). m.p: 80-82 °C, IR (ν_{max}/cm^{-1}):1733, 1691, 1553, 1525,1380. ^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.80 (s, 3H, CH_3), 3.10 (s, 2H, 2xCH, H-6 & H-10), 7.20 - 7.23(m, 1H, H-27), 7.24-7.27 (m,6H, H-20,21,22,20',21',22'), 7.38-7.43(m, 4H, H-19,23,19',23'), 7.45(s, 2H, 2x =CH, H-11 & H-11'), 7.47(dd, 2H, *J*=4.0 Hz, 1.2Hz, H-25 & H-29), 7.53-7.56 (m, 2H, H-26,28), 7.79(d, 4H, *J*=8.0 Hz, H-13,17,13',17'), 8.27(d, 4H, *J*=8.0 Hz, H-14,16,14',16'). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 189.91, 179.85, 158.68, 143.86, 142.89, 141.15, 137.97, 137.55, 133.86, 129.91, 128.42, 127.81, 127.34, 125.92, 124.82, 121.7, 111.82, 63.63, 48.54, 17.82. Combustion analysis for $C_{41}H_{30}N_4O_6$: Calculated. C 72.99, H 4.48, N 8.3; found C 72.95, H 4.46, N 8.29. (+) LCMS (*m*/*z*): calculated for $[C_{41}H_{30}N_4O_6 + H]^+$ 674.7, observed 675.6.

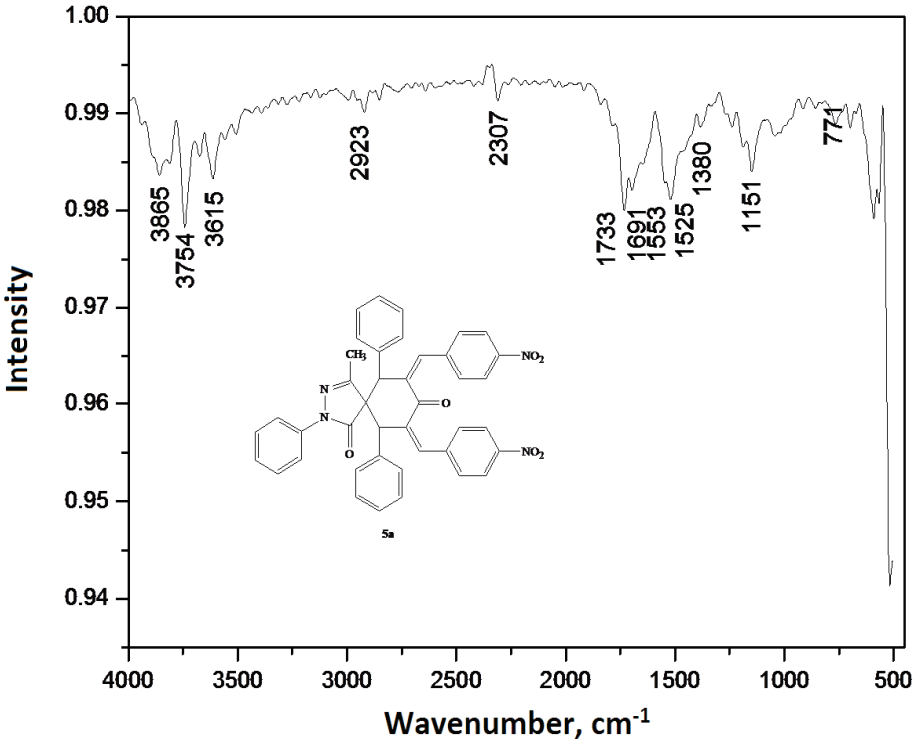

Figure S-4. IR spectrum of 4-methyl-7,9-bis-(4-nitro-benzylidene)-2,6,10-triphenyl-2,3--diaza-spiro[4.5]dec-3-ene-1,8-dione (**5a**)

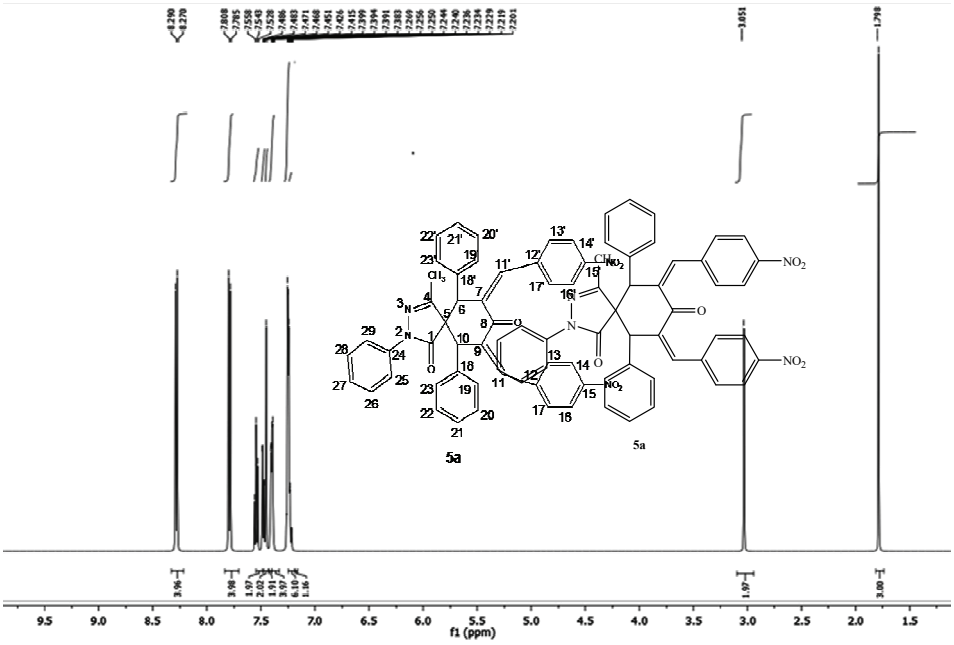

Figure S-5. ^{1}H NMR spectrum of 4-methyl-7,9-bis-(4-nitro-benzylidene)-2,6,10-triphenyl--2,3-diaza-spiro[4.5]dec-3-ene-1,8-dione (**5a**) ($CDCl_3$, 400 MHz)

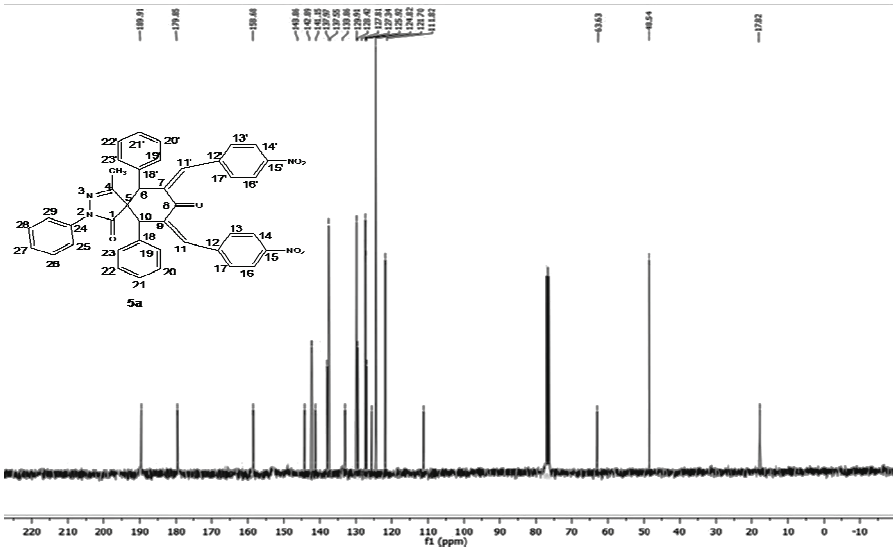

Figure S-6. ^{13}C NMR pectrum of 4-methyl-7,9-bis-(4-nitro-benzylidene)-2,6,10-triphenyl--2,3-diaza-spiro[4.5]dec-3-ene-1,8-dione (**5a**) ($CDCl_3$, 100 MHz)

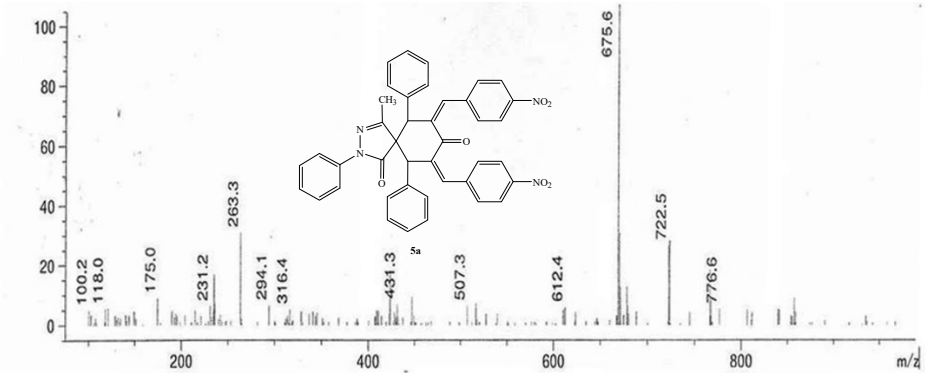

Figure S-7. Mass spectrum of 4-methyl-7,9-bis-(4-nitro-benzylidene)-2,6,10-triphenyl-2,3--diaza-spiro[4.5]dec-3-ene-1,8-dione (**5a**)

*4-Methyl-7,9-bis-(4-cyano-benzylidiene)-2,6,10-triphenyl-2,3-diazaspiro[4,5]dec-3-ene-1,8-dione(**5b**).* Yellow solid. Yield: 475 mg, 75% (Conventional) and 551 mg, 87 % (MW). m.p.: 110-112 °C, IR (ν_{max}/cm^{-1}):2304, 1730, 1690, 1546, 1512. ^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.90 (s, 3H, CH_3), 3.08(s, 2H, 2xCH, H-6 & H-10), 7.20-7.23 (m, 1H, H-27), 7.25-7.29 (m, 6H, H-20,21,22,20',21',22'), 7.33 (s, 2H,2x =CH, H-11 & H-11'), 7.39-7.43 (m, 4H, H-19,23,19',23'), 7.44 (dd, 2H, *J*=4.0Hz, 1.2Hz, H-25 & H-29), 7.51-7.54 (m, 2H, H-26,28), 7.69 (d, 4H, *J*=8.0 Hz, H-13,17,13',17'), 7.72 (d, 4H, *J*=8.0Hz, H-14,16,14',16'). ^{13}C NMR (100 MHz, $CDCl_3$, δ):189.83, 180.12, 157.34, 143.12, 141.26, 139.76, 137.48, 134.18, 129.53, 128.45, 127.41, 127.09, 125.26, 124.18, 121.29, 119.12, 111.29, 62.83, 48.26, 16.76. Combustion analysis for $C_{43}H_{30}N_4O_2$: Calculated. C, 81.37, H 4.76, N 8.83; found C 81.36, H 4.74, N 8.8. (+) LCMS (*m*/*z*): calculated for $[C_{43}H_{30}N_4O_2 + H]^+$ 634.7, observed 635.4.

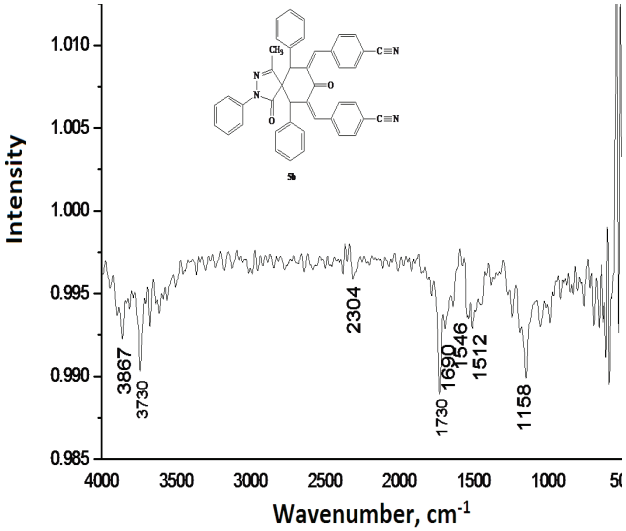

Figure S-8. IR spectrum of 4-methyl-7,9-bis-(4-cyano-benzylidiene)-2,6,10-triphenyl-2,3 diazaspiro[4,5]dec-3-ene-1,8-dione (**5b**)

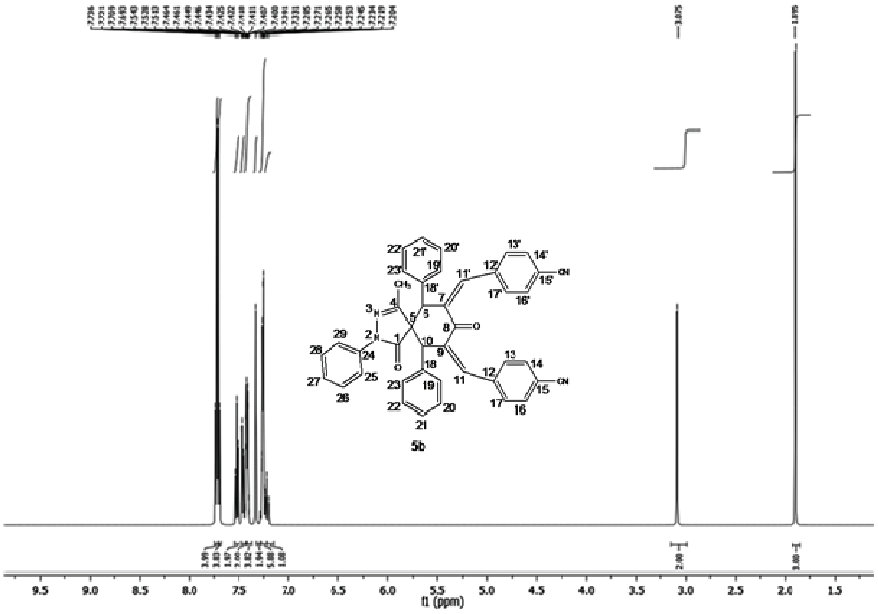

Figure S-9. ^{1}H NMR spectrum of 4-Methyl-7,9-bis-(4-cyano-benzylidiene)-2,6,10-triphenyl--2,3 diazaspiro[4,5]dec-3-ene-1,8-dione (**5b**) ($CDCl_3$, 400 MHz)

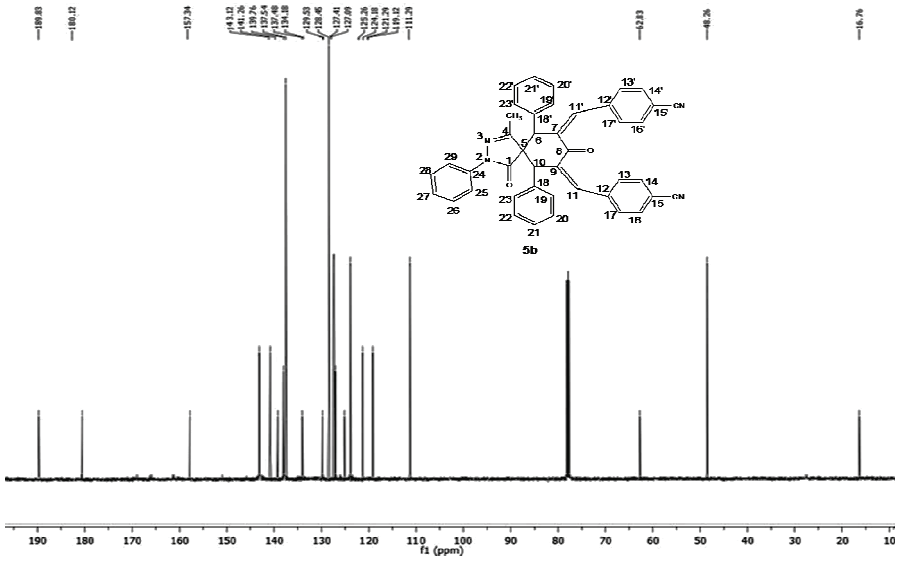

Figure S-10. ^{13}C NMR spectrum of 4-methyl-7,9-bis-(4-cyano-benzylidiene)-2,6,10-triphenyl--2,3-diazaspiro[4,5]dec-3-ene-1,8-dione (**5b**) ($CDCl_3$, 100 MHz).

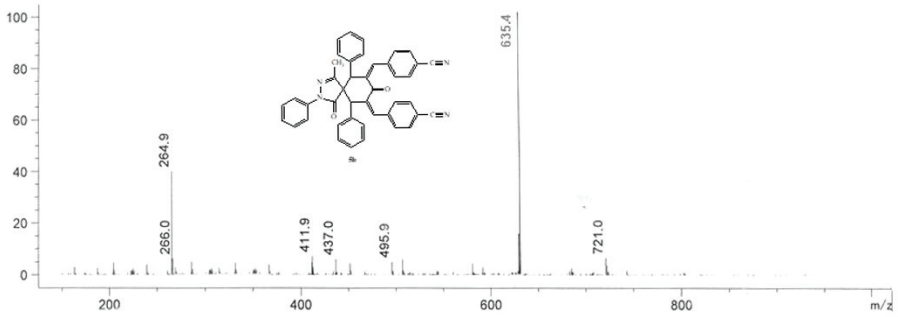

Figure S-11. Mass spectrum of 4-methyl-7,9-bis-(4-cyano-benzylidiene)-2,6,10-triphenyl-2,3-diazaspiro[4,5]dec-3-ene-1,8-dione (**5b**)

*7,9-Bis-(5-bromo-2-hydroxy-benzylidene)-4-methyl-2,6,10-triphenyl-2,3-diazaspiro[4.5] dec-3-ene-1,8-dione(**5c**).* Reddish brown solid. Yield: 557 mg, 72%(Conventional) and 658 mg, 85% (MW). m.p.: 90-92 °C, IR (ν_{max}/cm^{-1}):3614, 1731, 1683, 1546, 1512. ^{1}H NMR (400 MHz, $CDCl_3$ δ): 1.97(s, 3H, CH_3), 3.10 (s, 2H, 2xCH, H-6 & H-10), 6.84(d, 2H, *J*=8.0 Hz, H-16 & 16'), 7.21-7.24(m,1H, H-27), 7.25-7.28(m, 6H, H-20,21,22,20',21',22'), 7.37(d, *J*=8.0 Hz, 2H, H-26 & 28), 7.40-7.43 (m, 4H, H-19,23,19',23'), 7.44(dd, 2H, *J*=4.0 Hz, 1.2Hz, H-25& H-29), 7.50 (s, 2H, 2x =CH, H-11 & H-11'), 7.51-7.54 (m, 2H, H-15&15'), 7.59(s, 2H, H-13 &13'), 9.77(bs, 2H, 2x OH). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 187.02, 177.62, 156.0, 155.26, 145.37, 139.53, 138.9, 137.55, 133.13, 131.39, 129.53, 128.45, 127.41, 127.34, 125.26, 123.13, 121.29, 119.52, 113.18, 63.9, 48.55, 16.33. Combustion analysis for $C_{41}H_{30}Br_2N_2O_4$: Calculated. C 63.58, H 3.9, N 3.62; found C 63.56, H 3.87, N 3.59. (+) LCMS (*m*/*z*): calculated for $[C_{41}H_{30}Br_2N_2O_4 + H]^{2+}$ 774.4, observed 776.1.

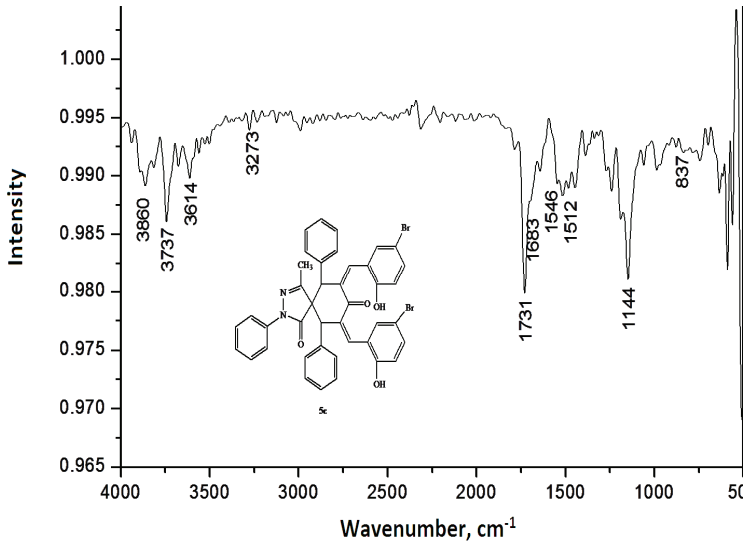

Figure S-12. IR spectrum of 7,9-bis-(5-bromo-2-hydroxy-benzylidene)-4-methyl-2,6,10--triphenyl-2,3-diazaspiro[4.5]dec-3-ene-1,8-dione (**5c**)

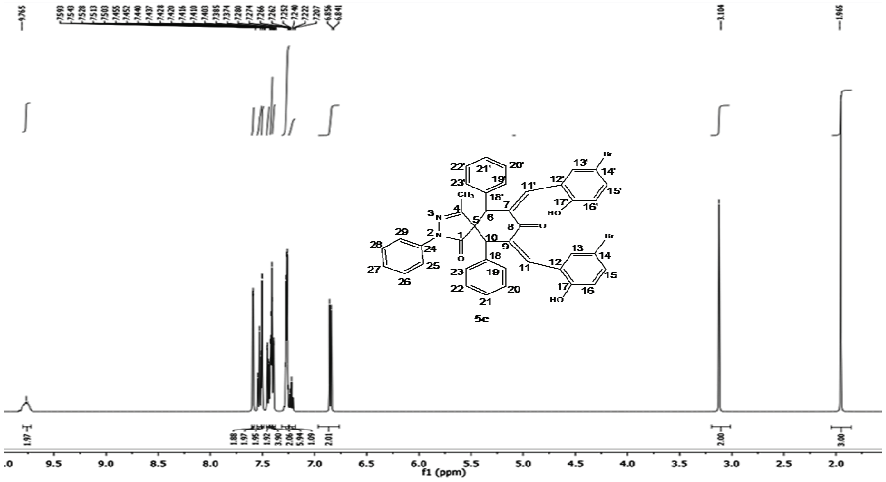

Figure S-13. ^{1}H NMR spectrum of 7,9-bis-(5-bromo-2-hydroxy-benzylidene)-4-methyl--2,6,10-triphenyl-2,3-diazaspiro[4.5]dec-3-ene-1,8-dione (**5c**) ($CDCl_3$, 400 MHz).

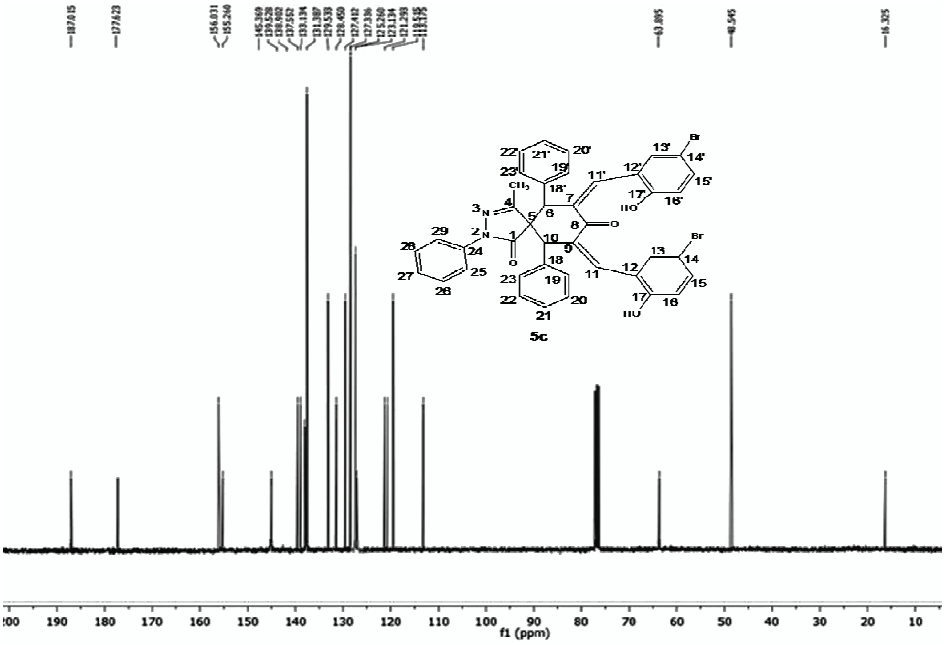

Figure S-14. ^{13}C NMR spectrum of 7,9-bis-(5-bromo-2-hydroxy-benzylidene)-4-methyl--2,6,10-triphenyl-2,3-diazaspiro[4.5]dec-3-ene-1,8-dione (**5c**) ($CDCl_3$, 100 MHz).

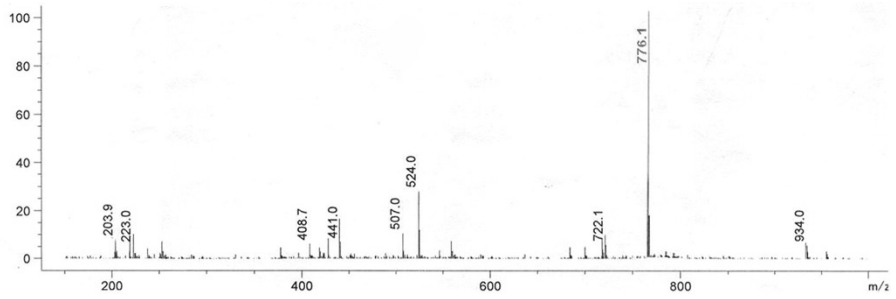

Figure S-15. Mass spectrum of 7,9-bis-(5-bromo-2-hydroxy-benzylidene)-4-methyl-2,6,10--triphenyl-2,3-diazaspiro[4.5]dec-3-ene-1,8-dione (**5c**).

*7,9-Bis-(3,4-dimethoxy-benzylidene)-4-methyl-2,6,10-triphenyl-2,3-diazaspiro[4.5]dec-3-ene-1,8-dione(**5d**).* Pale yellow solid. Yield: 478 mg, 68 % (Conventional) and 570 mg, 81 % (MW). m.p.: 98-101 °C, IR (ν_{max}/cm^{-1}):1730, 1690, 1553, 1499, 1144. ^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.96(s, 3H, CH_3), 3.09(s, 2H, 2xCH, H-6 & H-10), 3.82 (s, 12H, 4xOCH_3), 7.09 (d, 2H, *J*=8.0 Hz, H-14 &14'), 7.18-7.21 (m,1H, H-27), 7.22 (s, 2H, H-17&17'), 7.23-7.27(m, 6H, H-20,21,22,20',21',22'), 7.31 (s, 2H, 2x =CH, H-11 & H-11'), 7.36 (dd, 2H, *J*=4.0 Hz, 1.2Hz, H-13 & H-13'), 7.41-7.44 (m, 4H, H-19,23,19',23'), 7.45 (d, 2H, *J*=8.0 Hz, H-25 & 29), 7.51-7.54 (m,2H, H-26 & 28), ^{13}C NMR (100 MHz, $CDCl_3$, δ): 187.07, 176.26, 155.45, 144.92, 140.43, 150.94, 150.04, 140.26, 137.92, 137.51, 129.42, 128.26, 127.41, 127.03, 126.41, 123.57, 121.23, 113.34, 112.51, 64.62, 56.78, 48.5, 16.35. Combustion analysis for $C_{45}H_{40}N_2O_6$: Calculated. C 76.68, H 5.72, N 3.97; found C 76.65, H 5.69, N 3.95. (+) LCMS (*m*/*z*): calculated for $[C_{45}H_{40}N_2O_6 + H]^{2+}$ 704.8, observed 706.5.

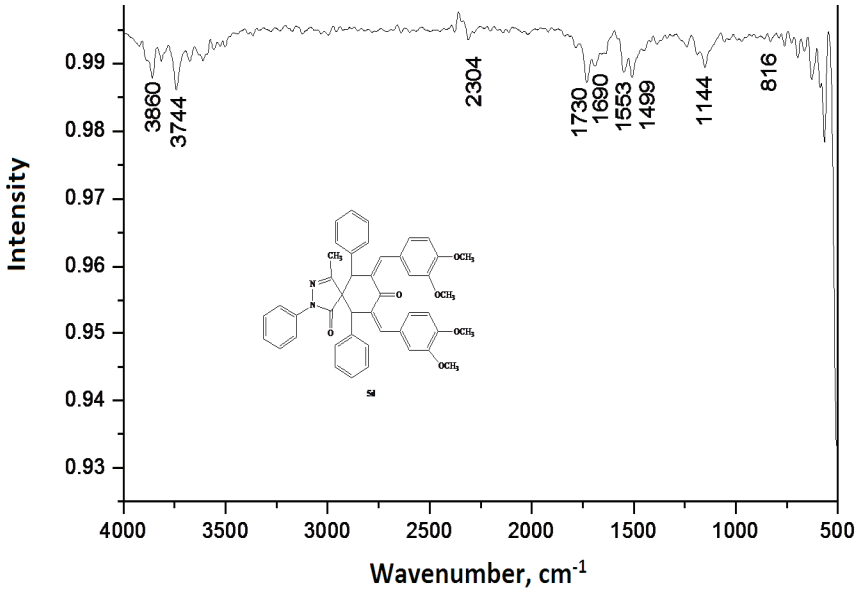

Figure S-16. IR spectrum of 7,9-bis-(3,4-dimethoxy-benzylidene)-4-methyl-2,6,10-triphenyl--2,3-diaza-spiro[4.5]dec-3-ene-1,8-dione (**5d**).

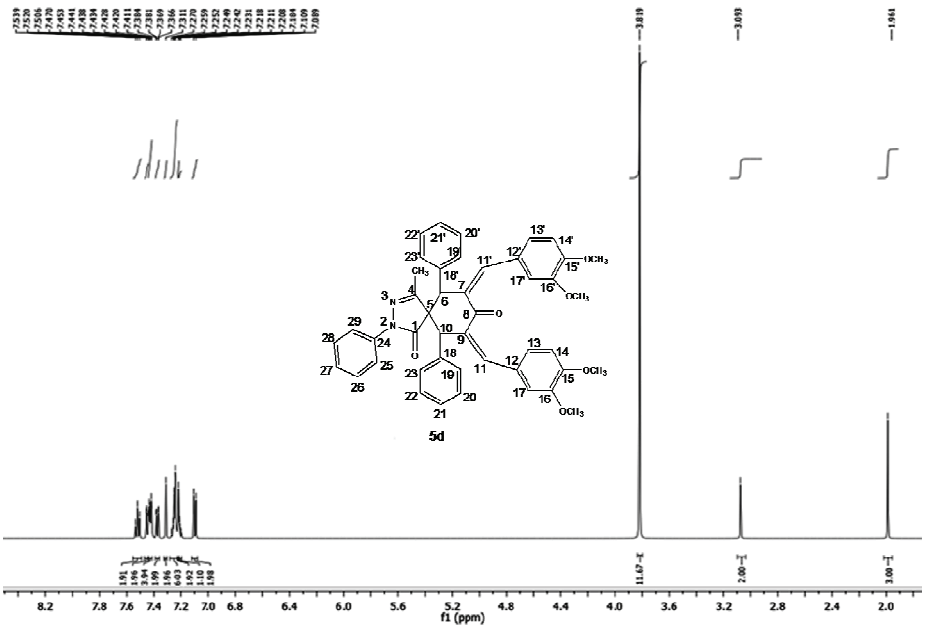

Figure S-17. ^{1}H NMR spectrum of 7,9-bis-(3,4-dimethoxy-benzylidene)-4-methyl-2,6,10--triphenyl-2,3-diaza-spiro[4.5]dec-3-ene-1,8-dione (**5d**) ($CDCl_3$, 400 MHz).

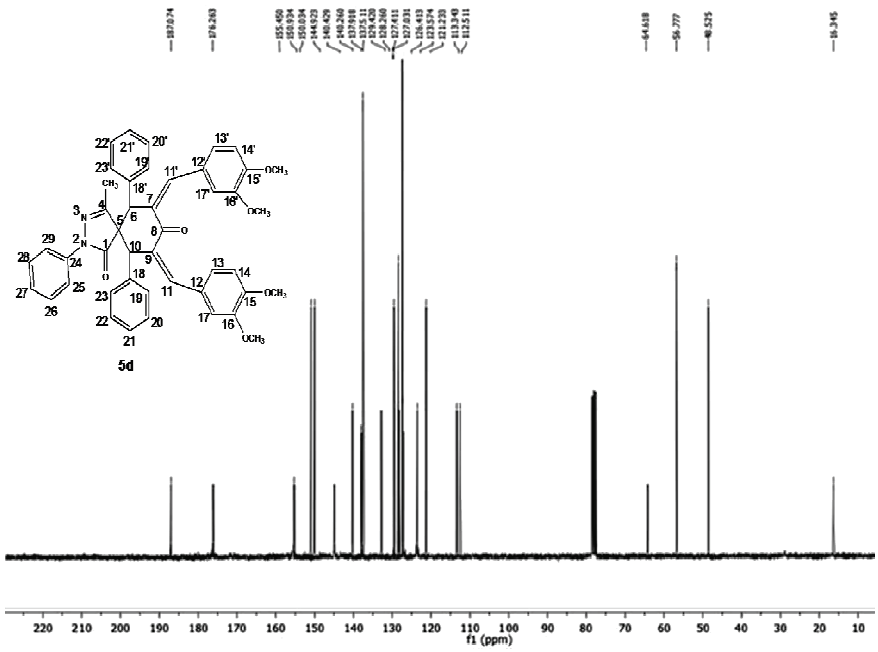

Figure S-18. ^{13}C NMR spectrum of 7,9-bis-(3,4-dimethoxy-benzylidene)-4-methyl-2,6,10--triphenyl-2,3-diaza-spiro[4.5]dec-3-ene-1,8-dione (**5d**) ($CDCl_3$, 100 MHz).

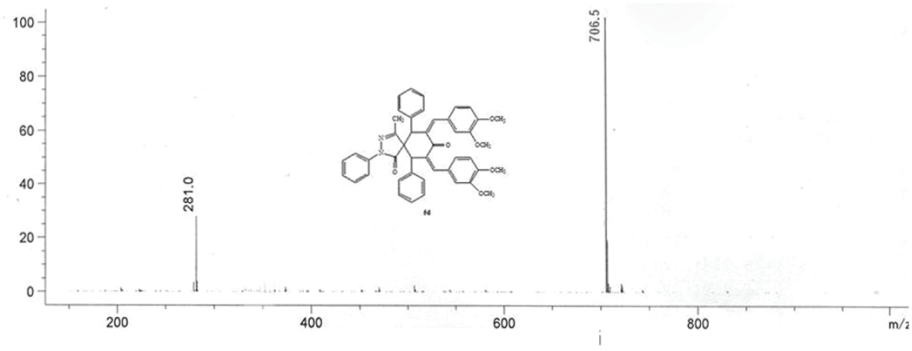

Figure S-19. Mass spectrum of 7,9-bis-(3,4-dimethoxy-benzylidene)-4-methyl-2,6,10--triphenyl-2,3-diaza-spiro[4.5]dec-3-ene-1,8-dione (**5d**).

*4-Methyl-2,6,10-triphenyl-7,9-bis-(2,4,6-trimethoxybenzylidene)-2,3-diazaspiro[4.5]dec-3-ene-1,8-dione (5e).*Pale yellow solid. Yield: 534 mg, 70% (Conventional) and 626 mg, 82% (MW). m.p.: 85-87 °C, IR (ν_{max}/cm^{-1}):1751, 1683, 1546, 1505, 1096. ^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.88 (s, 3H, CH_3), 3.11 (s, 2H, 2xCH, H-6 & H-10), 3.81 (s, 12H, 4xOCH_3), 3.83 (s, 6H, 2xOCH_3), 6.40 (s, 4H, H-14,16,14',16'), 7.21-7.24 (m, 1H, H-27), 7.25-7.28 (m, 6H, H-20,21,22,20',21',22'), 7.36 (s, 2H,2x =CH, H-11 & H-11'), 7.40-7.44 (m, 4H, H-19,23,19',23'), 7.48 (dd, 2H, *J*=4.0Hz, 1.2Hz, H-25 & H-29), 7.53-7.56 (m, 2H, H-26 & 28). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 187.07, 177.55, 160.62, 158.95, 155.45, 144.07, 141.55, 139.54, 137.29, 129.53, 128.09, 127.41, 127.29, 127.06, 121.49, 107.73, 90.97, 64.62, 56.78, 56.03, 48.42, 16.34. Combustion analysis for $C_{47}H_{44}N_2O_8$: Calculated. C 73.8, H 5.8, N 3.66; found C 73.78, H 5.77, N 3.62. (+) LCMS (*m*/*z*): calculated for $[C_{47}H_{44}N_2O_8 + H]^+$ 764.8, observed 765.9.

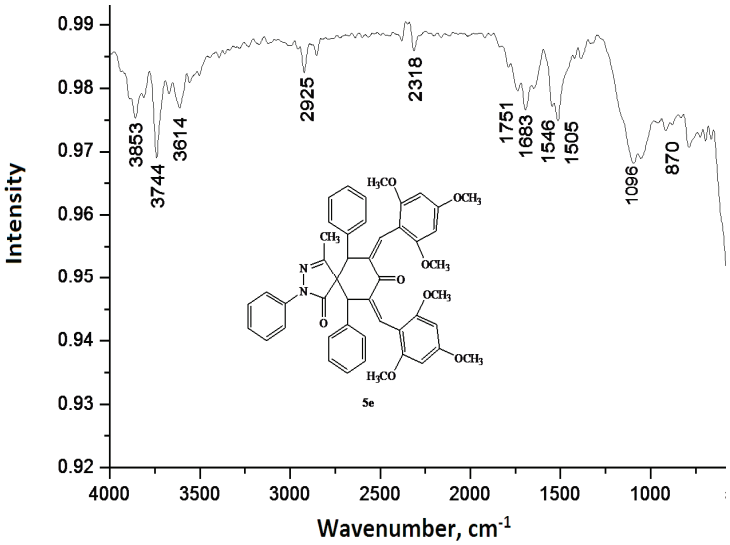

Figure S-20. IR spectrum of 4-methyl-2,6,10-triphenyl-7,9-bis-(2,4,6-trimethoxy--benzylidene)-2,3-diazaspiro[4.5]dec-3-ene-1,8-dione (**5e**).

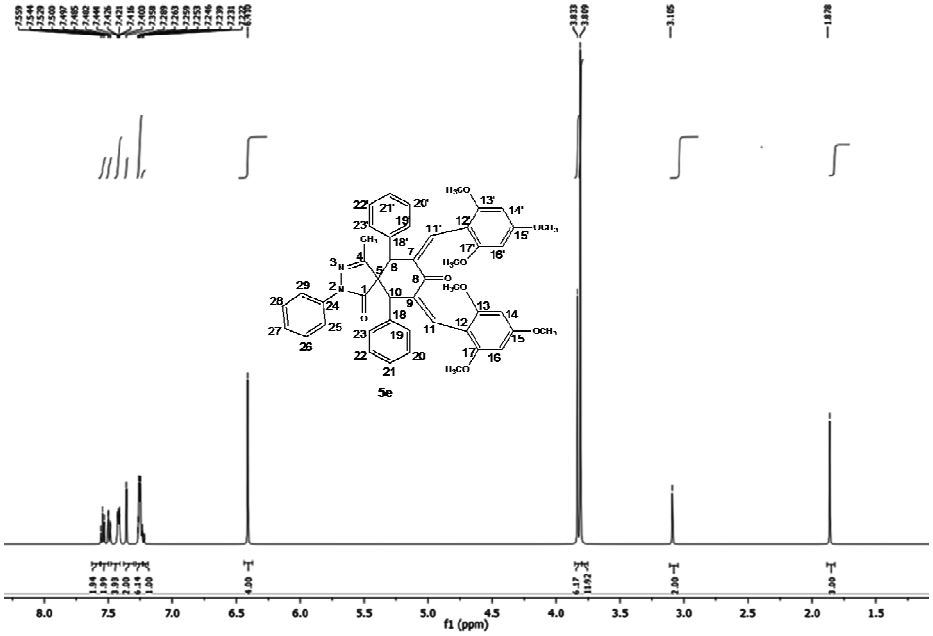

Figure S-21. ^{1}H NMR spectrum of 4-methyl-2,6,10-triphenyl-7,9-bis-(2,4,6-trimethoxy--benzylidene)-2,3-diazaspiro[4.5]dec-3-ene-1,8-dione (**5e**) ($CDCl_3$, 400 MHz).

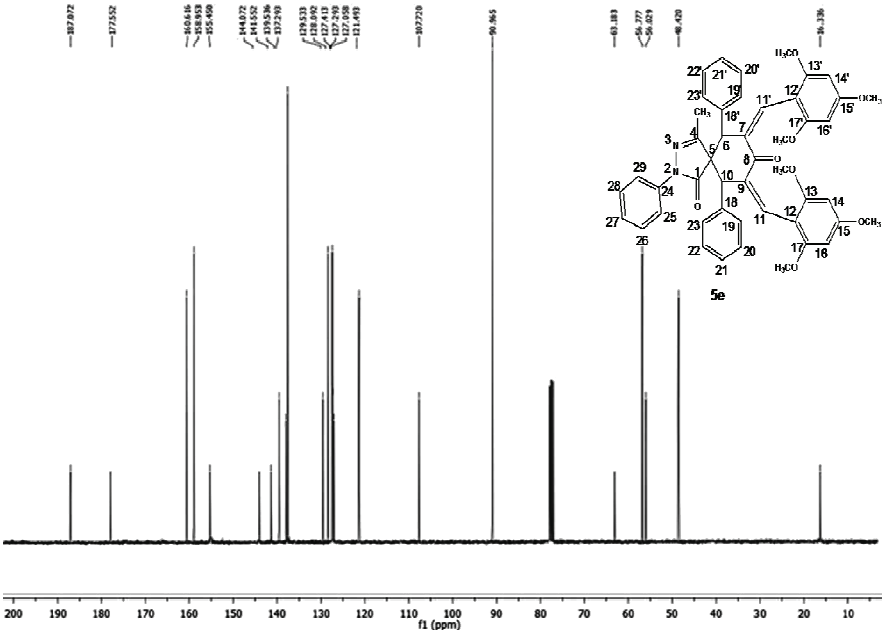

Figure S-22. ^{13}C NMR spectrum of 4-methyl-2,6,10-triphenyl-7,9-bis-(2,4,6-trimethoxy-benzylidene)-2,3-diazaspiro[4.5]dec-3-ene-1,8-dione (**5e**) ($CDCl_3$, 100 MHz).

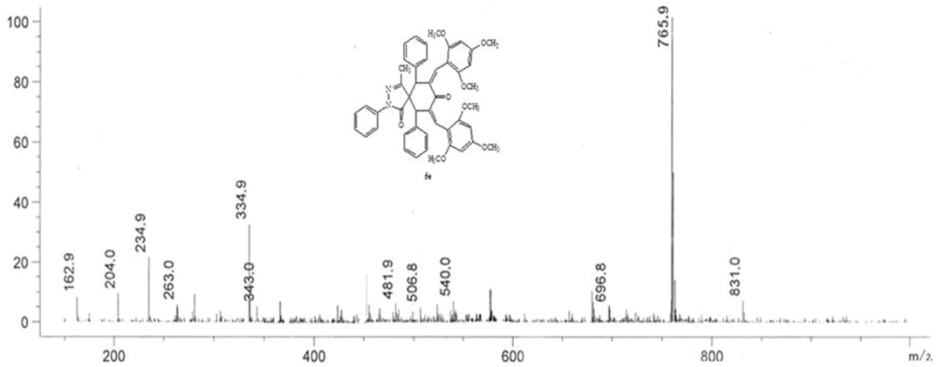

Figure S-23. Mass spectrum of 4-methyl-2,6,10-triphenyl-7,9-bis-(2,4,6-trimethoxy--benzylidene)-2,3-diazaspiro[4.5]dec-3-ene-1,8-dione (**5e**).

*7,9-Bis-(4-hydroxy-benzylidene)-4-methyl-2,6,10-triphenyl-2,3-diazaspiro [4.5]dec-3-ene-1,8-dione(**5f**).* Reddish brown solid. Yield: 425 mg, 69 % (Conventional) and 493 mg, 80 % (MW). m.p.: 104-106 °C, IR (ν_{max}/cm^{-1}):3608, 1751, 1696, 1560, 1505. ^{1}H NMR (400 MHz, $CDCl_3$, δ): 2.02 (s, 3H, CH_3), 3.05 (s, 2H, 2xCH, H-6 & H-10), 6.86 (d, 4H, *J*=8.0 Hz, H-14,16,14',16'), 7.21-7.24 (m, 1H, H-27),7.25 (s,2H,2x =CH, H-11&H-11'), 7.26-7.29(m, 6H, H-20,21, 22,20',21', 22'), 7.35(d, 4H, *J*=8.0 Hz, H-13,17,13',17'), 7.40-7.44 (m, 4H, H-19,23,19',23'), 7.47 (dd, 2H, *J*= 4.0 Hz, 1.2Hz, H-25 & H-29), 7.52-7.55 (m, 2H, H-26 &28), 9.59 (bs, 2H, 2xOH). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 187.04, 177.54, 155.26, 145.36, 141.12, 140.43, 137.97, 137.55, 130.65, 129.53, 128.45, 127.41, 127.34, 126.57, 121.29, 116.11, 63.51, 48.95, 16.42. Combustion analysis for $C_{41}H_{32}N_2O_4$: Calculated. C 79.85, H 5.23, N 4.54; found. C 79.81, H 5.2, N 4.51. (+) LCMS (*m*/*z*): calculated for $[C_{41}H_{32}N_2O_4 + H]^+$ 616.7, observed 617.2.

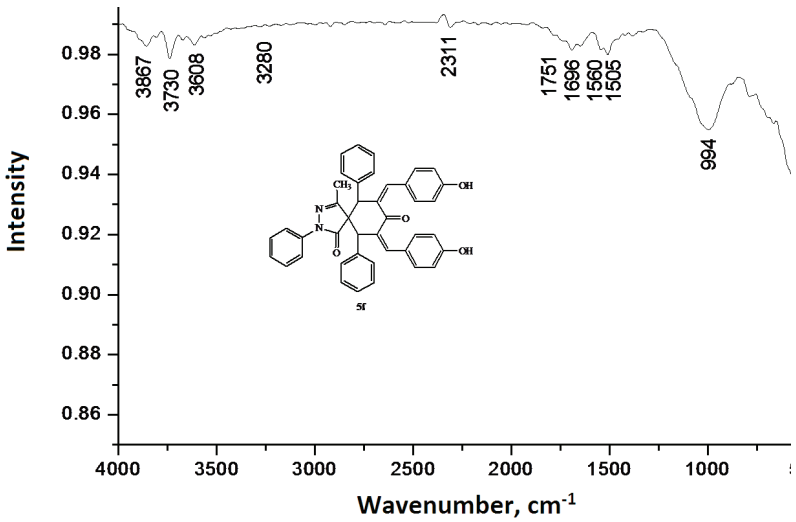

Figure S-24. IR spectrum of 7,9-bis-(4-hydroxy-benzylidene)-4-methyl-2,6,10-triphenyl-2,3--diazaspiro[4.5]dec-3-ene-1,8-dione (**5f**).

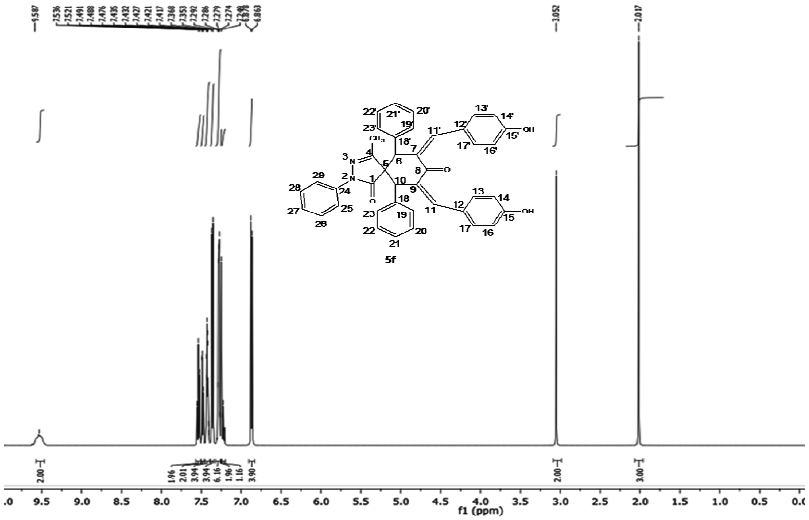

Figure S-25. ^{1}H NMR spectrum of 7,9-bis-(4-hydroxy-benzylidene)-4-methyl-2,6,10--triphenyl-2,3-diazaspiro[4.5]dec-3-ene-1,8-dione (**5f**) ($CDCl_3$, 400 MHz).

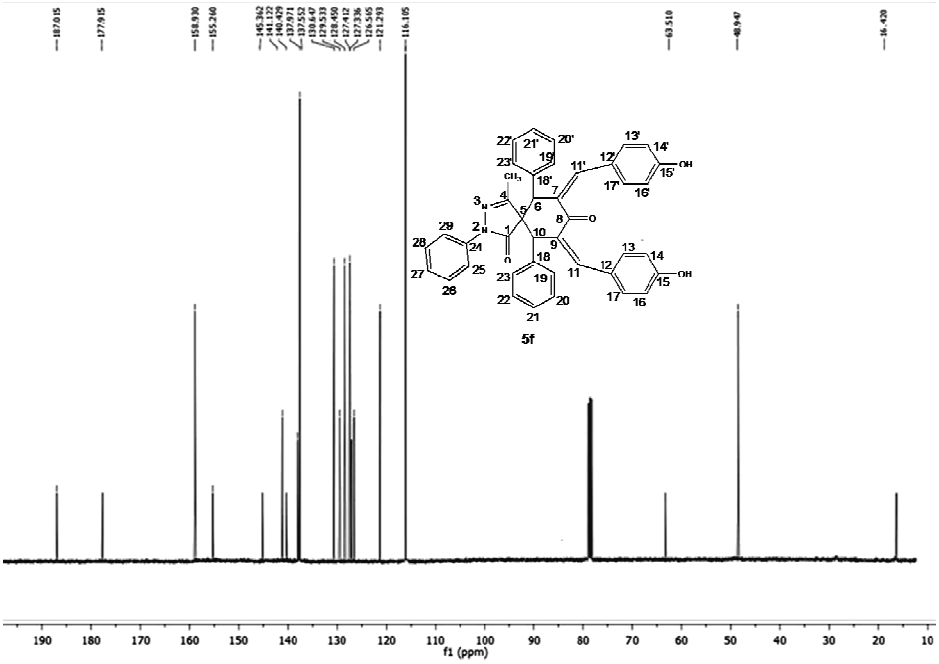

Figure S-26. ^{13}C NMR spectrum of 7,9-bis-(4-hydroxy-benzylidene)-4-methyl-2,6,10--triphenyl-2,3-diazaspiro[4.5]dec-3-ene-1,8-dione (**5f**) ($CDCl_3$, 100 MHz).

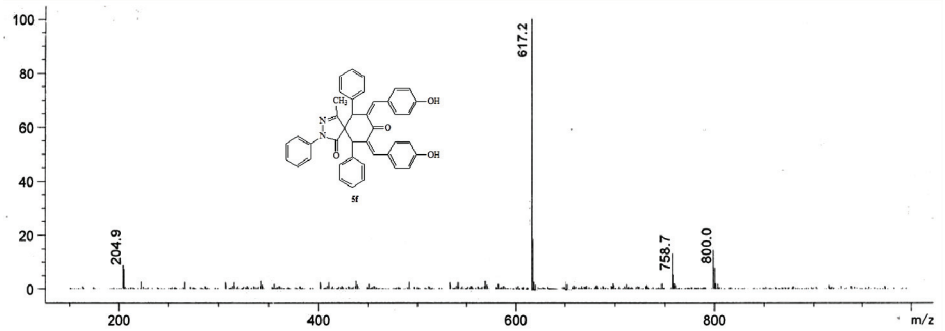

Figure S-27. Mass spectrum of 7,9bBis-(4-hydroxy-benzylidene)-4-methyl-2,6,10-triphenyl--2,3-diazaspiro[4.5]dec-3-ene-1,8-dione (**5f**).

TABLE S-I. Bond length and bond angle of compound 3 after Optimization using DFT

Parameters	Bond length, Å	Parameters	Bond angle, º
N1-N2	1.4034	A (2,1,5)	108.907
N1-C5	1.2876	A (1,2,3)	111.9807
N2-C3	1.3782	A (1,2,13)	118.6363
N2-C13	1.4202	A (3,2,13)	129.3763
C3-C4	1.537	A (2,3,4)	106.2208
C3-O12	1.2264	A (2,3,12)	127.7026
C4-C5	1.5158	A (4,3,12)	126.0575
C4-C6	1.5877	A (3,4,5)	99.9198
C4-C10	1.5842	A (3,4,6)	111.219
C5-C11	1.495	A (5,4,6)	110.2337
C6-C7	1.5429	A (5,4,10)	116.6476
C6-C14	1.525	A (6,4,10)	110.582
C6-H32	1.0966	A (1,5,4)	112.8982
C7-C8	1.5193	A (1,5,11)	120.0156
C7-H33	1.0933	A (4,5,11)	127.0484
C7-H34	1.0978	A (4,6,7)	110.9684
C8-C9	1.5236	A (4,6,14)	114.5591
C8-O16	1.2175	A (4,6,32)	105.0213
C9-C10	1.5393	A (7,6,14)	113.1489
C9-H35	1.0991	A (7,6,32)	106.4349
C9-H36	1.0935	A (14,6,32)	105.8892
C10-C15	1.5267	A (6,7,8)	110.6872
C10-H37	1.0972	A (6,7,33)	111.0992
C11-H38	1.0958	A (6,7,34)	110.6249
C11-H39	1.0921	A (8,7,33)	108.6975
C11-H40	1.0944	A (8,7,34)	108.3323
C13-C27	1.404	A (33,7,34)	107.286
C13-C31	1.4049	A (7,8,9)	115.0769
C14-C17	1.4029	A (7,8,16)	122.7311
C14-C21	1.4045	A (9,8,16)	122.1899

Parameters	Bond length, Å	Parameters	Bond angle, º
C15-C22	1.4029	A (8,9,10)	111.1029
C15-C26	1.4052	A (8,9,35)	107.5767
C17-C18	1.397	A (8,9,36)	108.264
C17-H41	1.0871	A (10,9,35)	112.0241
C18-C19	1.3962	A (10,9,36)	111.0201
C18-H42	1.0862	A (35,9,36)	106.6448
C19-C20	1.3973	A (4,10,9)	112.2182
C19-H43	1.086	A (4,10,15)	113.7583
C20-C21	1.3965	A (4,10,37)	103.3626
C20-H44	1.0861	A (9,10,15)	114.1925
C21-H45	1.0846	A (9,10,37)	106.1228
C22-C23	1.3981	A (15,10,37)	106.0509
C22-H46	1.0858	A (5,11,38)	111.6091
C23-C24	1.396	A (5,11,39)	109.4596
C23-H47	1.0863	A (5,11,40)	111.0081
C24-C25	1.3974	A (38,11,39)	108.6075
C24-H48	1.086	A (38,11,40)	107.4932
C25-C26	1.3958	A (39,11,40)	108.5749
C25-H49	1.0861	A (2,13,27)	119.172
C26-H50	1.0865	A (2,13,31)	120.876
C27-C28	1.3944	A (27,13,31)	119.9518
C27-H51	1.0818	A (6,14,17)	119.5823
C28-C29	1.3974	A (6,14,21)	122.2029
C28-H52	1.0862	A (17,14,21)	118.1997
C29-C30	1.3964	A (10,15,22)	122.6511
C29-H53	1.0858	A (10,15,26)	119.3265
C30-C31	1.3963	A (22,15,26)	118.0131
C30-H54	1.0863	A (14,17,18)	121.2142
C31-H55	1.0809	A (14,17,41)	119.5772
		A (18,17,41)	119.2071
		A (17,18,19)	119.9803
		A (17,18,42)	119.7536
		A (19,18,42)	120.2656
		A (18,19,20)	119.4519
		A (18,19,43)	120.2837
		A (20,19,43)	120.2641
		A (19,20,21)	120.4235
		A (19,20,44)	120.1077
		A (21,20,44)	119.4688
		A (14,21,20)	120.728
		A (14,21,45)	120.0704
		A (20,21,45)	119.1973
		A (15,22,23)	121.0508
		A (15,22,46)	120.2589
		A (23,22,46)	118.6841

Parameters	Bond length, Å	Parameters	Bond angle, º
		A (22,23,24)	120.248
		A (22,23,47)	119.5832
		A (24,23,47)	120.168
		A (23,24,25)	119.3597
		A (23,24,48)	120.3056
		A (25,24,48)	120.3314
		A (24,25,26)	120.223
		A (24,25,49)	120.1859
		A (26,25,49)	119.5889
		A (15,26,25)	121.0917
		A (15,26,50)	119.5846
		A (25,26,50)	119.3194
		A (13,27,28)	119.7234
		A (13,27,51)	119.5329
		A (28,27,51)	120.7436
		A (27,28,29)	120.7846
		A (27,28,52)	119.0485
		A (29,28,52)	120.1668
		A (28,29,30)	119.1113
		A (28,29,53)	120.4466
		A (30,29,53)	120.4422
		A (29,30,31)	121.0673
		A (29,30,54)	120.1087
		A (31,30,54)	118.8239
		A (13,31,30)	119.3616
		A (13,31,55)	119.9719
		A (30,31,55)	120.6665

TABLE S-II. Bond length and bond angle of compound 5b after optimization using DFT

Parameters	Bond length, Å	Parameters	Bond angle, º
N1-N2	1.4032	A (2,1,5)	108.7814
N1-C5	1.2874	A (1,2,3)	112.0698
N2-C3	1.3801	A (1,2,13)	118.581
N2-C13	1.4222	A (3,2,13)	129.2761
C3-C4	1.538	A (2,3,4)	105.8661
C3-O12	1.2254	A (2,3,12)	127.6833
C4-C5	1.5125	A (4,3,12)	126.3661
C4-C6	1.5714	A (3,4,5)	100.0674
C4-C10	1.6059	A (3,4,6)	116.8856
C5-C11	1.4955	A (3,4,10)	103.9681
C6-C7	1.527	A (5,4,6)	110.69
C6-C14	1.5309	A (5,4,10)	116.1912
C6-H32	1.1008	A (6,4,10)	108.9623
C7-C8	1.501	A (1,5,4)	112.9752
C7-C53	1.3501	A (1,5,11)	120.5944

Parameters	Bond length, Å	Parameters	Bond angle, º
C8-C9	1.5185	A (4,5,11)	126.2983
C8-O16	1.2245	A (4,6,7)	112.0152
C9-C10	1.5278	A (4,6,14)	119.2836
C9-C52	1.35	A (4,6,32)	101.1835
C10-C15	1.5235	A (7,6,14)	116.4093
C10-H33	1.0983	A (7,6,32)	101.5681
C11-H34	1.0969	A (14,6,32)	102.6732
C11-H35	1.0921	A (6,7,8)	110.0794
C11-H36	1.0949	A (6,7,53)	133.0574
C13-C27	1.4038	A (8,7,53)	116.5527
C13-C31	1.4046	A (7,8,9)	114.7374
C14-C17	1.407	A (7,8,16)	123.1589
C14-C21	1.3995	A (9,8,16)	122.0901
C15-C22	1.403	A (8,9,10)	111.5635
C15-C26	1.4045	A (8,9,52)	114.9494
C17-C18	1.3933	A (10,9,52)	133.2194
C17-H37	1.0874	A (4,10,9)	112.304
C18-C19	1.3987	A (4,10,15)	113.1059
C18-H38	1.0861	A (4,10,33)	100.4324
C19-C20	1.3935	A (9,10,15)	119.6461
C19-H39	1.0858	A (9,10,33)	103.5288
C20-C21	1.3997	A (15,10,33)	105.0397
C20-H40	1.086	A (5,11,34)	110.5294
C21-H41	1.0819	A (5,11,35)	109.7297
C22-C23	1.3957	A (5,11,36)	111.7205
C22-H42	1.0833	A (34,11,35)	108.1118
C23-C24	1.397	A (34,11,36)	107.2061
C23-H43	1.086	A (35,11,36)	109.4457
C24-C25	1.3963	A (2,13,27)	119.1241
C24-H44	1.0859	A (2,13,31)	120.8388
C2-C26	1.397	A (27,13,31)	120.0366
C25-H45	1.0861	A (6,14,17)	116.3387
C26-H46	1.0868	A (6,14,21)	125.7841
C27-C28	1.3945	A (17,14,21)	117.8156
C27-H47	1.0818	A (10,15,22)	123.9801
C28-C29	1.3973	A (10,15,26)	117.989
C28-H48	1.0861	A (22,15,26)	118.0046
C29-C30	1.3963	A (14,17,18)	121.4329
C29-H49	1.0857	A (14,17,37)	119.335
C30-C31	1.3963	A (18,17,37)	119.2305
C30-H50	1.0861	A (17,18,19)	120.0581
C31-H51	1.0809	A (17,18,38)	119.6995
C52-C54	1.4798	A (19,18,38)	120.2415
C52-H78	1.0916	A (18,19,20)	119.1928
C53-C64	1.4694	A (18,19,39)	120.3875

Parameters	Bond length, Å	Parameters	Bond angle, º
C53-H79	1.0907	A (20,19,39)	120.4194
C54-C55	1.4071	A (19,20,21)	120.5448
C54-C56	1.4051	A (19,20,40)	120.2345
C55-C57	1.3913	A (21,20,40)	119.2204
C55-H58	1.0864	A (14,21,20)	120.9482
C56-C59	1.3912	A (14,21,41)	121.2696
C56-H60	1.0839	A (20,21,41)	117.7814
C57-C61	1.4059	A (15,22,23)	120.9784
C57-H62	1.0849	A (15,22,42)	120.4495
C59-C61	1.4052	A (23,22,42)	118.5619
C59-H63	1.0847	A (22,23,24)	120.3509
C61-C74	1.4348	A (22,23,43)	119.5321
C64-C65	1.4098	A (24,23,43)	120.116
C64-C66	1.4063	A (23,24,25)	119.4142
C65-C67	1.3893	A (23,24,44)	120.2394
C65-H68	1.0865	A (24,25,26)	120.0172
C66-C69	1.3916	A (24,25,45)	120.2959
C66-H70	1.0835	A (26,25,45)	119.6834
C67-C71	1.4067	A (15,26,25)	121.2324
C67-H72	1.0848	A (15,26,46)	119.3911
C69-C71	1.4054	A (25,26,46)	119.3721
C69-H73	1.0849	A (13,27,28)	119.6648
C71-C75	1.4346	A (13,27,47)	119.6188
C74-N76	1.1641	A (28,27,47)	120.7162
C75-N77	1.1643	A (27,28,29)	120.7765
		A (27,28,48)	119.0551
		A (29,28,48)	120.1683
		A (28,29,30)	119.158
		A (28,29,49)	120.4237
		A (30,29,49)	120.4183
		A (29,30,31)	121.0361
		A (29,30,50)	120.1218
		A (31,30,50)	118.842
		A (13,31,30)	119.3279
		A (13,31,30)	119.3279
		A (13,31,51)	120.0464
		A (30,31,51)	120.6257
		A (9,52,54)	133.5168
		A (9,52,78)	113.1699
		A (54,52,78)	113.2648
		A (7,53,64)	132.4845
		A (7,53,79)	113.4806
		A (64,53,79)	114.0253
		A (52,54,55)	119.2816
		A (52,54,56)	121.8042

Parameters	Bond length, Å	Parameters	Bond angle, º
		A (55,54,56)	118.566
		A (54,55,57)	121.0637
		A (54,55,58)	119.5439
		A (57,55,58)	119.3916
		A (54,56,59)	120.8575
		A (54,56,60)	119.6222
		A (59,56,60)	119.5198
		A (55,57,61)	119.7622
		A (55,57,62)	120.4638
		A (61,57,62)	119.7697
		A (56,59,61)	120.0456
		A (56,59,63)	120.2196
		A (61,59,63)	119.7339
		A (57,61,59)	119.659
		A (57,61,74)	120.1163
		A (59,61,74)	120.2233
		A (53,64,65)	118.0672
		A (53,64,66)	123.2136
		A (65,64,66)	118.6022
		A (64,65,67)	121.1653
		A (64,65,68)	119.381
		A (67,65,68)	119.4469
		A (64,66,69)	120.5948
		A (64,66,70)	119.7266
		A (69,66,70)	119.6186
		A (65,67,71)	119.6505
		A (65,67,72)	120.5281
		A (71,67,72)	119.8191
		A (66,69,71)	120.2362
		A (66,69,73)	120.1135
		A (71,69,73)	119.649
		A (67,71,69)	119.6896
		A (67,71,75)	120.1196
		A (69,71,75)	120.1859