ELECTRONIC SUUPLEMENTRAY INFORMATION

Design and one-pot synthesis of hybrid thiazolidin-4-one-1,3,5-triazines as potent antibacterial agent against human disease causing pathogens

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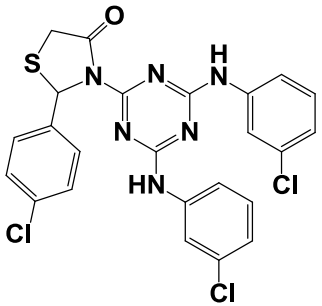
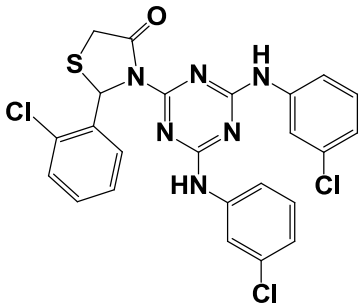
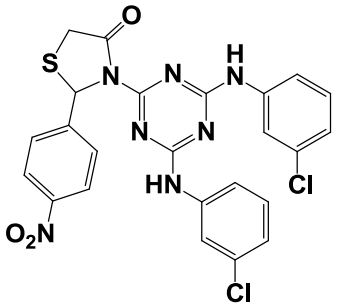
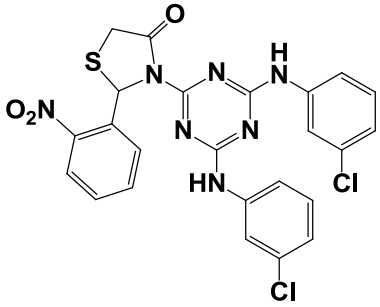
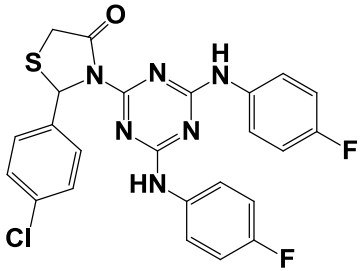
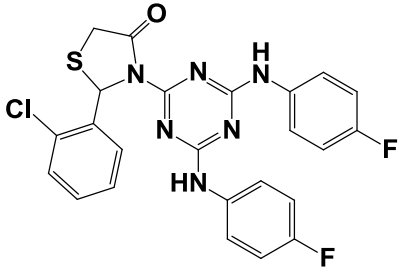
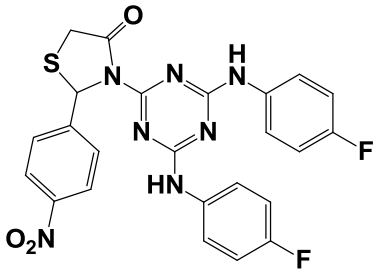
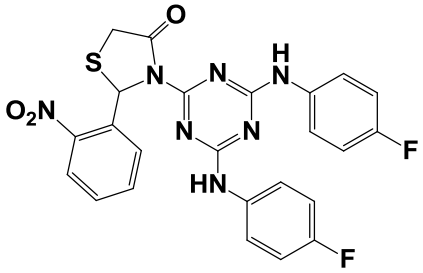
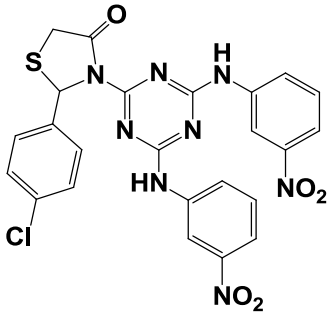
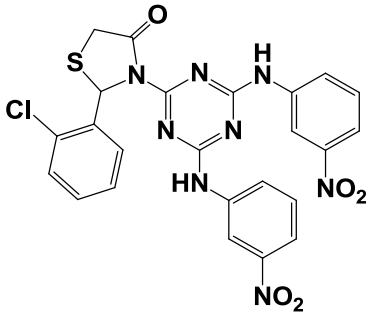
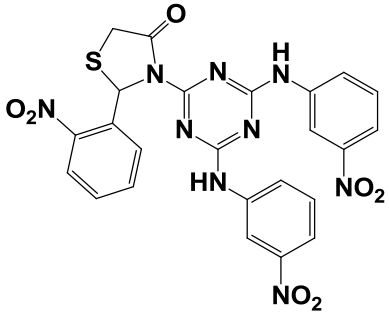
Table 1 Physical and spectral properties of synthesized target compounds.

Compound	Structure	State	Melting point (°C)	Percentage Yeild	R_f	FT-IR (KBr) ν_{max} cm^{-1}	^{1}H-NMR (400MHz, DMSO, TMS) δ ppm	Mass (m/z)
7a		Yellow Powder	245-275	76	0.55	3450-3384 (N-H_{str}), 3112-2863 (Ar C-H_{str}), 1757(C=O_{str}), 1690-1625(Ar C=C_{str}), 1576-1523 (C=N_{str}), 1325-1253 (Ar C-N_{str}), 1017-770 (Ar C-H_{def}), 870-673 (Ar C-Cl_{str})	2.50 (s, 1H, -NH), 3.24-3.20 (d, 1H, J= 16 Hz, -NH), 5.34 (s, 1H, -CH), 7.10-7.04 (t, 3H, J= 20Hz, Ar-H), 7.30-7.20 (m, 3H, Ar-H), 7.41-7.32 (m, 2H, Ar-H), 7.60-7.55 (d, 2H, J= 12 Hz, Ar-H), 7.76 (s, 1H, Ar-H),	457 (100%), 459, 348, 350.

							7.88 (s, 1H, Ar-H).	
7b		Dark Yellow Powder	250-252	80	0.90	3294 (N-H_{str}), 3115-2865 (Ar C-H_{str}), 1754(C=O_{str}), 1684-1627(Ar C=C_{str}), 1570-1510 (C=N_{str}), 1336-1250 (Ar C-N_{str}), 910-790 (Ar C-H_{def}), 780-695 (Ar C-Cl_{str}).	2.10 (s, 1H, -NH), 2.36 (s, 1H, -NH), 7.08-7.04 (d, 2H, J=8Hz, Ar-H), 7.14-7.10 (d, 2H, J=8Hz, Ar-H), 7.48-7.24 (m, 4H, Ar-H), 7.65 (s, 1H, Ar-H), 7.76 (s, 1H, Ar-H), 7.80 (s, 1H, Ar-H).	348 (100%), 350, 368.
7c		Brown Powder	240-242	56	0.60	3281 (N-H_{str}), 3118-2930 (Ar C-H_{str}), 1750 (C=O_{str}), 1698-1370 (Ar C=C_{str}), 1583-1540 (C=N_{str}), 1526 (Ar C-NO_{2str}), 1359-1270 (Ar C-N_{str}), 921-669(Ar C-H_{def}), 770-611 (Ar C-Cl_{str}).	3.49-3.44 (t, 1H, J=16Hz, -NH), 3.70-3.59 (t, 1H, J=36Hz, -NH), 7.09-7.05 (t, 2H, J=24Hz, Ar-H), 7.30-7.27(d, 2H, J=4Hz, Ar-H), 7.58-7.57(d, 2H, J=8Hz, Ar-H), 7.80-7.71 (m, 3H, Ar-H), 8.10-8.08 (d, 2H, J=8Hz, Ar-H), 8.21-8.18 (d, 2H, J= 8Hz, Ar-H), 8.25-8.22 (d, 2H, J=8Hz, Ar-H)	348 (100%), 350, 459.
7d		Yellow Powder	193-195	62	0.75	3312 (N-H_{str}), 3105 (Ar C-H_{str}), 1759 (C=O_{str}), 1618-1579 (Ar C=C_{str}), 1520-1486(Ar C-NO_{2str}), 1290-1228 (Ar C-N_{str}), 996-667 (Ar C-H_{def}), 791-600 (Ar C-Cl_{str}).	2.60 (s, 1H, -NH), 3.51 (s, 1H, -NH), 7.09-7.06 (d, 2H, J=8Hz, Ar-H), 7.37-7.29 (t, 3H, J=16Hz, Ar-H), 7.91-7.68 (m, 4H, Ar-H).	348 (100%), 369, 368, 350.

7e		Brown powder	301-303	72	0.59	3210 (N-H_{str}), 3128-2945 (Ar C-H_{str}), 1759 (C=O_{str}), 1678 (Ar C=C_{str}), 1379 (Ar C-N_{str}), 1014-1098 (C-F_{str}), 760 - 839 (Ar C-H_{def}).	2.63 (s, 1H, -NH), 3.22-3.17 (d, 1H, J=16Hz, -NH), 7.20-7.09 (m, 2H, Ar-H), 7.27 (s, 1H, Ar-H), 7.34-7.33 (d, 2H, J=8Hz, Ar-H), 7.48-7.45 (d, 2H, J=8Hz, Ar-H), 7.67 (s, H, Ar-H), 7.80 (s, 1H, Ar-H), 7.94 (s, 1H, Ar-H).	222 (100%), 316, 180.
7f		Dark brown powder	290-292	45	0.81	3233 (N-H_{str}), 3129-2869 (Ar C-H_{str}), 1760 (C=O_{str}), 1680 - 1589 (Ar C=C_{str}), 1329-1296 (Ar C-N_{str}), 1119-1010(C-F_{str}), 1149 (C-N_{str}), 870-720 (Ar, C-H_{def}), 740 -727 (Ar C-Cl_{str}).	3.18 (s, 1H, -NH), 3.28 (s, 1H, -NH), 7.19-6.95 (m, 4H, Ar-H), 7.40-7.24 (m, 2H, Ar-H), 7.49-7.40 (t, 2H, J= 12Hz , Ar-H), 7.52-7.50(d, 2H, J=8Hz, Ar-H), 7.64 (s, 1H, Ar-H), 7.81 (s, 1H, Ar-H).	222 (100%), 316, 180.
7g		Brown powder	.>360			3300-3286 (N-H_{str}), 3128-2878 (Ar C-H_{str}), 1760 (C=O_{str}), 1680 -1510 (Ar C=C_{str}), 1421 (Ar C-NO_{2str}), 1336 (Ar C-Nstr), 1001(C-F_{str}), 900-670 (Ar C-H_{def}).	3.29-3.20 (d, 1H, J=16Hz, -N-H), 3.49-3.42 (d, H, J=15 Hz, -NH), 7.10-7.03 (t, 2H, J=16Hz, Ar-H), 8.06 (s, 1H, Ar-H), 8.21-8.24 (d, 2H, J=12Hz, Ar-H).	316 (100%), 222, 317.

7h		Yellowish Powder	295-297	78	0.88	3310 (N-H_{str}), 3110-2864 (Ar C-H_{str}), 1745 (C=O_{str}), 1691-1584 (Ar C=C_{str}), 1495 (Ar C-NO_{2str}), 1334-1290 (Ar C-N_{str}), 1021 (C-F_{str}), 843-730 (Ar C-H_{def}).	3.29 (s, 1H, -NH), 3.34-3.28 (t, 1H, J=16Hz, -NH), 7.15-7.05 (m, 4H, Ar-H), 7.24-7.21 (d, 2H, J=8Hz, Ar-H), 7.39 (s, 1H, Ar-H), 7.80-7.74 (t, 2H, J=16Hz, Ar-H).	316 (100%), 315, 317, 409.
7i		Dark yellow	130-132	66	0.83	3324 (N-H_{str}), 3059 (Ar C-H_{str}), 1641 (C=O_{str}), 1645-1571 (Ar C=C_{str}), 1540 (Ar C-NO_2str), 1332-1300 (Ar C-Nstr), 893-746 (Ar C-H_{str}), 628-795 (Ar C-C_{str}).	2.22 (s, 1H, -N-H), 2.39 (s, 1H, -NH), 7.40-7.36 (m, 3H, Ar-H), 7.60-7.49 (m, 3H, Ar-H), 7.96-7.83(m, 2H, Ar-H), 8.18 (s, 1H, Ar-H), 8.64-8.61 (d,2H, J=12Hz, Ar-H)	369 (100%), 370, 248.
7j		Dark brown powder	255-257	56	0.69	3320 (N-H_{str}), 3129-2300 (Ar C-H_{str}), 1759 (C=O_{str}), 1665-1566 (Ar C=C_{str}), 1516 (Ar C-NO_{2str}), 1350-1310 (Ar C-N_{str}), 889-736 (Ar C-H_{def}), 677 (Ar C-Cl_{str}).	3.18 (s, H, >NH), 3.29 (s, H, NH), 3.50 (s, H, NH), 3.60(s, H, NH), 7.18-7.14 (d, H, J=8Hz, Ar-H), 7.44-7.30 (m, H, Ar-H), 7.59-7.49 (m, H, Ar-H), 7.69-7.66 (m, H, Ar-H), 7.86-7.80 (m, H, Ar-H), 8.10 (s, H, Ar-H), 8.20-8.18 (d, H, J=4Hz, Ar-H), 8.69-8.66 (d, H, J=8Hz, Ar-H)	369 (100%), 370, 248.
7k		Brown Powder	220-223	75	0.69	3386 (N-H_{str}), 3080 (Ar C-H_{str}), 1701 (C=O_{str}), 1614-1576 (Ar C=C_{str}), 1513 (Ar C-NO_{2str}), 1349 (Ar C-N_{str}), 885-735 (Ar C-H_{def})	2.20 (s, 1H, -NH), 2.39 (s, 1H, -NH), 7.57-7.45 (m, 4H, Ar-H), 7.80-7.76 (m, 3H, Ar-H), 7.96-7.88 (m, 3H, Ar-H), 8.75 (s, 1H, Ar-H)	369 (100%), 370, 248, 475, 388.

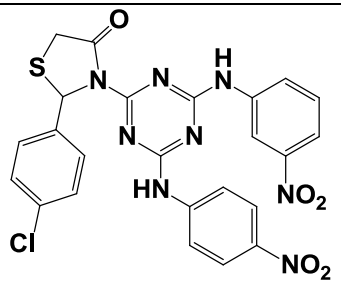
7l		Brownish black powder	140-142	80	0.88	3335 (N-H_{str}), 2930 (Ar C-H_{str}), 1634-1596 (Ar C=Cstr), 1690 (C=O_{str}), 1470 (Ar C-NO_{2str}), 1305(C-N_{str}), 891-696 (Ar C-H_{def}), 751-631(Ar C-Cl_{str})	2.39 (s, 1H, -NH), 2.63 (s, 1H, -NH), 6.66-6.63 (m, 3H, Ar-H), 7.60-7.54 (m, 2H, Ar-H), 7.95-7.89 (m, 2H, Ar-H).	369 (100%), 139, 231, 475.

Table 2 Elemental analysis of the synthesized title compounds 7 (a-l).

Compound	Carbon		Hydrogen		Nitrogen	
	Calculated	Found	Calculated	Found	Calculated	Found
7a	53.00	53.02	3.15	3.12	15.45	15.42
7b	53.00	52.99	3.15	3.13	15.45	15.44
7c	51.99	51.97	3.09	3.10	17.68	17.65
7d	51.99	52.00	3.09	3.07	17.68	17.69
7e	56.42	56.42	3.35	3.33	16.45	16.47
7f	56.42	56.40	3.35	3.36	16.45	16.43
7g	55.27	55.25	3.29	3.29	18.80	18.78
7i	51.02	51.02	3.03	3.00	19.83	19.85
7j	51.02	51.03	3.03	3.02	19.83	18.84
7k	50.09	50.07	2.98	2.97	21.90	21.92
7l	51.02	51.00	3.03	3.03	19.83	19.81