Synthesis, Characterization and Exploration of Photovoltaic Behavior of Hydrazide Based Scaffolds: A Concise Experimental and DFT Study

Muhammad Haroon*[a,b] Tashfeen Akhtar*[a], Muhammad Khalid[c,d], Hasnain Mehmood[a], Muhammad Adnan Asghar[e], Rabia Baby[f], Raha Orfali[g*], Shagufta Perveen[h]

[a]Department of Chemistry, Mirpur University of Science and Technology (MUST), 10250-Mirpur (AJK) Pakistan.

[b]Department of Chemistry, Government Major Muhammad Afzal Khan (Shaheed), Boys Degree College Afzalpur, Mirpur (Affiliated with Mirpur University of Science and Technology (MUST), 10250-Mirpur (AJK) Pakistan).

[c]Institute of Chemistry, Khwaja Fareed University of Engineering & Information Technology, Rahim Yar Khan, 64200, Pakistan.

[d]Center for Theoretical and Computational Research, Khwaja Fareed University of Engineering & Information Technology, Rahim Yar Khan, 64200, Pakistan.

[e]Department of Chemistry, Division of Science and Technology, University of Education Lahore, Pakistan

[f]Department of education, Sukkur IBA university, zip code. 65200

[g]Department of Pharmacognosy, Collage of Pharmacy, King Saud University, PO Box 2457, Riyadh 11451, Saudi Arabia

[h]Department of Chemistry, School of Computer, Mathematical and Natural Sciences, Morgan State University, Baltimore, MD, 21251, USA

*Corresponding author's E-mail addresses:

Muhammad Khalid (muhammad.khalid@kfueit.edu.pk; Khalid@iq.usp.br)

Tashfeen Akhtar (tashfeenchem@must.edu.pk),

Raha Orfali (rorfali@ksu.edu.sa)

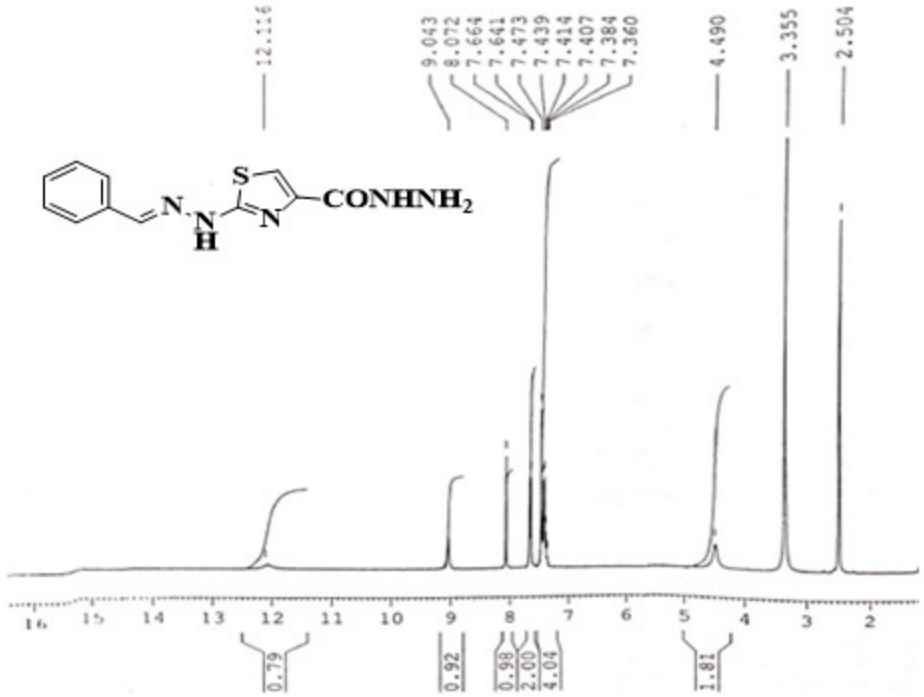


Figure S1: ^{1}H-NMR spectrum of **BDTC1**

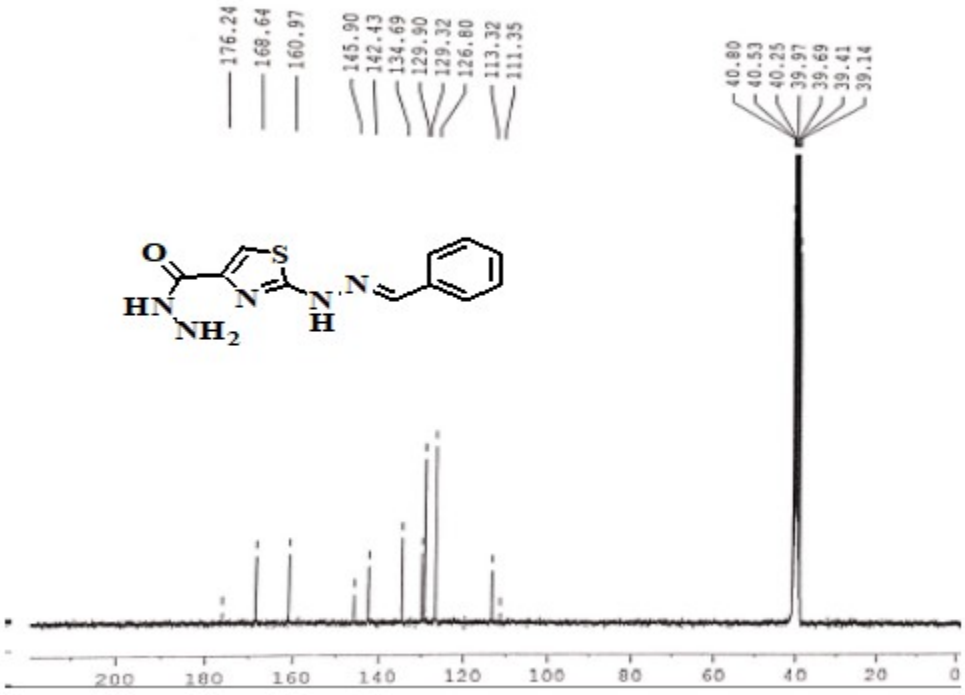
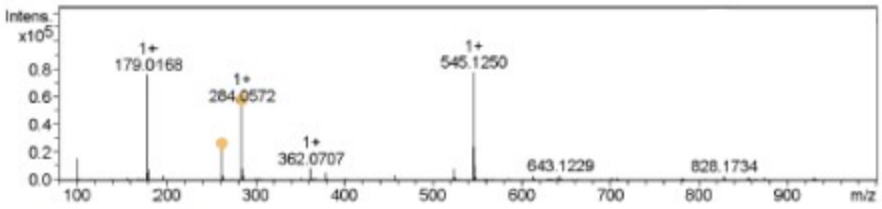
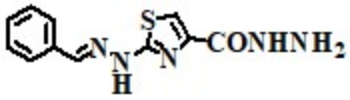


Figure S2: ^{13}C-NMR spectrum of **BDTC1**



#	m/z	I %
1	101.0019	20.7
2	179.0168	97.6
3	180.0189	6.3
4	181.0133	9.6
5	196.0258	4.1
6	262.0753	28.9
7	263.0778	4.4
8	284.0572	68.8
9	285.0598	10.4
10	286.0551	3.9
11	362.0707	11.0
12	379.1406	7.0
13	457.1043	4.3
14	523.1436	10.7
15	545.1250	100.0
16	546.1278	31.0
17	547.1245	13.9
18	613.1123	3.8
19	643.1229	4.3
20	828.1734	3.7



Generate Molecular Formula Parameters

Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE

Expected Formula C11 H11 N5 O1 S1 **Adduct(s):** H, Na, NH4, C3H5N2, radical

#	meas. m/z	theo. m/z	|Err|[ppm]	Sigma	Formula	Adduct	Adduct Mass
1	262.0753	262.0757	1.60	0.0031	C11H12N5OS	M+H	1.0078
1	284.0572	284.0577	1.50	0.0024	C11H11N5NaOS	M+Na	22.9898

Note: Sigma fits < 0.05 indicates high probability of correct MF

Figure S3: HRMS spectrum of **BDTC1**

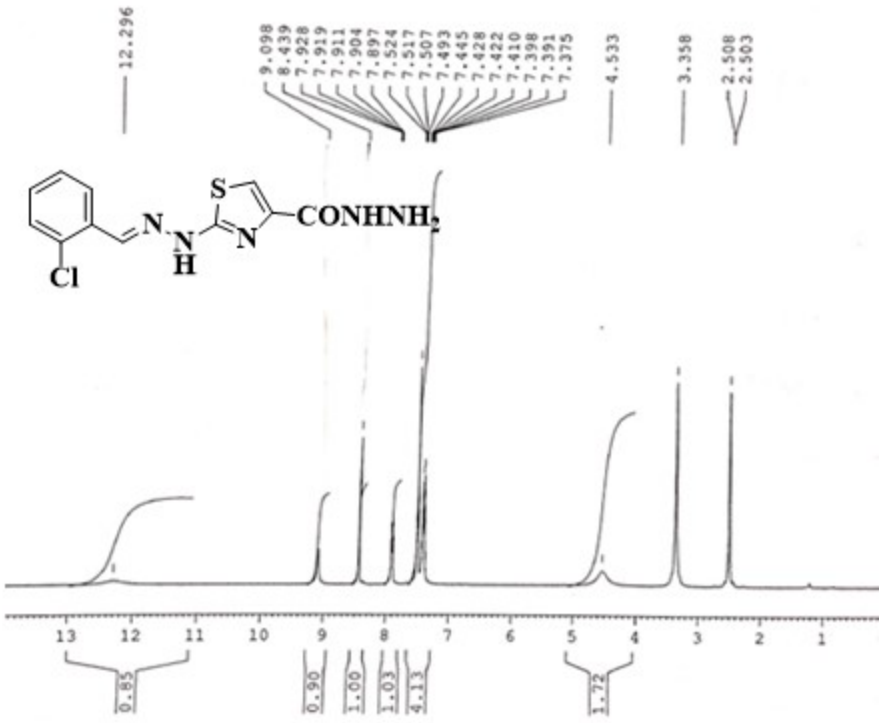


Figure S4: ^{1}H-NMR spectrum of **BDTC2**

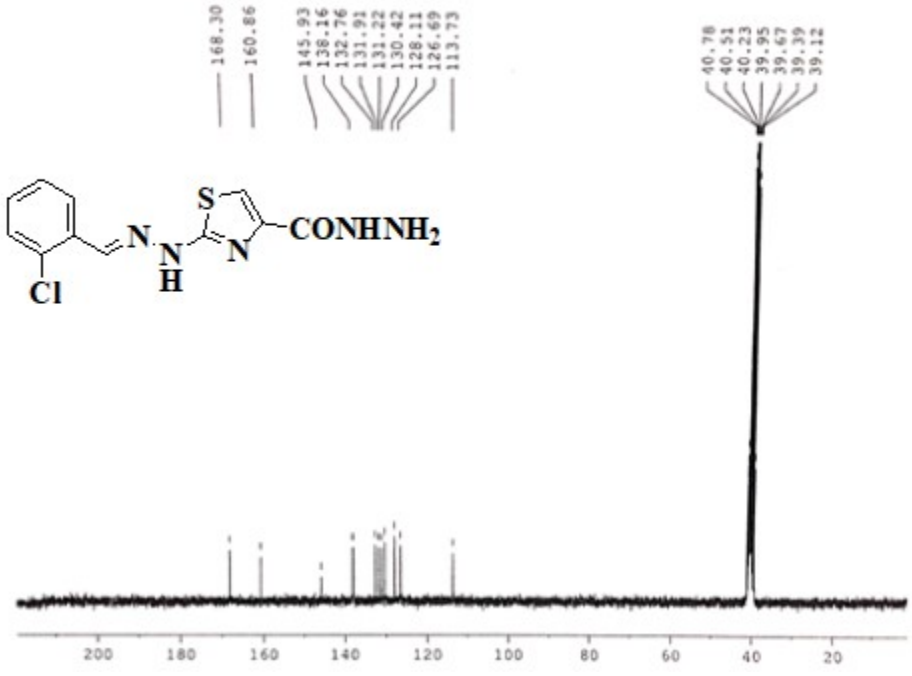
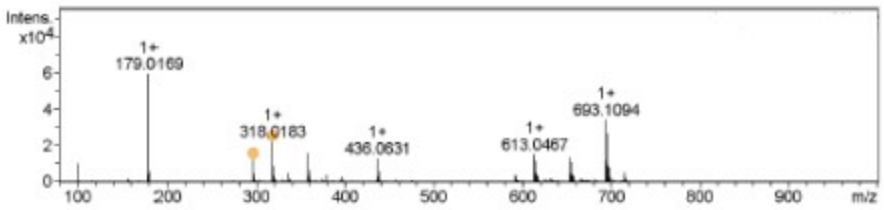
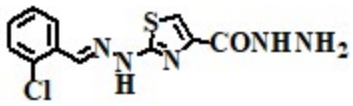


Figure S5: ^{13}C-NMR spectrum of **BDTC2**



#	m/z	I %
1	101.0021	17.4
2	179.0169	100.0
3	181.0133	9.5
4	296.0363	20.8
5	318.0183	37.4
6	320.0163	14.4
7	358.0498	26.4
8	360.0468	10.4
9	436.0631	21.8
10	438.0602	9.5
11	613.0467	25.3
12	615.0444	19.7
13	653.0774	23.0
14	655.0760	18.0
15	693.1094	57.3
16	694.1114	20.2
17	695.1064	44.6
18	696.1092	15.4
19	697.1038	12.6
20	714.2000	8.1



Generate Molecular Formula Parameters

Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE

Expected Formula C11 H10 Cl1 N5 O1 S1 **Adduct(s):** H, Na, NH4, C3H5N2, radical

#	meas. m/z	theo. m/z	|Err|[ppm]	Sigma	Formula	Adduct	Adduct Mass
1	296.0363	296.0367	1.50	0.0091	C11H11ClN5OS	M+H	1.0078
1	318.0183	318.0187	1.10	0.0039	C11H10ClN5NaOS	M+Na	22.9898

Note: Sigma fits < 0.05 indicates high probability of correct MF

Figure S6: HRMS spectrum of **BDTC2**

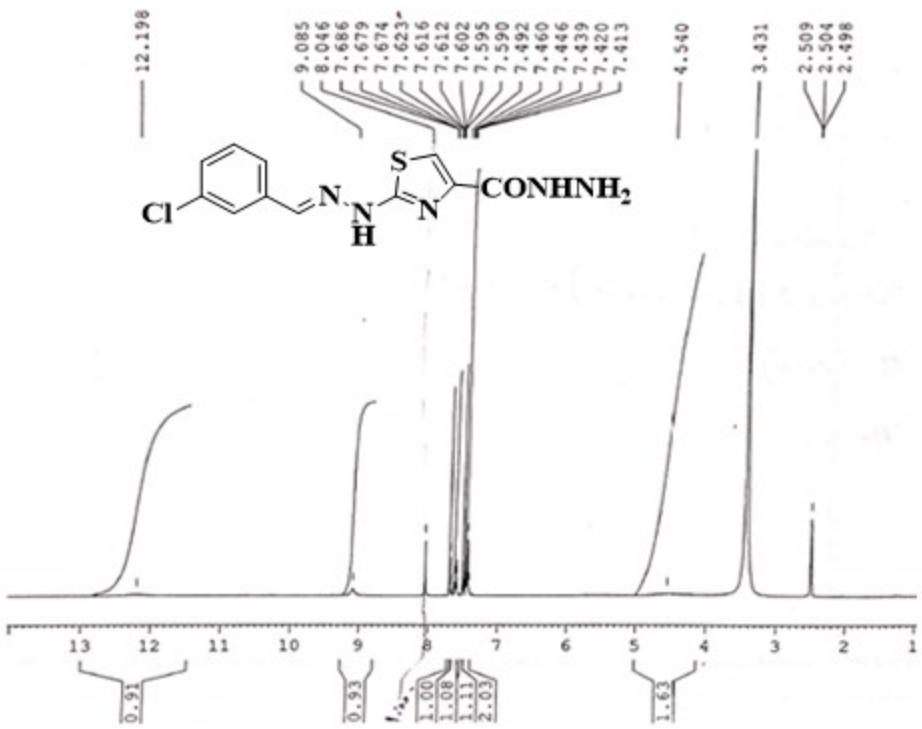


Figure S7: ^{1}H-NMR spectrum of **BDTC3**

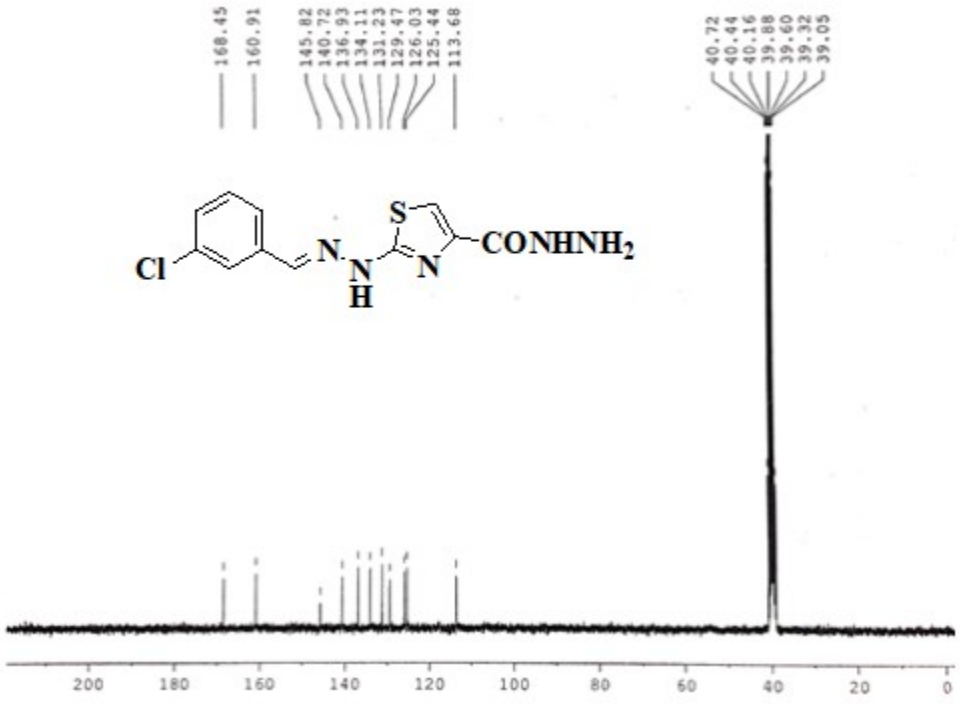
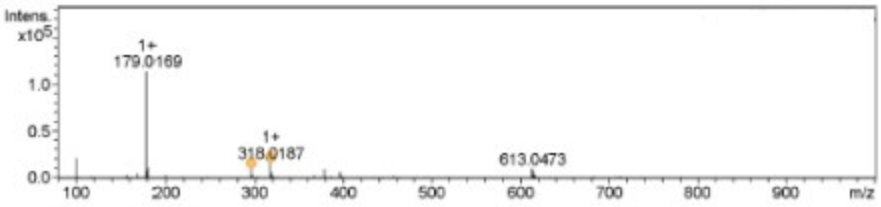
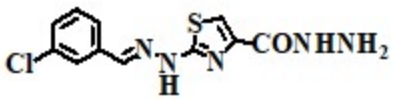


Figure S8: ^{13}C-NMR spectrum of **BDTC3**



#	m/z	I %
1	101.0011	18.5
2	157.0347	2.8
3	168.9908	3.9
4	179.0169	100.0
5	180.0192	6.1
6	181.0134	9.7
7	199.0005	2.6
8	296.0369	8.6
9	298.0341	3.3
10	318.0187	14.3
11	319.0210	2.1
12	320.0163	5.4
13	367.1407	2.4
14	379.1419	7.9
15	396.0325	5.4
16	398.0300	2.3
17	457.1551	2.3
18	613.0473	8.5
19	614.0505	2.5
20	615.0452	6.6



Generate Molecular Formula Parameters

Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE

Expected Formula C11 H10 Cl1 N5 O1 S1 **Adduct(s):** H, Na, NH4, C3H5N2, radical

#	meas. m/z	theo. m/z	|Err|[ppm]	Sigma	Formula	Adduct	Adduct Mass
1	296.0369	296.0367	0.50	0.0049	C11H11ClN5OS	M+H	1.0078
1	318.0187	318.0187	0.10	0.0015	C11H10ClN5NaOS	M+Na	22.9898

Note: Sigma fits < 0.05 indicates high probability of correct MF

Figure S9: HRMS spectrum of **BDTC3**

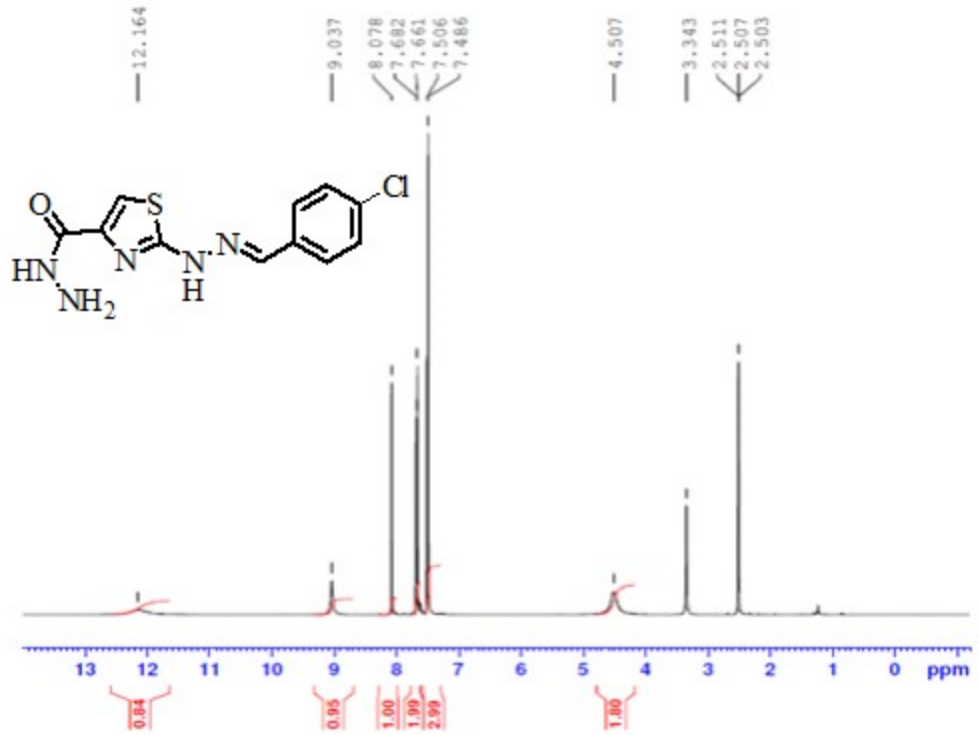


Figure S10: ^{1}H-NMR spectrum of **BDTC4**

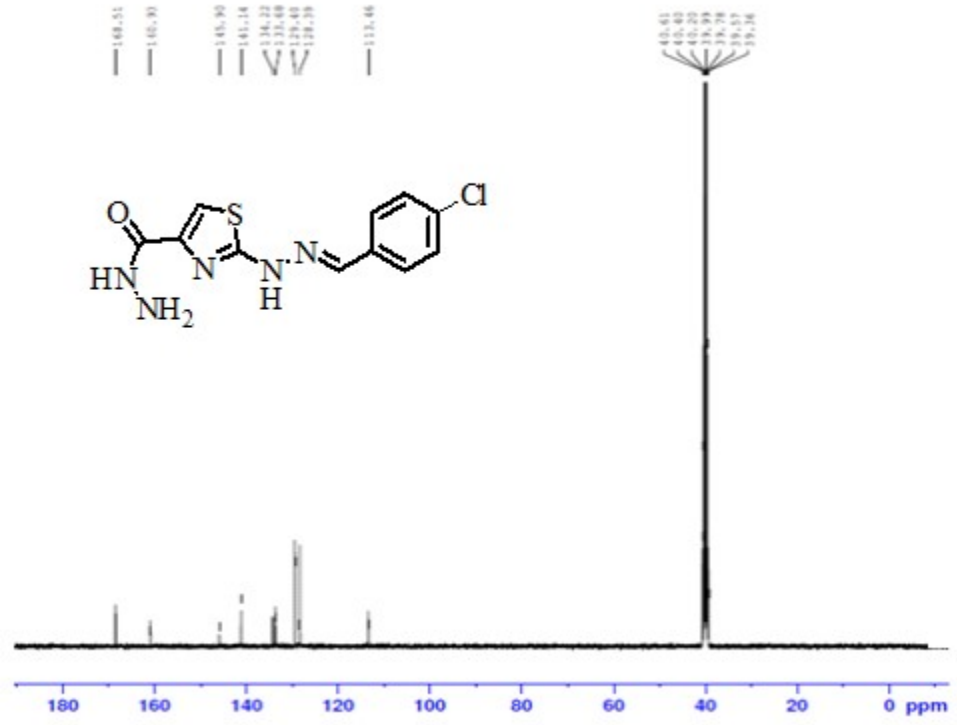
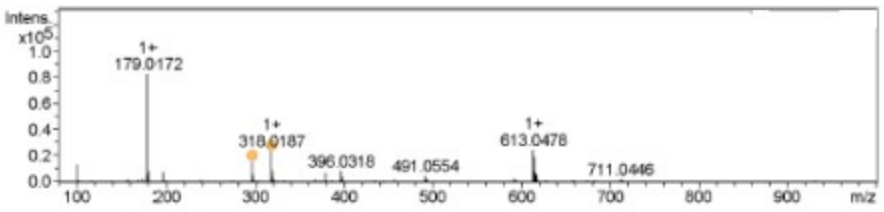
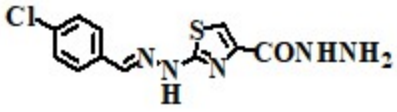


Figure S11: ^{13}C-NMR spectrum of **BDTC4**



#	m/z	I %
1	101.0025	16.2
2	174.0446	3.2
3	179.0172	100.0
4	180.0195	6.2
5	181.0135	9.8
6	196.0258	8.8
7	296.0366	19.1
8	298.0344	6.9
9	318.0187	28.8
10	319.0212	4.2
11	320.0160	10.5
12	379.1415	8.2
13	396.0318	10.0
14	398.0297	4.6
15	491.0554	5.4
16	613.0478	29.7
17	614.0496	9.0
18	615.0447	23.2
19	616.0474	6.9
20	617.0428	6.3



Generate Molecular Formula Parameters

Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	5 ppm	0.08	3 - 0	both	false	false	TRUE

Expected Formula C11 H10 Cl1 N5 O1 S1 **Adduct(s):** H, Na, NH4, C3H5N2, radical

#	meas. m/z	theo. m/z	[Err][ppm]	Sigma	Formula	Adduct	Adduct Mass
1	296.0366	296.0367	0.30	0.0086	C11H11ClN5OS	M+H	1.0078
1	318.0187	318.0187	0.10	0.0056	C11H10ClN5NaOS	M+Na	22.9898

Note: Sigma fits < 0.05 indicates high probability of correct MF

Figure S12: HRMS spectrum of **BDTC4**

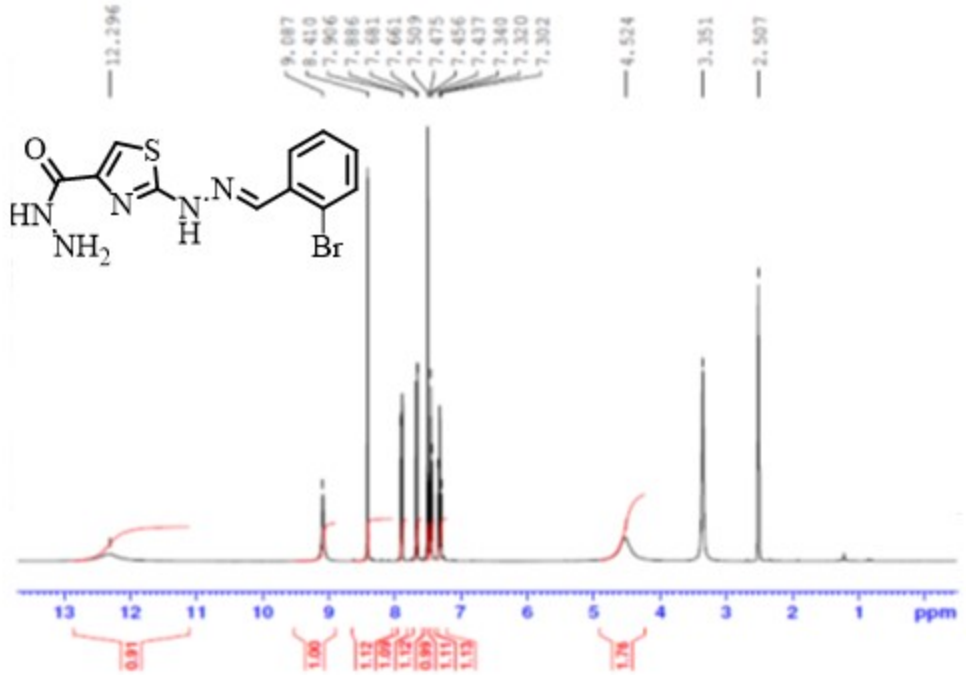


Figure S13: ^{1}H-NMR spectrum of **BDTC5**

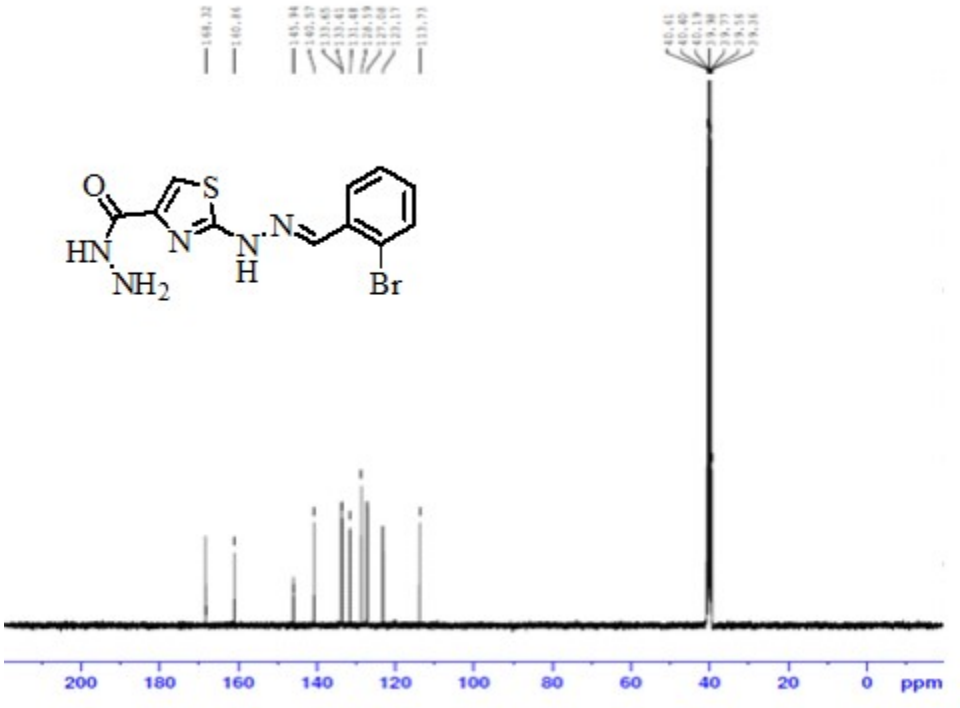
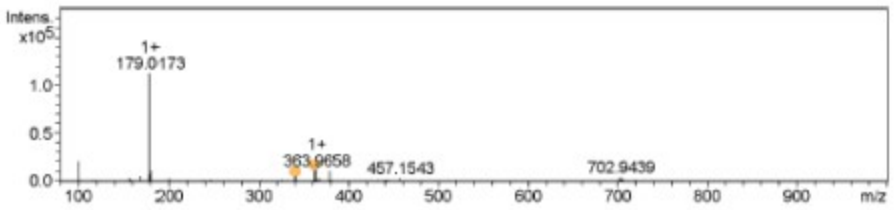
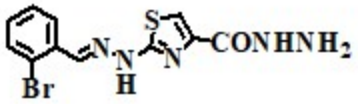


Figure S14: ^{13}C-NMR spectrum of **BDTC5**



#	m/z	I %
1	101.0034	18.7
2	157.0355	3.4
3	168.9909	4.8
4	179.0173	100.0
5	180.0195	6.0
6	181.0138	9.8
7	199.0006	2.7
8	339.9864	3.8
9	341.9835	3.9
10	361.9681	9.5
11	362.9701	1.5
12	363.9658	10.2
13	364.9683	1.5
14	367.1406	2.6
15	379.1416	9.1
16	380.1450	1.5
17	457.1543	2.9
18	700.9449	1.9
19	702.9439	3.8
20	704.9417	2.2



Generate Molecular Formula Parameters

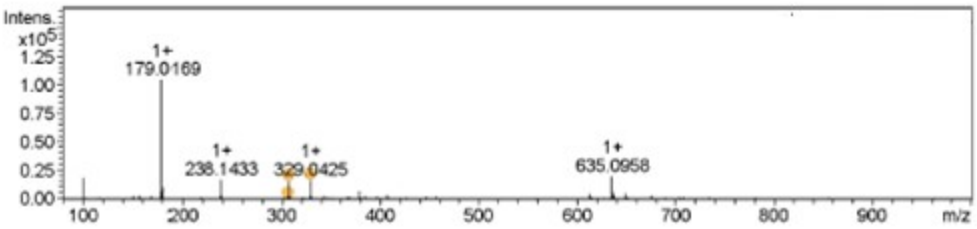
Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE

Expected Formula C11 H10 Br1 N5 O1 S1 **Adduct(s):** H, Na, NH4, C3H5N2, radical

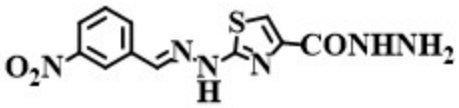
#	meas. m/z	theo. m/z	[Err][ppm]	Sigma	Formula	Adduct	Adduct Mass
1	339.9864	339.9862	0.70	0.0080	C11H11BrN5OS	M+H	1.0078
1	361.9681	361.9682	0.20	0.0163	C11H10BrN5NaOS	M+Na	22.9898

Note: Sigma fits < 0.05 indicates high probability of correct MF

Figure S15: HRMS spectrum of **BDTC5**



#	m/z	I %
1	101.0019	18.1
2	157.0354	3.3
3	168.9904	2.6
4	179.0169	100.0
5	180.0192	6.1
6	181.0131	9.6
7	238.1433	16.6
8	239.1466	2.6
9	307.0608	15.0
10	329.0425	16.0
11	343.0467	2.8
12	379.1413	6.6
13	385.0741	2.7
14	407.0567	3.6
15	613.1126	4.0
16	635.0958	19.0
17	636.0980	5.7
18	637.0954	2.9
19	649.1007	4.4
20	675.1271	3.3



Generate Molecular Formula Parameters

Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE

Expected Formula C11 H10 N6 O3 S1 **Adduct(s):** H, Na, NH4, C3H5N2, radical

#	meas. m/z	theo. m/z	[Err][ppm]	Sigma	Formula	Adduct	Adduct Mass
1	307.0608	307.0608	0.00	0.0025	C11H11N6O3S	M+H	1.0078
1	329.0425	329.0427	0.70	0.0043	C11H10N6NaO3S	M+Na	22.9898

Note: Sigma fits < 0.05 indicates high probability of correct MF

Figure S16: ^{1}H-NMR spectrum of **BDTC6**

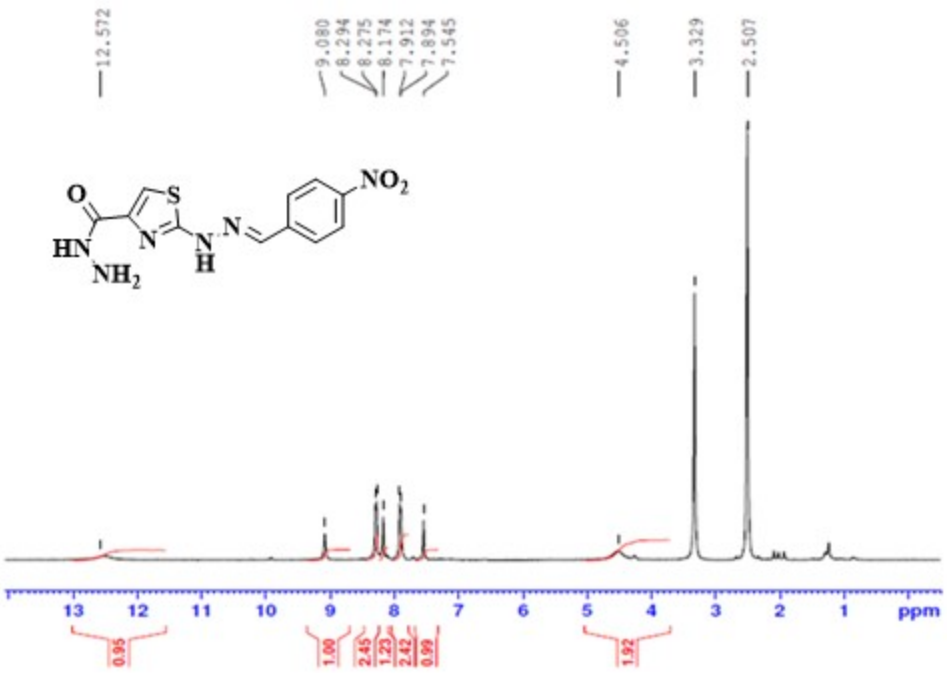
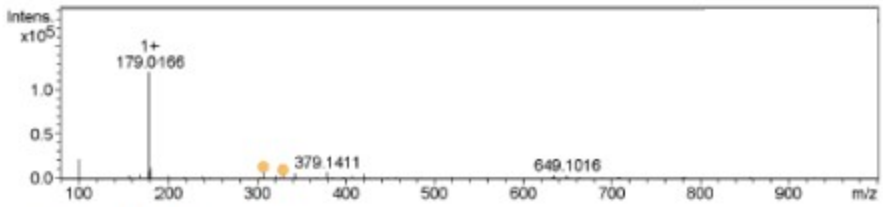
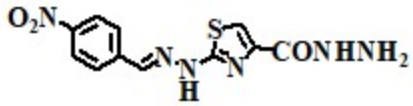


Figure S17: ^{1}H-NMR spectrum of **BDTC7**



#	m/z	I %
1	101.0000	18.4
2	157.0345	3.0
3	168.9899	3.8
4	179.0166	100.0
5	180.0191	6.3
6	181.0128	10.0
7	199.0003	2.6
8	238.1433	2.2
9	307.0608	5.5
10	321.0655	2.3
11	329.0429	2.8
12	343.0471	4.4
13	367.1405	1.5
14	379.1411	5.7
15	407.0568	2.1
16	421.0611	4.1
17	457.1546	1.5
18	635.1021	2.5
19	649.1016	3.4
20	707.1647	1.5



Generate Molecular Formula Parameters

Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE

Expected Formula C11 H10 N6 O3 S1 **Adduct(s):** H, Na, NH4, C3H5N2, radical

#	meas. m/z	theo. m/z	[Err[ppm]	Sigma	Formula	Adduct	Adduct Mass
1	307.0608	307.0608	0.00	0.0034	C11H11N6O3S	M+H	1.0078
1	329.0429	329.0427	0.60	0.0017	C11H10N6NaO3S	M+Na	22.9898

Note: Sigma fits < 0.05 indicates high probability of correct MF

Figure S18: HRMS spectrum of **BDTC7**

Spectroscopic data

2-(2-Benzylidenehydrazinyl)thiazole-4-carbohydrazide (BDTC1)

Light green solid; Yield: 53%; R_f: 0.29 (acetone/*n*-hexane, 1:2); Melting point: 232-233˚C; IR (ATR, cm^{-1}): 3394 (-NH_2 stretching), 3310 (-NH stretching), 1666 (C=O stretching), 1473 (C-H bending, aliphatic), 1499, 1515, 1561, 1593 (C=C ring stretching), HRMS: calculated for $C_{11}H_{11}N_5OS$: 261.0684 $[M+H]^+$, found: 262.0753 $[M+H]^+$, 284.0572 $[M+Na]^+$, 545.1250 $[2M+Na]^+$; ^{1}H-NMR (300 MHz): δ 12.11 (s, 1H, -N-NH-C-), 9.04 (s, -CO-NH-, 1H), 8.07 (s, 1H, -CH=N- azomethines), 7.65 (m, 2H, Ar-H), 7.41 (m, 4H, Ar-H+1,3-thiazole ring C-5), 4.49 (s, 2H, -NH_2); ^{13}C-NMR (75 MHz): δ 168.6 (1,3-thiazole ring C-2), 160.9 (C=O), 145.9 (1,3-thiazole ring C-4), 142.4 (-CH=N- azomethine), 134.7, 129.9, 129.3, 126.8, 111.3 (Ar-C), 113.3 (1,3-thiazole ring C-5).

2-(2-(2-Chlorobenzylidene)hydrazinyl)thiazole-4-carbohydrazide (BDTC2)

Light green solid; Yield: 51%; Melting point: 250-251˚C; R_f: 0.27 (acetone/*n*-hexane, 1:2); IR (ATR, cm^{-1}): 3433 (-NH_2 stretching), 3310 (-NH stretching), 1662 (C=O stretching), 1442 (C-H bending, aliphatic), 1581, 1556, 1511, 1497 (C=C ring stretching); HRMS: calculated for $C_{11}H_{10}ClN_5OS$: 295.0295 $[M+H]^+$, found: 296.0363 $[M+H]^+$, 318.0183 $[M+Na]^+$, 615.0444 $[2M+Na]^+$; ^{1}H-NMR (300 MHz): δ 12.29 (s, 1H, -N-NH-C-), 9.09 (s, 1H, -CO-NH-), 8.43 (s, 1H, -CH=N- azomethine), 7.91 (m, 1H, Ar-H), 7.44 (m, 4H, Ar-H+1,3-thiazole ring C-5), 4.53 (s, 2H, -NH_2); ^{13}C-NMR (75 MHz): δ 168.3 (1,3-thiazole ring C-2), 160.9 (C=O), 145.9 (1,3-thiazole ring C-4), 138.2 (-CH=N- azomethine), 132.8, 131.9, 131.2, 130.4, 128.1, 126.7 (Ar-C), 113.7 (1,3-thiazole ring C-5).

2-(2-(3-Chlorobenzylidene)hydrazinyl)thiazole-4-carbohydrazide (BDTC3)

Light green solid; Yield: 55%; Melting point: 248-249 ˚C; R_f: 0.28 (acetone/*n*-hexane, 1:2); IR (ATR, cm^{-1}): 3305 (-NH stretching), 1631 (C=O stretching), 1454 (C-H bending, aliphatic), 1599, 1570, 1521, 1502 (C=C ring stretching); HRMS: Calcd for $C_{11}H_{10}ClN_5OS$: 295.0295 $[M+H]^+$, found: 296.0369 $[M+H]^+$, 318.0187 $[M+Na]^+$, 615.0452 $[2M+Na]^+$; ^{1}H-NMR (300 MHz): δ 12.19 (s, 1H, -N-NH-C-), 9.08 (s, 1H, -CO-NH-), 8.04 (s, 1H, -CH=N- azomethine), 7.68 (s, 1H, 1,3-thiazole ring C-5), 7.67 (m, 1H, Ar-H), 7.60 (m, 1H, Ar-H), 7.44 (m, 2H, Ar-H), 4.54 (s, 2H, -NH_2); ^{13}C-NMR (75 MHz): δ 168.6 (1,3-thiazole ring C-2), 160.9 (C=O), 145.8 (1,3-thiazole ring C-4), 140.7 (-CH=N- azomethine), 136.9, 134.1, 131.2, 129.5, 126.0, 125.4 (Ar-C), 113.7 (1,3-thiazole ring C-5).

2-(2-(4-Chlorobenzylidene)hydrazinyl)thiazole-4-carbohydrazide (BDTC4)

Light green solid; Yield: 48%; Melting point: 253-254 ˚C; R_f: 0.24 (acetone/*n*-hexane, 1:2); IR (ATR, cm^{-1}): 3402 (-NH_2 stretching), 3309 (-NH stretching), 1608 (C=O stretching), 1465 (C-H bending, aliphatic), 1589, 1550, 1525, 1500 (C=C ring stretching); HRMS: Calcd for $C_{11}H_{10}ClN_5OS$: 295.0295 $[M+H]^+$, found: 296.0366 $[M+H]^+$, 318.0187 $[M+Na]^+$, 615.0447 $[2M+Na]^+$; ^{1}H-NMR (300 MHz): δ 12.16 (s, 1H, -N-NH-C-), 9.03 (s, 1H, -CO-NH-), 8.07 (s, 1H, -CH=N- azomethine), 7.67 (d, 2H, Ar-H, *J*= 8.4 Hz), 7.45 (s, 1H, 1,3-thiazole ring C-5), 7.49 (d, 2H, Ar-H, *J*= 8.0 Hz), 4.50 (s, 2H, -NH_2); ^{13}C-NMR (75 MHz): δ 168.5 (1,3-thiazole ring C-2), 160.9 (C=O), 145.9 (1,3-thiazole ring C-4), 141.1 (-CH=N- azomethine), 134.2, 133.7, 129.4, 128.4 (Ar-C), 113.5 (1,3-thiazole ring C-5).

2-(2-(2-Bromobenzylidene)hydrazinyl)thiazole-4-carbohydrazide (BDTC5)

Light green solid; Yield: 54%; Melting point: 239-240 ˚C; R_f: 0.25 (acetone/*n*-hexane, 1:2); IR (ATR, cm^{-1}): 3394 (-NH_2 stretching), 3298 (-NH stretching), 1658 (C=O stretching), 1435 (C-H bending, aliphatic), 1579, 1544, 1520, 1495 (C=C ring stretching); HRMS: Calcd for $C_{11}H_{10}BrN_5OS$: 338.9789 $[M+H]^+$, found: 339.9864 $[M+H]^+$, 361.9681 $[M+Na]^+$, 700.9449 $[2M+Na]^+$; ^{1}H-NMR (400 MHz): δ 12.31 (s, 1H, -N-NH-C-), 9.08 (s, 1H, -CO-NH-), 8.41 (s, 1H, -CH=N- azomethine), 7.89 (d, 1H, Ar-H, *J*= 8.0 Hz), 7.67 (d, 1H, Ar-H, *J*= 8.0 Hz), 7.51 (s, 1H, 1,3-thiazole ring C-5), 7.45 (t, 1H, Ar-H, *J*= 7.6 Hz), 7.32 (t, 1H, Ar-H, *J*= 8.0 Hz), 4.52 (s, 2H, -NH_2); ^{13}C-NMR (100 MHz): δ 168.3 (1,3-thiazole ring C-2), 160.9 (C=O), 145.9 (1,3-thiazole ring C-4), 140.6 (-CH=N- azomethine), 133.7, 133.4, 131.5, 128.6, 127.1, 123.2 (Ar-C), 113.7 (1,3-thiazole ring C-5).

2-(2-(3-Nitrobenzylidene)hydrazinyl)thiazole-4-carbohydrazide (BDTC6)

Light green solid; Yield: 62%; Melting point: 258-259 ˚C; R_f: 0.29 (acetone/*n*-hexane, 1:2); IR (ATR, cm^{-1}): 3375 (-NH_2 stretching), 3272 (-NH stretching), 1735 (C=O stretching), 1462 (C-H bending, aliphatic), 1589, 1561, 1523, 1501 (C=C ring stretching); HRMS: Calcd for $C_{11}H_{10}N_6O_3S$: 306.0535 $[M+H]^+$, found: 307.0608 $[M+H]^+$, 329.0425 $[M+Na]^+$, 635.0958 $[2M+Na]^+$; ^{1}H-NMR (400 MHz): δ 12.40 (s, 1H, -N-NH-C-), 9.06 (s, 1H, -CO-NH-), 8.10 (s, 1H, -CH=N- azomethine), 8.46 (s, 1H, Ar-H), 8.21 (d, 1H, Ar-H, *J*= 7.2 Hz), 8.09 (d, 1H, Ar-H, *J*= 7.6 Hz), 7.73 (t, 1H, Ar-H, *J*= 8.0 Hz), 7.52 (s, 1H, 1,3-thiazole ring C-5), 4.51 (s, 2H, -NH_2); ^{13}C-NMR (100 MHz): δ 168.5 (1,3-thiazole ring C-2), 160.9 (C=O), 141.2 (-CH=N- azomethine), 134.0, 132.3, 128.6, 122.9 (Ar-C), 113.5 (1,3-thiazole ring C-5).

2-(2-(4-Nitrobenzylidene)hydrazinyl)thiazole-4-carbohydrazide (BDTC7)

Light green solid; Yield: 55%; Melting point: 298-299 ˚C; R_f: 0.30 (acetone/*n*-hexane, 1:2); IR (ATR, cm^{-1}): 3398 (-NH_2 stretching), 3282 (-NH stretching), 1728 (C=O stretching), 1454 (C-H bending, aliphatic), 1581, 1566, 1535, 1513 (C=C ring stretching); HRMS: Calcd for $C_{11}H_{10}N_6O_3S$: 306.0535 $[M+H]^+$, found: 307.0608 $[M+H]^+$, 329.0429 $[M+Na]^+$, 635.1021 $[2M+Na]^+$; ^{1}H-NMR (400 MHz): δ 12.57 (s, 1H, -N-NH-C-), 9.08 (s, 1H, -CO-NH-), 8.28 (d, 2H, Ar-H, *J*= 7.6 Hz), 8.17 (s, 1H, -CH=N- azomethine), 7.90 (d, 2H, Ar-H, *J*= 7.2 Hz), 7.54 (s, 1H, 1,3-thiazole ring C-5), 4.50 (s, 2H, -NH_2); ^{13}C-NMR (100 MHz): δ solubility issue.

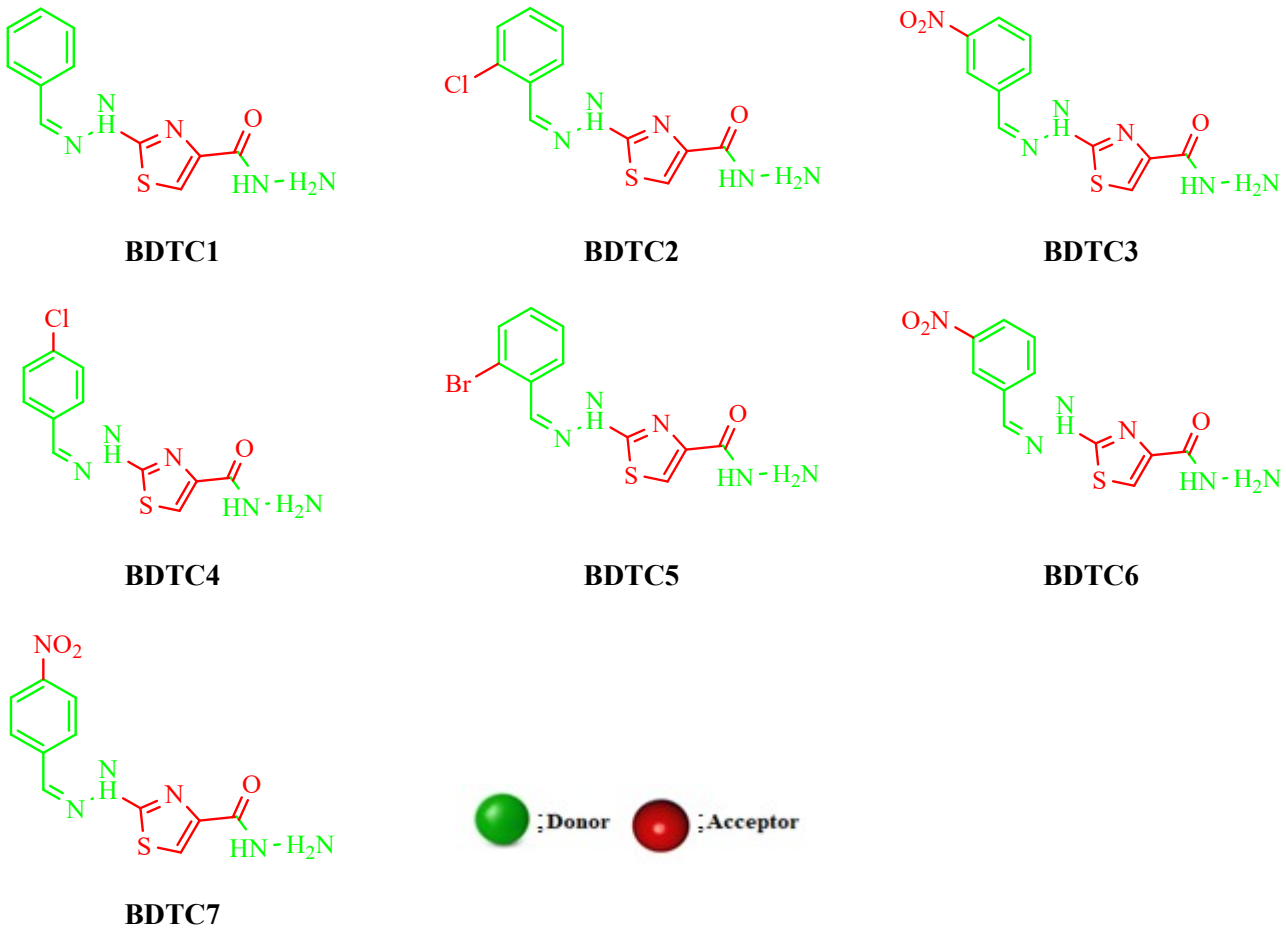


Figure S19: The optimized structures of **BDTC1-BDTC7** compounds.

Table S1: Wave length, excitation energy and oscillator strength of investigated compound **BDTC1**.

No.	*E* (*eV*)	λ_{max}(*nm*)	*f*	MO transitions
1	372.593	3.328	0.064	H→L (96%)
2	272.738	4.546	0.043	H-1→L (16%), H→L+1 (75%)
3	264.579	4.686	0.015	H-4→L (20%), H-1→L (26%), H→L+1 (11%)
4	262.567	4.722	0.009	H-2→L (12%), H-2→L+1 (44%), H→L+2 (16%)
5	260.608	4.758	0.071	H-1→L (31%), H→L+2 (31%)
6	250.782	4.944	0.022	H-4→L (45%), H→L+2 (27%), H-6→L+2 (2%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength

Table S2: Wave length, excitation energy and oscillator strength of investigated compound **BDTC2.**

No.	*E* (*eV*)	λ_{max}(*nm*)	*f*	MO transitions
1	362.888	3.417	0.087	H→L (97%)
2	274.581	4.515	0.004	H-3→L (15%), H→L+1 (23%), H→L+2 (54%)
3	270.962	4.576	0.037	H-2→L (21%), H→L+1 (54%), H→L+2 (12%)
4	262.946	4.715	0.010	H-2→L+1 (14%), H-1→L (25%), H-1→L+1 (45%)
5	260.318	4.763	0.018	H-3→L (53%), H→L+2 (22%)
6	258.365	4.799	0.091	H-2→L (31%), H-1→L (15%), H→L+1 (16%)

MO=molecular orbital, H=HOMO, L=LUMO, f= oscillator strength

Table S3: Wave length, excitation energy and oscillator strength of investigated compound **BDTC3.**

No.	*E* (*eV*)	λ_{max}(*nm*)	*f*	MO transitions
1	380.180	3.261	0.075	H→L (96%)
2	280.026	4.428	0.026	H-1→L (47%), H→L+1 (29%)
3	268.271	4.622	0.020	H-1→L (24%), H→L+1 (60%)
4	267.871	4.629	0.048	H-4→L (13%), H→L+2 (73%)
5	264.015	4.696	0.001	H-2→L (30%), H-2→L+1 (37%)
6	257.005	4.824	0.015	H-4→L (37%), H→L+2 (14%)

MO=molecular orbital, H=HOMO, L=LUMO, f= oscillator strength

Table S4: Wave length, excitation energy and oscillator strength of investigated compound **BDTC4.**

No.	*E* (*eV*)	λ_{max}(*nm*)	*f*	MO transitions
1	381.197	3.253	0.076	H→L (96%)
2	278.792	4.447	0.029	H-1→L (20%), H→L+1 (72%)
3	271.259	4.571	0.119	H-1→L (37%), H→L+2 (51%)
4	265.127	4.676	0.042	H-2→L+1 (12%), H-1→L (22%), H→L+2 (20%)
5	262.695	4.720	0.025	H-2→L (17%), H-2→L+1 (27%), H-2→L+2 (16%)
6	254.467	4.872	0.016	H-2→L (66%), H-2→L+1 (13%)

MO=molecular orbital, H=HOMO, L=LUMO, f= oscillator strength

Table S5: Wave length, excitation energy and oscillator strength of investigated compound **BDTC5.**

No.	*E* (*eV*)	λ_{max}(*nm*)	*f*	MO transitions
1	360.902	3.435	0.067	H→L (97%)
2	276.226	4.489	0.007	H→L+1 (61%), H→L+2 (12%)
3	269.818	4.595	0.026	H-2→L (10%), H→L+2 (74%), H-1→L (8%)
4	263.847	4.699	0.057	H-3→L (11%), H-2→L+2 (11%), H-1→L (29%), H→L+1 (22%)
5	262.256	4.728	0.015	H-3→L (15%), H-2→L (16%), H-1→L+2 (25%)
6	257.394	4.817	0.054	H-3→L (35%), H-1→L (13%), H→L+2 (10%)

MO=molecular orbital, H=HOMO, L=LUMO, f= oscillator strength

Table S6: Wave length, excitation energy and oscillator strength of investigated compound **BDTC6.**

No.	*E* (*eV*)	λ_{max}(*nm*)	*f*	MO transitions
1	382.809	3.239	0.038	H→L (93%), H→L+1 (5%)
2	332.942	3.724	0.058	H→L+1 (91%), H→L (5%)
3	311.581	3.979	0.000	H-9→L (87%), H-9→L+1 (7%), H-9→L+3 (3%)
4	295.757	4.192	0.013	H-2→L (89%), H-5→L (3%)
5	283.587	4.372	0.000	H-10→L (75%), H-10→L+1 (5%)
6	281.450	4.405	0.000	H-1→L (82%), H-10→L (5%)

MO=molecular orbital, H=HOMO, L=LUMO, f= oscillator strength

Table S7: Wave length, excitation energy and oscillator strength of investigated compound **BDTC7.**

No.	*E* (*eV*)	λ_{max}(*nm*)	*f*	MO transitions
1	448.990	2.761	0.070	H→L (97%), H→L+1 (2%)

2	327.308	3.788	0.000	H-9→L (86%), H-9→L+1 (11%)
3	311.604	3.979	0.079	H-3→L (13%), H-2→L (29%), H-1→L (44%)
4	307.531	4.032	0.028	H-3→L (10%), H-2→L (26%), H-1→L (54%)
5	295.729	4.193	0.043	H-2→L (11%), H→L+1 (63%), H-10→L (6%)
6	293.370	4.226	0.004	H-10→L (81%), H-10→L+1 (10%)

MO=molecular orbital, H=HOMO, L=LUMO, f= oscillator strength

Table S8: Computed E_{HOMO}, E_{LUMO} and energy gap (E_{LUMO}-E_{HOMO}) of **BDTC1-BDTC7**.

Comp.	E_{HOMO}	E_{LUMO}	E_{gap}
BDTC1	-5.843	-1.365	4.478
BDTC2	-5.954	-1.450	4.504
BDTC3	-6.010	-1.636	4.374
BDTC4	-5.979	-1.619	4.360
BDTC5	-5.935	-1.389	4.546
BDTC6	-6.385	-2.327	4.058
BDTC7	-6.249	-2.666	3.583

Units in *eV*