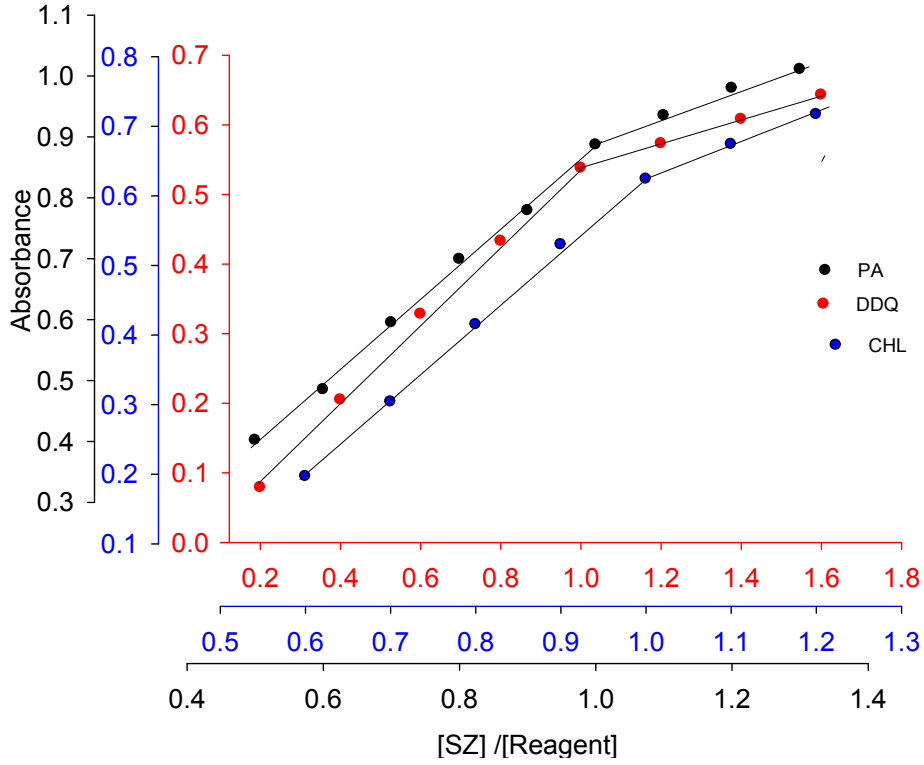


Fig. S1†: Molar ratio plots of SZ→DDQ, SZ→CHL and SZ→PA charge transfer complexes.

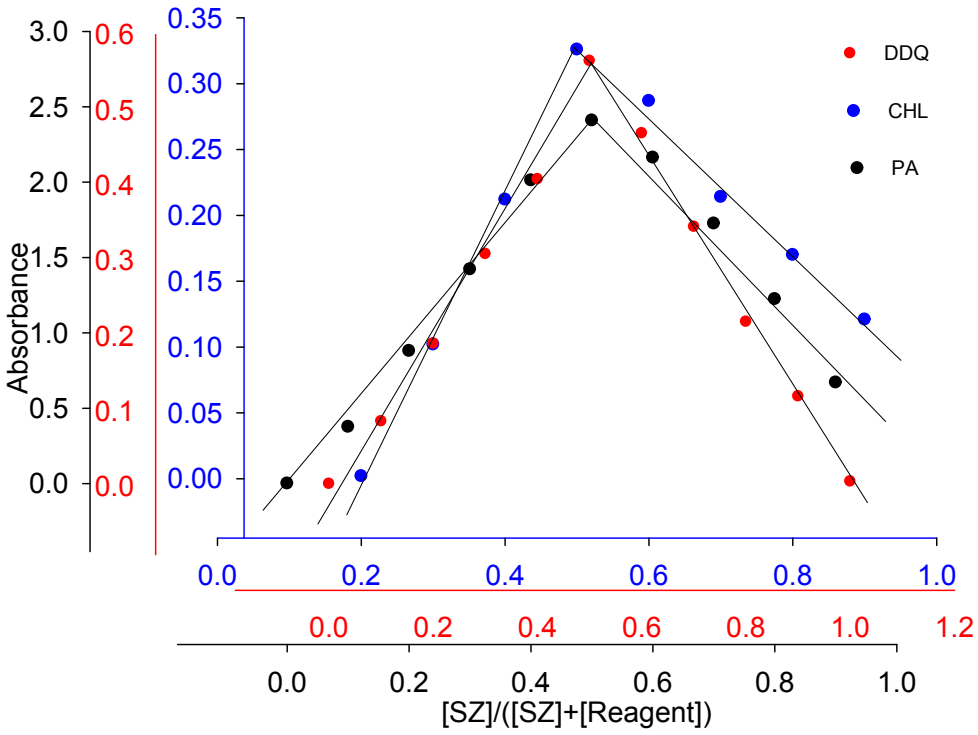


Fig. S2†: Continuous variation plots of SZ→DDQ, SZ→CHL and SZ→PA charge transfer complexes.

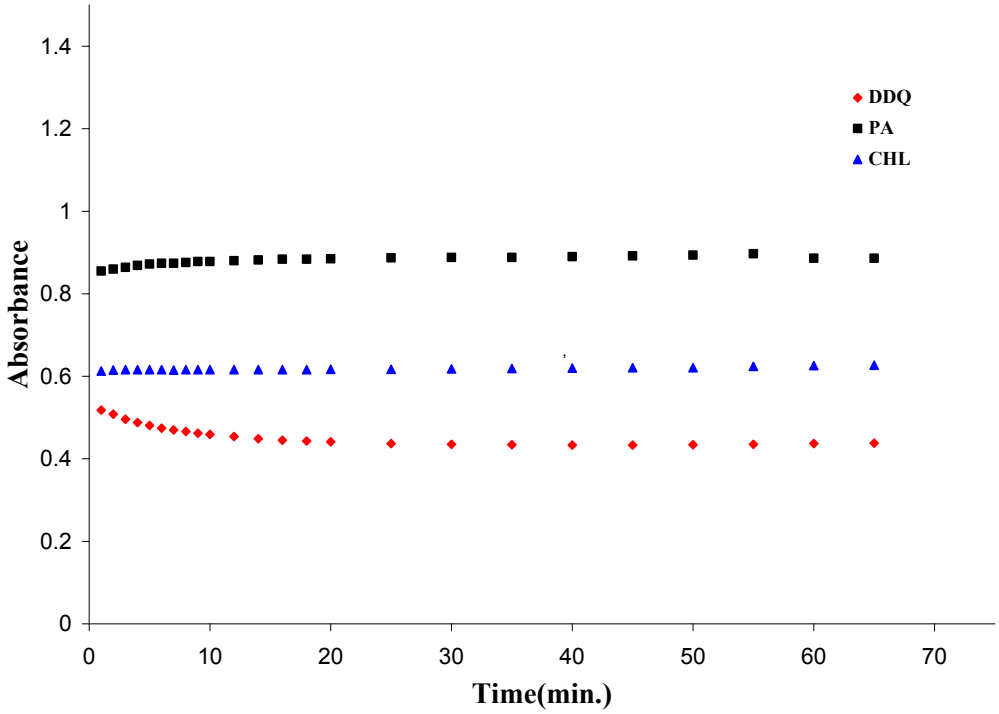


Fig. S3†: Effect of time on the stability of SZ→DDQ, SZ→CHL and SZ→PA charge transfer complexes.

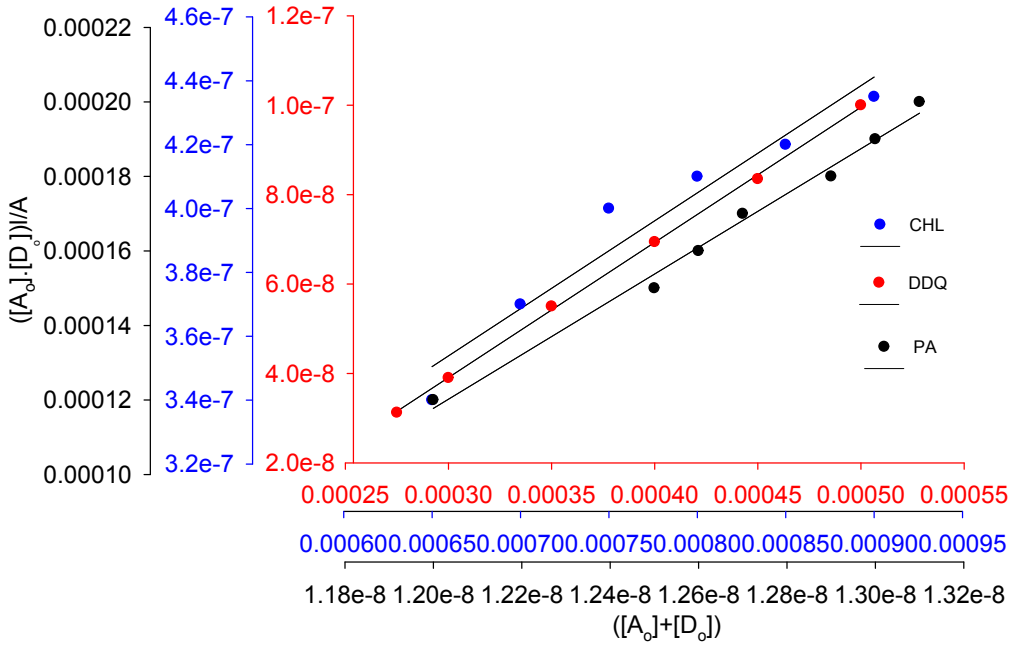


Fig. S4†: Modified benesi-Hildbrand plots of the studied CT complexes.

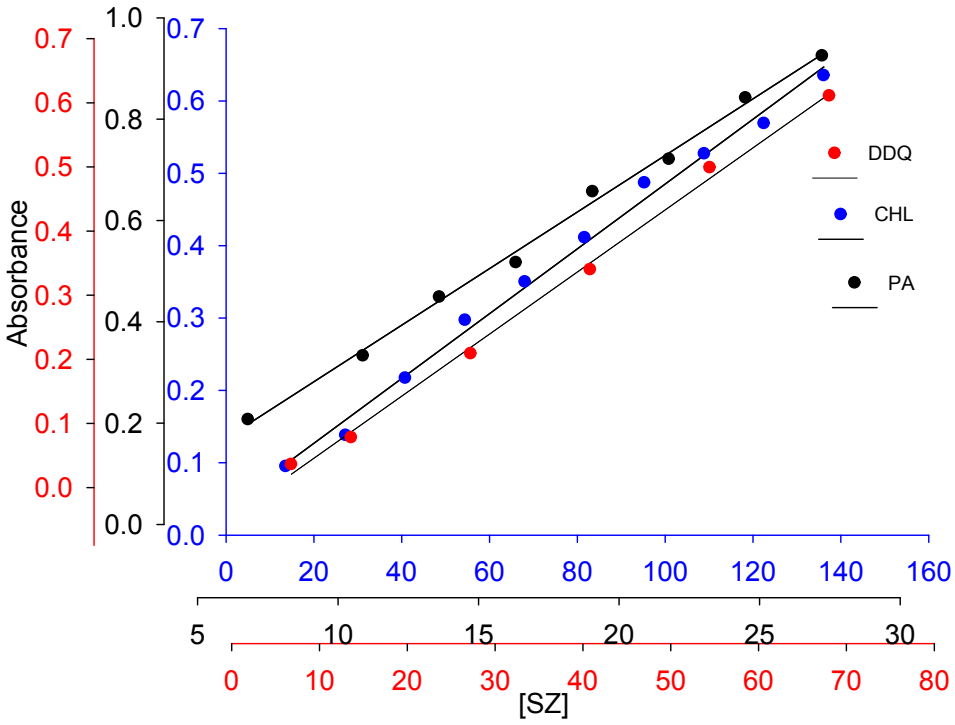


Fig. S5†: Calibration curves of the CT complexes (absorbance vs. [SZ, μg]).

Table S1†: Effect of interferants on SZ-CT complexes

Interferant	Amount taken (mg mL^{-1})	DDQ* Recovery% ±RSD%	CHL** Recovery% ±RSD%	PA*** Recovery% ±RSD%
Glucose	0.54	98.0± 0.37	99.83 ± 1.28	101.0 ± 1.27
Fructose	0.54	98.92± 0.58	99.68 ± 1.77	100.0 ± 1.39
Lactose	0.40	98.27± 1.32	99.60 ± 1.38	99.99 ± 1.43
Starch	0.30	97.12± 0.64	98.74 ± 1.74	99.31± 1.36
Sodium citrate	0.37	97.55± 0.56	99.82 ± 1.54	99.98 ± 1.30

*= Average of four determinations at 0.068 mg mL^{-1}
**= Average of four determinations at 0.109 mg mL^{-1}
***= Average of four determinations at 0.027 mg mL^{-1}

Table S2†: The intra-day and inter-day precision and accuracy of data obtained for the developed method

Intra-day (n=5)				Inter -day (n=5)
Acceptor	NO.	SZ taken µgmL^{-1}	Recovery % ± RSD%	Recovery % ± RSD%
DDQ	1.	40.83	99.87±1.57	98.99±2.00
	2.	54.45	101.0±1.63	99.25±1.93
	3.	68.06	99.61±1.65	99.40±1.95
CHL	1.	108.90	99.86±0.64	99.69±1.22
	2.	122.51	100.01±0.73	99.61±1.25
	3.	136.12	100.2±0.89	99.70±1.46
PA	1.	21.78	99.86±1.48	99.36±1.22
	2.	24.50	100.02±0.99	99.30±1.25
	3.	27.22	99.82±1.01	99.89±1.46

Table S3†**:** Ruggedness and robustness (RSD%) of the complexes

Method of robustness				Method of ruggedness
Parameters				Inter-analyst (n=4)
Acceptor	SZ taken μgmL^{-1}	Volume of DDQ (n=3)	Time Reaction(n=3)	
DDQ	40.83	1.72	1.89	2.35
	54.45	2.00	1.72	2.22
	68.06	1.90	1.76	2.42
CHL	108.90	1.84	1.69	2.12
	122.51	1.70	1.52	2.32
	136.12	1.74	1.75	2.30
PA	21.78	1.89	1.47	2.30
	24.50	1.99	1.86	2.05
	27.22	1.90	1.79	2.14

n, number of determinations, RSD%, percentage relative standard deviation.

Table S4†: Spectrophotometric determination of SZ in Dermazin cream.

Acceptor	NO.	SZ taken (μgmL^{-1})	Pure solution (Recovery% ±RSD%)	Dermazin cream (Recovery% ±RSD%)
DDQ	1.	40.83	99.87±1.57	99.60± 1.19
	2.	54.45	101.0±1.63	100.05 ± 1.56
	3.	68.06	99.61±1.65	99.29± 1.63
CHL	1.	108.90	99.86±0.64	100.0 ±1.38
	2.	122.51	100.01±0.73	100.2 ±1.05
	3.	136.11	100.2±0.89	99.99±0.95
PA	1.	22.78	99.86±1.48	99.72± 1.97
	2.	24.50	100.02±0.99	99.67 ± 1.37
	3.	27.22	99.82±1.01	100.1± 1.72

Table S5†: The bond lengths (Å) and angles (º) of SZ, DDQ, and SZ→DDQ complex.							
Bond lengths (Å)				Bond angles (º)			
	SZ→DDQ	**SZ**	**DDQ**		**SZ→DDQ**	**SZ**	**DDQ**
C(1)-C(4)	1.38616	1.38453		C(1)-C(4)-C(3)	115.38809	118.88118	
C(4)-C(3)	1.39093	1.39358		C(4)-C(3)-N9)	123.27641	116.93078	
C(3)-N(9)	1.32273	1.4060		C(3)-N(9)-C(2)	116.81128	121.33824	
C(2)-N(8)	1.37138	1.35160		C(2)-N(10)-N(8)	121.58736	120.96026	
C(1)-N(10)	1.34803	1.3887		C(2)-N(8)-N(9)	113.94503	110.40788	
C(2)-N(9)	1.34909	1.40763		C(2)-N(8)-S(11)	124.24213	122.51940	
S(11)-N(8)	1.59749	1.62038		N(8)-S(11)-O(12)	108.93510	105.95889	
S(11)-O(12)	1.45662	1.47982		N(8)-S(11)-O(13)	117.76914	114.88774	
S(11)-O(13)	1.45901	1.47899		S(11)-C14)-C(15)	118.81637	121.07442	
S(11)-C(14)	1.77225	1.81534		S(11)-C(14)-C(16)	118.85324	119.22627	
C(14)-C(15)	1.42372	1.39796		C(14)-C16C(19)	119.65284	120.39587	
C(14)-C(16)	1.42370	1.39542		C(16)-C(19)C(21)	120.15976	120.38631	
C(16)-C(19)	1.35495	1.39410		C(19)-C(21)-C(17)	117.98626	118.79583	
C(19)-C(21)	1.46475	1.40233		C(21)-C(17)-C(15)	121.2350	120.82363	
C(21)-C(17)	1.46103	1.40345		C(17)-C(15)-C(14)	118.72942	119.92339	
C(21)-N(24)	1.28514	1.41430		C(15)-C(14)-C(16)	122.22479	119.67412	
C(15)-C(17)	1.35341	1.39299		C(17)-C(21)-N(24)	117.82040	120.58308	
C(27)-C28)	1.34714		1.34497	C(19)-C(21)-N(24)	124.19032	120.57889	
C(28)-C(29)	1.48441		1.49391	C(26)-C(27)-C(28)	124.37996		121.42560
C(29)-C(30)	1.47302		1.49925	C(27)-C(28)-C(29)	122.27169		121.42562
C(30)-C(31)	1.46410		1.34687	C(28)-C(29)-C(30)	114.81621		117.31593
C(30)-C(37)	1.30680		1.28760	C(29)-C(30)-C(31)	121.25202		121.25832
C(31)-C(36)	1.39746		1.42876	C(30)-C(31)-C(26)	122.24800		121.25866
C(36)-N(39)	1.16648		1.15543	C(27)-C(26)-O(35)	119.17231		122.33320
C(37)-N(38)	1.21821		1.15543	C(31)-C(26)-O(35)	126.31956		120.35093
C(26)-O(35)	1.23312		1.20605	C(28)-C(29)-O(34)	121.74147		122.33277
C(29)-O(34)	1.22283		1.20605	C(30)-C(29)-O(34)	123.44214		120.35130
C(27)-Cl(32)	1.72620		1.70845	C(26)-C(27)-Cl(32)	114.34912		115.28931
C(28)-Cl(33)	1.73493		1.70845	C(29)-C(28)-Cl(33)	114.83107		115.28911
C(26)-C(27)	1.51520		1.49390	C(31)-C(30)-C(37)	124.08253		122.59523
C(26)-C(31)	1.41578		1.49925	C(30)-C(37)-N(38)	174.37418		179.67912
				C(29)-C(30)-C(37)	114.14970		116.14645
				C(26)-C(31)-C(36)	118.02293		116.14621
				C(30)-C(31)-C(36)	119.72900		122.59513
				C(31)-C(36)-N(39)	177.77485		179.67944
				C(27)-C(28)-Cl(32)	121.27075		123.28509
				C(27)-C(28)-Cl(33)	122.89591		123.28526
				C(26)-C(27)-C(31)	114.50803		117.31587

Table S6†: The bond lengths (Å) and angles (º) of SZ, CHL, and SZ→CHL complex.							
Bond lengths (Å)				Bond angles (º)			
	SZ→CHL	**SZ**	**CHL**		**SZ→CHL**	**SZ**	**CHL**
C(1)-C(2)	1.38643	1.39410		C(1)-C(2)-C(3)	119.95506	120.39587	
C(2)-C(3)	1.39050	1.39542		C(2)-C(3)-C(4)	119.94374	119.67412	
C(3)-C(4)	1.38697	1.39796		C(3)-C(4)-C(5)	120.18501	119.92339	
C(4)-C(5)	1.38772	1.39299		C(4)-C(5)-C(6)	120.41733	120.82363	
C(5)-C(6)	1.39664	1.40345		C(5)-C(6)-C(1)	118.90253	118.79583	
C(6)-C(1)	1.39803	1.40233		C(6)-C(1)-C(2)	120.59010	120.38631	
C(6)-N(11)	1.40463	1.41430		C(5)-C(6)-N(11)	120.57292	120.58308	
S(14)-O(16)	1.46777	1.47982		C(1)-C(6)-N(11)	120.47680	120.57889	
S(14)-O(17)	1.46709	1.47899		C(2)-C(3)-S(14)	120.46048	119.22627	
S(14)-N(15)	1.62194	1.62038		C(3)-C(4)-S(14)	106.12206	121.07442	
C(3)-S(14)	1.79251	1.81534		C(3)-S(14)-O(16)	106.45576	104.48066	
N(15)-C(18)	1.33182	1.35160		C(3)-S(14)-O(17)	105.58368	105.85533	
C(18)-N(23)	1.37068	1.40763		C(3)-S(14)-N(15)	114.56657	107.98337	
C(18)-C(24)	1.36120	1.32046		S(14)-N(15)-C(18)	121.43562	122.51940	
C(20)-N(23)	1.32314	1.40608		N(15)-C(18)-N(23)	114.70649	110.40788	
C(19)-N(24)	1.31738	1.38875		N(15)-C(18)-N(24)	123.51545	128.59683	
C(19)-C(21)	1.39401	1.39358		C(18)-N(23)-C(20)	121.76676	121.33824	
C(20)-C(21)	1.38495	1.38495		N(23)-C(20)-C(21)	118.67088	116.93078	
C(27)-C(28)	1.51118		1.51412	C(20)-C(21)-C(19)	117.67640	118.88118	
C(28)-C(29)	1.45453		1.46968	C(21)-C(19)-N(24)	124.10086	123.32431	
C(29)-C(30)	1.35830		1.35650	C(19)-N(24)-C(18)	114.96460	117.88225	
C(31)-C(32)	1.46384		1.46967	C(27)-C(28)-C(29)	116.37755		116.09620
C(27)-C(32)	1.34243		1.35648	C(28)-C(29)-C(30)	122.72526		122.61715
C(27)-O(39)	1.33281		1.33251	C(29)-C(30)-C(31)	119.41595		121.28685
C(28)-O(35)	1.21556		1.21591	C(30)-C(31)-C(32)	116.71596		116.09539
C(30)-O(36)	1.30193		1.33247	C(31)-C(32)-C(27)	121.89066		122.61928
C(31)-O(34)	1.21271		1.21592	C(32)-C(27)-C(28)	121.34698		121.28512
C(29)-Cl(33)	1.73630		1.74533	C(27)-C(32)-Cl(38)	120.05962		120.13128
C(32)-Cl(38)	1.73983		1.74540	C(31)-C(32)-Cl38)	118.02436		117.24943
C(30)-C(31)	1.51964		1.51409	C(28)-C(27)-O(39)	118.77179		113.09496
				C(32)C(27)-O(39)	125.08832		125.61992
				C(27)-C(28)-O(35)	118.77179		120.05370
				C(29)-C(28)-O(35)	124.85019		123.85010
				C(28)-C(29)-Cl(33)	116.68898		117.25092
				C(30)-C(29)-Cl(33)	120.43570		120.13192
				C(29)-C(30)-O(36)	123.09848		125.61839
				C(31)-C(30)-O(36)	117.09461		113.09476
				C(30)-C(31)-O(34)	119.78775		120.05461
				C(32)-C(31)-O(34)	123.34497		123.85000

Table S7†: The bond lengths (Å) and angles (º) of SZ, PA, and SZ→PA complex.							
Bond lengths (Å)				Bond angles (º)			
	SZ→PA	***SZ***	**PA**		**SZ→PA**	***SZ***	**PA**
C(1)-C(2)	1.38397	1.39410		C(1)-C(2)-C(3)	119.72586	120.39587	
C(2)-C(3)	1.39356	1.39542		C(2)-C(3)-C(4)	120.38479	119.67412	
C(3)-C(4)	1.38730	1.39796		C(3)-(C4)-C(5)	119.84115	119.92339	
C(4)-C(5)	1.38764	1.39299		C(4)-C(5)-C(6)	120.44615	120.82363	
C(5)-C(6)	1.39830	1.40345		C(5)-C(6)-C(1)	119.05147	118.79583	
C(6)-C(1)	1.40018	1.40233		C(6)-C(1)-C(2)	120.54127	120.38631	
C(6)-N(11)	1.39763	1.41430		C(5)-C(6)-N(11)	120.50759	120.58308	
S(14)-O(16)	1.45883	1.47982		C(1)-C(6)-N(11)	120.38469	120.57889	
S(14)-O(17)	1.46401	1.47899		C(2)-C(3)-S(14)	119.76878	119.22627	
S(14)-N(15)	1.65181	1.62038		C(3)-C(4)-S(14)	119.83422	121.07442	
C(3)-S(14)	1.78224	1.81534		C(3)-S(14)-O(16)	108.29701	104.48066	
N(15)-C(18)	1.29876	1.35160		C(3)-S(14)-O(17)	107.94484	105.85533	
C18)-N(23)	1.38816	1.40763		C(3)-S(14)-N(15)	102.3045	107.98337	
C(18)-C(24)	1.37011	1.32046		S(14)-N(15)-C(18)	121.53282	122.51940	
C(20)-N(23)	1.34307	1.40608		N(15)-C(18)-N(23)	115.34206	110.40788	
C(19)-N(24)	1.30587	1.38875		N(15)-C(18)-N(24)	127.05689	128.59683	
C(19)-C(21)	1.41240	1.39358		C(18)-N(23)-C(20)	122.83582	121.33824	
C(20)-C(21)	1.36514	1.38453		N(23)-C(20)-C(21)	119.70546	116.93078	
C(27)-C(28)	1.39919		1.39410	C(20)-C(21)-C(19)	115.55154	118.8811	
C(28)-C(29)	1.39919		1.38294	C(21)-C(19)-N(24)	125.06077	123.32431	
C(29)-C(30)	1.46001		1.42030	C(19)-N(24)-C(18)	118.55810	117.88225	
C(30)-C(31)	1.43246		1.4266	C(27)-C(28)-C(29)	119.14016		119.37484
C(31)-C(32)	1.39396		1.39197	C(28)-C(29)-C(30)	122.53926		122.12266
C(27)-C(32)	1.37535		1.38376	C(29)-C(30)-C(31)	114.22825		115.90678
C(27)-N(38)	1.44785		1.46965	C(30)-C(31)-C(32)	122.87499		122.35401
N(38)-O(42)	1.22679		1.22866	C(27)-C(31)-C(32)	119.41415		118.80492
N(38)-O(43)	1.22711		1.22846	C(27)-C(28)-C(32)	121.68633		121.41706
C(31)-N(39)	1.44687		1.45878	C(27)-N(38)-O(42)	117.94550		117.25588
N(39)-O(44)	1.23181		1.22017	C(27)-N(38)-O(43)	118.36614		117.17227
N(39)-O(45)	1.22575		1.24992	C(29)-N(37)-O(40)	123.46144		116.34884
C(30)-O(33)	1.27058		1.31804	C(29)-N(37)-O(41)	119.17001		117.80575
C29N(37)	1.39805		1.47592	C(31)-N(39)-O(44)	117.91469		118.80988
N(37)-O(40)	1.24505		1.22984	C(31)-N(39)-O(45)	119.46037		117.96654
N(37)-O(41)	1.38218		1.22420	C(29)-C(30)-O(33)	120.23945		120.38603
				C(27)-C(28)-N(38)	119.19420		119.25901
				C(27)-C(32)-N(38)	119.11491		119.32351
				C(28)-C(29)-N(37)	117.49473		116.87453
				C(29)-C(30)-N(37)	119.93460		121.00231
				C(30)-C(31)-N(39)	121.03523		120.48848
				C(31)-C(32)-N(39)	116.08973		117.15743

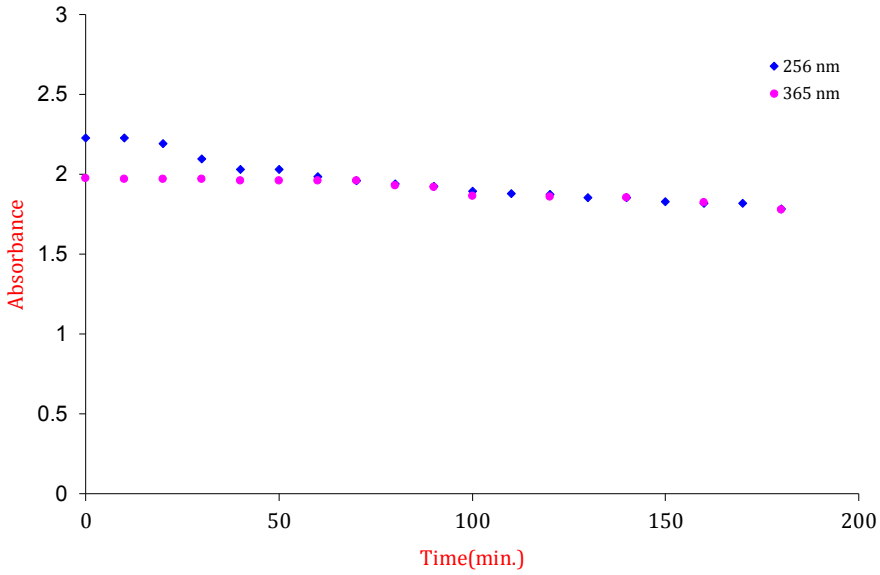
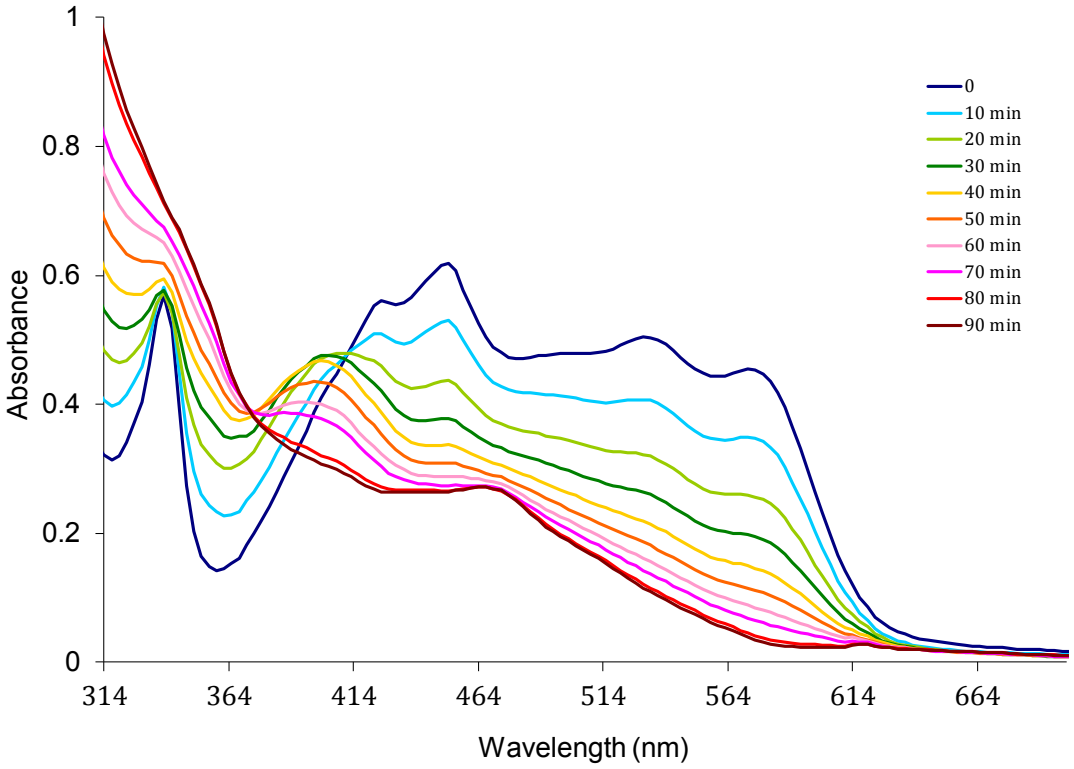


Fig. S6†: Change in the absorbance value of SZ at 239 nm upon the exposure to 256 and 365 nm light source.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Wavelength (nm)
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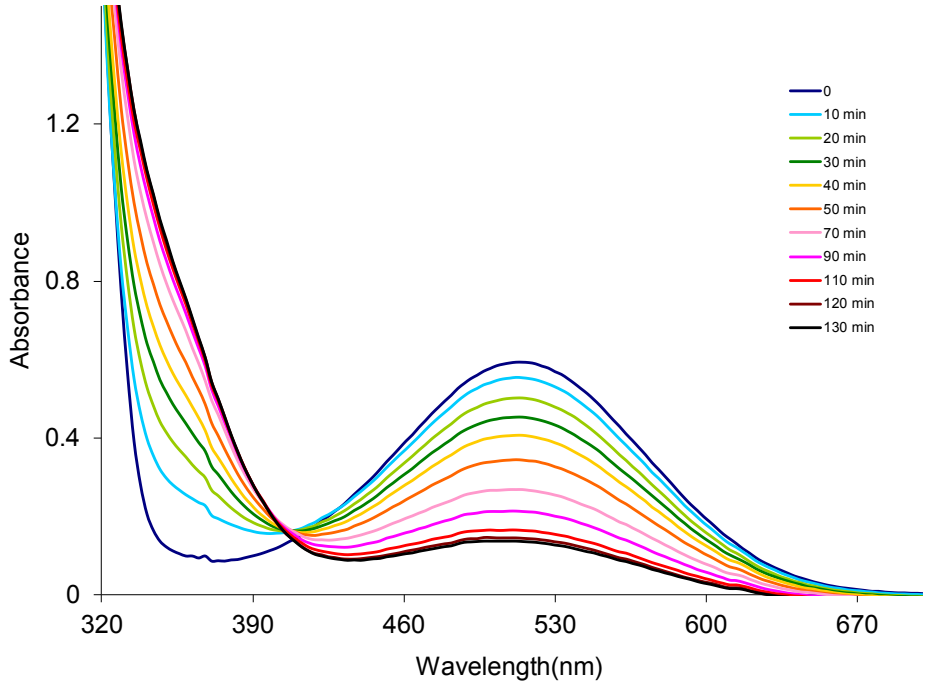
10 min
20 min
30 min
40 min
50 min
60 min
70 min
80 min
90 min

a)


Absorbance
Wavelength(nm)
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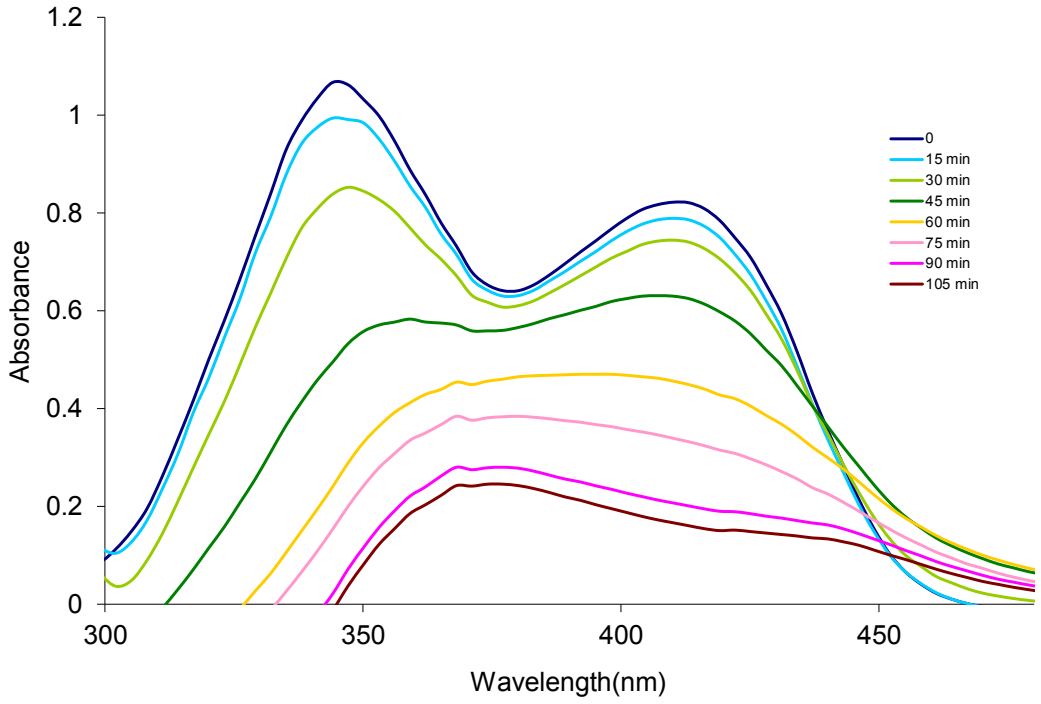
10 min
20 min
30 min
40 min
50 min
70 min
90 min
110 min
120 min
130 min

b)



c)

Fig. S7†: Ultraviolet light photodegradation of a) SZ→DDQ, b) SZ→CHL and c) SZ→PA upon the exposure at 256 nm.

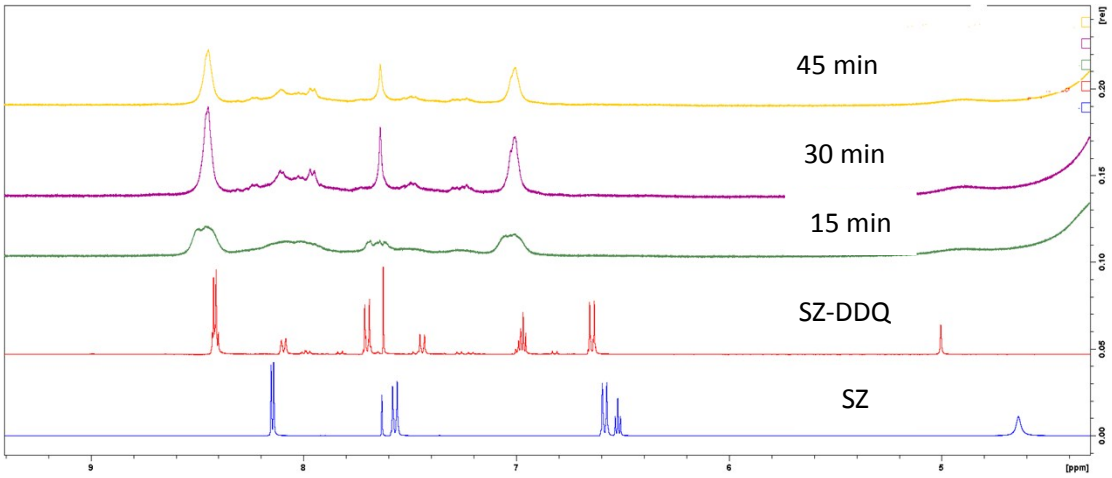


Fig. S8†: ^{1}H NMR spectral changes upon the illumination of SZ→DDQ/$NaNO_2$ system at 256 nm.