Supporting Information for

Triplet-Sensitized Photodegradation of Sulfa Drugs Containing Six-Membered Heterocyclic Groups: Identification of an SO_2 Extrusion Photoproduct

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Section S1. Characterization of the Lake Josephine natural water sample.

Filtered (0.2 µm) natural water samples were analyzed for dissolved organic carbon (DOC) on a Shimadzu TOC-V CSH total organic carbon analyzer. The filtered water was also analyzed for anions with a Dionex ion chromatography system with an AS14 column and carbonate buffered eluent. Cations in the water sample were monitored by a ThermoElemental PQ ExCell inductively coupled plasma mass spectrometer. The results from these analyses for Lake Josephine can be found in Table S1.

Ion Concentrations					
Cations			Anions		
Na	37.1	ppm	F	0.069	ppm
Mg	8.13	ppm	Cl	62.84	ppm
Al	4.12	ppb	NO_2	0.009	ppm
Si	2.51	ppm	Br	0.023	ppm
P	1.76	ppb	NO_3	0.096	ppm
K	3.22	ppm	PO_4	<0.005	ppm
Ca	27.2	ppm	SO_4	3.784	ppm
Fe	0	ppb	ClO_3	<0.010	ppm
Mn	4.89	ppb			
Sr	45.5	ppb			
Ba	50.3	ppb			
pH = 8.0					
DOC = 5.9 mg/L					

Table S1. Ion, DOC, and pH analysis of Lake Josephine natural water sample. Unit of ppm is by mass.

Section S2. Photodegradation of **5** in LJW and DI H_2O.

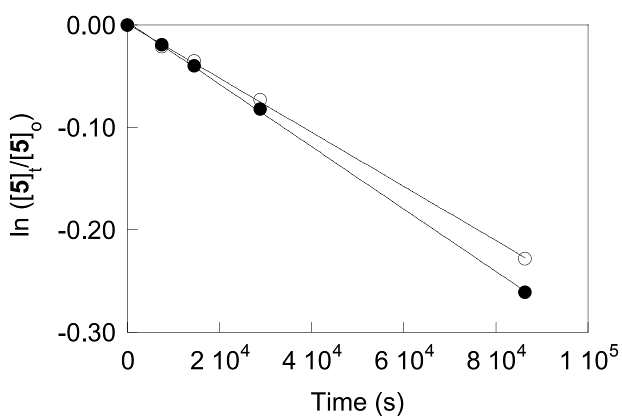

Figure S1. Photodegradation of **5** in LJW (○) and DI H_2O (●). The slight decrease in the LJW photolysis rate is due to light screening by the dissolved organic matter.

Section S3. Thermal generation of $^1O_2$ via the reaction of MoO_4^{2-} and H_2O_2 for **1-4**.

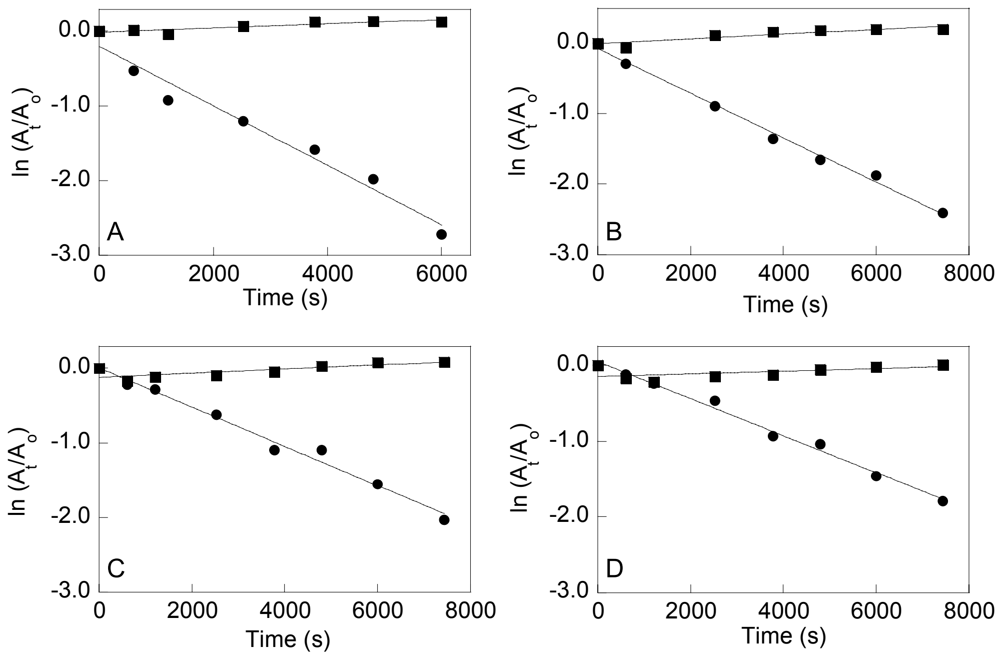

Figure S2. Degradation of FFA (●) via reaction with thermally generated $^1O_2$. The sulfa drugs (■) do not appear to react with $^1O_2$. The maximum reaction rate constants for **1-4** with $^1O_2$, all of which are statistically indiscernible from zero, were calculated to be 6.0×10^6 M^{-1} s^{-1} (**1**, A), 9.1×10^6 M^{-1} s^{-1} (**2**, B), 8.9×10^6 M^{-1} s^{-1} (**3**, C), and 6.8×10^6 M^{-1} s^{-1} (**4**, D).

Section S4. Competitive hydroxyl radical oxidation of sulfa drugs **1-5** versus the reference compound acetophenone using Fenton's reagent.

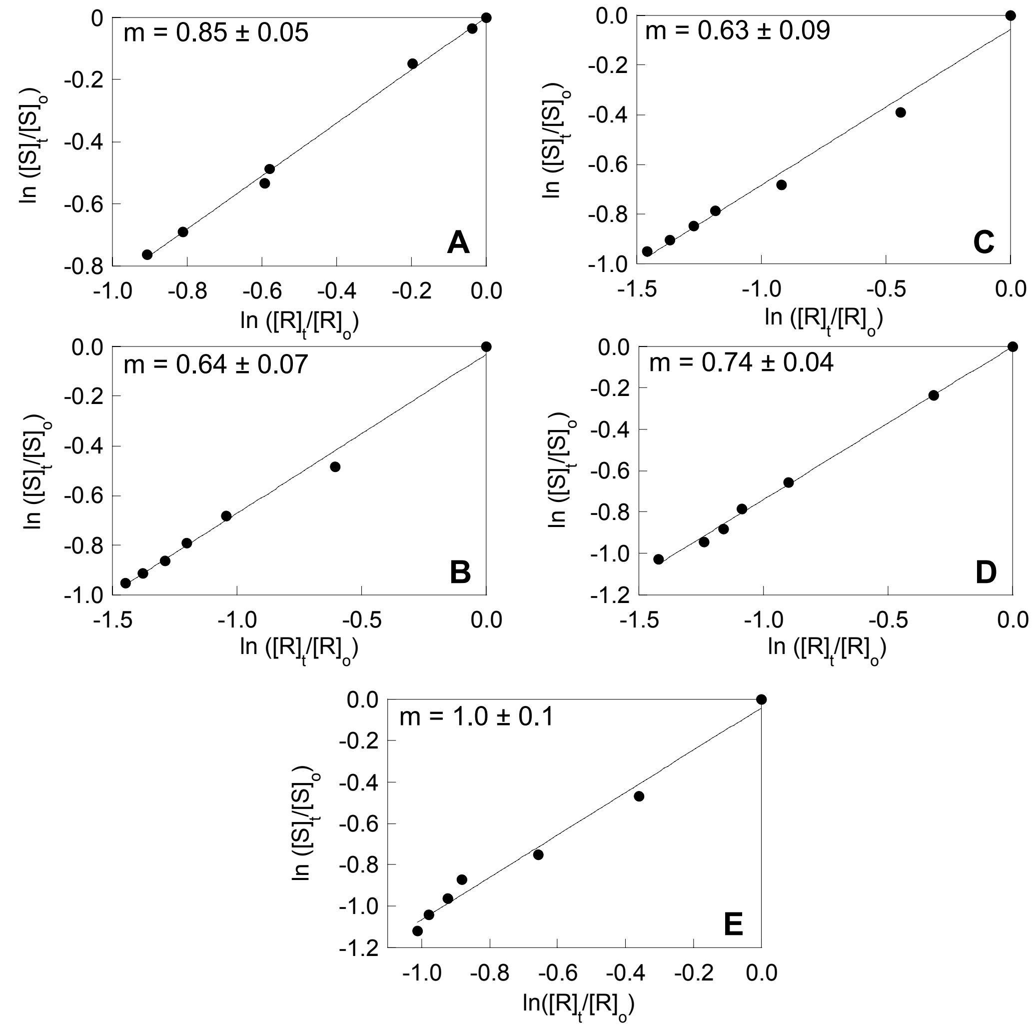

Figure S3. Competitive hydroxyl radical oxidation of substrates (S): sulfamethazine (**1**, A); sulfamerazine (**2**, B); sulfadiazine (**3**, C); sulfachloropyridazine (**4**, D); and sulfadimethoxine (**5**, E) versus the reference compound (R; acetophenone, $k_{rxn} = 5.9 \times 10^9$ M^{-1} s^{-1} (*1*)) using Fenton's reagent.

Section S5. pK_a determination for **1**-**5**.

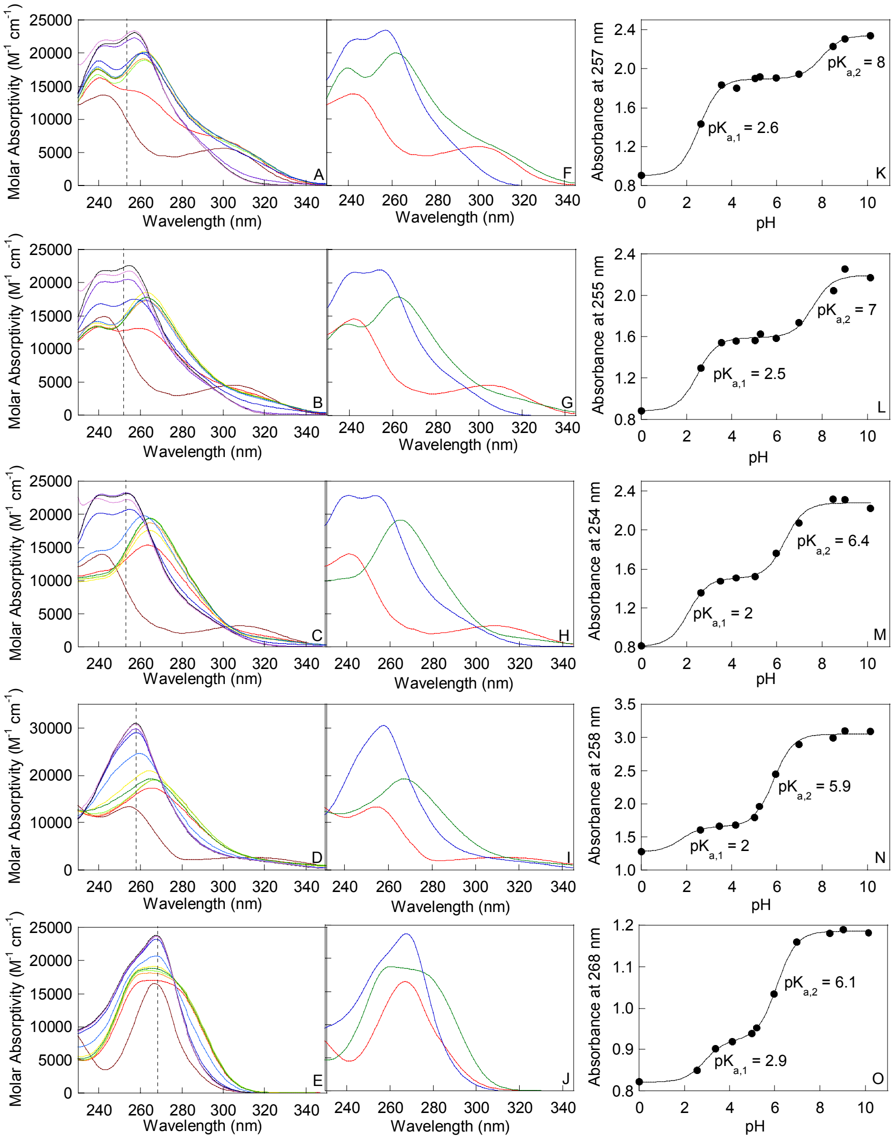

Figure S4. The absorbance spectra of 100 μM solutions of sulfamethazine (**1**, A), sulfamerazine (**2**, B), sulfadiazine (**3**, C), sulfachloropyridazine (**4**, D), and 50 μM solutions of sulfadimethoxine (**5**, E) in various pH buffers (red = low pH, purple = high pH) are shown in panels A-E, respectively. Panels F-J show the molar absorptivity of the components of each compound (**1**, F; **2**, G; **3**, H; **4**, I; **5**, J; blue = anionic component, green = neutral component, red = cationic component) calculated using matrix deconvolution as described previously (*2*). Panels A-E were used to determine panels K-O, and show the corresponding absorbance intensity at a single wavelength versus pH (**1**, K; **2**, L; **3**, M; **4**, N; **5**, O). The solid line represents a fit of the data to obtain the pK_as of the compounds.

Table S2. Tabulated absorption spectra of the components of **1-5**.

Molar absorptivities (M^{-1} cm^{-1}) of the components of 1-5.

		1			2			3			4			5	
Wavelength (nm)	**SH_2^+**	**SH**	**S^-**	**SH_2^+**	**SH**	**S^-**	**SH_2^+**	**SH**	**S^-**	**SH_2^+**	**SH**	**S^-**	**SH_2^+**	**SH**	**S^-**
400	0	0	0	2	5	0	0	13	27	3	81	0	0	0	0
399	0	0	0	2	5	0	0	13	27	2	81	0	0	0	0
398	0	0	0	3	5	0	1	13	27	3	82	0	0	0	0
397	0	0	0	2	5	0	1	13	27	3	84	0	0	0	0
396	0	0	0	1	5	0	2	17	27	3	87	1	0	0	0
395	0	0	0	2	5	0	3	17	27	4	92	2	0	0	0
394	0	0	0	2	6	0	2	17	28	4	97	2	0	0	0
393	0	0	0	2	6	0	3	18	28	4	102	2	0	0	0
392	0	0	0	1	6	0	2	19	28	4	108	1	0	0	0
391	0	0	0	0	6	0	3	19	29	4	115	1	0	0	0
390	0	0	0	0	7	0	2	20	29	4	121	1	0	0	0
389	0	0	0	0	7	0	1	21	29	3	129	1	0	0	0
388	0	0	0	1	8	0	2	22	30	4	136	1	0	0	0
387	0	0	0	1	8	0	2	23	30	6	144	1	0	0	0
386	0	0	0	0	9	0	4	24	31	8	152	1	0	0	0
385	0	0	0	1	9	0	4	25	31	11	162	1	0	0	0
384	0	0	0	0	10	0	3	27	32	13	171	2	0	0	0
383	0	0	0	0	11	0	3	28	32	13	180	2	0	0	0
382	0	0	0	0	11	0	2	29	32	15	191	2	0	0	0
381	0	0	0	0	12	0	3	30	33	17	201	2	0	0	0
380	0	0	0	0	13	0	4	32	34	20	213	2	0	0	0
379	0	0	0	0	14	0	6	34	34	24	225	2	0	0	0
378	0	0	0	0	15	0	5	37	34	28	238	2	0	0	0
377	0	0	0	0	17	0	4	38	35	32	251	3	0	0	0
376	0	0	0	0	19	0	4	40	36	38	264	3	0	0	0
375	0	0	0	0	22	0	4	43	36	47	279	3	0	0	0
374	0	0	0	0	23	0	6	46	36	57	294	5	0	0	0
373	0	0	0	0	25	0	8	49	37	69	310	7	0	0	0
372	0	0	0	0	27	0	10	52	37	83	326	8	0	0	0
371	0	0	0	0	30	0	12	55	37	94	344	9	0	0	0
370	0	0	0	0	32	0	11	58	38	107	362	12	0	0	0
369	0	0	0	0	35	0	12	63	39	122	383	13	0	0	0
368	0	0	0	0	38	0	11	67	39	134	402	16	0	0	0
367	0	0	0	0	41	0	10	71	40	153	422	18	0	0	0
366	0	0	0	0	45	0	14	76	40	175	443	20	0	0	0
365	0	0	0	0	54	0	14	87	42	194	484	29	0	0	0

Molar absorptivities (M^{-1} cm^{-1}) of the components of 1-5.

		1			2			3			4			5	
Wavelength (nm)	SH_2^+	SH	S^-	SH_2^+	SH	S^-	SH_2^+	SH	S^-	SH_2^+	SH	S^-	SH_2^+	SH	S^-
364	0	0	0	0	63	0	14	98	43	221	523	39	0	0	0
363	0	0	0	0	72	0	15	109	44	249	557	50	0	0	0
362	0	0	0	0	81	0	14	119	44	276	588	62	0	0	0
361	0	0	0	0	91	0	17	131	44	305	618	74	0	0	0
360	0	0	0	6	109	0	34	142	44	372	650	92	0	0	0
359	0	34	0	11	112	0	47	145	44	398	655	96	0	0	0
358	0	44	0	18	118	0	52	151	44	418	665	100	0	0	0
357	0	48	0	21	126	0	59	160	45	453	674	106	0	0	0
356	0	55	0	26	138	0	76	171	44	500	697	121	0	0	0
355	0	69	0	32	163	0	77	195	46	546	747	153	0	0	0
354	0	89	0	36	196	0	86	220	47	601	800	189	0	0	0
353	0	104	0	48	222	0	105	243	46	659	840	224	0	0	0
352	0	120	0	67	245	0	122	263	45	719	880	258	0	0	0
351	0	140	0	84	277	0	153	284	50	792	923	283	0	0	0
350	30	209	0	124	356	0	205	336	56	894	965	346	0	0	0
349	45	227	0	140	371	0	225	349	59	931	968	358	8	0	0
348	66	252	0	167	397	0	252	369	61	967	978	373	19	23	0
347	86	279	0	195	425	0	289	388	65	1025	992	386	40	40	0
346	100	312	0	225	460	0	328	412	67	1093	1020	420	37	39	0
345	115	351	0	259	499	0	372	439	68	1159	1050	459	38	39	0
344	131	395	0	296	543	0	419	468	69	1225	1082	503	37	42	0
343	152	447	0	339	592	0	472	500	69	1294	1116	549	35	42	0
342	178	505	0	388	645	0	531	533	70	1364	1151	598	38	43	0
341	207	568	0	442	702	0	594	568	71	1432	1186	651	40	45	0
340	240	639	0	503	762	0	661	603	73	1503	1223	704	42	46	0
339	274	717	0	570	825	0	733	640	75	1574	1258	760	45	48	0
338	314	803	0	644	892	0	809	677	77	1641	1295	817	47	50	0
337	360	896	0	725	961	0	890	716	79	1711	1333	875	48	49	0
336	412	997	0	814	1034	0	977	754	82	1779	1370	935	47	47	0
335	469	1106	0	908	1109	0	1065	794	87	1846	1409	994	44	50	0
334	537	1223	0	1011	1187	0	1162	833	94	1912	1449	1053	45	49	0
333	613	1350	0	1125	1268	0	1260	874	102	1977	1490	1113	44	52	0
332	699	1484	0	1245	1350	0	1363	915	111	2040	1532	1172	47	57	0
331	799	1628	0	1376	1435	0	1470	956	122	2101	1575	1229	53	58	0
330	908	1779	0	1513	1520	0	1576	997	135	2159	1620	1287	54	61	0
329	1028	1937	0	1654	1607	0	1686	1037	150	2213	1665	1343	57	62	0
328	1163	2104	0	1804	1695	0	1798	1077	167	2268	1713	1397	63	62	0
327	1307	2279	0	1956	1784	0	1908	1118	188	2317	1762	1451	63	66	0

Molar absorptivities (M^{-1} cm^{-1}) of the components of 1-5.

	1			2			3			4			5		
Wavelength (nm)	SH_2^+	SH	S^-	SH_2^+	SH	S^-	SH_2^+	SH	S^-	SH_2^+	SH	S^-	SH_2^+	SH	S^-
326	1465	2459	0	2113	1872	0	2019	1157	212	2364	1813	1504	65	72	0
325	1637	2645	0	2274	1960	12	2129	1196	240	2409	1866	1555	68	77	0
324	1821	2835	0	2437	2047	28	2233	1234	272	2447	1922	1605	68	87	0
323	2017	3029	0	2602	2133	48	2338	1272	309	2484	1980	1654	73	96	0
322	2226	3225	4	2770	2217	73	2441	1310	351	2519	2040	1703	80	107	0
321	2445	3424	15	2936	2301	102	2540	1349	399	2551	2105	1749	86	121	0
320	2672	3622	32	3101	2383	139	2634	1387	454	2580	2174	1797	94	135	0
319	2904	3819	53	3262	2463	181	2722	1427	515	2604	2246	1844	103	155	0
318	3141	4013	81	3416	2543	230	2800	1469	583	2623	2323	1890	113	181	0
317	3382	4206	118	3566	2622	290	2873	1514	658	2640	2406	1937	125	214	0
316	3625	4395	163	3707	2701	357	2940	1563	741	2654	2495	1985	142	259	0
315	3866	4579	218	3840	2780	434	2999	1616	833	2666	2591	2035	162	314	0
314	4102	4760	283	3963	2860	521	3052	1675	933	2674	2695	2086	186	381	3
313	4327	4936	361	4074	2941	619	3094	1741	1040	2677	2807	2139	213	465	17
312	4543	5108	452	4175	3026	729	3127	1817	1156	2678	2929	2194	244	568	34
311	4747	5276	558	4263	3113	851	3154	1903	1281	2675	3062	2252	282	691	59
310	4939	5440	678	4339	3206	983	3171	2001	1413	2670	3207	2312	328	836	94
309	5115	5600	815	4403	3304	1127	3181	2112	1553	2661	3364	2376	384	1007	134
308	5274	5758	967	4452	3409	1281	3182	2239	1698	2649	3536	2443	449	1208	180
307	5416	5913	1135	4488	3521	1446	3174	2381	1851	2636	3721	2513	526	1441	233
306	5538	6066	1318	4512	3643	1621	3161	2542	2009	2619	3924	2588	613	1709	294
305	5640	6218	1516	4526	3773	1805	3141	2722	2173	2601	4142	2668	711	2013	365
304	5723	6370	1730	4529	3914	1997	3117	2923	2340	2579	4378	2753	827	2358	446
303	5786	6524	1959	4522	4067	2196	3086	3145	2511	2554	4632	2843	958	2743	539
302	5828	6680	2202	4503	4231	2401	3048	3389	2688	2527	4904	2941	1109	3170	644
301	5852	6838	2457	4474	4410	2611	3005	3655	2868	2497	5196	3047	1279	3641	766
300	5858	7000	2726	4436	4601	2829	2956	3943	3052	2465	5508	3163	1468	4153	904
299	5850	7167	3005	4393	4807	3051	2907	4255	3238	2434	5841	3290	1681	4707	1065
298	5829	7340	3294	4343	5028	3276	2855	4588	3428	2402	6192	3428	1916	5301	1246
297	5795	7520	3591	4288	5264	3503	2801	4943	3620	2368	6564	3580	2176	5930	1452
296	5753	7706	3896	4228	5513	3732	2742	5315	3816	2335	6954	3746	2462	6591	1685
295	5701	7901	4205	4161	5776	3962	2680	5707	4014	2300	7363	3929	2773	7282	1943
294	5644	8104	4518	4092	6053	4193	2617	6115	4213	2265	7789	4130	3108	8000	2235
293	5582	8315	4833	4021	6343	4424	2554	6539	4413	2229	8230	4348	3471	8737	2560
292	5515	8536	5151	3951	6646	4654	2492	6976	4616	2192	8686	4587	3858	9486	2924
291	5449	8767	5471	3882	6961	4884	2431	7427	4821	2157	9154	4848	4266	10240	3330
290	5379	9008	5795	3814	7287	5115	2373	7889	5028	2122	9634	5133	4694	10986	3785
289	5307	9261	6121	3743	7625	5346	2316	8359	5238	2089	10123	5445	5133	11718	4289

Molar absorptivities (M^{-1} cm^{-1}) of the components of 1-5.

		1			2			3			4			5	
Wavelength (nm)	**SH_2^+**	**SH**	**S^-**	**SH_2^+**	**SH**	**S^-**	**SH_2^+**	**SH**	**S^-**	**SH_2^+**	**SH**	**S^-**	**SH_2^+**	**SH**	**S^-**
288	5235	9527	6449	3673	7975	5581	2264	8841	5452	2058	10623	5785	5582	12435	4849
287	5159	9807	6782	3606	8337	5818	2217	9330	5671	2028	11129	6155	6033	13125	5466
286	5081	10103	7120	3542	8711	6061	2173	9826	5898	2002	11639	6557	6487	13782	6148
285	5002	10416	7464	3482	9097	6309	2134	10330	6133	1985	12153	6994	6944	14400	6902
284	4922	10748	7817	3425	9496	6566	2098	10841	6377	1976	12672	7466	7404	14972	7727
283	4839	11099	8180	3373	9907	6833	2066	11356	6636	1979	13191	7977	7867	15500	8629
282	4758	11472	8554	3326	10332	7114	2040	11878	6909	2002	13710	8527	8349	15980	9605
281	4680	11868	8946	3288	10769	7411	2019	12406	7202	2045	14226	9119	8851	16410	10655
280	4604	12288	9354	3256	11219	7726	2006	12939	7517	2123	14738	9753	9391	16792	11780
279	4537	12728	9787	3234	11681	8064	2001	13477	7856	2242	15246	10431	9989	17119	12977
278	4484	13192	10244	3226	12153	8429	2010	14018	8225	2412	15747	11155	10648	17393	14236
277	4450	13677	10733	3240	12634	8825	2040	14559	8625	2648	16235	11926	11376	17618	15538
276	4441	14181	11253	3282	13122	9252	2097	15100	9061	2959	16708	12744	12161	17793	16866
275	4462	14702	11809	3355	13614	9717	2189	15635	9536	3350	17159	13613	12977	17930	18185
274	4504	15240	12404	3457	14107	10221	2312	16162	10054	3811	17593	14529	13777	18039	19455
273	4552	15782	13037	3569	14593	10766	2450	16673	10613	4313	17992	15497	14507	18128	20629
272	4588	16330	13710	3672	15074	11354	2575	17162	11216	4826	18355	16514	15126	18208	21663
271	4607	16879	14424	3752	15544	11984	2670	17620	11865	5333	18671	17581	15615	18281	22509
270	4620	17418	15180	3816	15993	12655	2733	18040	12556	5850	18927	18693	15983	18349	23138
269	4654	17932	15959	3892	16415	13361	2800	18404	13289	6406	19120	19841	16252	18407	23535
268	4732	18417	16768	4007	16796	14102	2902	18708	14060	7023	19237	21032	16427	18456	23705
267	4857	18859	17600	4170	17130	14875	3054	18941	14863	7692	19272	22244	16498	18498	23678
266	5024	19241	18446	4375	17408	15665	3250	19092	15690	8377	19219	23490	16460	18535	23489
265	5217	19560	19279	4601	17626	16467	3467	19154	16534	9044	19084	24710	16298	18572	23182
264	5429	19803	20108	4842	17774	17270	3688	19130	17382	9674	18863	25923	16016	18612	22803
263	5667	19963	20876	5100	17848	18056	3917	19012	18225	10271	18571	27093	15637	18655	22385
262	5945	20028	21570	5390	17848	18810	4173	18805	19044	10848	18216	28162	15174	18700	21957
261	6275	19999	22192	5733	17765	19516	4477	18510	19821	11403	17810	29093	14653	18736	21539
260	6661	19875	22711	6135	17607	20160	4843	18131	20541	11920	17383	29814	14080	18743	21140
259	7099	19660	23090	6598	17371	20724	5271	17681	21190	12374	16947	30285	13462	18699	20759
258	7579	19376	23320	7107	17079	21187	5755	17177	21737	12740	16517	30491	12805	18571	20394
257	8090	19028	23414	7654	16734	21535	6283	16626	22173	13007	16117	30430	12116	18338	20034
256	8626	18639	23386	8236	16346	21772	6853	16043	22497	13183	15739	30169	11410	17988	19668
255	9183	18230	23271	8849	15936	21906	7462	15443	22708	13274	15384	29775	10694	17517	19282
254	9752	17820	23086	9491	15511	21944	8105	14837	22805	13287	15045	29328	9979	16934	18860
253	10328	17427	22873	10150	15092	21913	8778	14240	22811	13228	14724	28819	9273	16253	18391
252	10896	17073	22656	10813	14692	21836	9469	13663	22759	13108	14417	28272	8584	15489	17871
251	11440	16777	22451	11462	14328	21731	10161	13116	22670	12936	14123	27706	7924	14658	17300

Molar absorptivities (M^{-1} cm^{-1}) of the components of 1-5.

		1			2			3			4			5	
Wavelength (nm)	**SH_2^+**	**SH**	**S^-**	**SH_2^+**	**SH**	**S^-**	**SH_2^+**	**SH**	**S^-**	**SH_2^+**	**SH**	**S^-**	**SH_2^+**	**SH**	**S^-**
250	11951	16549	22283	12083	14009	21635	10840	12608	22575	12726	13841	27074	7301	13788	16694
249	12414	16405	22152	12660	13750	21556	11488	12149	22497	12489	13566	26408	6725	12899	16067
248	12821	16349	22076	13181	13556	21508	12094	11743	22442	12239	13299	25721	6204	12018	15439
247	13165	16379	22050	13632	13431	21487	12639	11399	22425	11990	13047	24966	5742	11164	14826
246	13441	16491	22060	14001	13373	21495	13107	11114	22441	11753	12810	24149	5345	10345	14236
245	13645	16675	22080	14280	13377	21526	13488	10889	22499	11540	12592	23273	5020	9573	13680
244	13779	16913	22091	14467	13432	21568	13771	10715	22591	11358	12396	22365	4765	8855	13165
243	13847	17177	22069	14565	13523	21596	13957	10588	22694	11216	12227	21423	4589	8194	12694
242	13851	17434	21988	14582	13629	21583	14052	10498	22790	11120	12088	20459	4490	7594	12269
241	13805	17639	21831	14522	13727	21514	14060	10436	22841	11076	11978	19487	4470	7052	11886
240	13716	17753	21559	14404	13796	21361	13996	10390	22832	11084	11900	18511	4525	6568	11540
239	13601	17745	21185	14236	13813	21117	13874	10353	22731	11143	11848	17555	4653	6142	11230
238	13465	17600	20719	14030	13768	20785	13705	10315	22527	11253	11824	16626	4847	5772	10950
237	13316	17318	20161	13801	13650	20351	13506	10275	22213	11409	11826	15733	5099	5456	10699
236	13159	16910	19547	13557	13466	19837	13290	10232	21771	11613	11852	14883	5396	5194	10471
235	12993	16406	18899	13310	13221	19263	13068	10186	21243	11858	11902	14090	5725	4984	10264
234	12825	15826	18237	13065	12928	18648	12851	10142	20631	12139	11978	13356	6071	4822	10076
233	12659	15196	17582	12827	12597	18011	12648	10104	19983	12452	12081	12692	6423	4711	9901
232	12495	14536	16959	12606	12242	17378	12464	10076	19330	12790	12214	12102	6779	4645	9738
231	12342	13865	16390	12404	11874	16794	12307	10059	18725	13145	12381	11591	7135	4628	9588
230	12208	13197	15923	12230	11501	16294	12183	10051	18301	13516	12580	11169	7499	4658	9449
229	12099	12537	15707	12094	11129	16048	12107	10005	18584	13890	12810	10859	7874	4741	9329
228	12036	11869	16260	12010	10733	16712	12123	9754	21354	14267	13069	10688	8266	4884	9236
227	12106	10927	22212	12031	10163	21160	12089	9955	20153	14648	13341	10747	8679	5095	9191
226	12077	10491	20807	11997	9963	19807	12089	10221	18892	15038	13559	11502	9117	5390	9223
225	12060	9888	17359	11997	9761	16576	12108	10963	16041	15464	13921	14301	9581	5774	9411
224	11932	10117	5306	11918	10208	5906	12024	12475	7671	15650	15689	8017	10094	6184	10263
223	12051	9943	4981	12044	10303	5478	12132	13347	7123	15973	16504	8552	10866	5927	16265
222	12199	10031	4817	12198	10566	5231	12256	14235	6798	16271	17316	9165	11197	7335	12747
221	12366	10318	4786	12369	10946	5136	12395	15093	6657	16563	18157	9819	11459	9153	7599

1

Section S6. Growth of product **6** over the course of photolysis of **1**.

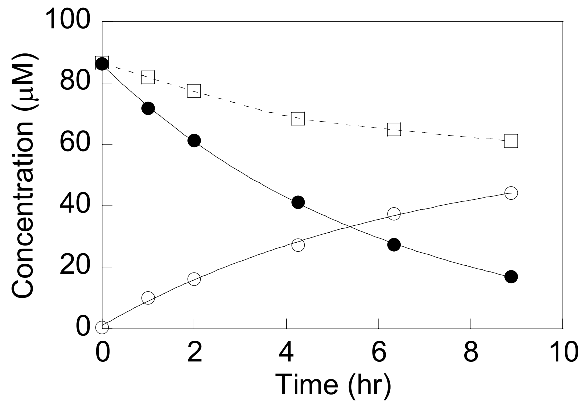

Figure S5. Growth of **6** (○) during the photolysis of **1** (●). Product **6** accounts for 63.6% of the loss of **1**. The amount of **1** and **6** are unable to account for the entire mass balance (□, ---) of the photolysis, and this may be due to inherent errors in the quantification of **6** or additional photoproduct formation that was not quantified.

Section S7. pH dependent direct photolysis of **5**, both buffered and unbuffered.

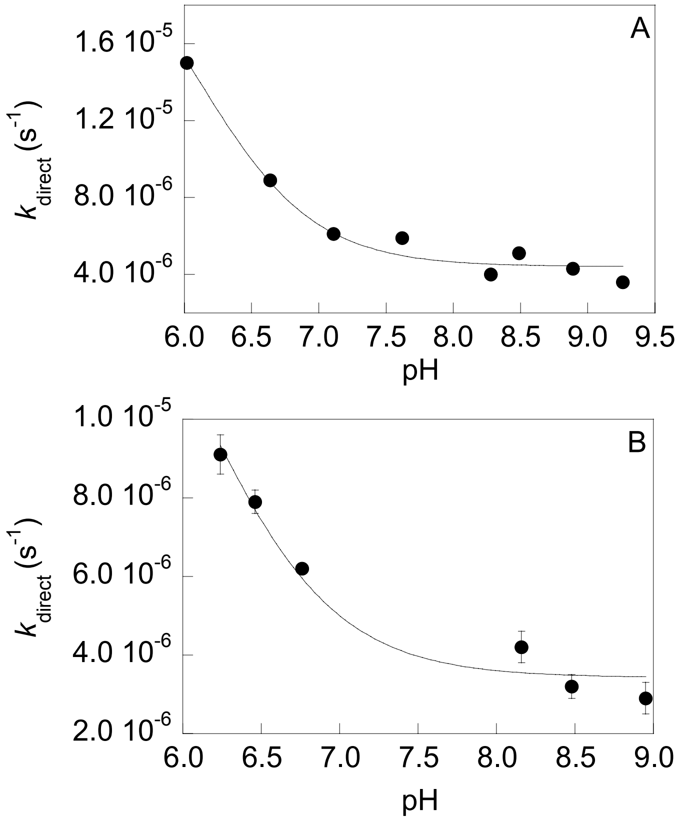

Figure S6. (A) pH dependent photolyses of 10 μM solutions of **5** in buffered H_2O solutions (pH 6 – 9.5). $k_{SH} = (2.4 \pm 0.1) \times 10^{-5}$ s^{-1}, $k_{S-} = (4.4 \pm 0.3) \times 10^{-6}$ s^{-1}. (B) pH dependent photolyses of 10 μM solutions of **5** in unbuffered H_2O solutions (pH 6-9). $k_{SH} = (1.8 \pm 0.1) \times 10^{-5}$ s^{-1}, $k_{S-} = (3.4 \pm 0.3) \times 10^{-6}$ s^{-1}. The solid line represents a fit to the data based on speciation as described previously (*2*).

Supporting Information References

(1) Buxton, G. V.; Greenstock, C. L.; Helman, W. P.; Ross, A. B. Critical review of rate constants for reactions of hydrated electrons, hydrogen atoms and hydroxyl radicals (·OH/·O-) in aqueous solution. *J. Phys. Chem. Ref. Data* **1988**, *17*, 513-886.

(2) Boreen, A. L.; Arnold, W. A.; McNeill, K. Photochemical fate of sulfa drugs in the aquatic environment: Sulfa drugs containing five-membered heterocyclic groups. *Environ. Sci. Technol.* **2004**, *38*, 3933-3940.