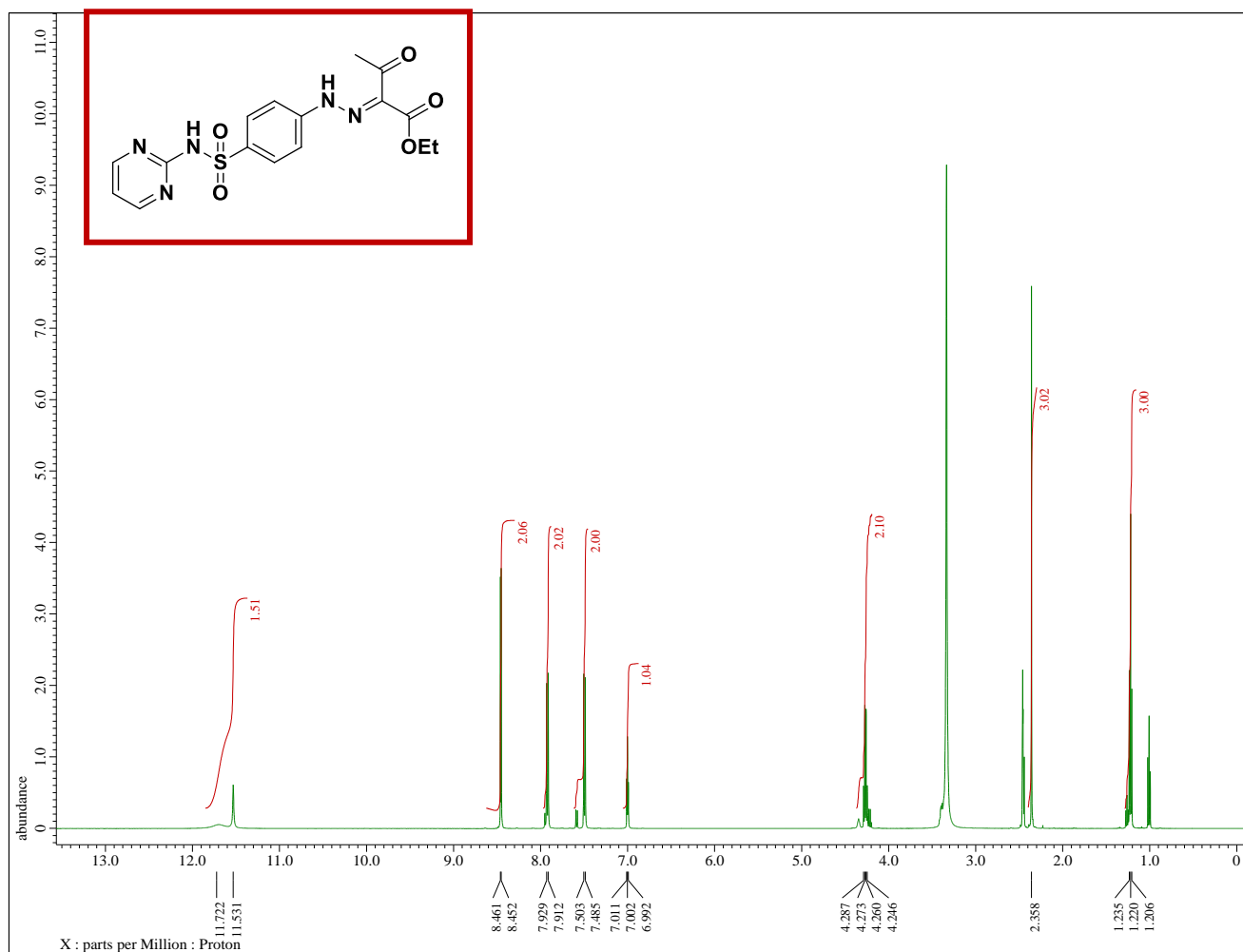
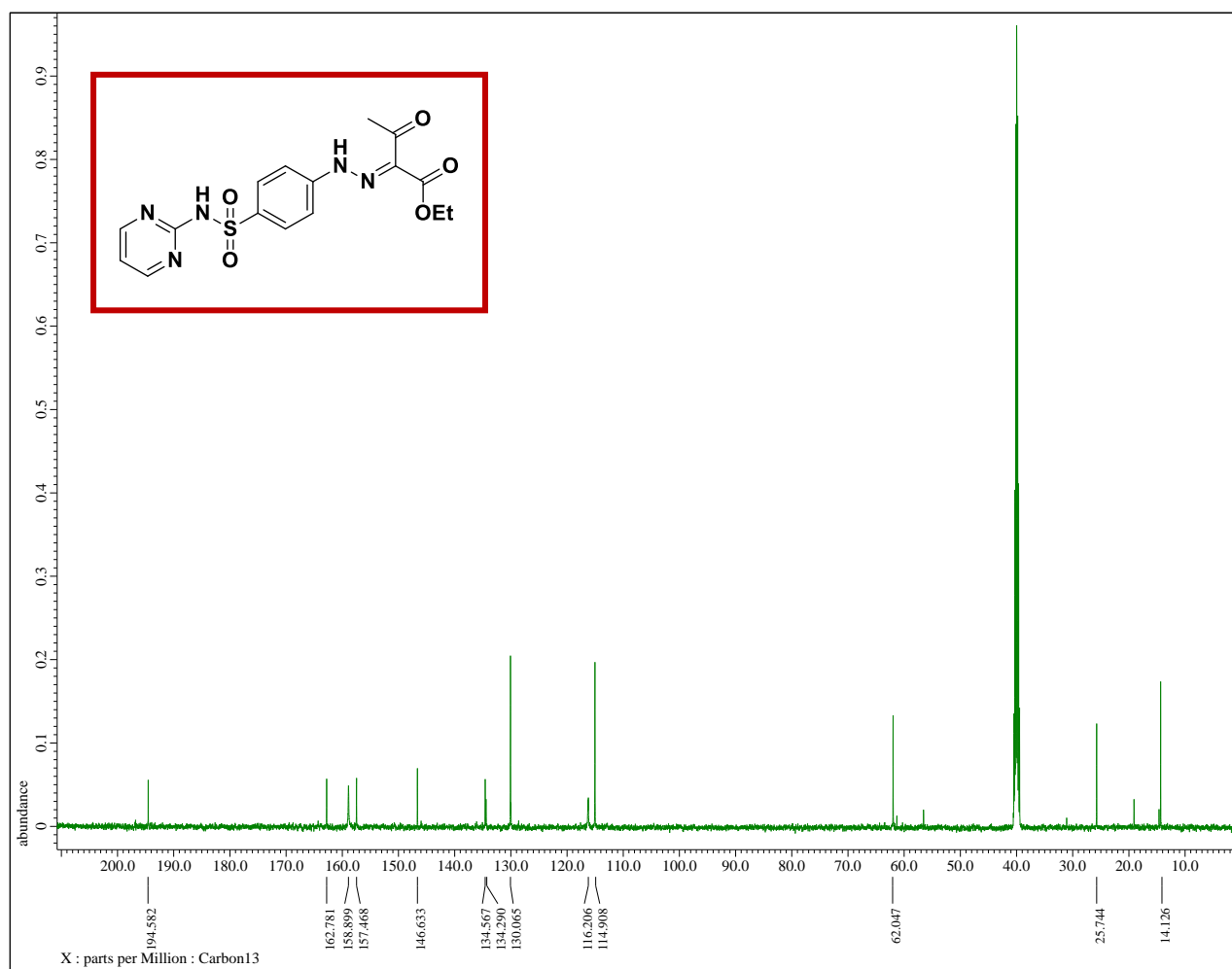


# Supplementary Materials: New Bioprecursor Prodrugs of Sulfadiazine: Synthesis, X-Ray structure and Hirshfeld Analysis

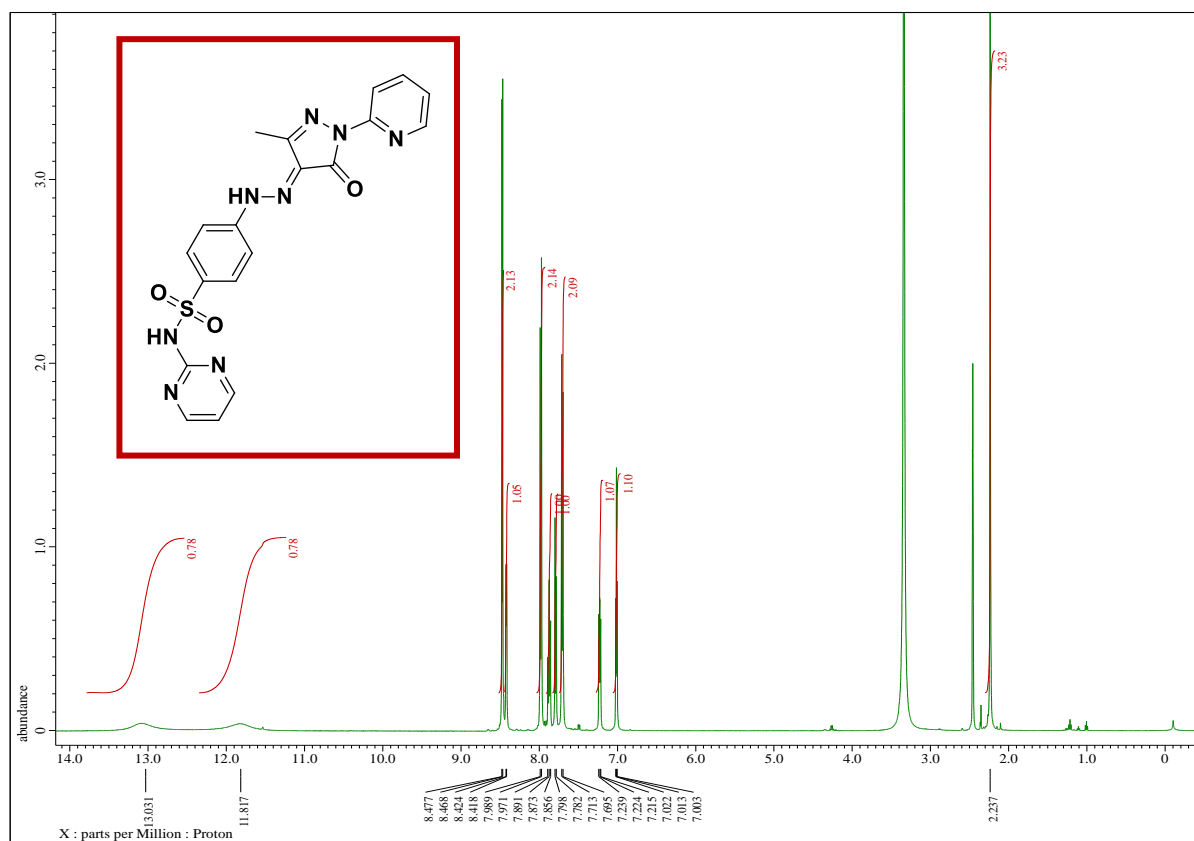
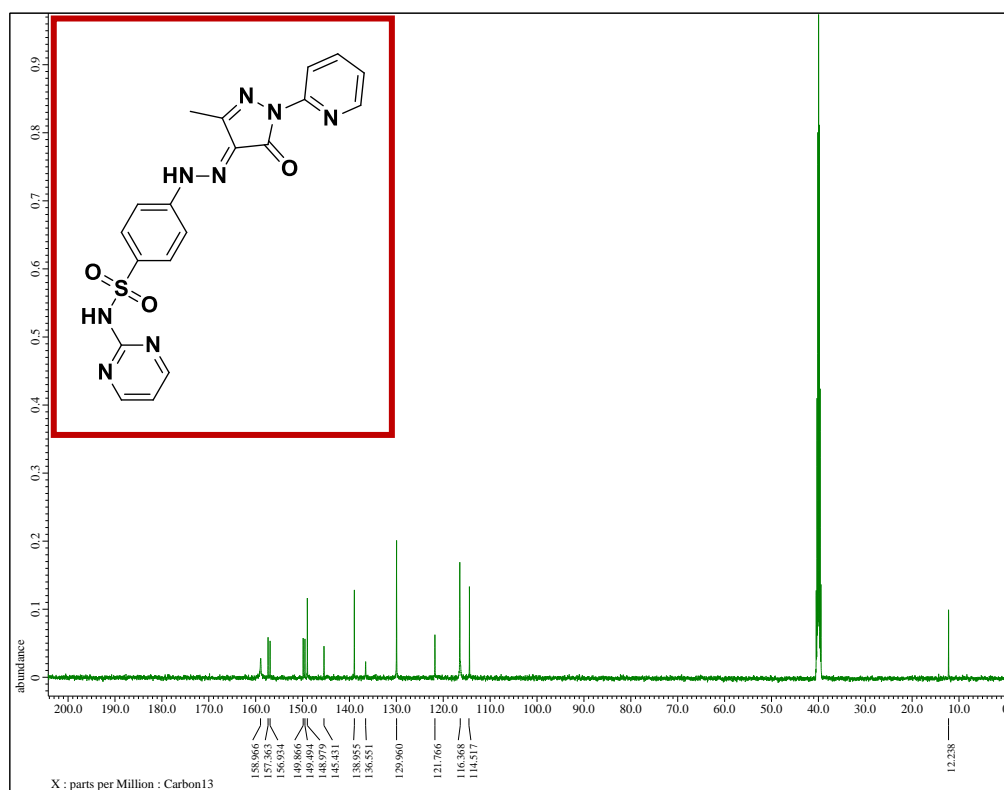
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**Figure S1:** <sup>1</sup>H NMR of 3 (DMSO-*d*<sub>6</sub>)



**Figure S2:**  $^{13}\text{C}$ NMR of **3** ( $\text{DMSO-d}_6$ )

Figure S3:  $^1\text{H}$ NMR of 5a (DMSO- $d_6$ )Figure S4:  $^{13}\text{C}$ NMR of 5 (DMSO- $d_6$ )

**Table S1** The calculated geometric parameters of **5<sup>a</sup>**.

Parameter	Calc	Exp	Parameter	Calc	Exp
<b>R(1-3)</b>	1.465	1.433	<b>A(3-1-4)</b>	121.932	118.696
<b>R(1-4)</b>	1.459	1.426	<b>A(3-1-10)</b>	101.858	103.466
<b>R(1-10)</b>	1.71	1.634	<b>A(3-1-34)</b>	108.485	109.687
<b>R(1-34)</b>	1.784	1.76	<b>A(4-1-10)</b>	110.129	110.776
<b>R(2-22)</b>	1.241	1.233	<b>A(4-1-34)</b>	108.47	108.384
<b>R(5-13)</b>	1.337	1.341	<b>A(10-1-34)</b>	104.569	104.95
<b>R(5-21)</b>	1.332	1.338	<b>A(1-10-39)</b>	126.514	125.517
<b>R(6-7)</b>	1.409	1.411	<b>A(1-10-47)</b>	111.816	115.975
<b>R(6-21)</b>	1.419	1.407	<b>A(1-34-32)</b>	118.999	118.308
<b>R(6-22)</b>	1.383	1.386	<b>A(1-34-35)</b>	119.76	120.387
<b>R(7-24)</b>	1.301	1.301	<b>A(2-22-6)</b>	129.311	128.141
<b>R(8-9)</b>	1.319	1.315	<b>A(2-22-23)</b>	126.924	127.952
<b>R(8-23)</b>	1.308	1.309	<b>A(13-5-21)</b>	117.564	116.218
<b>R(9-29)</b>	1.397	1.406	<b>A(5-13-14)</b>	115.574	117.878
<b>R(10-39)</b>	1.389	1.387	<b>A(5-13-15)</b>	123.885	124.241
<b>R(11-39)</b>	1.342	1.333	<b>A(5-21-6)</b>	115.929	115.303
<b>R(11-40)</b>	1.335	1.339	<b>A(5-21-19)</b>	123.767	124.204
<b>R(12-39)</b>	1.338	1.332	<b>A(7-6-21)</b>	119.479	119.172
<b>R(12-44)</b>	1.336	1.336	<b>A(7-6-22)</b>	112.047	111.726
<b>R(13-15)</b>	1.393	1.373	<b>A(6-7-24)</b>	107.796	107.33
<b>R(15-17)</b>	1.395	1.373	<b>A(21-6-22)</b>	128.474	128.949
<b>R(17-19)</b>	1.39	1.38	<b>A(6-21-19)</b>	120.304	120.49
<b>R(19-21)</b>	1.406	1.388	<b>A(6-22-23)</b>	103.764	103.907
<b>R(22-23)</b>	1.473	1.452	<b>A(7-24-23)</b>	110.884	110.85
<b>R(23-24)</b>	1.449	1.441	<b>A(7-24-25)</b>	121.854	122.507
<b>R(24-25)</b>	1.492	1.484	<b>A(9-8-23)</b>	117.447	117.999
<b>R(29-30)</b>	1.404	1.38	<b>A(8-9-29)</b>	121.578	118.855
<b>R(29-37)</b>	1.404	1.388	<b>A(8-9-46)</b>	117.765	119.327
<b>R(30-32)</b>	1.388	1.38	<b>A(8-23-22)</b>	127.431	128.26
<b>R(32-34)</b>	1.398	1.385	<b>A(8-23-24)</b>	127.061	125.531
<b>R(34-35)</b>	1.396	1.377	<b>A(29-9-46)</b>	120.656	121.07
<b>R(35-37)</b>	1.389	1.388	<b>A(9-29-30)</b>	121.683	120.934
<b>R(40-42)</b>	1.394	1.375	<b>A(9-29-37)</b>	117.835	118.082
<b>R(42-44)</b>	1.392	1.377	<b>A(9-46-2)</b>	135.313	134.246
			<b>A(39-10-47)</b>	115.405	118.152
			<b>A(10-39-11)</b>	114.695	114.618
			<b>A(10-39-12)</b>	117.974	117.457
			<b>A(39-11-40)</b>	115.558	115.008
			<b>A(11-39-12)</b>	127.298	127.923
			<b>A(11-40-41)</b>	116.08	118.652

	A(11-40-42)	122.737	122.688
	A(39-12-44)	115.487	114.736
	A(12-44-42)	122.866	123.104
	A(12-44-45)	116.058	118.452
	A(14-13-15)	120.541	117.88
	A(13-15-16)	120.709	121.038
	A(13-15-17)	117.635	117.936
	A(16-15-17)	121.656	121.026
	A(15-17-18)	120.673	119.886
	A(15-17-19)	119.762	120.231
	A(18-17-19)	119.565	119.882
	A(17-19-20)	122.062	121.43
	A(17-19-21)	117.386	117.147
	A(20-19-21)	120.551	121.424
	A(19-20-2)	122.734	124.101
	A(22-23-24)	105.508	106.168
	A(23-24-25)	127.261	126.619
	A(24-25-26)	110.804	109.471
	A(24-25-27)	110.812	109.48
	A(24-25-28)	109.672	109.467
	A(26-25-27)	107.201	109.474
	A(26-25-28)	109.15	109.462
	A(27-25-28)	109.146	109.473
	A(30-29-37)	120.481	120.979
	A(29-30-31)	119.53	120.275
	A(29-30-32)	119.389	119.443
	A(29-37-35)	120.023	119.477
	A(29-37-38)	119.881	120.267
	A(31-30-32)	121.08	120.282
	A(30-32-33)	120.524	120.208
	A(30-32-34)	119.755	119.577
	A(33-32-34)	119.714	120.215
	A(32-34-35)	121.216	121.301
	A(34-35-36)	119.751	120.429
	A(34-35-37)	119.133	119.154
	A(36-35-37)	121.115	120.418
	A(35-37-38)	120.096	120.256
	A(40-42-43)	121.992	121.735
	A(40-42-44)	116.041	116.533
	42-44)	121.966	121.732
	44-45)	121.075	118.444

<sup>a</sup>Atom numbering refer to **Fig. 6**

**Table S2** The calculated natural charges of **5<sup>a</sup>**.

Atom	Charge	Atom	Charge
S1	2.3582	C25	-0.7226
O2	-0.6363	H26	0.2560
O3	-0.9475	H27	0.2555
O4	-0.9180	H28	0.2655
N5	-0.4512	C29	0.1615
N6	-0.2774	C30	-0.2551
N7	-0.2271	H31	0.2684
N8	-0.1650	C32	-0.1952
N9	-0.3446	H33	0.2721
N10	-0.8910	C34	-0.3465
N11	-0.5071	C35	-0.1873
N12	-0.5157	H36	0.2817
C13	0.0286	C37	-0.2574
H14	0.2286	H38	0.2508
C15	-0.2934	C39	0.5956
H16	0.2460	C40	0.0658
C17	-0.1961	H41	0.2358
H18	0.2471	C42	-0.3494
C19	-0.2912	H43	0.2543
H20	0.2738	C44	0.0679
C21	0.3844	H45	0.2344
C22	0.6173	H46	0.4409
C23	0.0189	H47	0.4617
C24	0.2043		

<sup>a</sup>Atom numbering refer to **Fig. 6**