

## Supplementary Materials

### Synthesis of the Guanidine Derivative:

*N*-{[(7-(4,5-Dihydro-1*H*-imidazol-2-yl)-2-(*p*-tolyl)-6,7-dihydro-2*H*-imidazo[2,1-*c*][1,2,4]triazol-3(5*H*)-ylidene)amino]-(phenylamino)methylene}benzamide

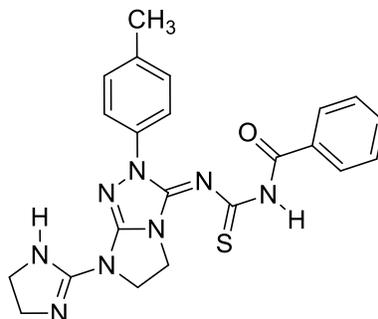
*Copies of IR, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, and MS spectra of compounds 2 and 3*

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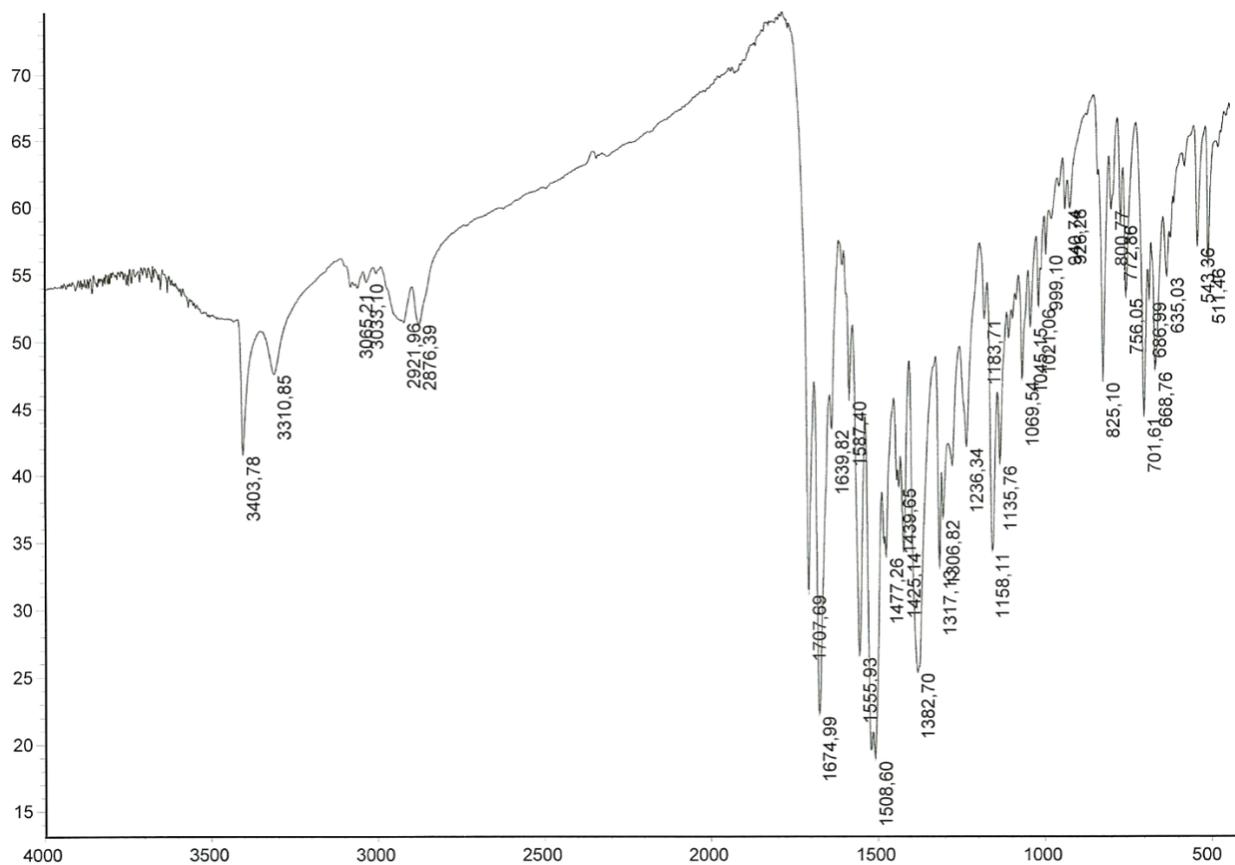
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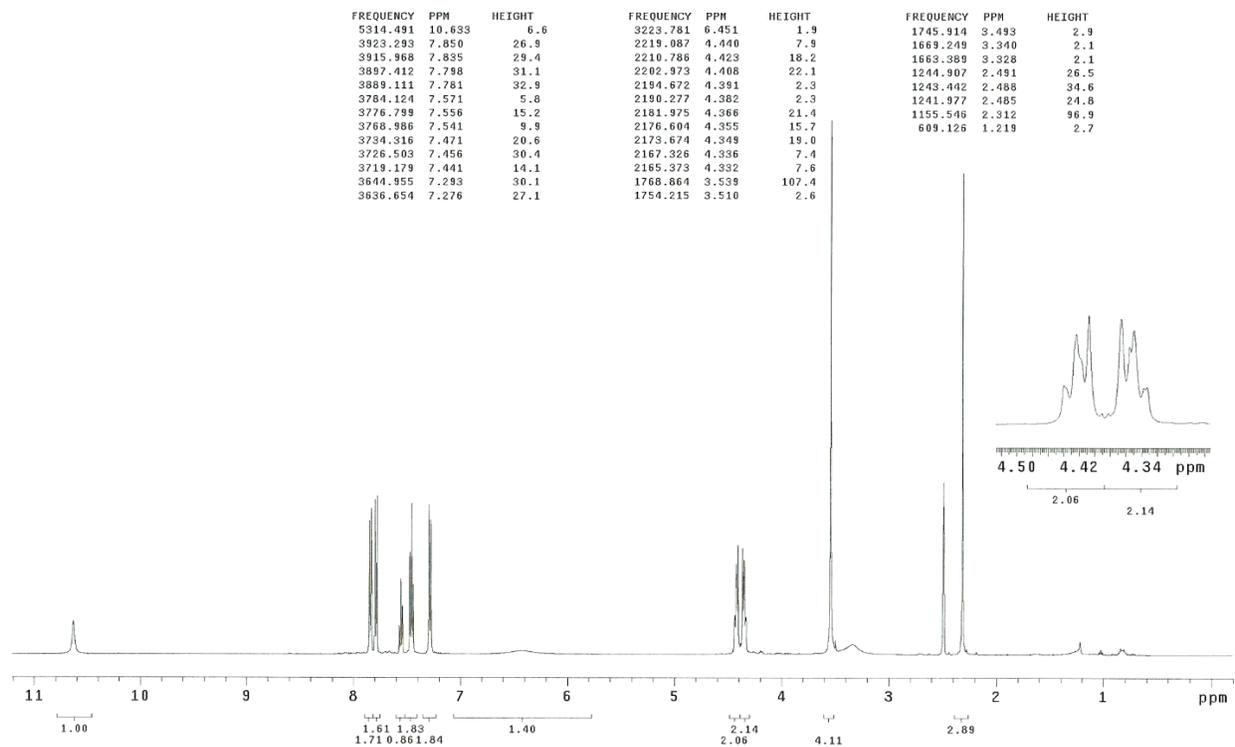
*N*-[7-(4,5-dihydro-1*H*-imidazol-2-yl)-2-(*p*-tolyl)-6,7-dihydro-2*H*-imidazo[2,1-*c*][1,2,4]triazol-3(5*H*)-ylidene]carbamothioyl]benzamide (**2**)



IR spectrum of **2** in KBr

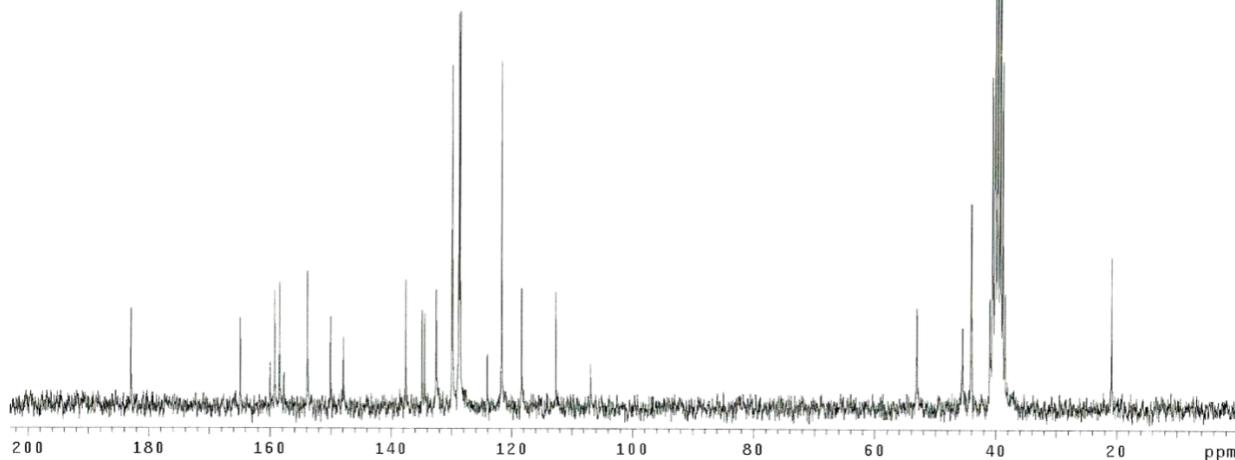


<sup>1</sup>H-NMR spectrum of 2 in DMSO-d<sub>6</sub> (500 MHz)



<sup>13</sup>C-NMR spectrum of **2** in DMSO-*d*<sub>6</sub> + TFA (125 MHz)

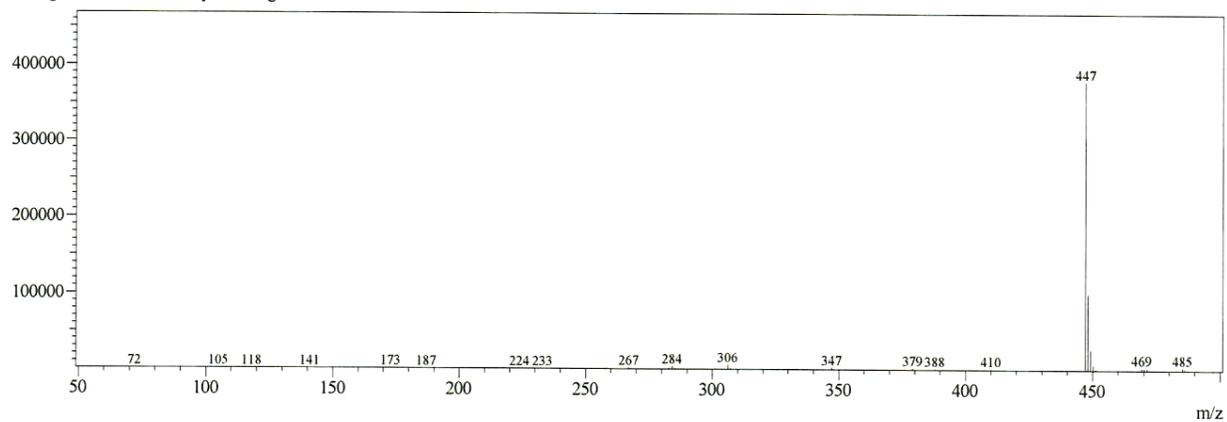
FREQUENCY	PPM	HEIGHT	FREQUENCY	PPM	HEIGHT
9197.819	182.927	18.4	5663.112	112.628	21.8
8289.989	164.872	16.6	5374.573	106.890	7.7
8043.229	159.964	8.0	2668.490	53.071	18.8
8004.932	159.203	21.8	2288.994	45.524	15.1
7966.634	158.441	23.4	2217.186	44.096	39.1
7928.336	157.679	5.9	2061.384	40.997	20.8
7735.977	153.854	25.7	2040.494	40.582	63.9
7545.359	150.063	16.9	2019.169	40.157	129.3
7437.429	147.916	12.8	1998.280	39.742	152.8
6917.798	137.582	24.0	1977.390	39.327	130.8
6781.145	134.864	18.1	1956.500	38.911	66.9
6759.385	134.431	17.4	1935.176	38.487	21.6
6663.235	132.518	22.1	1049.540	20.873	28.8
6530.904	129.887	65.9			
6476.069	128.797	76.1			
6466.929	128.615	76.6			
6239.754	124.097	9.6			
6120.074	121.717	66.6			
5951.216	118.358	22.5			



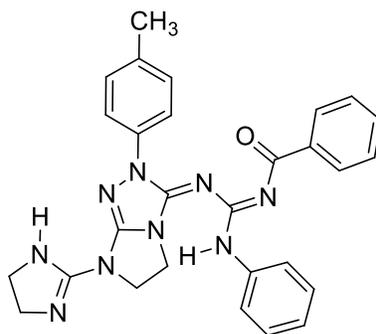
# MS spectrum of 2 (ESI)

## <Spectrum>

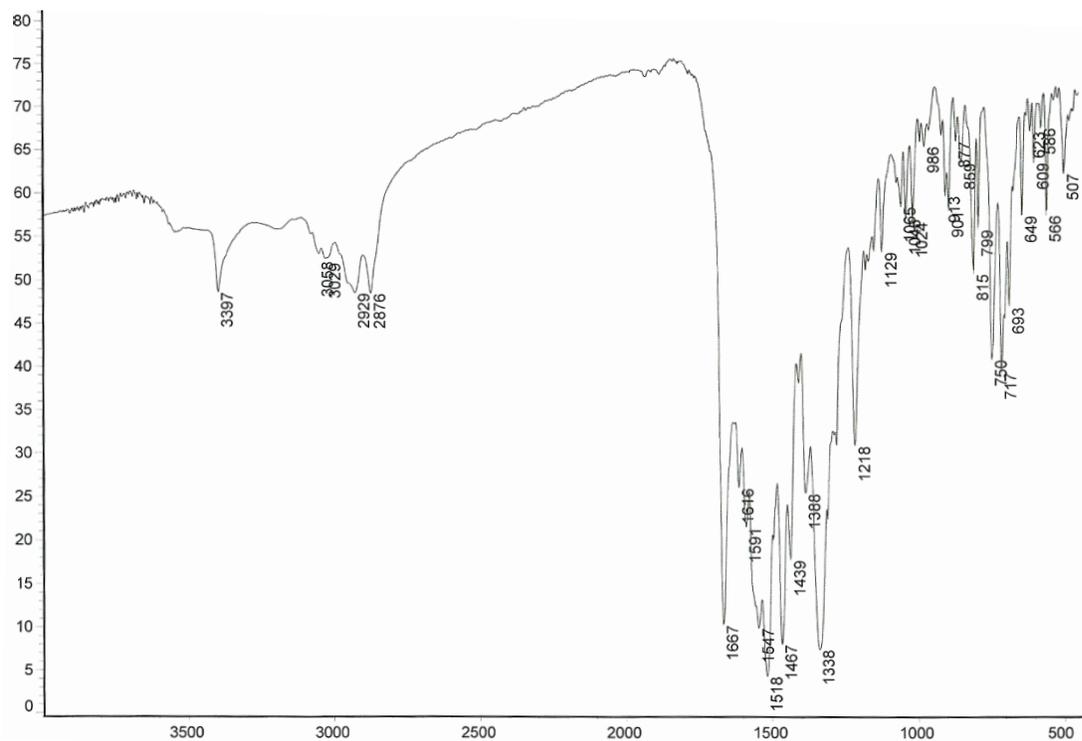
Retention Time: 2.817 (Scan#: 339)  
Max Peak: 449 Base Peak: 447.15 (379358)  
Spectrum: Single 2.817 (339)  
Background: None Polarity: Pos Segment: 1 - Event 1



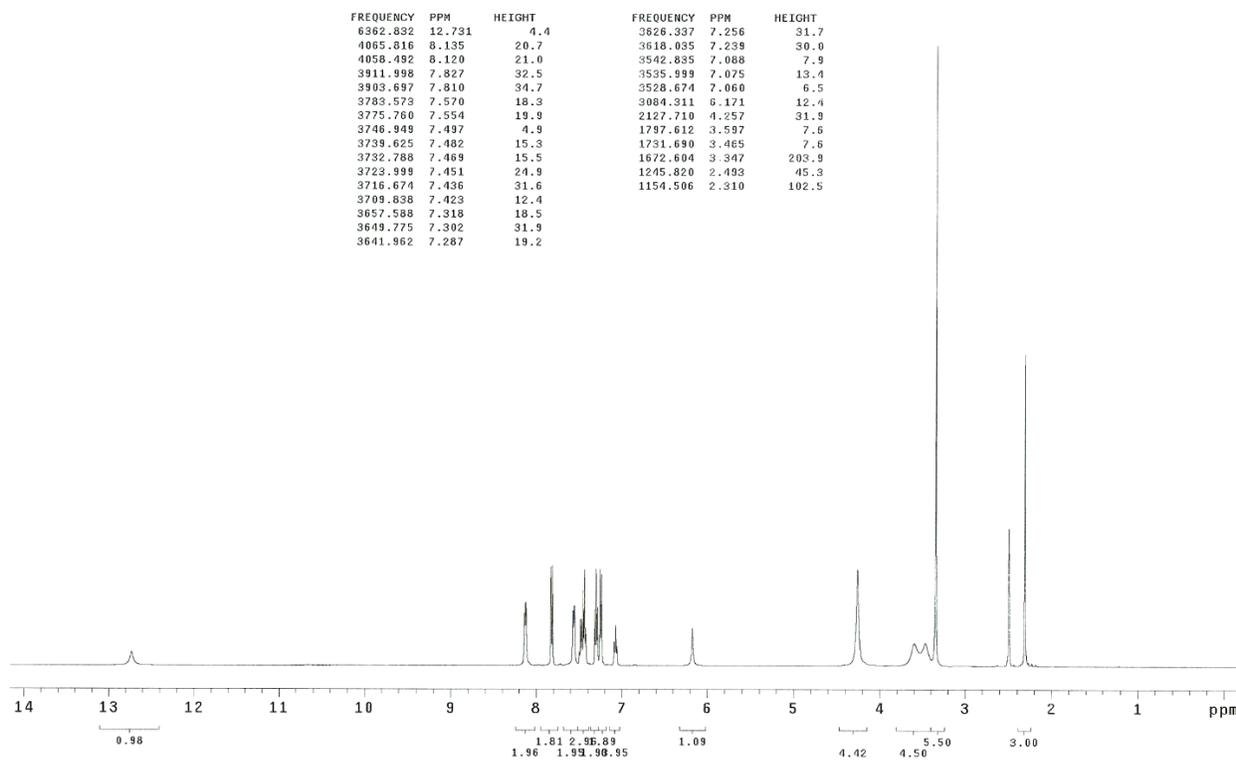
*N*-{[(7-(4,5-dihydro-1*H*-imidazol-2-yl)-2-(*p*-tolyl)-6,7-dihydro-2*H*-imidazo[2,1-*c*][1,2,4]triazol-3(5*H*)-ylidene)amino]-  
(phenylamino)methylene}benzamide (**3**)



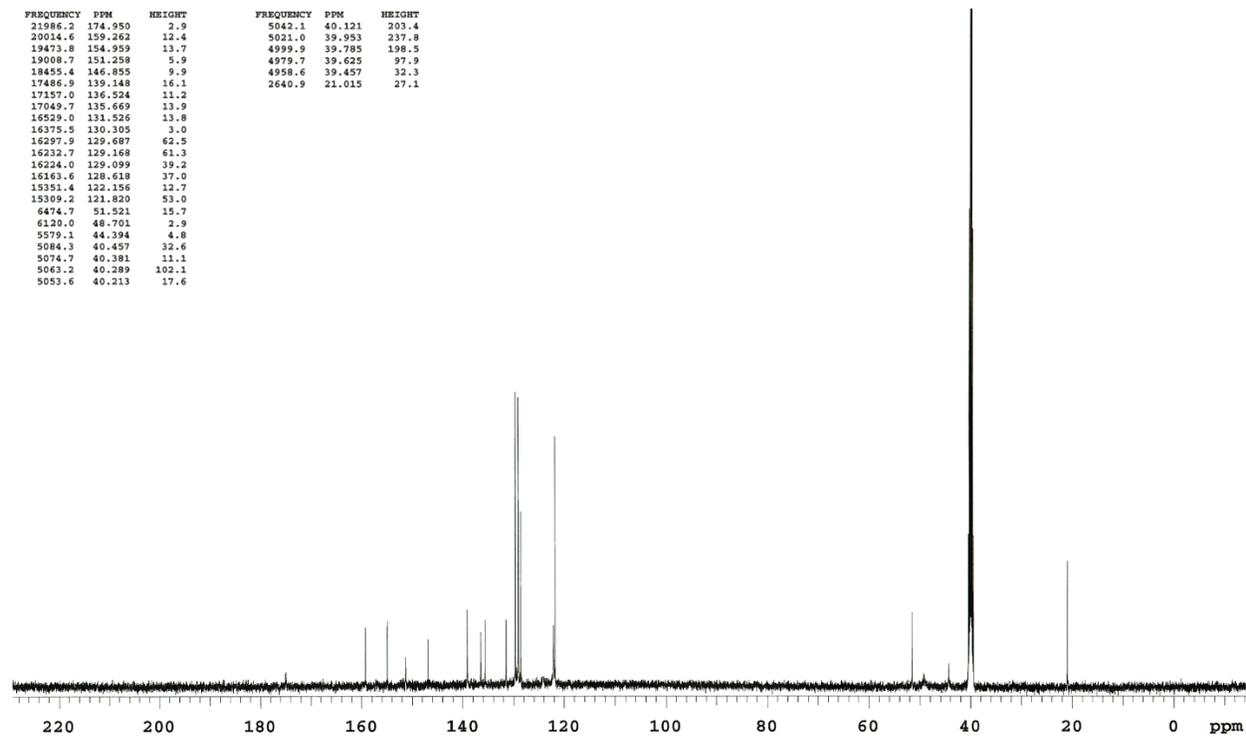
IR spectrum of **3** in KBr



<sup>1</sup>H-NMR spectrum of 3 in DMSO-d<sub>6</sub> (500 MHz)



$^{13}\text{C}$ -NMR spectrum of **3** in  $\text{DMSO-}d_6$  (125 MHz)



# MS spectrum of 3 (ESI)

## <Spectrum>

Retention Time: 2.233 (Scan#: 269)  
Max Peak: 695 Base Peak: 506.25 (467051)  
Spectrum: Single 2.233 (269)  
Background: None Polarity: Pos Segment1 - Event1

