

# Supplementary Materials

*Communication*

## 1-(Propane-2-ylidenehydrazono)-4-(*p*-tolyl)-2,3-diazaspiro[5.5]undec-3-ene

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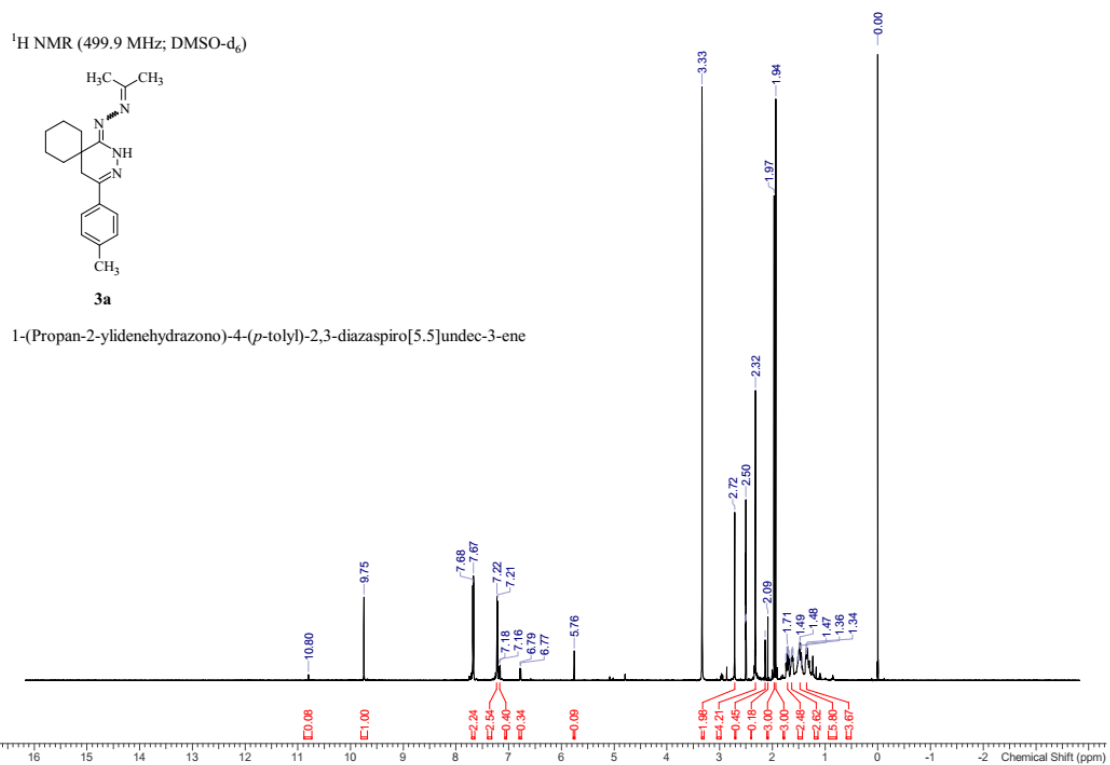
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**Abstract:** Earlier we published a new series of spiro[cycloalkane]pyridazinones with high Fsp<sup>3</sup> character. Our target was to synthesize further derivatives with nitrogen containing heterocycles, e.g., triazolo or tetrazolo rings. The corresponding thioxo derivatives (**1a,b**) were prepared too, which seemed to be good starting materials for the synthesis of tetrazolo derivatives. The reaction of the pyridazinethiones (**1a,b**) with hydrazine resulted surprisingly in the Schiff bases with acetone (**3a,b**) of the desired hydrazones (**2a,b**).

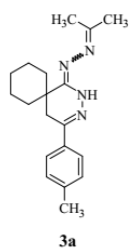
**Keywords:** pyridazinethione, spiro[cycloalkane]pyridazine, hydrazine, acetone, Schiff base

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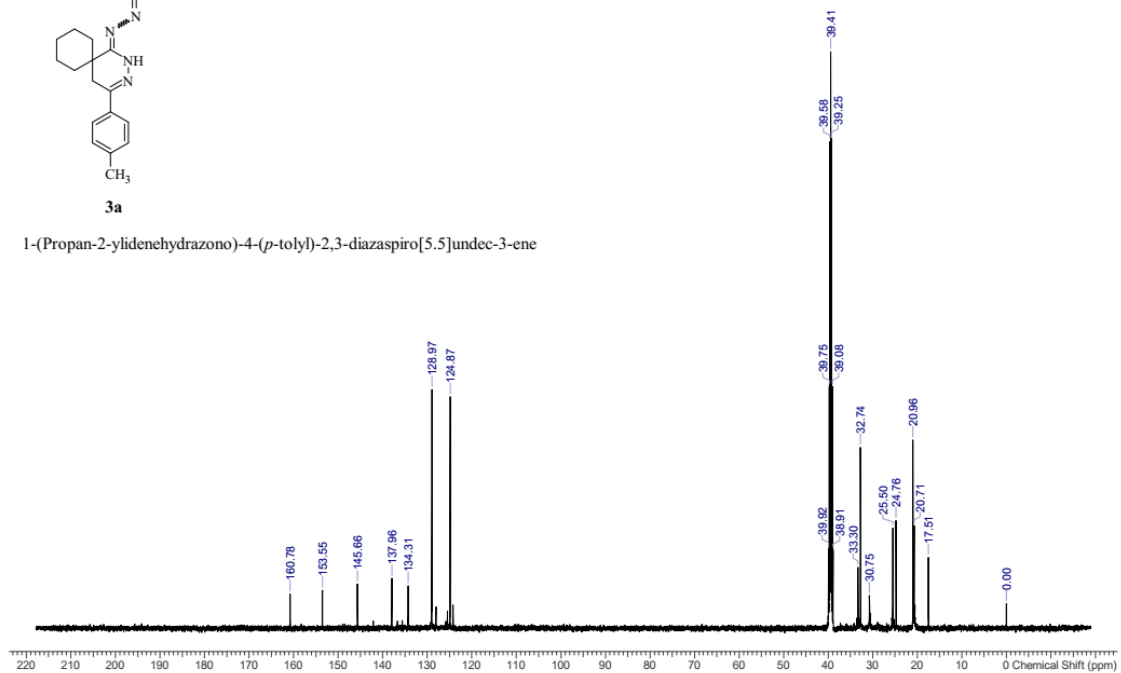


**Figure S1** The <sup>1</sup>H NMR spectrum of 1-(propan-2-ylidenehydrazono)-4-(*p*-tolyl)-2,3-diazaspiro[5.5]undec-3-ene (**3a**). The <sup>1</sup>H NMR spectrum was recorded in DMSO-d<sub>6</sub> solution with chemical shifts relative to tetramethylsilane.

<sup>13</sup>C NMR (125.7 MHz; DMSO-d<sub>6</sub>)

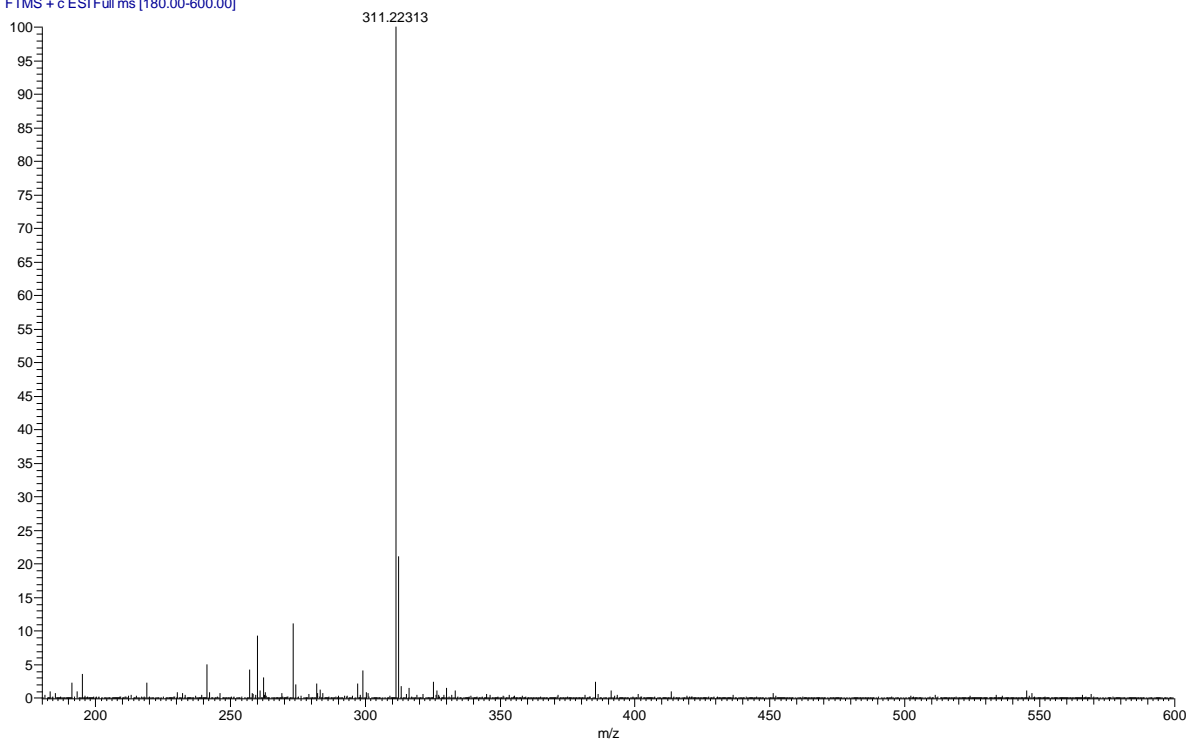


1-(Propan-2-ylidenehydrazono)-4-(*p*-tolyl)-2,3-diazaspiro[5.5]undec-3-ene

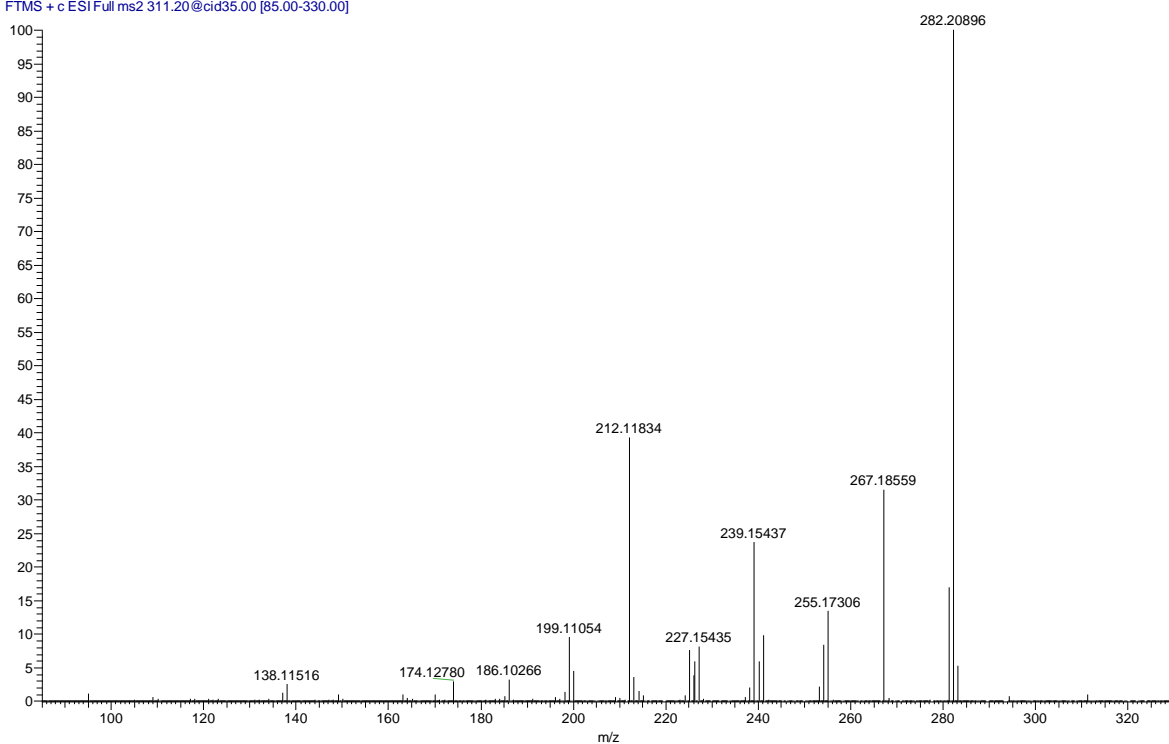


**Figure S2** The <sup>13</sup>C NMR spectrum of 1-(propan-2-ylidenehydrazono)-4-(*p*-tolyl)-2,3-diazaspiro[5.5]undec-3-ene (**3a**). The <sup>13</sup>C NMR spectrum was recorded in DMSO-d<sub>6</sub> solution with chemical shifts relative to tetramethylsilane.

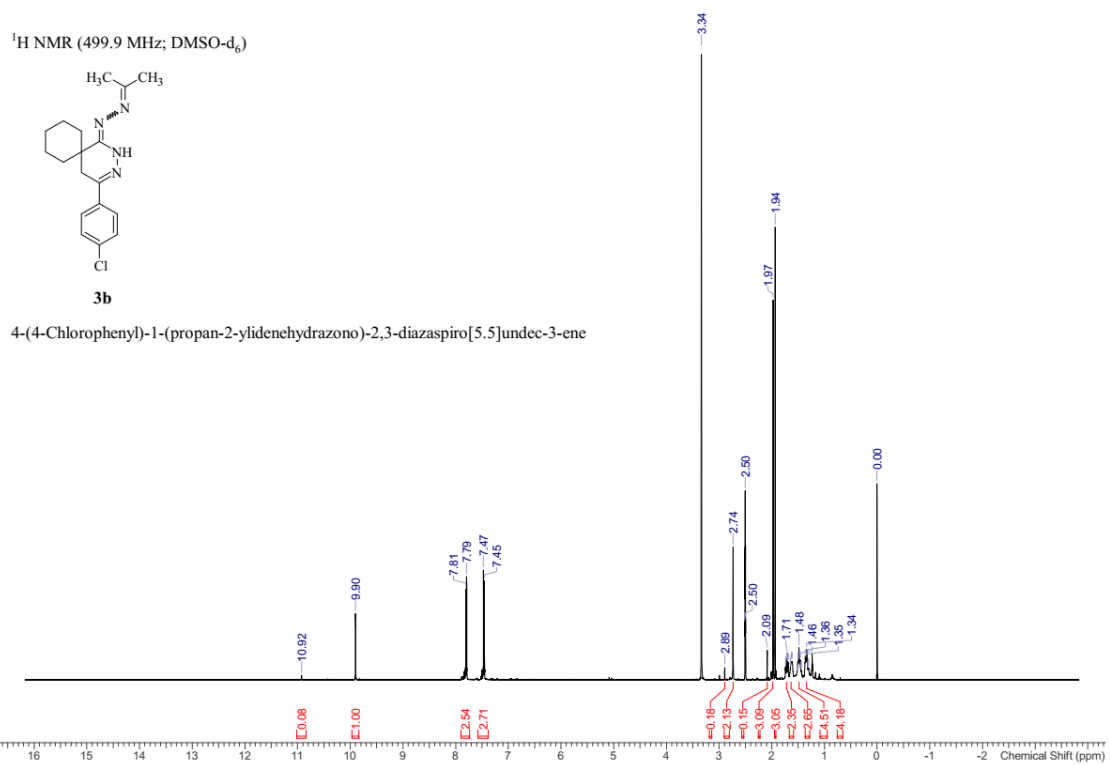
ku71205\_sfc-180-3\_d\_ve4234 #1-24 RT: 0.00-0.20 AV: 24 NL: 1.68E7  
T: FTMS + c ESI Full ms [180.00-600.00]



ku71205\_sfc-180-3\_d\_ve4235 #1-46 RT: 0.00-0.20 AV: 46 NL: 5.54E6  
T: FTMS + c ESI Full ms2 311.20@cid35.00 [85.00-330.00]

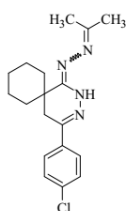


**Figure S3** The HR-MS and HR-MS-MS spectrum of 1-(propan-2-ylidenehydrazono)-4-(*p*-tolyl)-2,3-diazaspiro[5.5]undec-3-ene (**3a**)



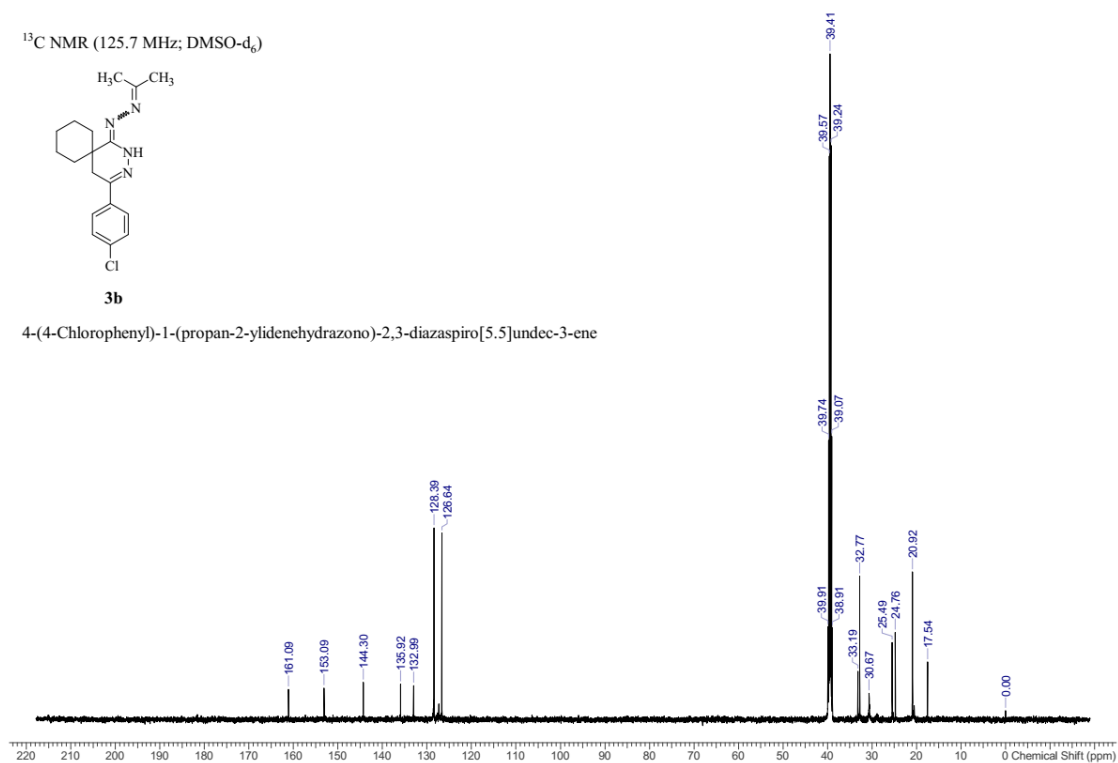
**Figure S4** The <sup>1</sup>H NMR spectrum of 4-(4-chlorophenyl)-1-(propan-2-ylidenehydrazono)-2,3-diazaspiro[5.5]undec-3-ene (**3b**). The <sup>1</sup>H NMR spectrum was recorded in DMSO-d<sub>6</sub> solution with chemical shifts relative to tetramethylsilane.

<sup>13</sup>C NMR (125.7 MHz; DMSO-d<sub>6</sub>)



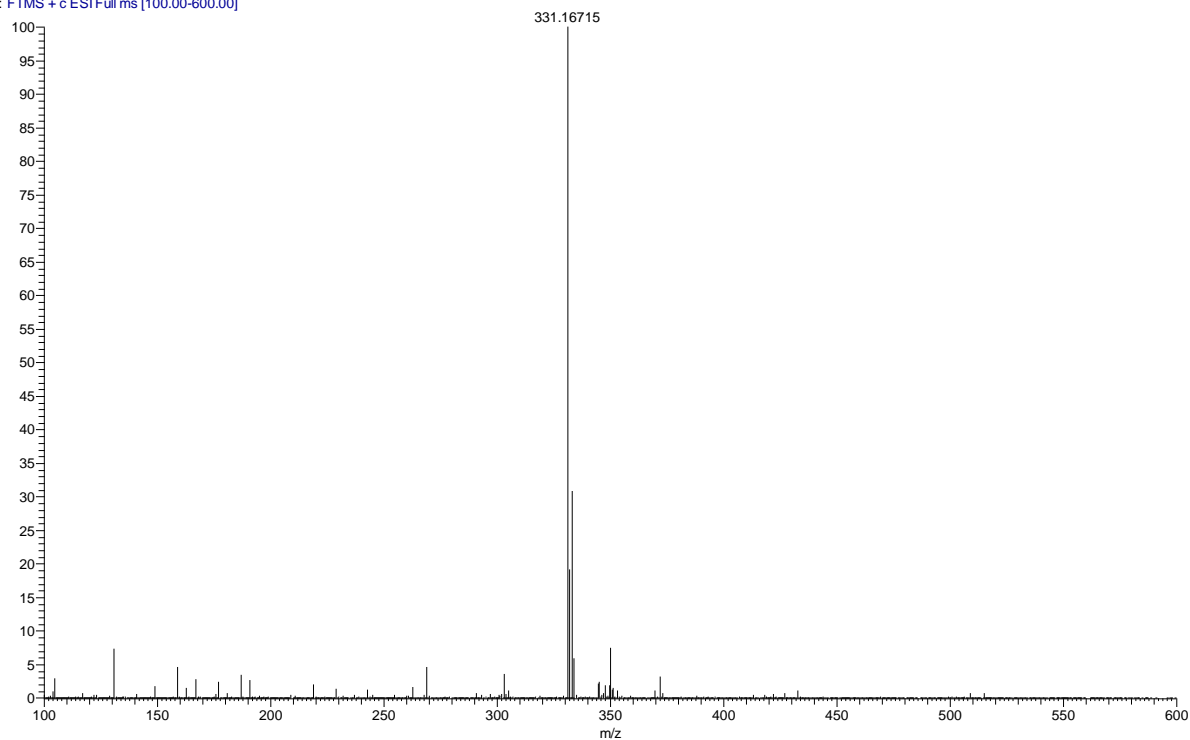
**3b**

4-(4-Chlorophenyl)-1-(propan-2-ylidenehydrazono)-2,3-diazaspiro[5.5]undec-3-ene



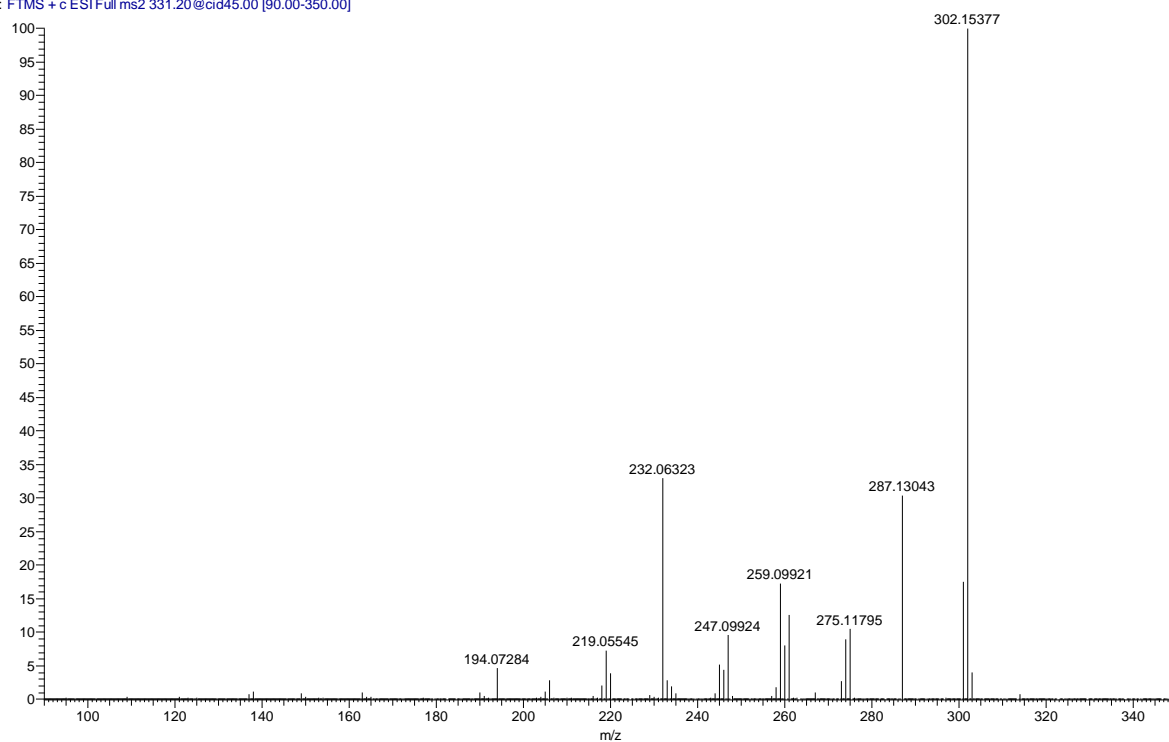
**Figure S5** The <sup>13</sup>C NMR spectrum of 4-(4-chlorophenyl)-1-(propan-2-ylidenehydrazono)-2,3-diazaspiro[5.5]undec-3-ene (**3b**). The <sup>13</sup>C NMR spectrum was recorded in DMSO-d<sub>6</sub> solution with chemical shifts relative to tetramethylsilane.

ku70811\_sfc-170-1\_d\_ve3866 #1-24 RT: 0.00-0.19 AV: 24 NL: 1.59E7  
T: FTMS + c ESI Full ms [100.00-600.00]



### HR-MS-MS spectrum (SFC-170-1)

ku70811\_sfc-170-1\_d\_ve3867 #1-46 RT: 0.00-0.20 AV: 46 NL: 7.79E6  
T: FTMS + c ESI Full ms2 331.20@cid45.00 [90.00-350.00]



**Figure S6** The HR-MS and HR-MS-MS spectrum of 4-(4-chlorophenyl)-1-(propan-2-ylidenehydrazono)-2,3-diazaspiro[5.5]undec-3-ene (**3b**)