

## 1 Supplementary information

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16	complex (L <sub>1b</sub> Pt-b).....	23
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### 23 4. Supplementary figures for biological studies

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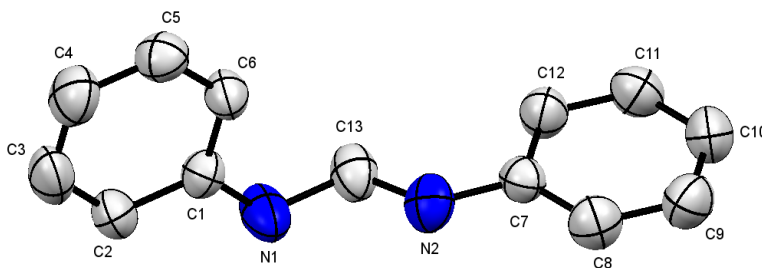
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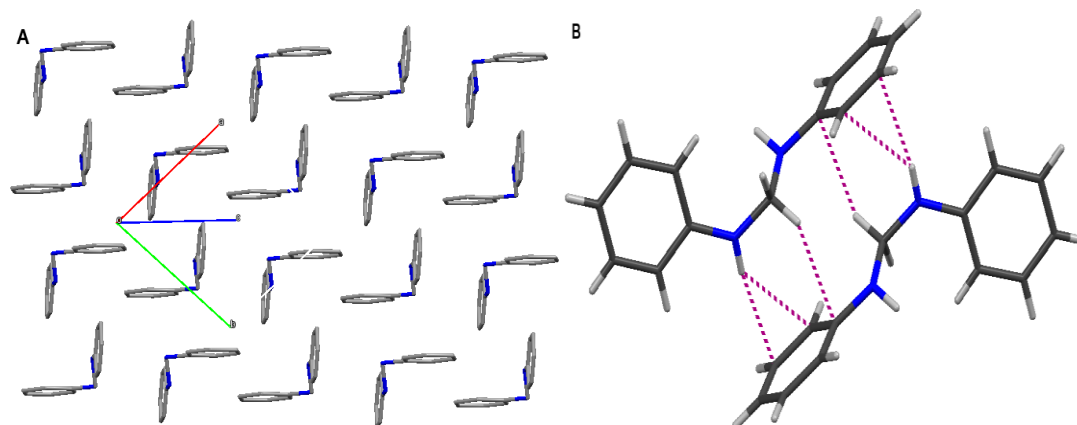
1 **1. X-ray data collection, structure resolution and model refinement of 2a**

2 The crystal data were obtained with Bruker APEX II QUAZAR three-circle  
3 diffractometer. Indexing was performed using APEX2 [S1]. Data integration and  
4 reduction were carried out with SAINT [S2]. Absorption correction was performed by  
5 multi-scan method implemented in SADABS [S3]. The structure was solved using  
6 SHELXT [S4] and then refined by full-matrix least-squares refinements on  $F^2$  using the  
7 SHELXL [S4] in OLEX2 [S5]. All nonhydrogen atoms were refined anisotropically  
8 using all reflections with  $I > 2\sigma(I)$ . Aromatic and aliphatic C-bound H atoms were  
9 positioned geometrically and refined using a riding mode. Crystallographic data and  
10 refinement details of the data collection for **2a** are given in **Table S** Mercury was used  
11 for visualization of the cif file [S6]. Additional crystallographic data with CCDC  
12 reference number 2306536 have been deposited within the Cambridge Crystallographic  
13 Data Center via the following link: [www.ccdc.cam.ac.uk/deposit](http://www.ccdc.cam.ac.uk/deposit)

14 N,N'-Diphenylmethanediamine **2a**,  $C_{13}H_{14}N_2$ , forms triclinic crystals. A view of the  
15 compound **2a** is shown on **Figure S1**. In the crystal structure, the intermolecular  
16 interactions are primarily of N—H $\cdots\pi$  and C—H $\cdots\pi$  character, without any  
17 contribution from N—H $\cdots$ N hydrogen bonding. Taken together, N—H $\cdots\pi$  and C—  
18 H $\cdots\pi$  interactions form crystal package of the structure (**Figure S2**).



19  
20 **Figure S1.** ORTEP plot of **2a**, with the atom-numbering scheme. Displacement ellipsoids drawn  
21 at the 50% probability level. All H atoms have been omitted.

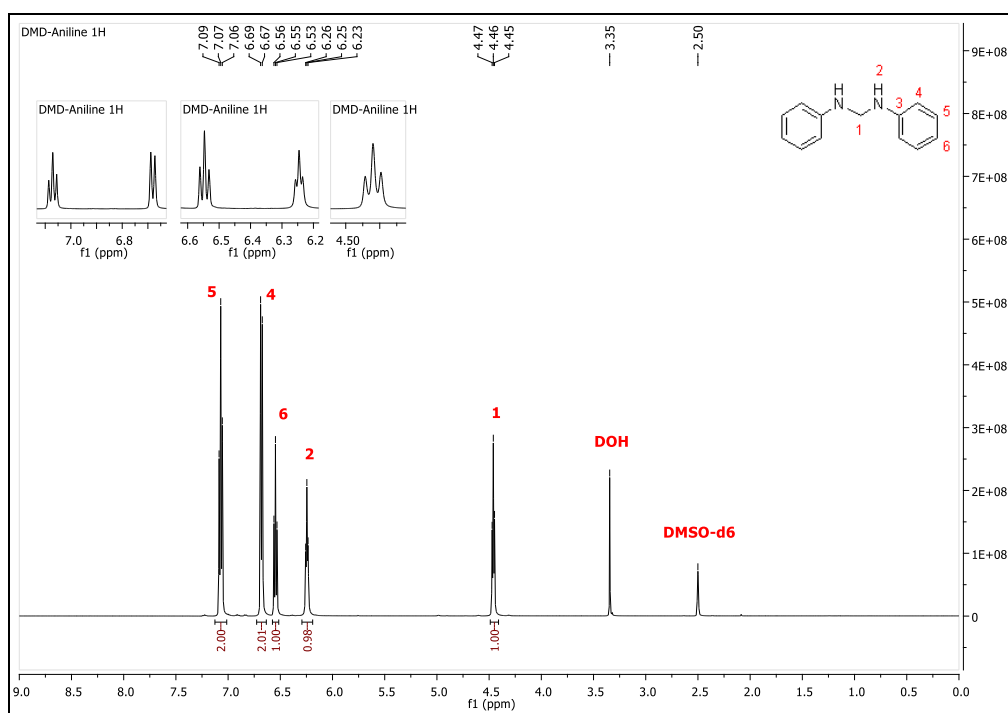


1  
 2 **Figure S2.** A) The pleated form of the layers, viewed in the direction of propagation of the  
 3 pleats. B) The N—H···π and C—H···π interactions indicated by dashed lines (symmetry code:  
 4  $-x, -y, -z$ ).

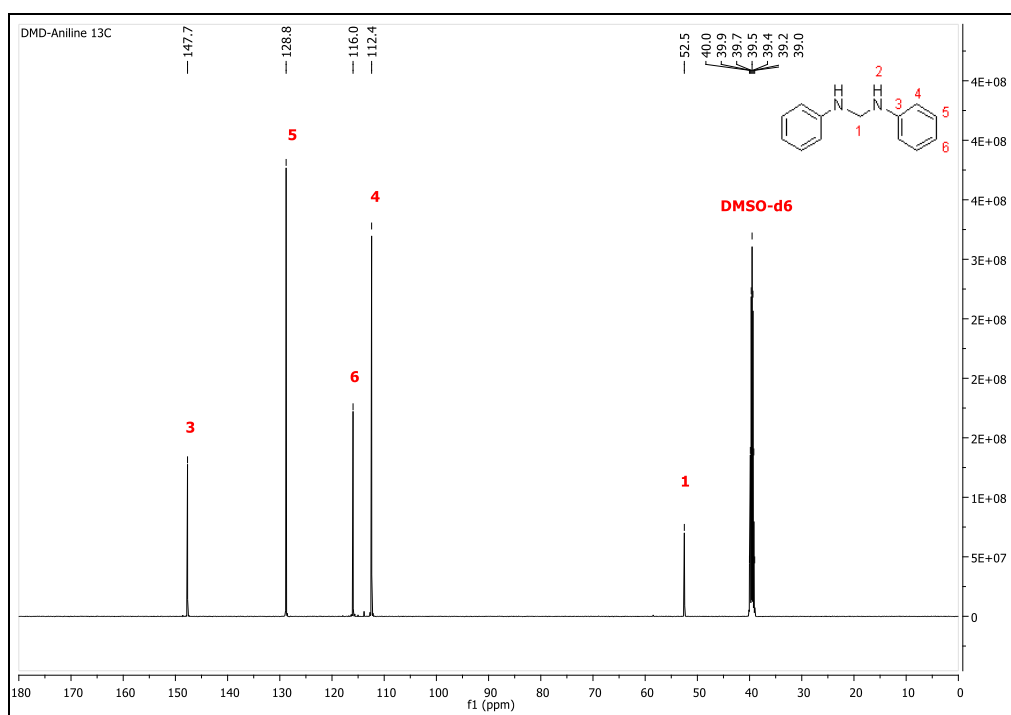
5 **Table S.** Crystal data and refinement parameters for 2a.

<b>Empirical formula</b>	0.5(C <sub>6.5</sub> H <sub>7</sub> N)
<b>Formula weight (g mol<sup>-1</sup>)</b>	99.13
<b>Temperature (K)</b>	296.15
<b>Crystal system</b>	Triclinic
<b>Space group</b>	<i>P</i> -1
<b><i>a</i> (Å)</b>	7.118 (4)
<b><i>b</i> (Å)</b>	7.596 (4)
<b><i>c</i> (Å)</b>	10.967 (6)
<b><math>\alpha</math> (°)</b>	72.24 (4)
<b><math>\beta</math> (°)</b>	77.59 (4)
<b><math>\gamma</math> (°)</b>	85.39 (4)
<b>Crystal size (mm)</b>	0.244 × 0.12 × 0.047
<b><i>V</i> (Å<sup>3</sup>)</b>	551.5(6)
<b><i>Z</i></b>	4
<b><math>\rho_{\text{calcd}}</math> (g cm<sup>-3</sup>)</b>	1.194
<b><math>\mu</math> (mm<sup>-1</sup>)</b>	0.072
<b><i>F</i>(000)</b>	212.0
<b>2 <math>\theta</math> range for data collection (°)</b>	3.98 to 49.996
<b><i>h</i>/<i>k</i>/<i>l</i></b>	$-8 \leq h \leq 8, -6 \leq k \leq 8, -13 \leq l \leq 13$
<b>Reflections collected</b>	4175
<b>Independent reflections</b>	1849 [Rint = 0.0772, Rsigma = 0.1122]
<b>Data/restraints/parameters</b>	1851/0/137
<b>Goodness-of-fit on <i>F</i><sup>2</sup></b>	0.892
<b>Final <i>R</i> indices [<i>I</i> &gt; 2<math>\sigma</math>(<i>I</i>)</b>	<i>R</i> 1 = 0.0748, <i>wR</i> 2 = 0.1759
<b><i>R</i> indices (all data)</b>	<i>R</i> 1 = 0.1607, <i>wR</i> 2 = 0.2143
<b>Largest diff. peak and hole (e.Å<sup>-3</sup>)</b>	0.46/−0.39
<b>CCDC</b>	2306536

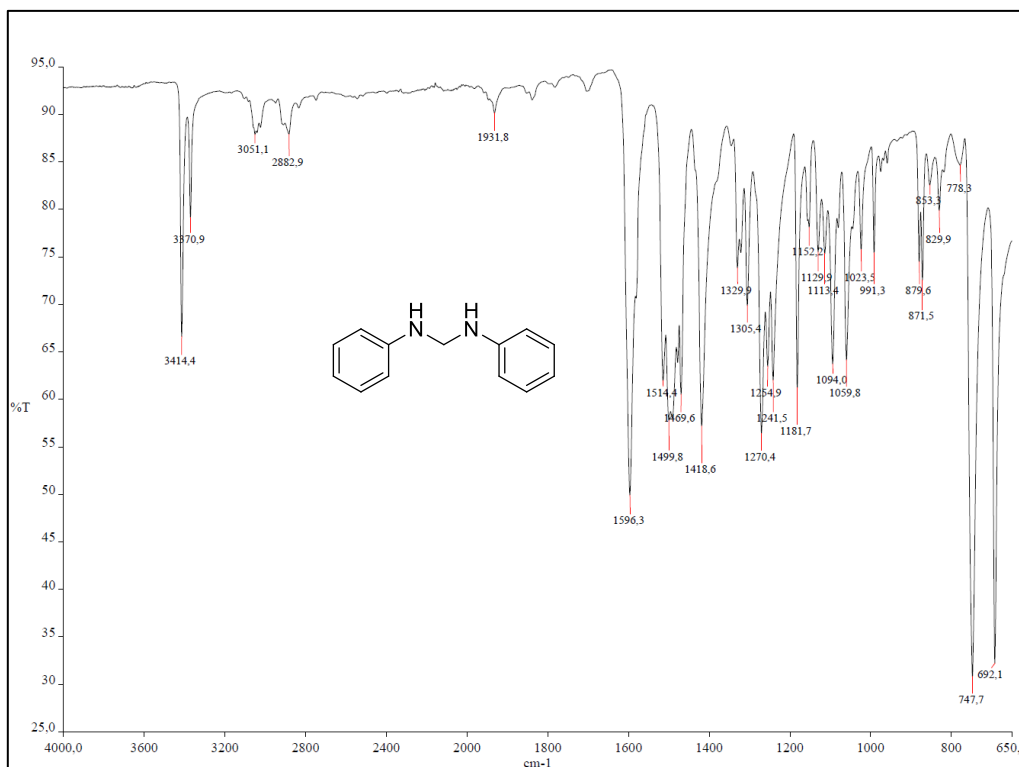
- 1 **2. Supplementary figures for synthetic parts**
- 2 **2.1 *N,N'*-diphenylmethanediamine (2a)**



3  
4 **Figure S3.**  $^1\text{H}$  NMR spectrum of *N,N'*-diphenylmethanediamine (2a).



5  
6 **Figure S4.**  $^{13}\text{C}$  NMR spectrum of *N,N'*-diphenylmethanediamine (2a).

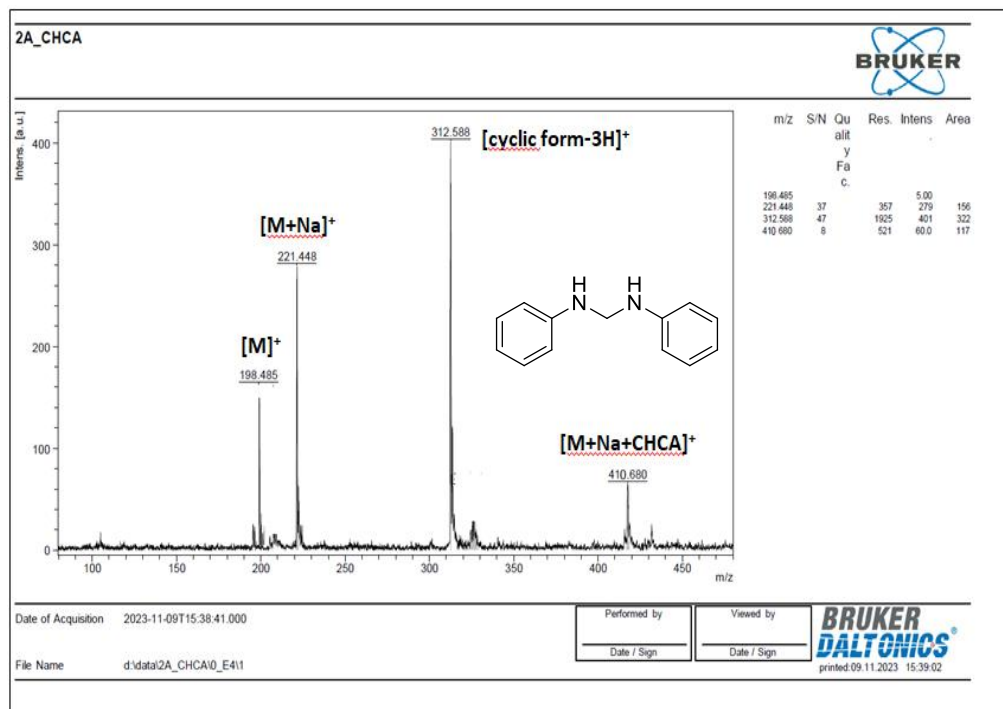


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Figure S5. FT-IR spectrum of *N,N'*-diphenylmethanediamine (2a).

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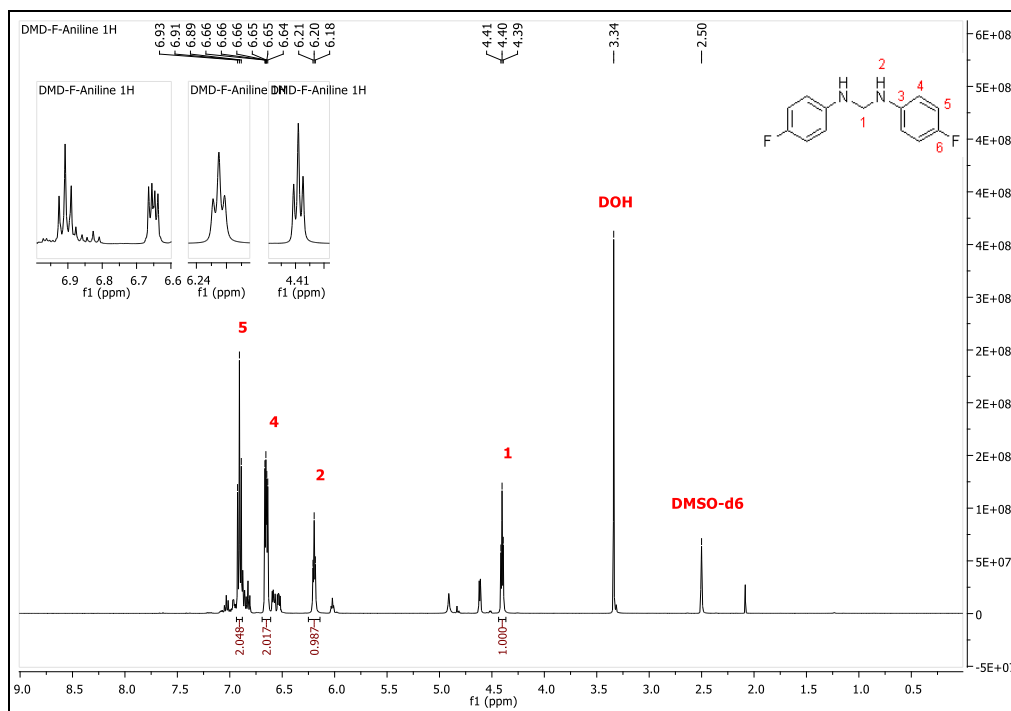


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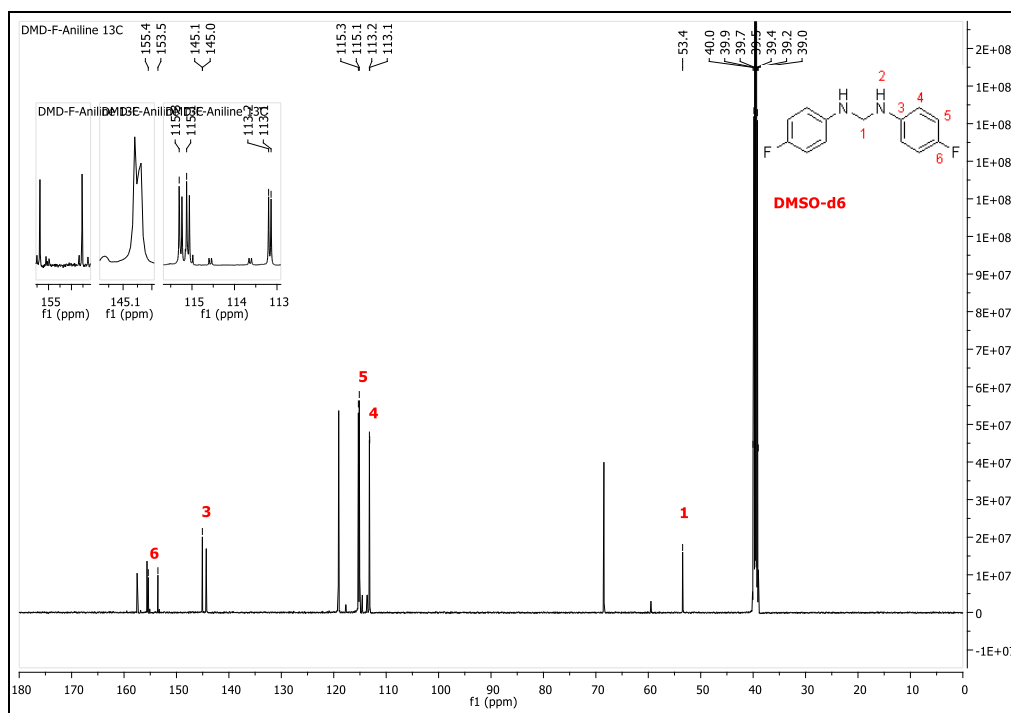
Figure S6. MS spectrum of *N,N'*-diphenylmethanediamine (2a).

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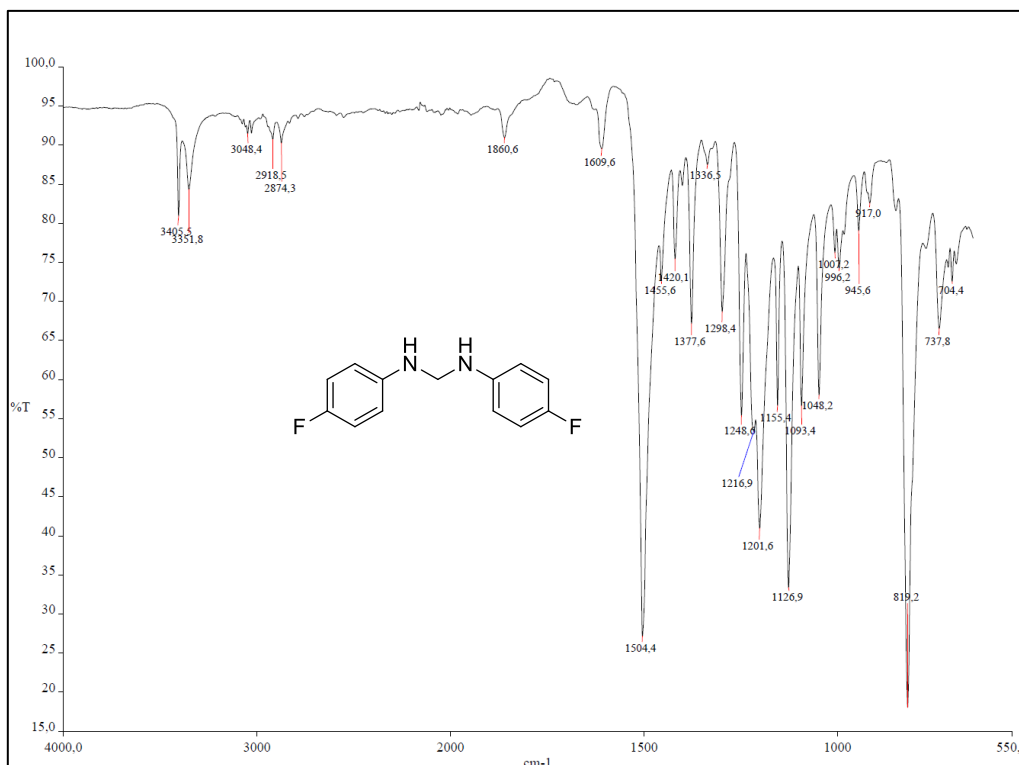
1 **2.2 *N,N'*-bis(4-fluorophenyl)methanediamine**



2  
3 **Figure S7.** <sup>1</sup>H NMR spectrum of *N,N'*-bis(4-fluorophenyl)methanediamine (2b).



4  
5  
6 **Figure S8.** <sup>13</sup>C NMR spectrum of *N,N'*-bis(4-fluorophenyl)methanediamine (2b).

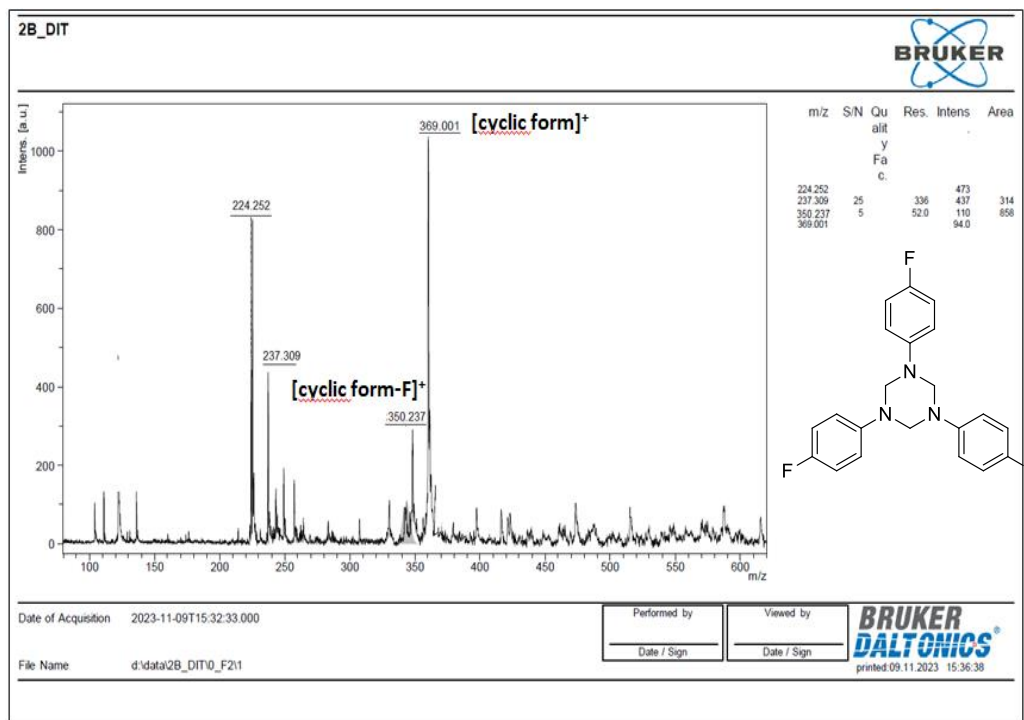


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**Figure S9.** FT-IR spectrum of *N,N'*-bis(4-fluorophenyl)methanediamine (2b).

3

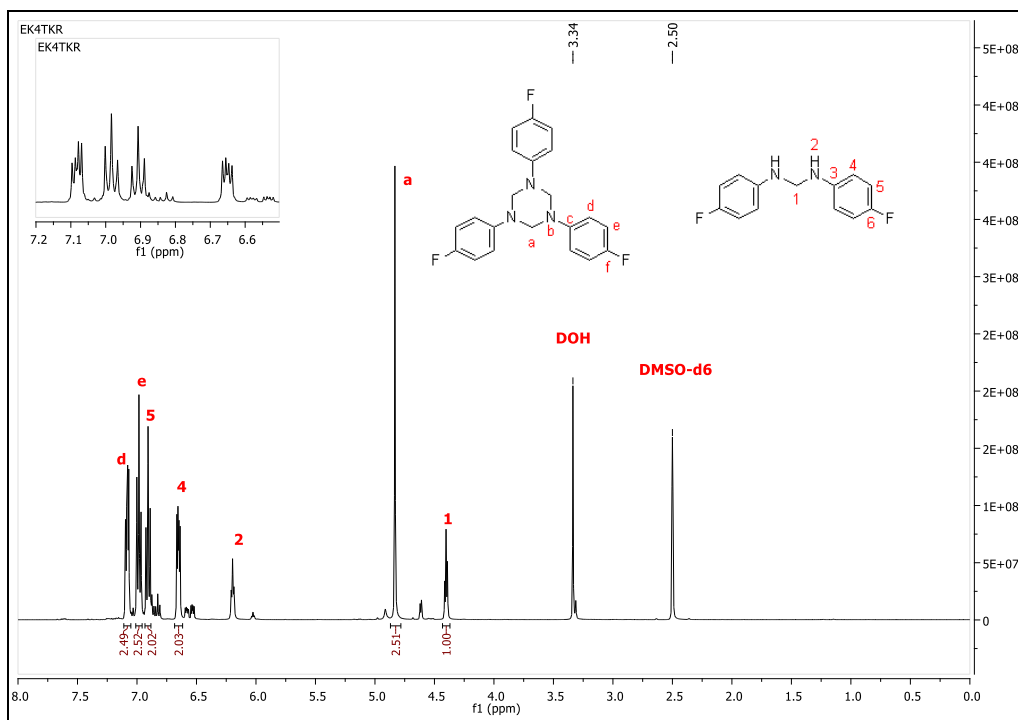


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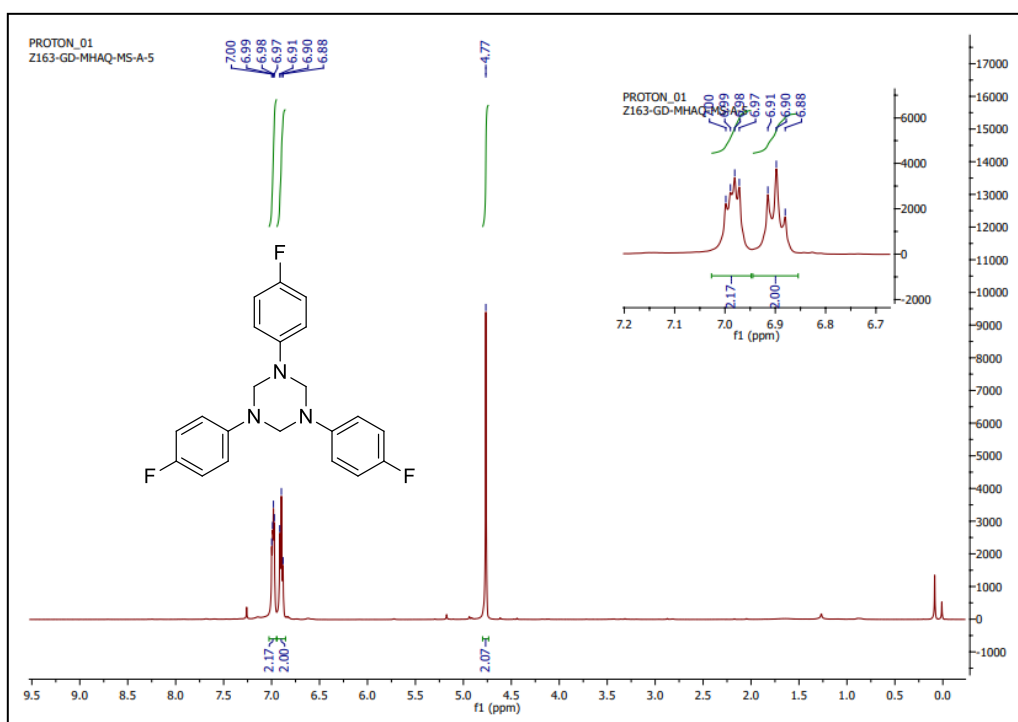
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**Figure S10.** MS spectrum of *N,N'*-bis(4-fluorophenyl)methanediamine (2b).

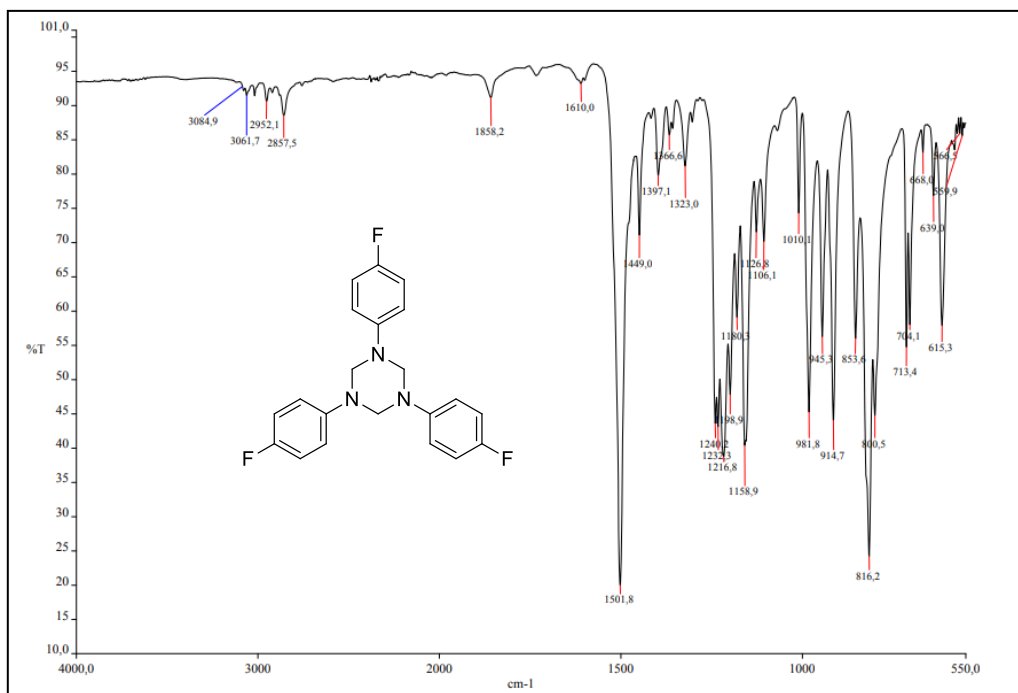




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2 **Figure S11.** <sup>1</sup>H NMR spectrum of *N,N'*-bis(4-fluorophenyl)methanediamine (2b) in  
3 DMSO-*d*<sub>6</sub> after 2 h.

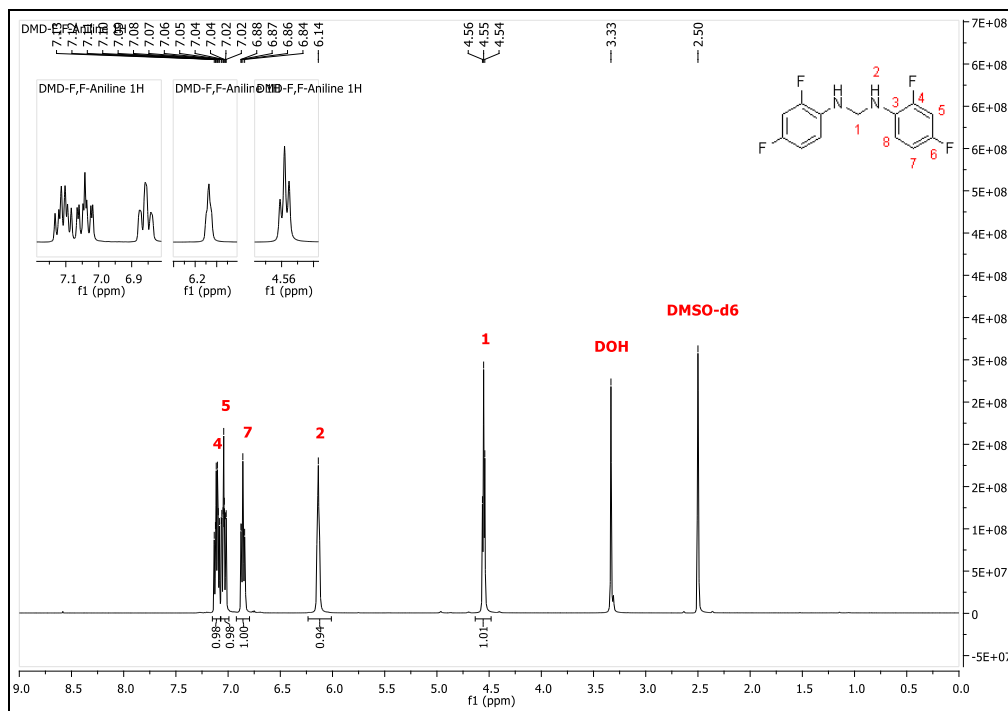


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5 **Figure S12.** <sup>1</sup>H NMR spectrum of *N,N'*-bis(4-fluorophenyl)methanediamine (2b) in  
6 CDCl<sub>3</sub> after 30 min.



1  
 2 **Figure S13.** FT-IR Spectrum of *N,N'*-bis(4-fluorophenyl)methanediamine (2b) after  
 3 cyclization.

4 **2.3 *N,N'*-bis(2,4-difluorophenyl)methanediamine**



5  
 6 **Figure S14.**  $^1\text{H}$  NMR spectrum of *N,N'*-bis(2,4-difluorophenyl)methanediamine (2c).

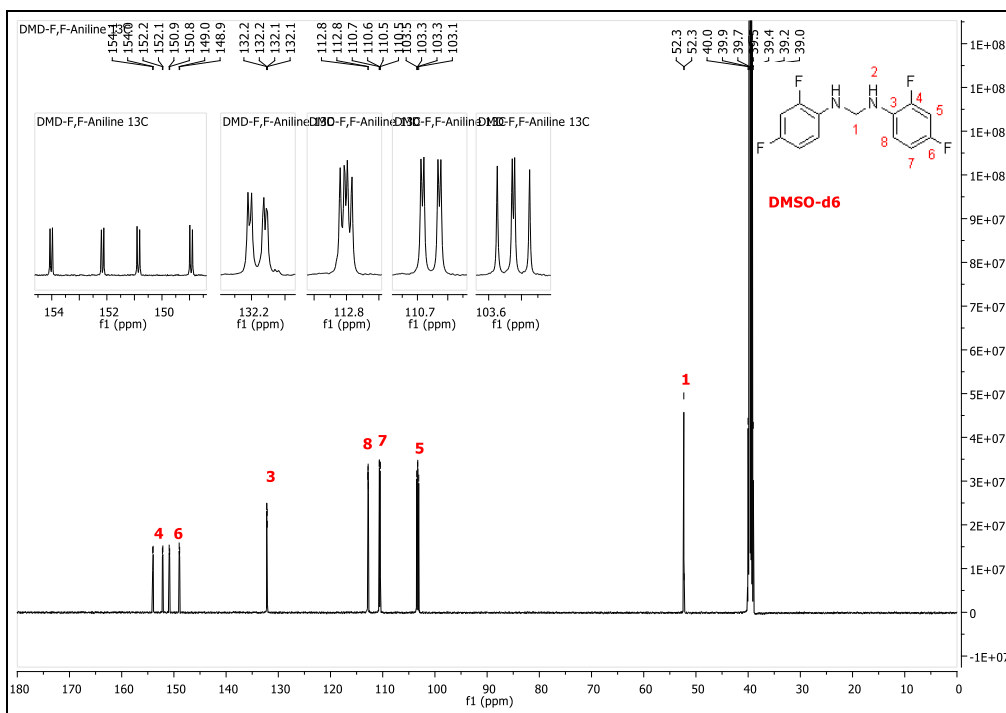


Figure S15.  $^{13}\text{C}$  NMR spectrum of *N,N'*-bis(2,4-difluorophenyl)methanediamine (2c).

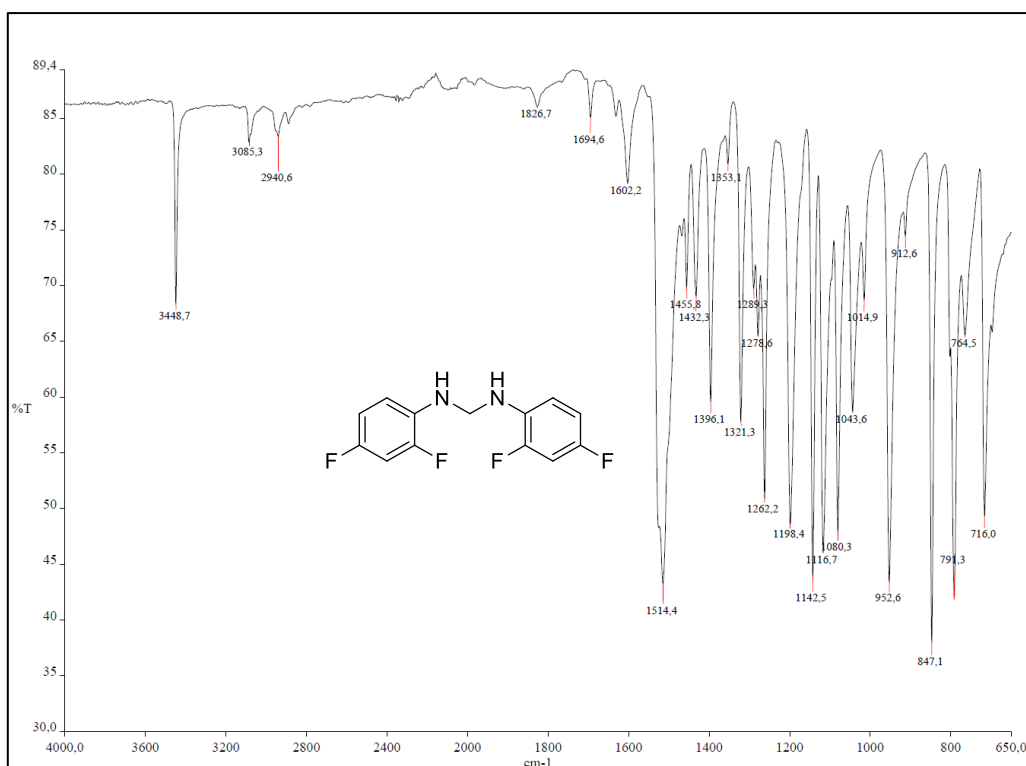
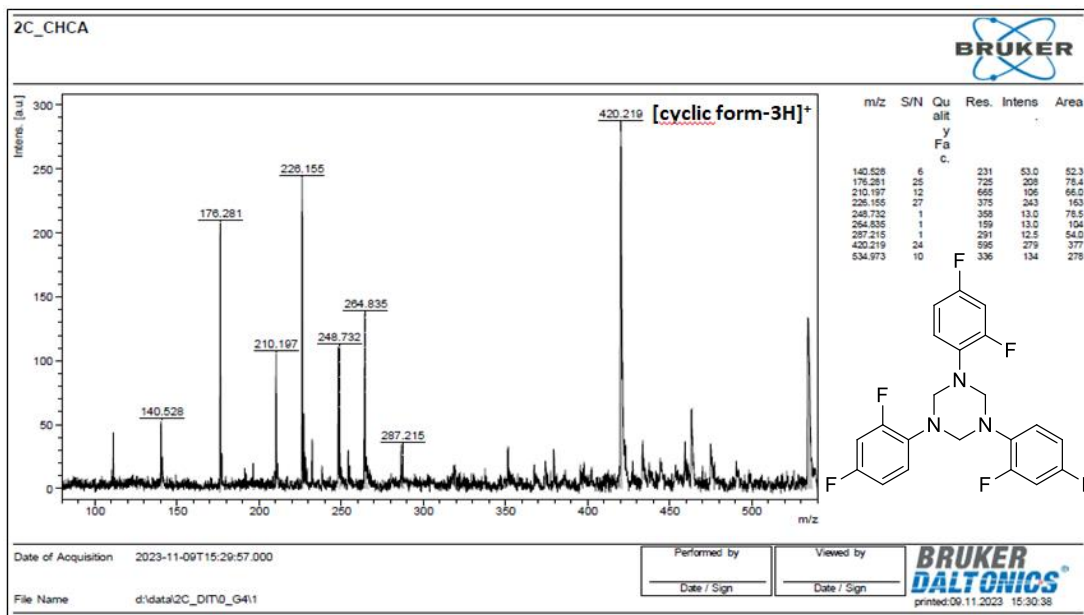


Figure S16. FT-IR spectrum of *N,N'*-bis(2,4-difluorophenyl)methanediamine (2c).



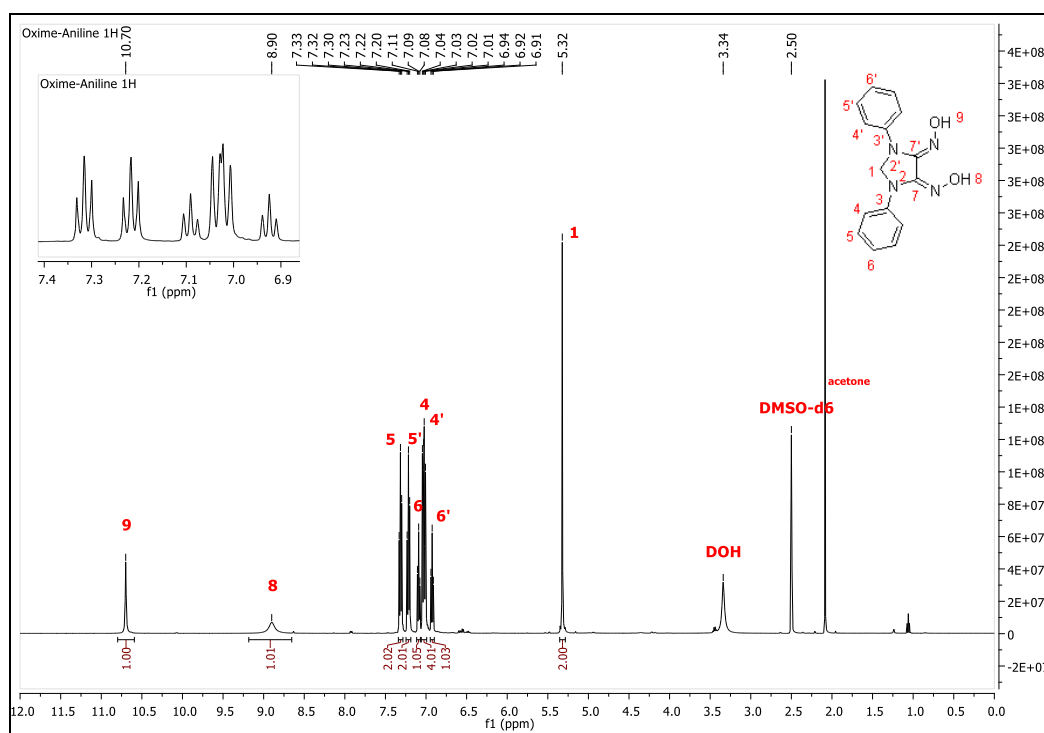
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**Figure S17.** MS spectrum of *N,N'*-bis(2,4-difluorophenyl)methanediamine (2c).

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**2.4 (4Z,5E)-1,3-diphenylimidazolidine-4,5-dionedioxime**



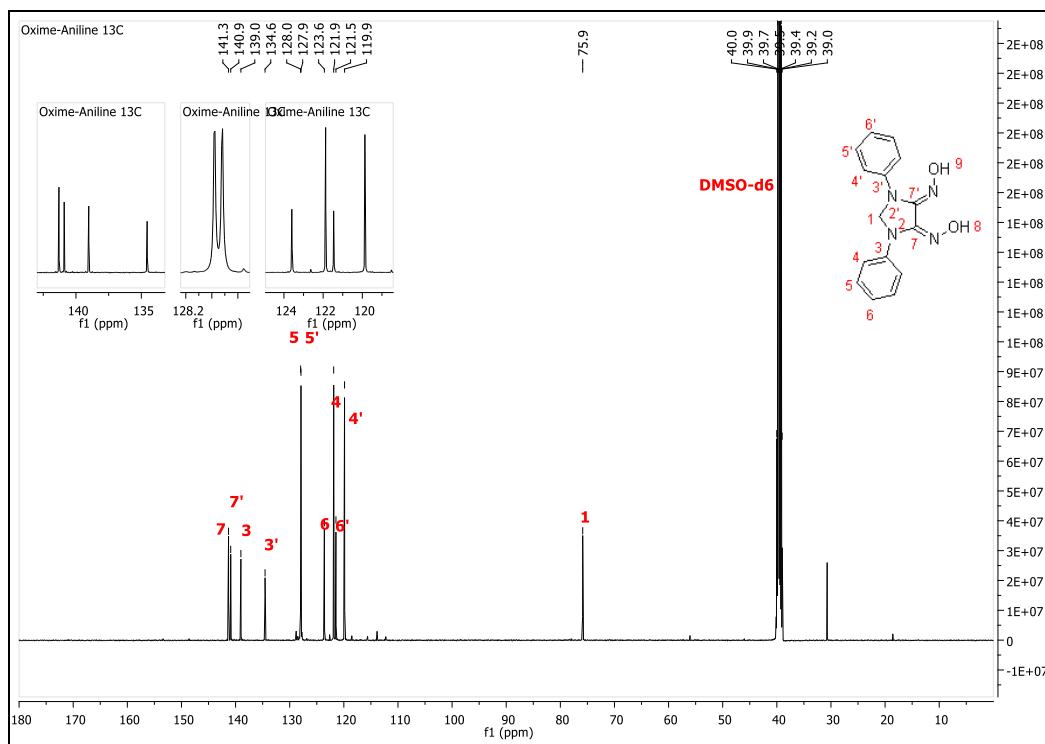
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**Figure S18.** <sup>1</sup>H NMR spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-

6

dionedioxime (*L*<sub>1a</sub>).

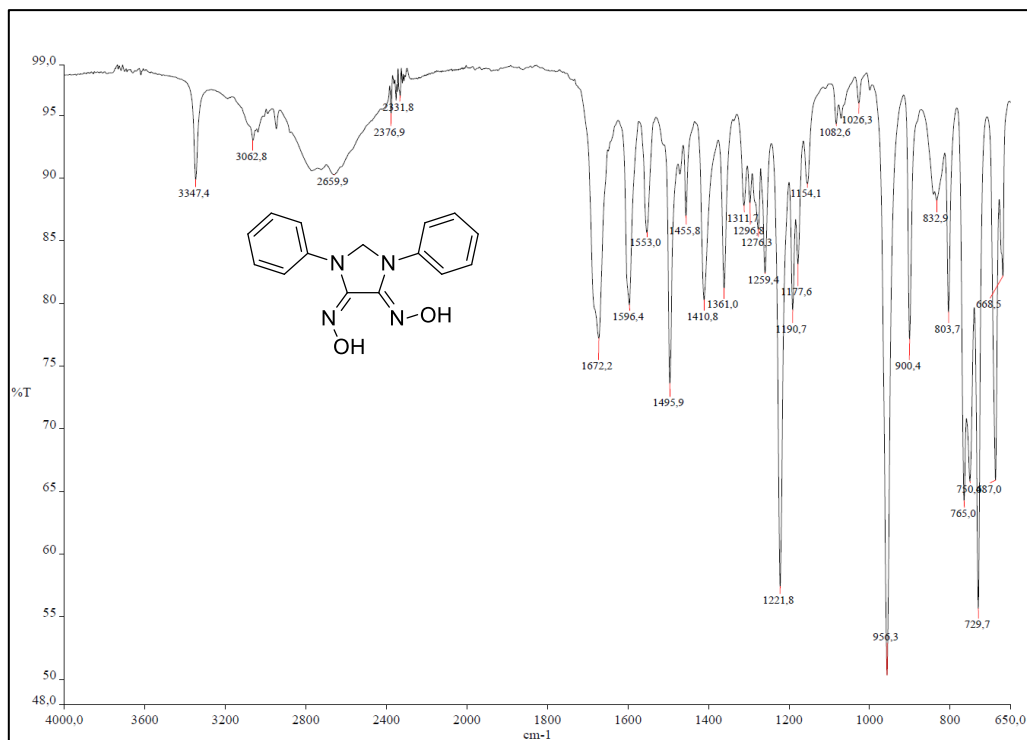


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**Figure S19.**  $^{13}\text{C}$  NMR spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-dionedioxime ( $\text{L}_{1a}$ ).

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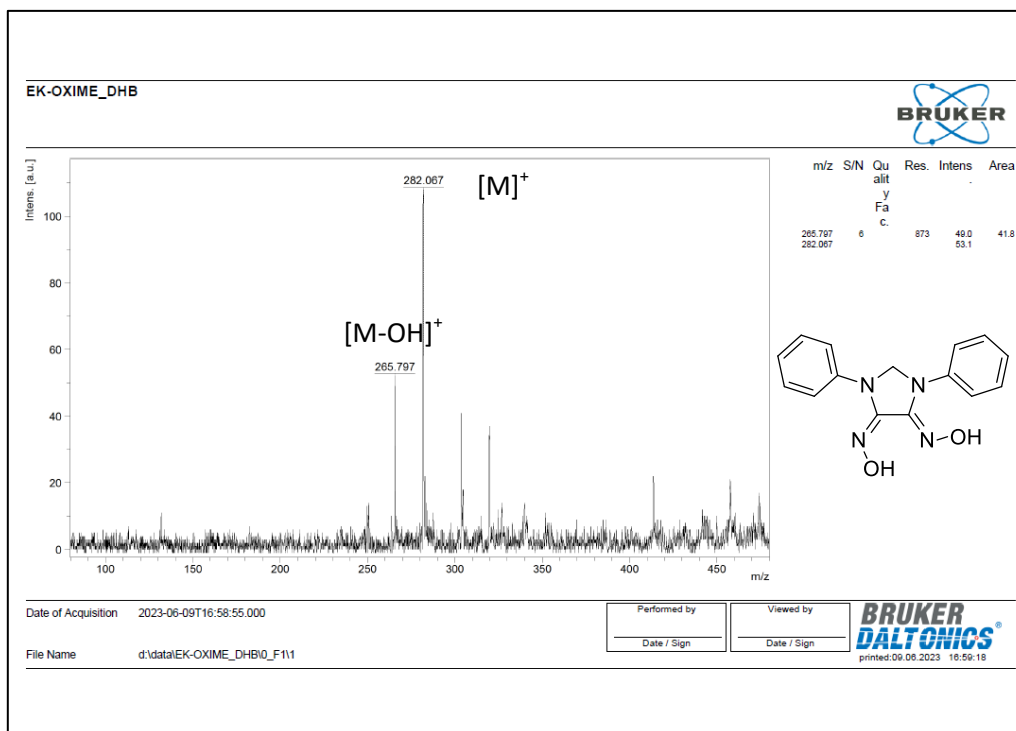
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**Figure S20.** FT-IR spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-dionedioxime ( $\text{L}_{1a}$ ).

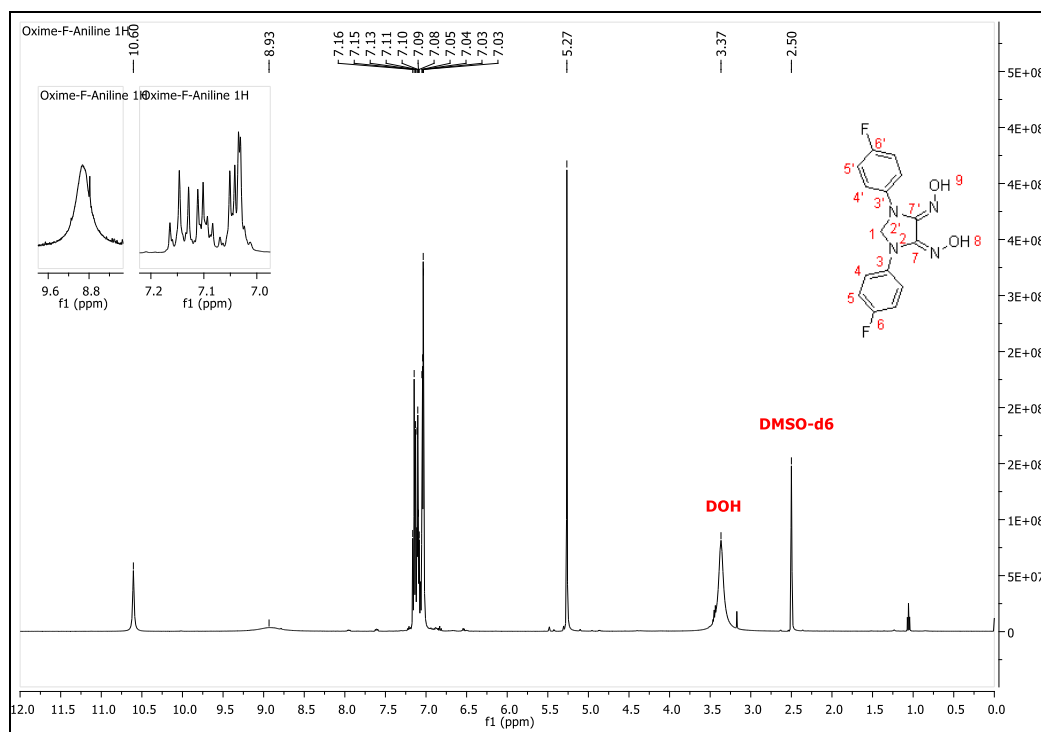
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1

2 **Figure S21.** MS spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-dionedioxime ( $L_{1a}$ ).

3 **2.5 (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-dionedioxime**

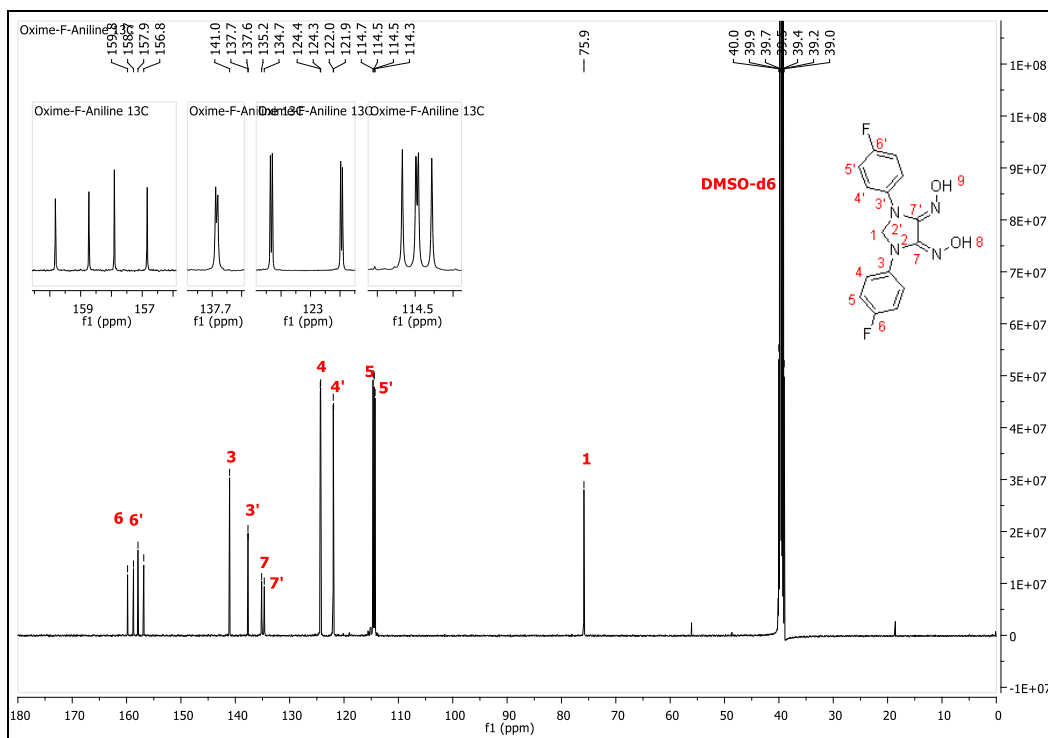


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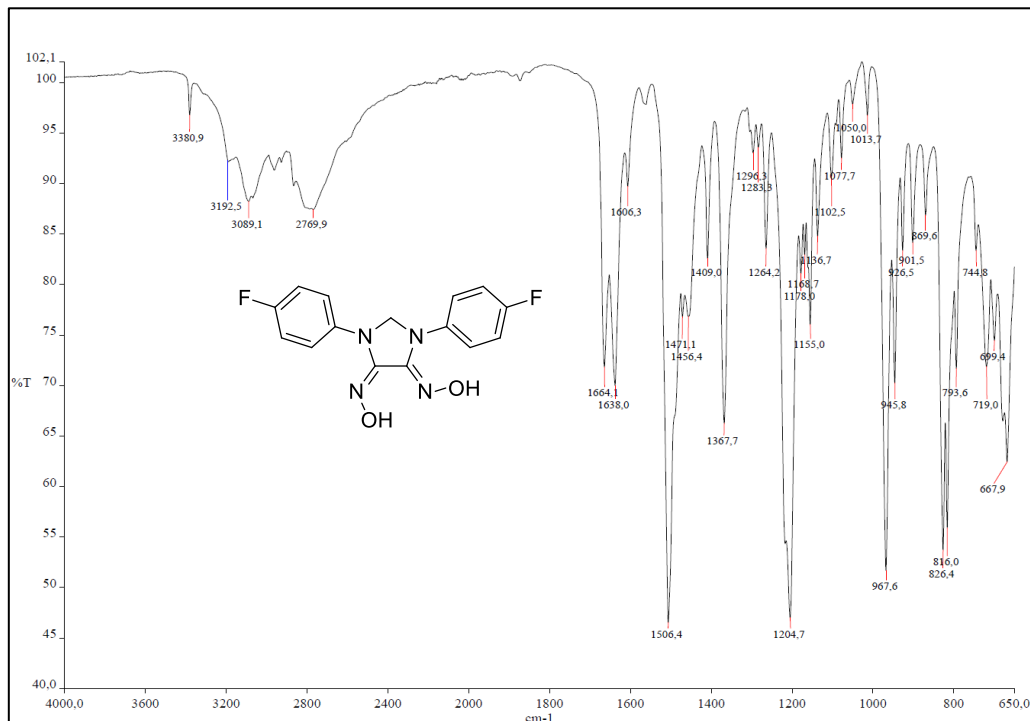
5 **Figure S22.**  $^1\text{H}$  NMR spectrum of (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-

6

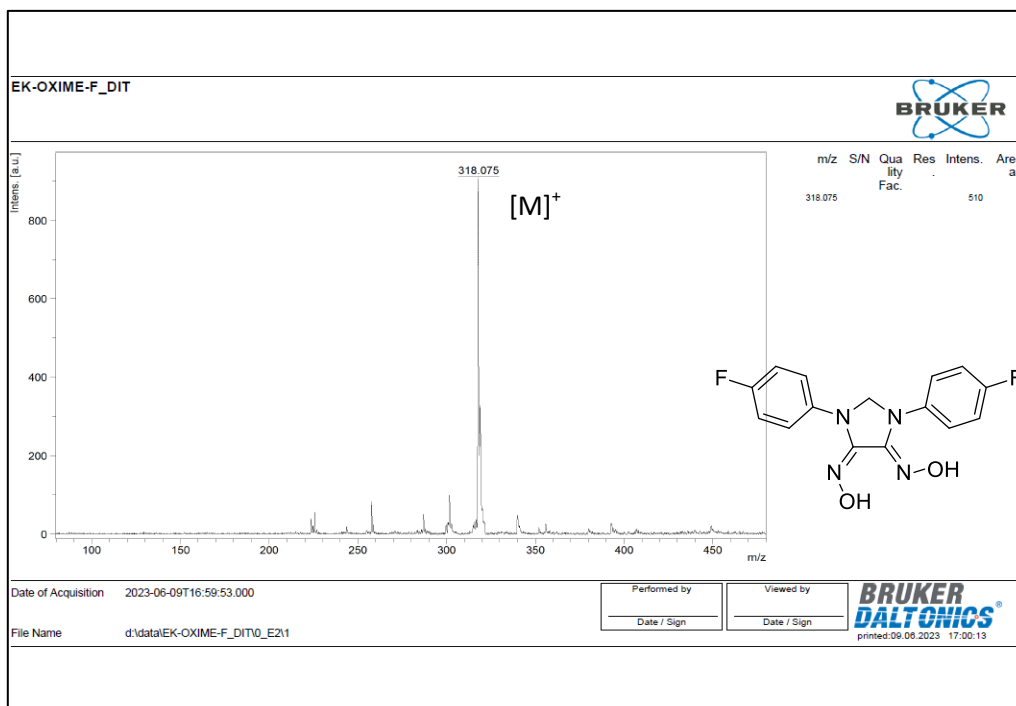
dionedioxime ( $L_{1b}$ ).



**Figure S23.**  $^{13}\text{C}$  NMR spectrum of (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-dionedioxime ( $\text{L}_{1b}$ ).



**Figure S24.** FT-IR spectrum of (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-dionedioxime ( $\text{L}_{1b}$ ).



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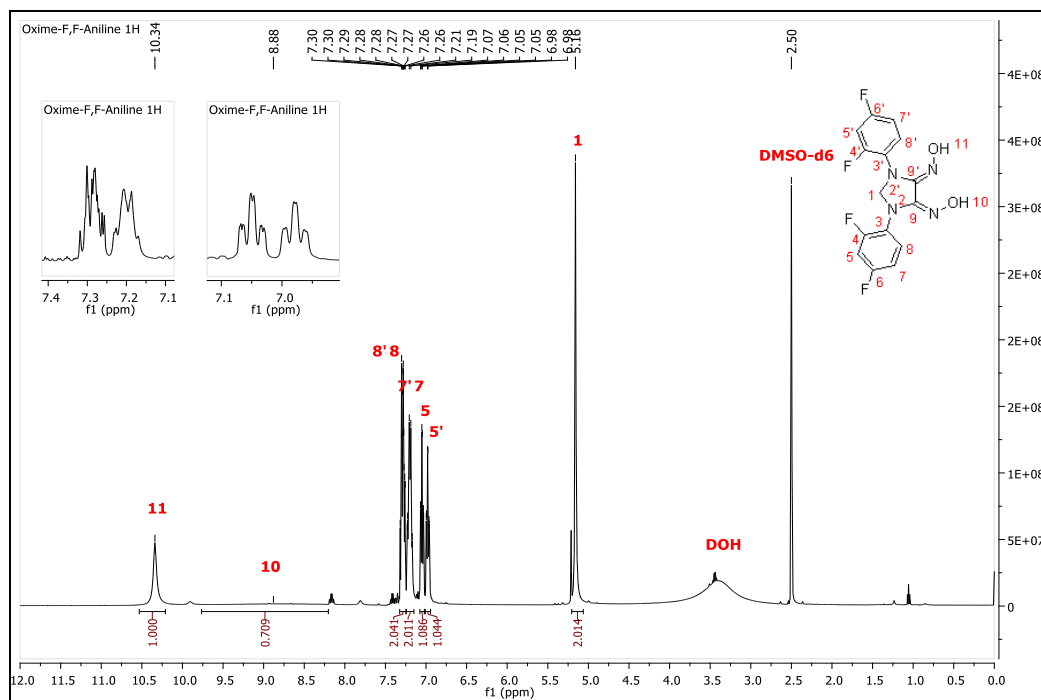
2 **Figure S25.** MS spectrum of (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-dionedioxime

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(L<sub>1b</sub>).

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**2.6 (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-dionedioxime**



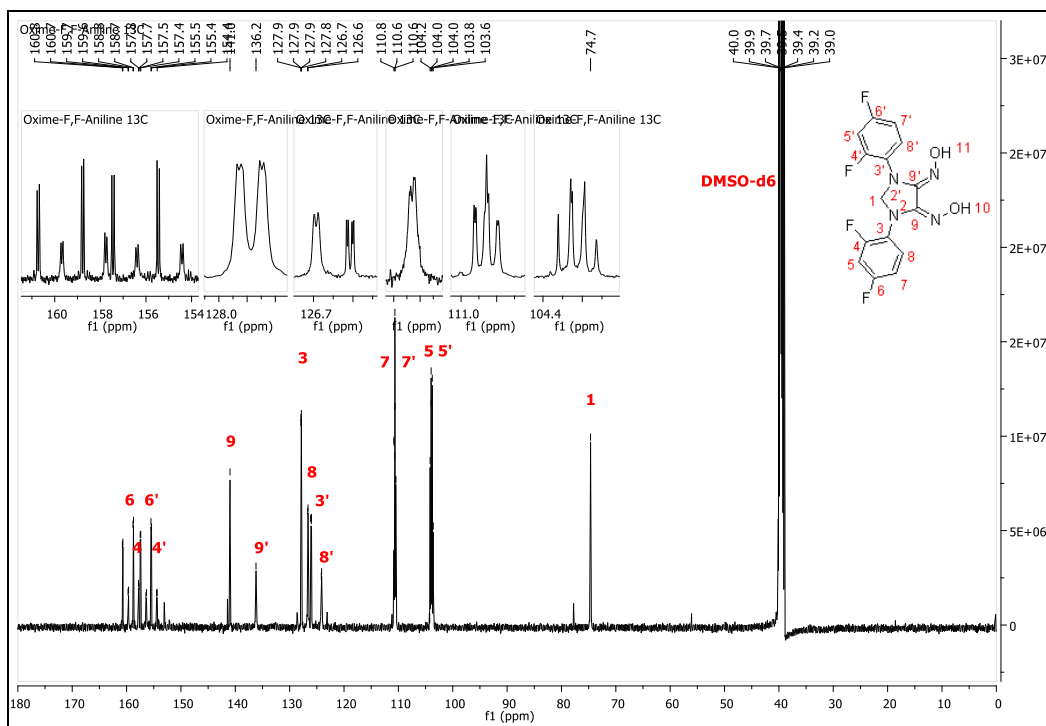
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6 **Figure S26.** <sup>1</sup>H NMR spectrum of (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-

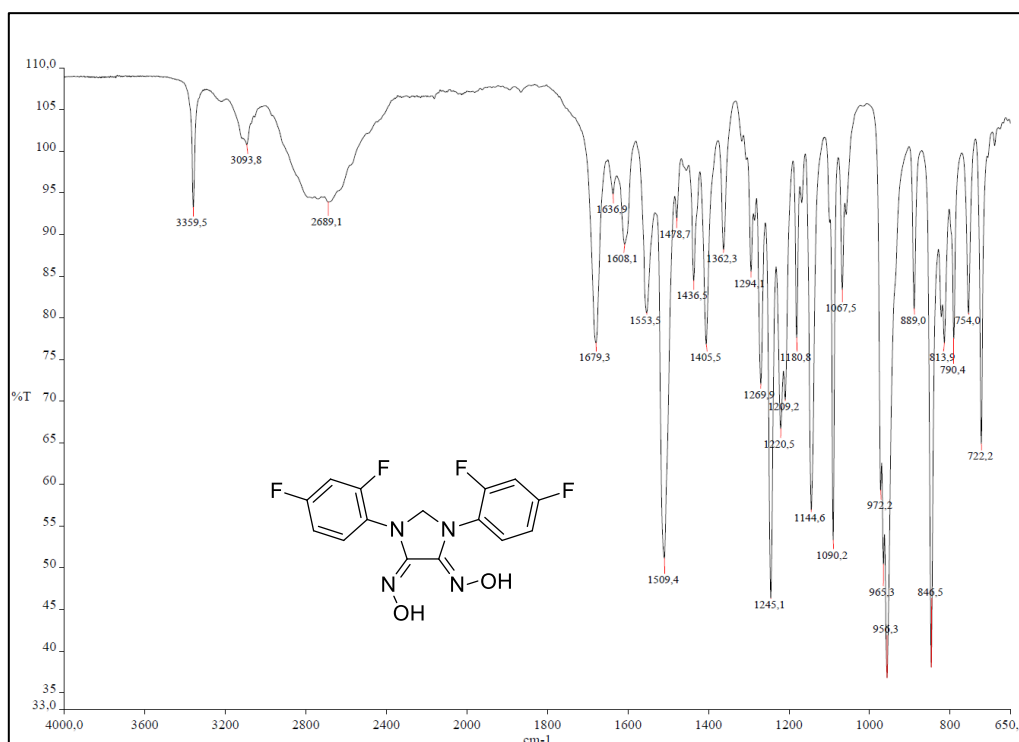
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dionedioxime (L<sub>1c</sub>).

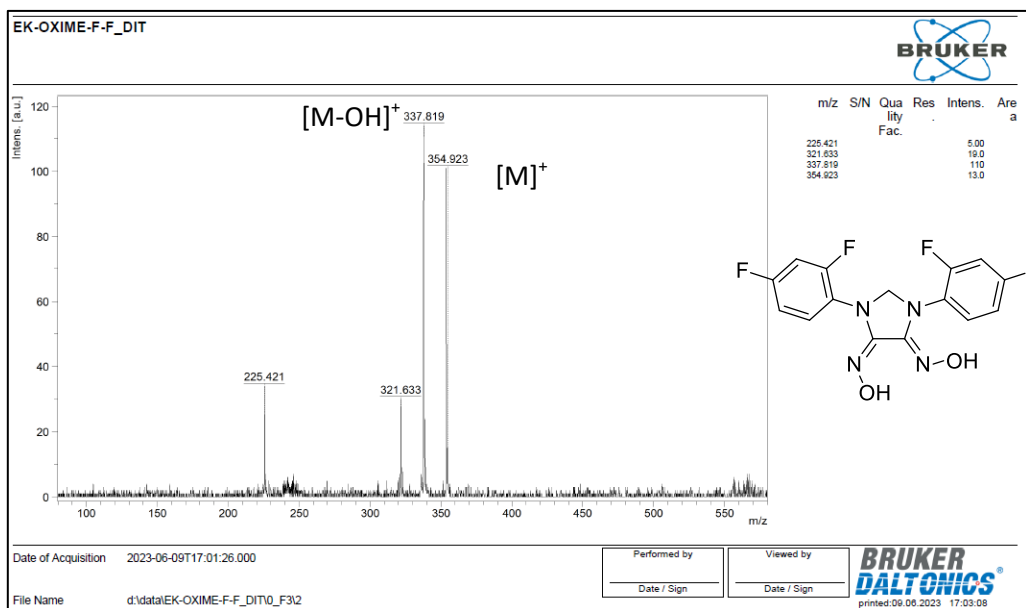




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2 **Figure S27.**  $^{13}\text{C}$  NMR spectrum of (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-  
3 dionedioxime ( $L_{1c}$ ).



4  
5 **Figure S28.** FT-IR spectrum of (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-  
6 dionedioxime ( $L_{1c}$ ).



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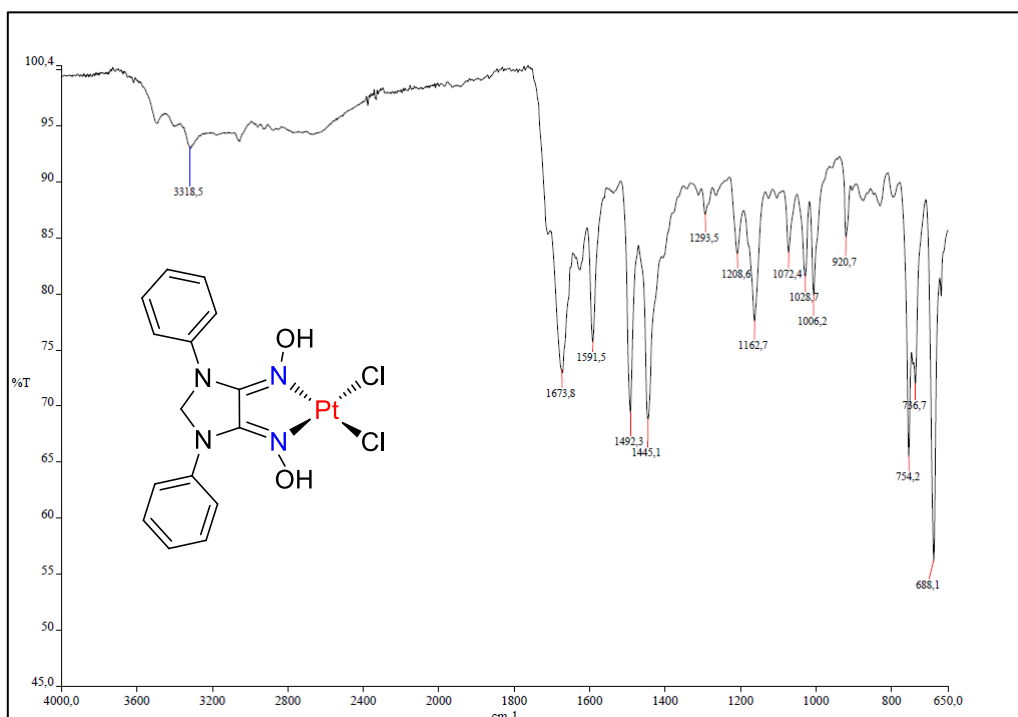
**Figure S29.** MS spectrum of (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-dionedioxime ( $L_{1c}$ ).

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## 2.7 Monoplatinum complexes of *vic*-dioximes

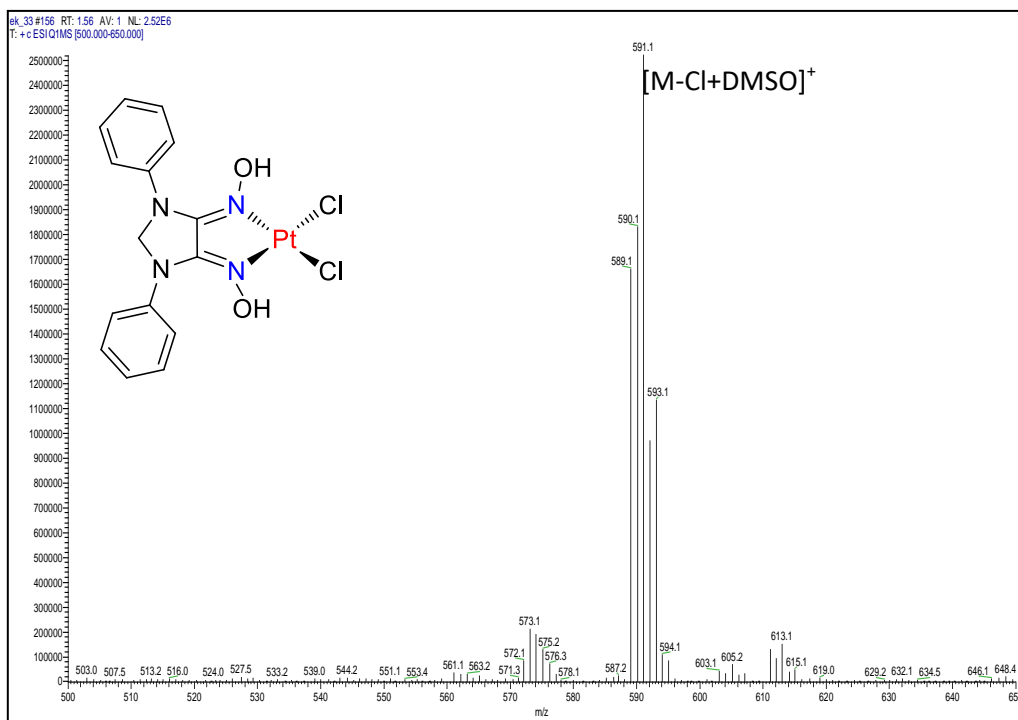


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**Figure S30.** FT-IR spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-dionedioxime mono-Pt(II) complex ( $L_{1a}Pt-m$ ).

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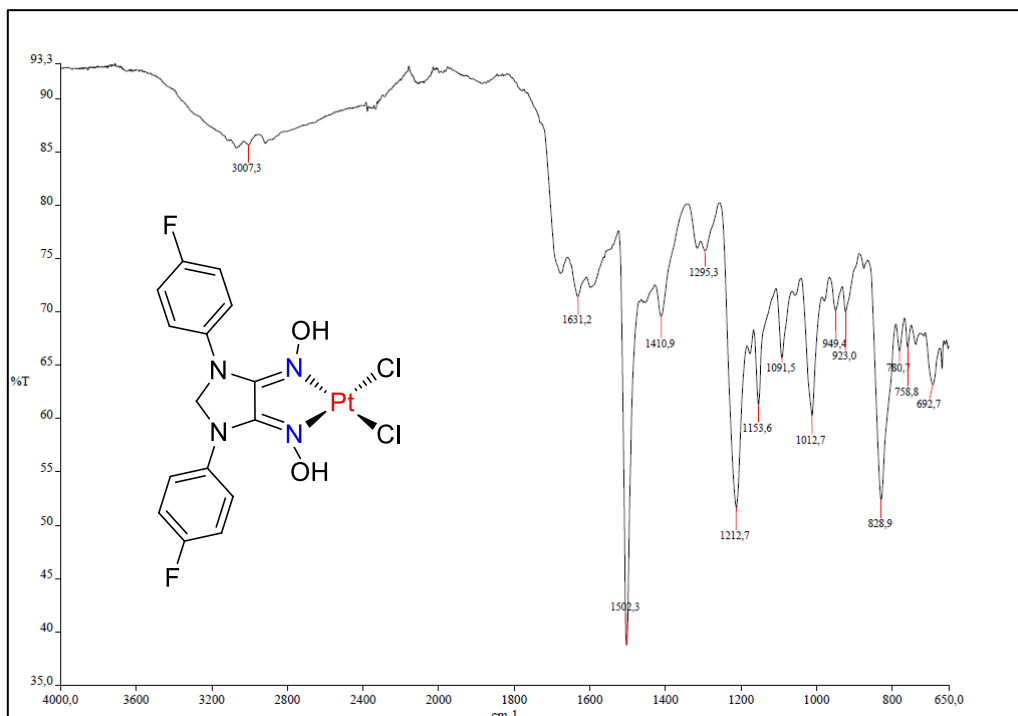


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**Figure S31.** MS spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-dione platinum(II) complex ( $L_{1a}Pt-m$ ).

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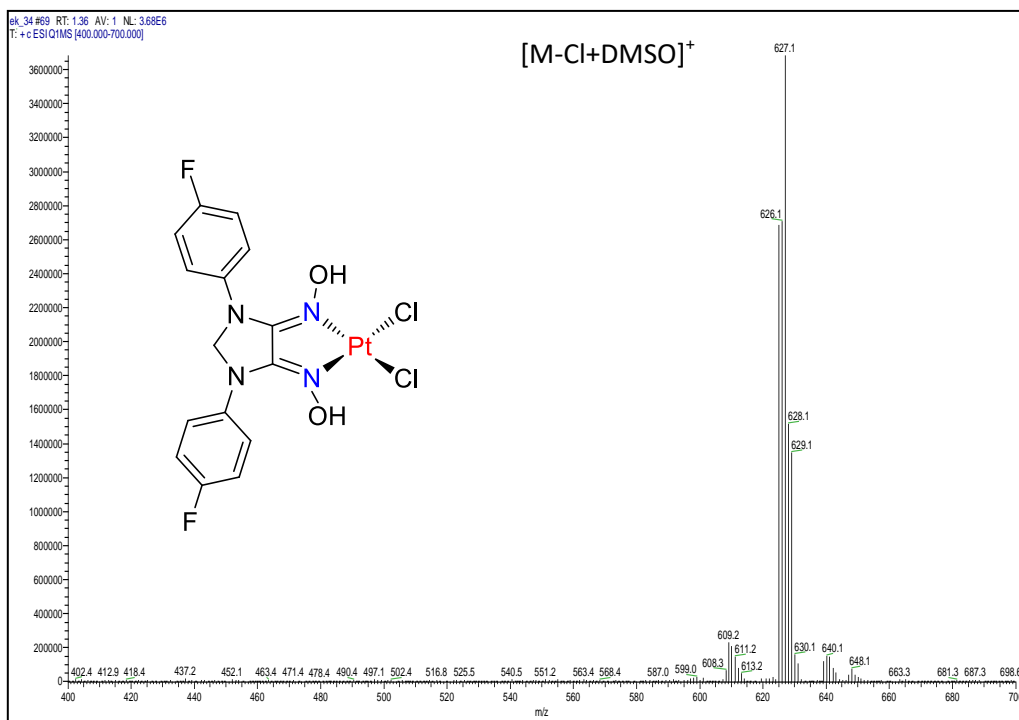


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**Figure S32.** FT-IR spectrum of (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-dione platinum(II) complex ( $L_{1b}Pt-m$ ).

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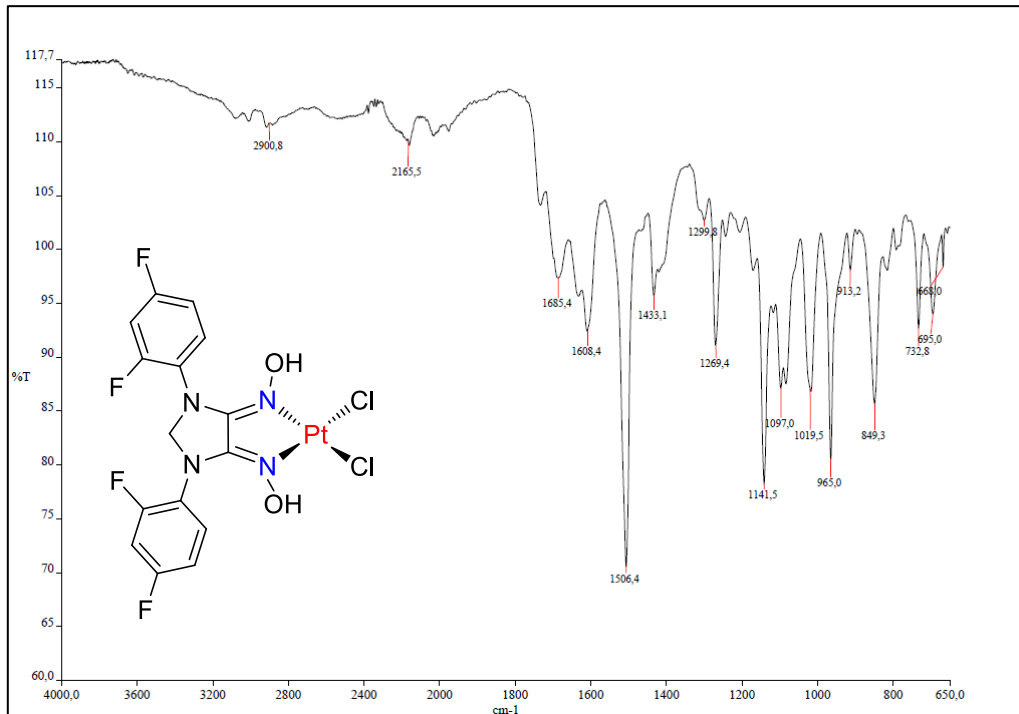


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**Figure S33.** MS spectrum of (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-dione platinum(II) complex ( $L_{1b}Pt-m$ ).

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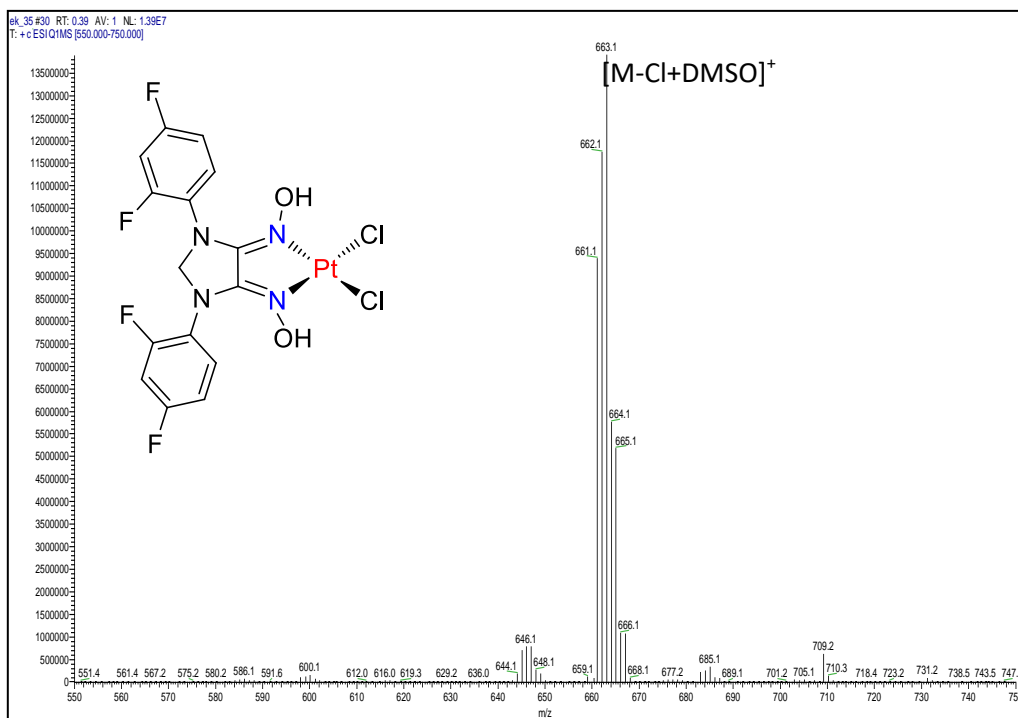


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**Figure S34.** FT-IR spectrum of (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-dione platinum(II) complex ( $L_{1c}Pt-m$ ).

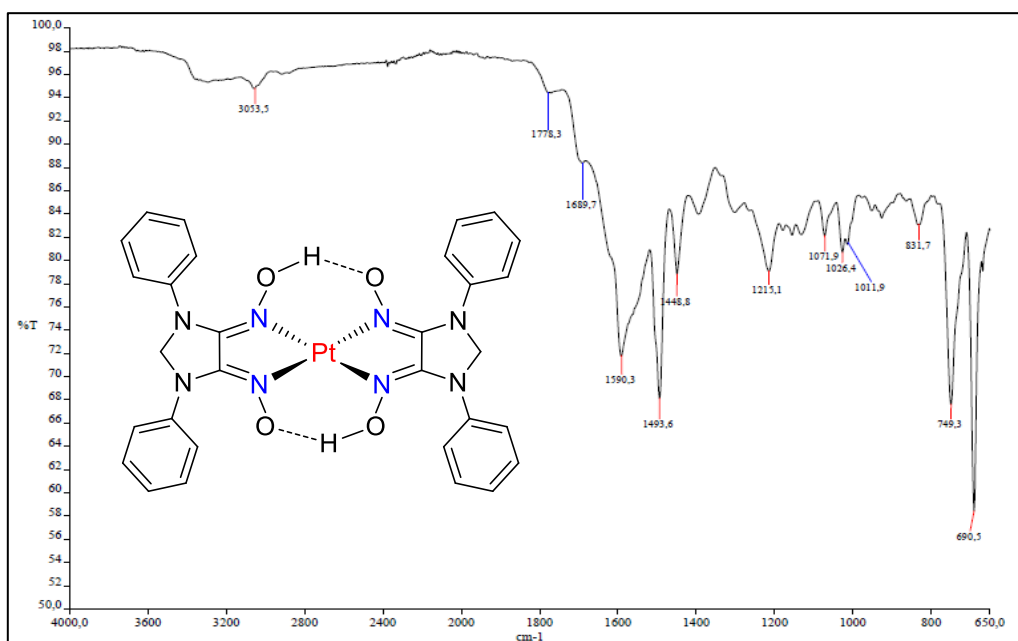
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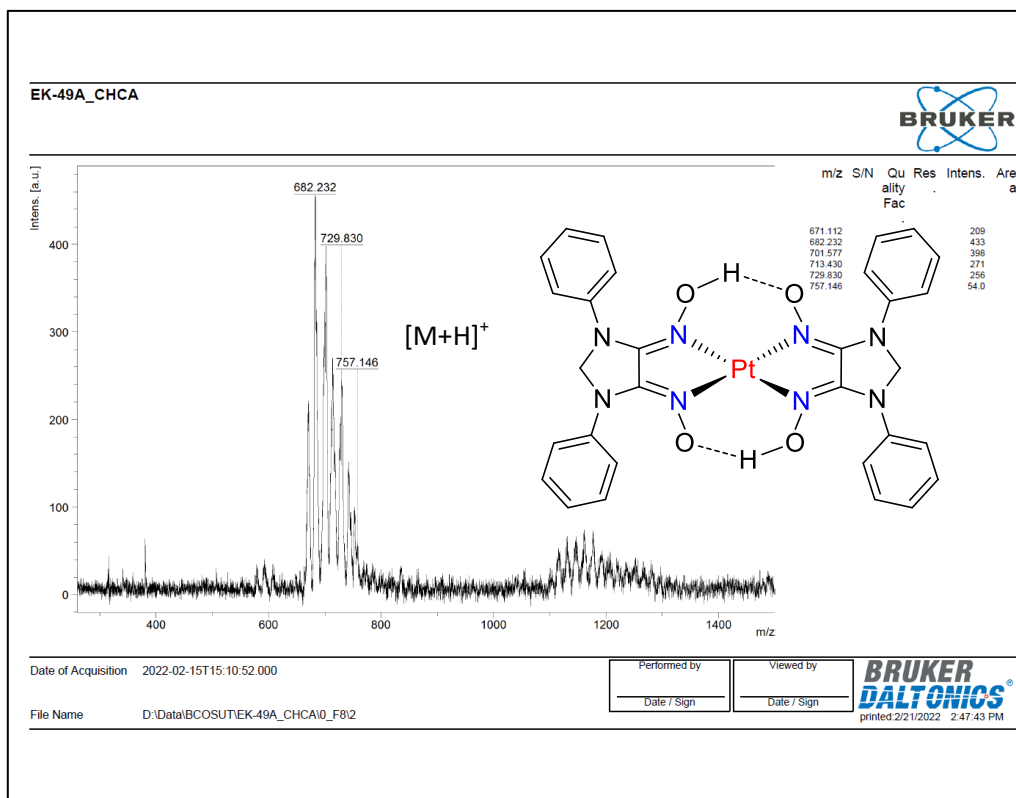
2 **Figure S35.** MS spectrum of (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-  
 3 dionedioxime mono-Pt(II) complex ( $L_{1c}Pt-m$ ).

4 **2.8 Bisplatinum complexes of vic-dioximes**



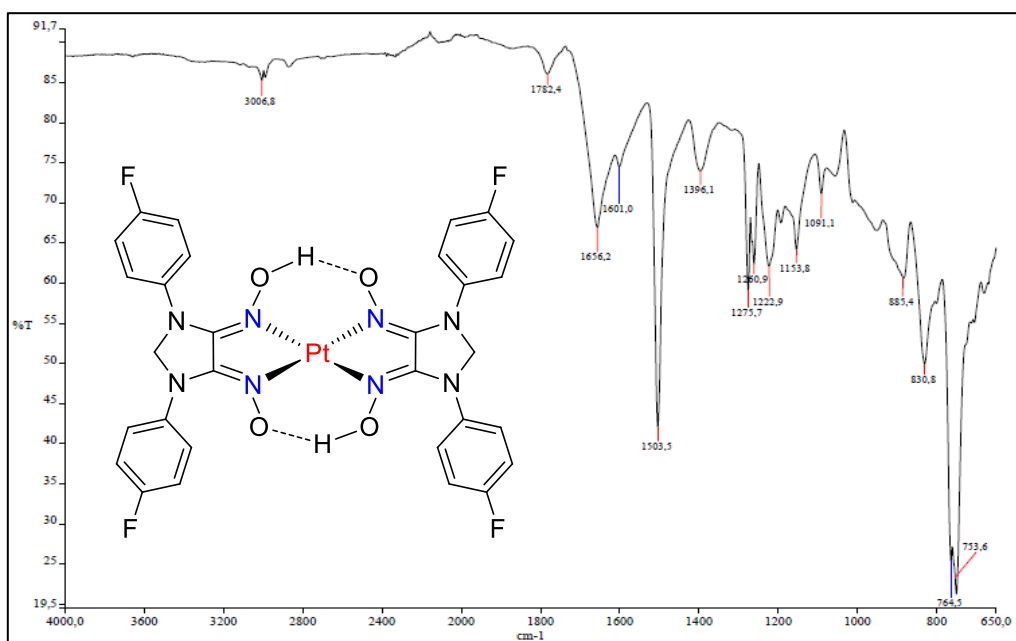
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6 **Figure S36.** FT-IR spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-dionedioxime  
 7 bis-Pt(II) complex ( $L_{1a}Pt-b$ ).



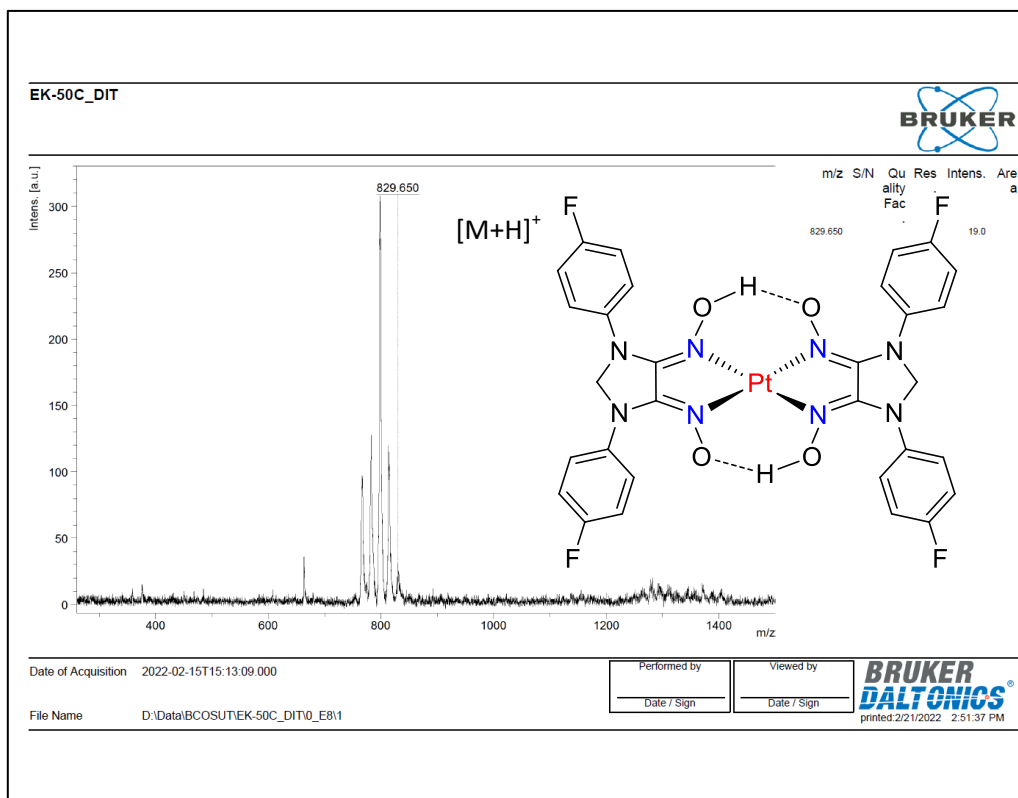
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2 **Figure S37.** MS spectrum of (4Z,5E)-1,3-diphenylimidazolidine-4,5-dione bis-  
3 Pt(II) complex (L<sub>1a</sub>Pt-b).



4

5 **Figure S38.** FT-IR spectrum of (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-  
6 dione bis-Pt(II) complex (L<sub>1b</sub>Pt-b).

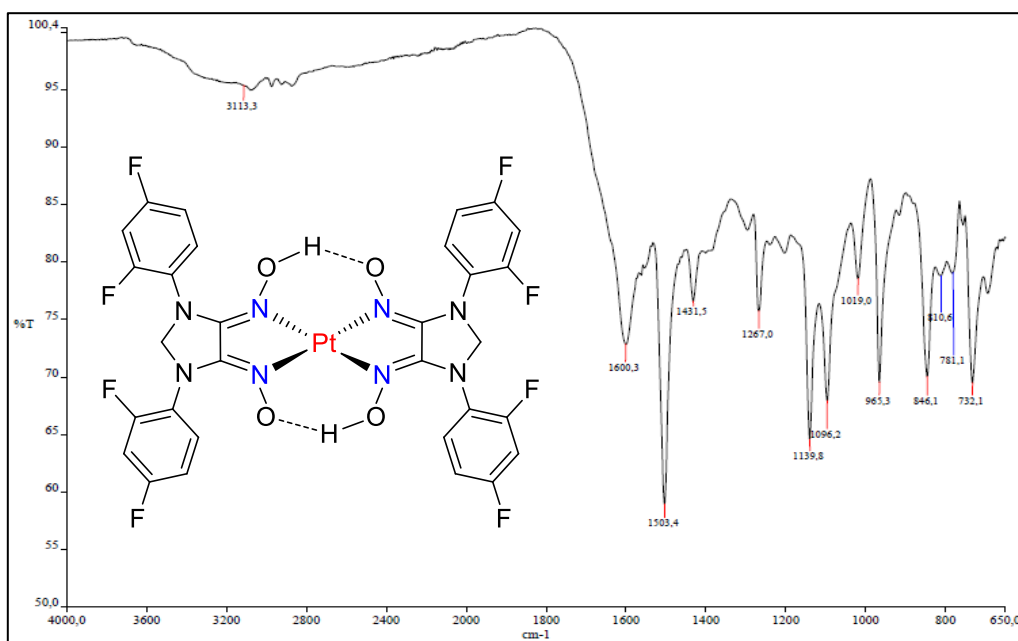


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2 **Figure S39.** MS spectrum of (4Z,5E)-1,3-bis(4-fluorophenyl)imidazolidine-4,5-

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dionedioxime bis-Pt(II) complex ( $L_{1b}Pt-b$ ).

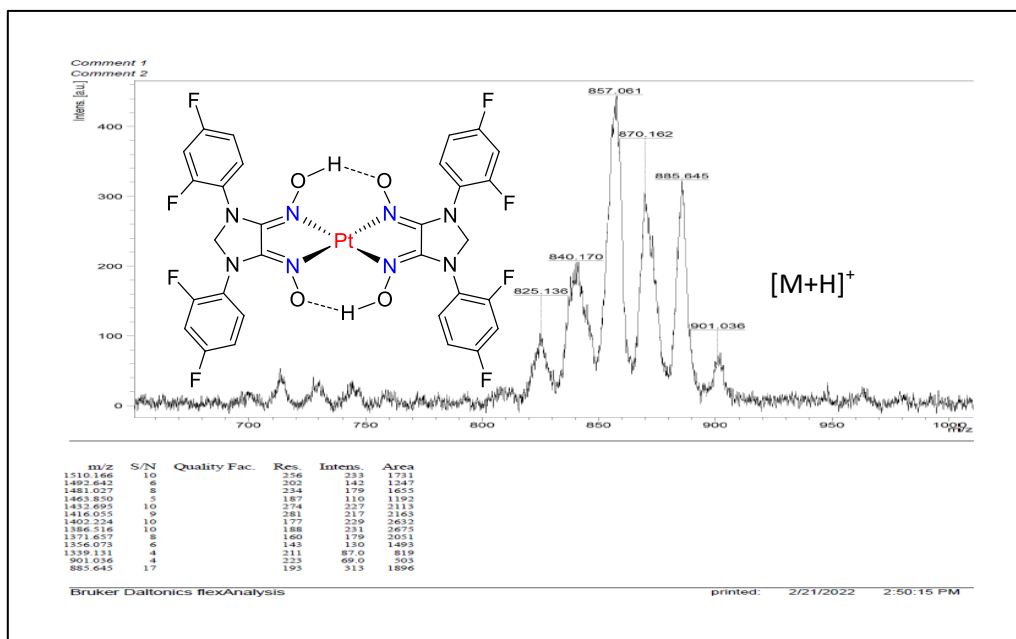


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5 **Figure S40.** FT-IR spectrum of (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-

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dionedioxime bis-Pt(II) complex ( $L_{1c}Pt-b$ ).



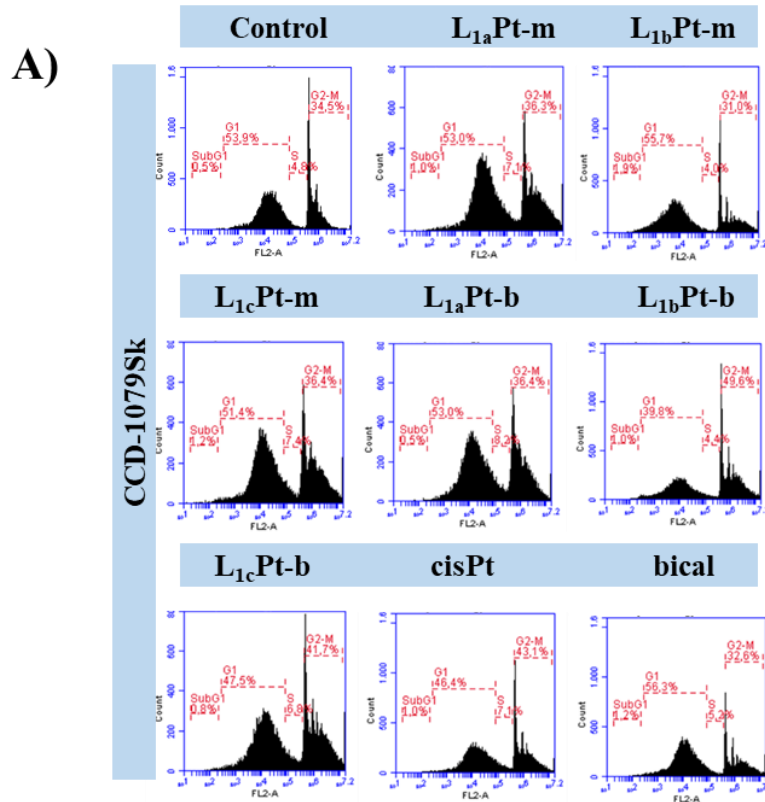
1  
2 **Figure S41.** MS spectrum of (4Z,5E)-1,3-bis(2,4-difluorophenyl)imidazolidine-4,5-  
3 dionedioxime bis-Pt(II) complex (L<sub>1c</sub>Pt-b).

4  
5 **3. Materials and methods for biological studies**

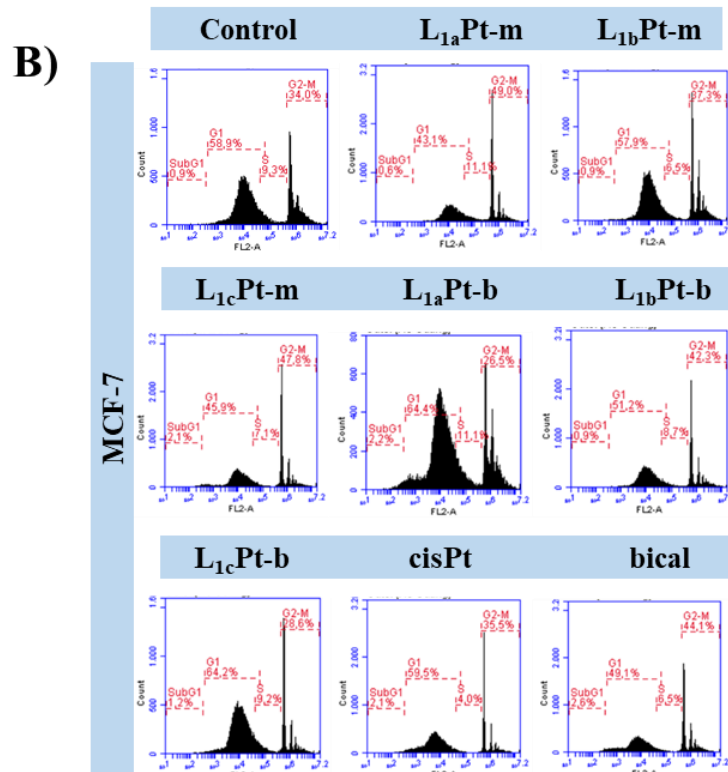
6 CCD-1079Sk (CRL-2097), MCF-7 (HTB-22) and MDA-MB-231 (HTB-26) cell lines  
7 were used for in vitro studies. MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-  
8 diphenyltetrazolium bromide) was purchased from Sigma Aldrich. Dulbecco's modified  
9 Eagle's medium/Nutrient Mixture F-12 culture Ham culture media, fetal bovine serum,  
10 %0.25 trypsin (1×), Penicillin streptomycin was purchased from Gibco. The apoptosis  
11 kit was purchased from BioLegend. The Cell Cycle kit was purchased from Thermo  
12 Scientific.



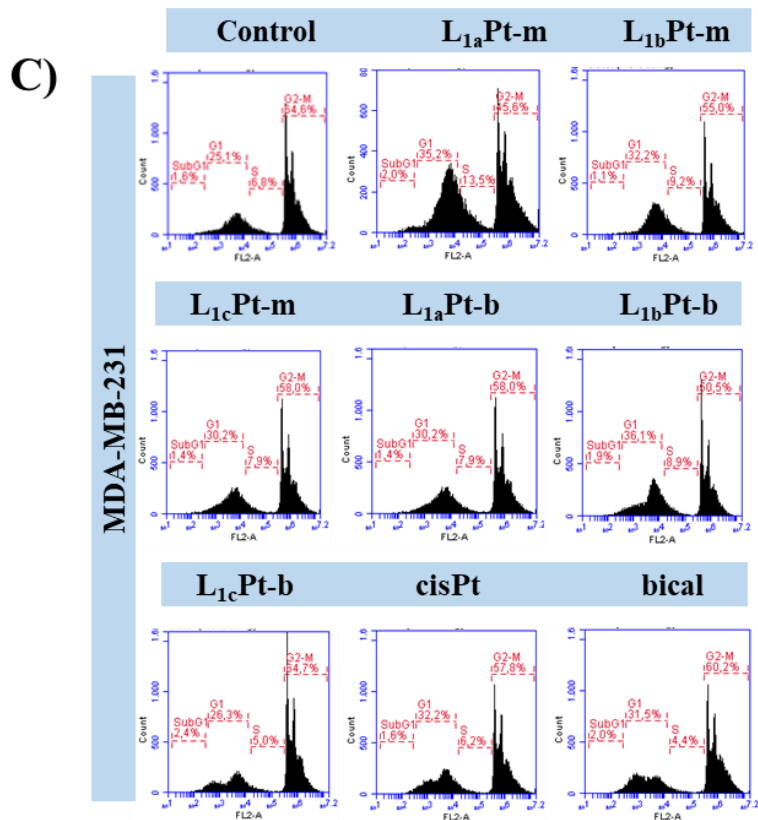
1 4. Supplementary figures for biological studies



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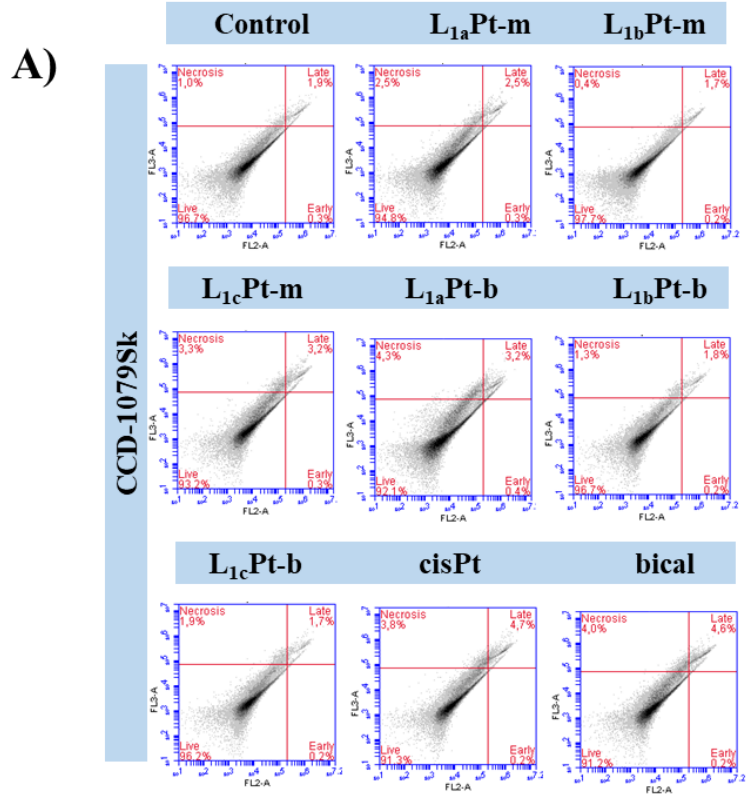
2 **Figure S42.** Cell cycle analysis of compounds treated A) CCD-1079Sk, B) MCF-7, and

3

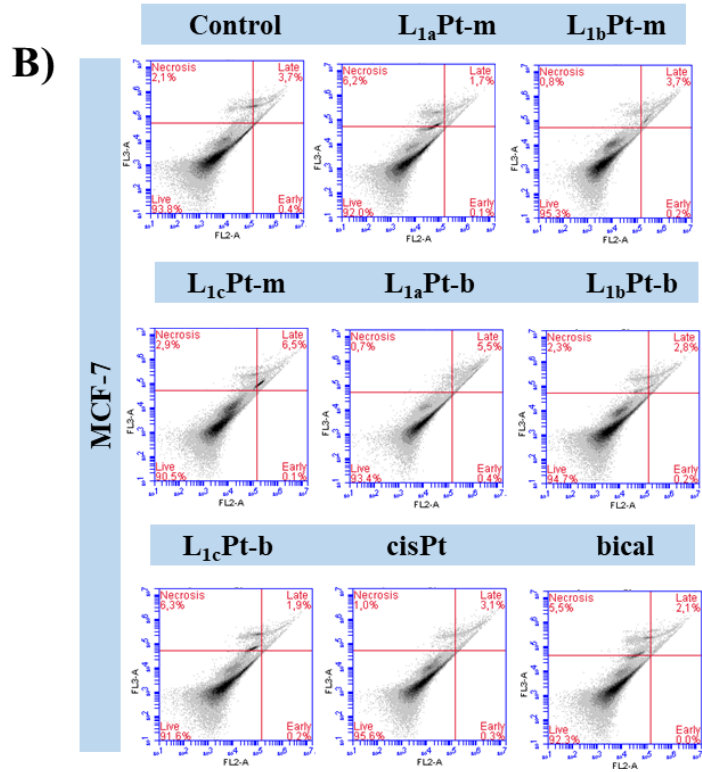
C) MDA-MB-231 cells.

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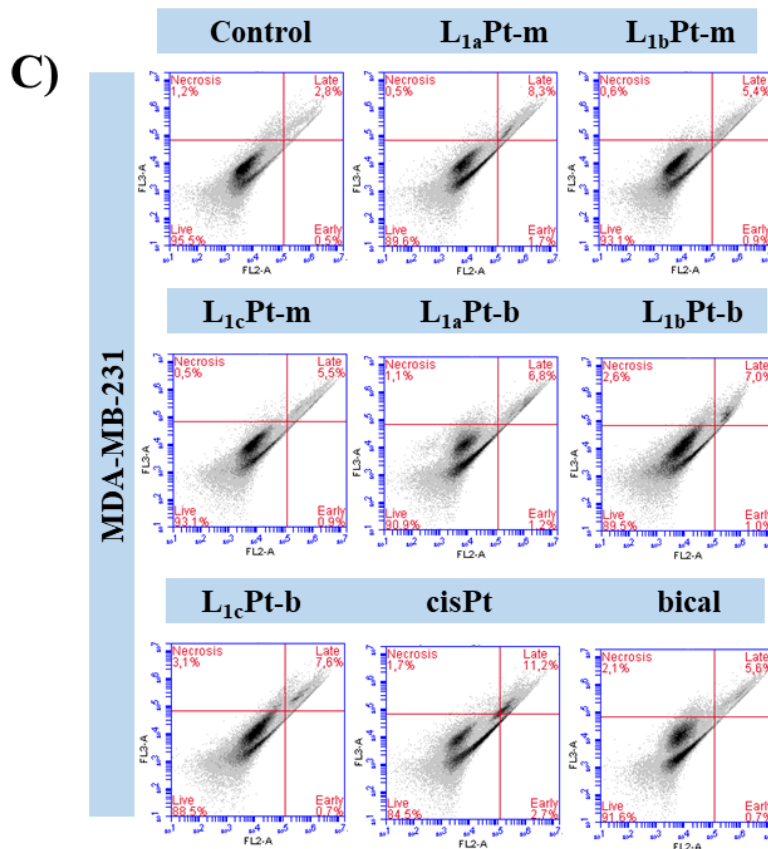
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2 **Figure S43.** Apoptosis assay results of compounds treated A) CCD-1079Sk, B) MCF-7,  
 3 and C) MDA-MB-231 cells.

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## 5 References

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